On three known deficiencies of Mathematical Quantum Field Theory

Cumulative habilitation
in the field of Mathematics

by

Dirk - André Deckert

presented in the habilitation procedure
at the Fakultät für Mathematik, Informatik und Statistik
of the Ludwig-Maximilians-Universität München

Dedicated to

my parents,
my wife,
my mentors,
my collaborators,
my colleagues,
my students,
my friends.

Über drei bekannte Mängel der Mathematischen Quantenfeldtheorie

Kumulative Habilitation
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Eidesstattliche Erklärung

Ich versichere hiermit an Eides statt, dass die vorgelegte Arbeit von mir selbständig und ohne unerlaubte Hilfe angefertigt wurde.

Dr. Dirk - André Deckert

Inhaltsverzeichnis / Table of Contents

1 Kumulative Habilitation

Gemäß der Zielvereinbarungen meines Habilitationsverfahrens, siehe Appendix B, lege ich folgende sechs wissenschaftliche Veröffentlichungen vor:

A1. *Consistency of multi-time Dirac equations with general interaction potentials*, D.-A. Deckert, L. Nickel, Journal of Mathematical Physics 57:072301, 15 pages, 2016

A2. *Multi-time dynamics of the Dirac-Fock-Podolsky model of QED*, D.-A. Deckert, L. Nickel, Journal of Mathematical Physics, 60:072301, 20 pages, 2019

A3. *The Mass Shell of the Nelson Model without Cut-offs*, S. Bachmann, D.-A. Deckert, A. Pizzo, Journal of Functional Analysis, 263(5):1224, 58 pages, 2012

A4. *Ultraviolet Properties of the Spinless, One-Particle Yukawa Model*, D.-A. Deckert, A. Pizzo, Communications in Mathematical Physics, 327(3):887, 33 pages, 2014

A5. *Relation Between the Resonance and the Scattering Matrix in the Massless Spin-Boson Model*, M. Ballesteros, D.-A. Deckert, F. Hänle, Communications in Mathematical Physics, 370:249–290, 41 pages, 2019

A6. *One-boson scattering processes in the massless Spin-Boson model – A non-perturbative formula*, M. Ballesteros, D.-A. Deckert, F. Hänle, Advances in Mathematics, 371:107248, 26 pages, 2020

Die oben genannten Arbeiten wurden, wie aufgelistet, in Zusammenarbeit mit meinen Kollaborationspartnern S. Bachmann (UBC Kanada), M. Ballesteros (UNAM Mexiko), A. Pizzo (U Tor Vergata Italien) sowie meinen Doktoranden L. Nickel und F. Hänle erstellt. Des Weiteren habe ich aus thematischen Gründen einen weiteren Bericht über folgende siebte und achte Arbeit

A7. *A Perspective on External Field QED.*, D.-A. Deckert, F. Merkl, book edition Quantum Mathematical Physics, Birkhäuser, 381-399, 18 pages, 2016

A8. *External Field QED on Cauchy Surfaces for Varying Electromagnetic Fields*, D.-A. Deckert, F. Merkl, Communications in Mathematical Physics, 345(3):973–1017, 44 pages, 2016

aufgenommen, welche zusammen mit Herrn F. Merkl (LMU) verfasst wurden. Da Herr Merkl in diesem Habilitationsverfahren die Rolle des Fachmentors einnimmt und gemäß genannter Zielvereinbarung nur sechs Arbeiten erforderlich sind, kann der Inhalt dieses letzten Berichts in der Begutachtung dieser Habilitation ausgeschlossen und nur die Arbeiten [A1-6] berücksichtigt werden.

Sämtliche Resultate in allen obig genannten Arbeiten sind aus gemeinsamen Diskussionen entstanden. Sie sind folglich Gemeinschaftsleistungen und können nicht den Autoren einzeln zugeordnet werden. Weiter beinhaltet Sektion 2 einen Bericht, in dem diese Arbeiten erläutert und in den wissenschaftlichen Zusammenhang gebracht und eingeordnet werden. Dieser Bericht ist in englischer Sprache verfasst und obige Arbeiten werden dort mit [A1-8] referenziert. Die elektronisch über das arXiv öffentlich zugänglichen Versionen aller oben genannten Arbeiten sind Appendix A beigefügt. Bis auf Kürzungen und kleineren editorischen Veränderungen stimmen die Inhalte der Veröffentlichungen [A1-8] mit den Versionen im Appendix A überein.

2 Main report

2.1 Introduction

In this habilitation thesis, I report on a series of works which were published jointly with my co-authors throughout the years 2012-20. The central topic of these works lies in a field of research that I would like to refer to as *mathematical quantum field theory* in the following. The motivation for this term is to separate the intended discussion about the involved mathematical difficulties in formulating a rigorous framework of quantum field theory from the undoubtedly successful but mostly informal computational methods that were developed to predict and explain the behavior of elementary particles.

As a matter of fact and despite these mathematical difficulties, quantum field theory has proven its predictive power to an astonishing level of accuracy in some experimentally accessible and interesting regimes. Together with the theory of general relativity, it has fundamentally shaped the face of modern physics in the past century and continues to do so in view of next-generation technologies. Experiments currently under construction, see for example the overview [21], promise to create unprecedented intense light and X-ray sources which may eventually allow to probe the structure of the quantum vacuum itself. This success story stands in strong contrast to the failure in finding a mathematically rigorous framework to describe at least one of the known relativistically interacting models of quantum field theory. One may ask how such a discrepancy is even possible. This seeming contradiction may be understood better by observing that there are two major approaches to quantum field theory, a so-called *perturbative* and a *non-perturbative* one.

The perturbative approach originated from the motivation to efficiently compute relativistic corrections to the predictions of quantum mechanics. Despite the missing mathematical justification, it works particularly well in the regime of high-energy scattering of particles. It has even exceeded its original motivation by predicting many new elementary particles that by now have all been confirmed and explored in the many famous collider experiments around the world. The non-perturbative approach to quantum field theory, on the contrary, seeks a mathematical framework of at least the level of sophistication of quantum mechanics, in which its computation rules can be derived from first principles. More precisely put, starting from a model definition in terms of a fundamental equation of motion equipped with an adequate sense of solutions, its objective is to answer concise questions about the existence and properties of its solutions.

As it has been the case in quantum mechanics, such a rigorous framework may not just be beneficial for the sake of mathematics but may also enable a deeper understanding of the physical theory itself. In non-perturbative quantum field theory, the motivation is of course not to avoid perturbation theory. On the contrary, analytic perturbation theory is probably still one of the most powerful tools to access properties of potential solutions. However, if employed, the emphasis lies not only on studying the first orders of perturbation, but also on the rigorous control of the truncation error. To avoid any confusion, I prefer the term *mathematical* over *non-perturbative quantum field theory*, as introduced above, although admittedly, both are somewhat peculiar.

In view of the mentioned next-generation experiments, there is also a physical motivation to go beyond the perturbative approach as it is unclear whether the latter will maintain its predictive power in these new and extreme regimes. Perturbative quantum field theory has foremost been applied in the regime of high-energy collision experiments in which scattering particles only see each other for a very short time in the impact zone, and therefore only interact weakly, relatively speaking, despite the high energies. New experiments may test quantum field theoretic systems, such as the quantum vacuum itself, under much more confined and extreme conditions in which also dynamic phenomena arising either from ultra-strong or long-time interactions may be observed and possibly even controlled. There is an increasing number of claims in the physical literature, see [33] for a review, that a non-perturbative description may have to be developed to describe such settings. Although I share this opinion, I need to emphasize that to this day none of them were sufficiently substantiated. The current epoch is hence particularly exciting since experiments may not just serve to repetitively reproduce theoretic predictions, as it has been the case for over half a century, but may in turn drive the development of the corresponding theory.

Before presenting the reports on the works [A1-8] in "mathematical quantum field theory" in the following sections, it may be valuable for the sake of perspective to briefly outline the informal perturbative approach in an introductory fashion starting from quantum mechanics. By analogy, this will allow me to emphasize what is missing in order to reach a non-perturbative understanding and enumerate three of the known fundamental deficiencies of mathematical quantum field theory. Specialists can of course safely skip this remaining part of the section as the following reports starting with Section 2.2 are self-contained.

For this introductory purpose, let us consider a quantum system, at first not necessarily containing quantum fields, and suppose its time evolution is characterized by a groupoid $(U(t_1, t_0))_{t_1,t_0\in\mathbb{R}}$ of unitary operators on a Hilbert space $\mathcal{H}$ of vectors Ψ such that the following Schrödinger-type equation

$$i\partial_t U(t, t_0)\Psi = HU(t, t_0)\Psi. \tag{1}$$

is fulfilled given a generating Hamiltonian, typically an unbounded self-adjoint linear operator, of the special form

$$H = H^0 + \alpha H^{\mathrm{I}}(t). \tag{2}$$

In the following, units are always chosen such that Planck's constant $\hbar$ equals one. In this special form, H^0 shall denote the Hamiltonian of the free system while $H^{\mathrm{I}}(t)$ is thought to encode the interaction, potentially depending on time t, and the coupling strength is given by $\alpha \in \mathbb{R}$, e.g., Sommerfeld's fine structure constant in the case of quantum electrodynamics.

In order to inquire about the full time evolution $U(t_1, t_0)$ from initial time t_0 to time t, one may attempt to expand it in terms of the mathematically well-understood free time evolution $U^0(t_1, t_0)$ generated by H^0 by means of iterating Volterra's integral equation corresponding to (1), i.e.,

$$U(t_1, t_0) = U^0(t_1, t_0) - i\alpha \int_{t_0}^{t_1} ds\, U^0(t_1, s)H^{\mathrm{I}}(s)U(s, t_0). \tag{3}$$

Thereby, one obtains an informal perturbation series of the so-called scattering matrix

$$S = \lim_{\substack{t_0\to-\infty \\ t_1\to+\infty}} U^0(0, t_1)U(t_1, t_0)U^0(t_0, 0) \tag{4}$$

$$=1 + (-i\alpha)^n \sum_{n=1}^{\infty} \int_{-\infty}^{+\infty} ds_1 \int_{-\infty}^{s_1} ds_2 \ldots \int_{\infty}^{s_{n-1}} ds_n U^0(0, s_1)H^{\mathrm{I}}(s_1)U^0(s_1, s_2)H^{\mathrm{I}}(s_2)\ldots H^{\mathrm{I}}(s_n)U^0(s_n, 0) \tag{5}$$

which is referred to as the Dyson series. Physically, the entity $|\langle\Psi_{\text{out}}, S\Psi_{\text{in}}\rangle_{\mathcal{H}}|^2$ describes the long-time transition probabilities between incoming and outgoing states in a scattering experiment which are modeled by the Hilbert space vectors Ψ_{in} and Ψ_{out}, respectively. Even for interacting quantum mechanical systems not containing quantum fields, giving a mathematical meaning to the expressions (4) and (5) is already a formidable mathematical task. This task is skipped entirely in the perturbative approach to quantum field theory. Rather than deriving those formulas from first principles, one regards (5) as a given symbolic expression for the scattering matrix and simply replaces the symbols H^0 and H^{I} by the desired quantum field theoretic operators describing the free evolution and interaction, respectively. The n-th order of the correction is then given by the matrix element corresponding to

$$S_n = (-i)^n \int_{-\infty}^{+\infty} ds_1 \int_{-\infty}^{s_1} ds_2 \ldots \int_{\infty}^{s_{n-1}} ds_n\, U^0(0, s_1)H^{\mathrm{I}}(s_1)U^0(s_1, s_2)H^{\mathrm{I}}(s_2)\ldots H^{\mathrm{I}}(s_n)U^0(s_n, 0) \tag{6}$$

which can quite efficiently be recast into explicit integral formulas by means of the so-called Feynman rules. Maybe not surprisingly, it turns out that those integrals are notoriously divergent for any relativistically interacting quantum field theory, and thus, render both the n-th order summand (6) as well as the

Dyson series (5) ill-defined. This may come as no surprise considering its informal origin. As discussed in more detail later, this is due to the ill-definedness of the interaction Hamiltonian H^{I}, and hence, the ill-posedness of the corresponding Schrödinger-type initial value problem (1). Leaving the Dyson series convergence aside, the perturbative approach then attempts to remedy the ill-defined behavior of the n-th order summand by means of a so-called renormalization procedure that introduces counter terms in order to cancel out these divergences at the expense of specifying additional parameters. If it is possible to render all orders n of corrections finite with only a set of finite many parameters, one calls the model *renormalizable*. Notably, whether the Dyson series is convergent or not is not even part of the definition of renormalizability in perturbative quantum field theory.

Given the algorithm that generates the symbolic expressions (6) for any particular order of perturbation and the corresponding integral formulas including the counter-terms providing the mathematical content, one has again a rigorous starting ground for mathematics, e.g., to prove whether a model of quantum field theory is renormalizable or not. As it is well-known, in the case of quantum electrodynamics, this question was answered affirmatively by several highly sophisticated proofs that in part employed quite distinct mathematical techniques; maybe most prominently [40]. To this day, there have been many arguments fought whether the renormalizability property is already sufficient to qualify a quantum field theory as a fundamental physical theory or not. Since this obviously depends on the definition of the term "fundamental theory", I do not enter this discussion here but instead point out two facts: First, as stated above, for many models of quantum field theory, the first couple of corrections already deliver quite accurate predictions, many of which have been experimentally verified. Second, it is unknown whether the resulting series of renormalized corrections converges or not, let alone how large the remainder after truncation is.

Nowadays, e.g., in the case of quantum electrodynamics, the folklore believe is that (5) may only be an asymptotic series similar to the following example motivated by the Euclidean φ^4 theory. For $\alpha > 0$, let us consider the following function

$$f(\alpha) := \int_{-\infty}^{\infty} dx\, e^{-x^2-\alpha x^4} = \int_{-\infty}^{\infty} dx \sum_{n=0}^{\infty} \alpha^n \frac{(-x^4)^n}{n!} e^{-x^2}, \tag{7}$$

for which it might seem tempting to commute the limits of the integral and summation to obtain

$$f(\alpha) \overset{?}{=} \sum_{n=0}^{\infty} \alpha^n f_n(\alpha) \qquad \text{for} \qquad f_n(\alpha) = \int_{-\infty}^{\infty} dx\, \frac{(-x^4)^n}{n!} e^{-x^2} = (-1)^n \frac{\Gamma(2n+\frac{1}{2})}{n!}. \tag{8}$$

However, as one may check by the ratio test, the series on the right hand side of $\overset{?}{=}$ in (8) does not converge for any $\alpha > 0$. Nevertheless, the first few summands $f_n(\alpha)$ already provide a reasonably good approximation of $f(\alpha)$ given α is sufficiently small. More precisely, the series is called asymptotic because the following property

$$\left| f(\alpha) - \sum_{n=0}^{N-1} f_n(\alpha) \right| = O_{\alpha\to 0}(f_N(\alpha)) \tag{9}$$

holds true. This property entails that keeping the order of approximation N fixed, the corresponding error vanishes as fast as $f_N(\alpha)$ does when α approaches zero. Of course, this may not be of much help physically as α is usually to be considered a natural constant. Nevertheless, this example shows that already an asymptotic series as likely produced by perturbative quantum field theory may provide a reasonably good prediction for small α when considering only the first few summands, even though the entire series (5) may not converge.

In studying the divergent integrals in (6), modern approaches introduce a regularization of the model of interest by cutting off the domains of integration below very small and above very large momenta of the interaction. These thresholds are usually referred to as infrared and ultraviolet cut-offs, respectively.

At best, this leads to a family of well-defined models and at least to converging integral formulas derived for the n-th order correction (6), both parametrized by the respective cut-offs. In order to remove the regularization, one attempts to define a group action that iteratively increases the allowed momentum range of the interaction scale by scale, enforcing a certain self-consistency condition. The latter condition is to ensure that the resulting models behave physically consistent. This is usually achieved by rescaling the underlying model parameters, such as particle masses and charges. Based on this imposed self-consistency condition, it is the hope that the renormalized flow of models consistently describes the interactions on the respective ranges of admitted momenta. This so-called renormalization group approach is clearly more appealing than subtracting similarly ill-defined counter-terms. However, when set up perturbatively in the case of quantum electrodynamics, it introduces another complication as the coupling constant α turns into a function of the ultraviolet cut-off which even exhibits a pole at a finite value, the so-called Landau pole. Disregarding the fact that a growing α makes the informal expansion used to define the renormalization group action even more questionable as in the first place, the Landau pole is yet another obstacle in removing the momenta cut-offs. To this day, the interpretation of this pole, whether it is only an artifact of the informally applied perturbation theory or whether it involves physics, is unclear. Without going into details of this discussion, I want to mention three facts: First, such a pole does not seem to show up in the similarly informal computations of quantum chromodynamics, describing the so-called strong interaction between quarks and gluons, although it remains present in the corresponding unification by means of the standard model. Second, in quantum electrodynamics, the Landau pole lies at a very high momentum that so far was not reached experimentally. And third, one often reads that by means of the Landau pole, quantum electrodynamics, and also the respective other theories that seem to exhibit such a pole, would predict their own breakdown at high energies, and this despite Hume's well-intentioned advice of 1739: *There is nothing in any object, consider'd in itself, which can afford us a reason for drawing a conclusion beyond it.*

Since this perturbative line of reasoning in reaching an evaluable expression of the n-th order correction (6) is rather informal, and since the series (5) can merely be regarded as an symbolic expression derived by an algorithm that mimics what one would hope to find for a well-behaved quantum system, one may ask for a formal derivation in mathematical quantum field theory. To put such an endeavor in perspective, it has to be emphasized again that already in the case of quantum mechanical models without quantum fields, deriving and proving the validity of an expansion such as (5) faces rather intricate mathematical questions. Is the initial value problem of the Schrödinger equation (1) well-posed? Is it possible to control the long-time evolution in view of (4) in any relevant sense? Does the power series (5) in α converge in any relevant sense? If not, are there other means to inquire about the time evolution $U(t_1, t_0)$ and the scattering matrix S? In the last century, great many efforts have been invested to address such questions, be it for one-particle quantum systems interacting with external potentials or many-particles systems including pair-interaction, and in many of those models the above questions have been answered satisfactorily. In mathematical quantum field theory, however, even for regularized, and therefore, mathematically well-behaved models, the tasks are at least as difficult and the additional desire to control their properties when removing the cut-offs makes their study even more cumbersome. Nevertheless, in the second half of the last century, many mathematical advances have been achieved, especially for models of persistent charges interacting with their quantum fields that address the well-posedness of their time evolution, the well-definedness of their scattering theory, and their behavior when removing the respective cut-offs. The selected works [A1-8] by my co-authors and myself presented in the following sections focus on the latter kind as well as on the type of equations of motion of relativistic interacting models of quantum field theory and how they provoke the divergences when removing the cut-offs. The encountered difficulties are well-known since the beginning of quantum field theory and may be categorized into what I would like to call the *three fundamental deficiencies of mathematical quantum field theory*:

D1. The *ultraviolet divergence* of bosonic fields mediating the interaction.

D2. The *infrared catastrophe* of massless bosonic fields mediating the interaction.

D3. The *ultraviolet divergence* of fermionic fields modeling matter and charges.

In principle, there may also occur an infrared catastrophe for fermionic fields provided they had no mass. In this report, however, I omit this problem entirely for two reasons. First, to this day, all known fermionic fields seem to have non-zero effective masses. Second, although ultimately one may like to start with a theory of only massless fields and let the Higgs mechanism act to assign appropriate masses, such a mechanism is far beyond the scope of the mathematical studies presented in this report.

Overview. Those three deficiencies D1-3 provide the road map which I will follow. While Section 2.2 focuses on D1 and D2, Section 2.3 concludes with a discussion of D3. The subsections 2.2.1 and 2.2.2 motivate the type of equations of motion that are to be expected in the case of models of persistent charges that feature a relativistic interaction which, contrary to non-relativistic quantum mechanics, are of multi-time nature. The given historical review is complemented by reports on the works [A1] and [A2] that provide rigorous results on the corresponding existence of multi-time dynamics. On the base of these multi-time equations of motion, a representative class of effective single-time models is derived. This so-called class of *scalar field models* turns out to be sufficiently sophisticated in order to analyze the mathematical nature of the deficiencies D1 and D2 on the same level as in quantum electrodynamics of persistent charges, however, without additional ballast of spin, polarization, and gauge freedom. Two central paragraphs in Section 2.2.2 labeled "Deficiency D1" and "Deficiency D2" review the mathematical implications of deficiencies D1 and D2, the well-definedness of the models when imposing the infrared and ultraviolet regularization, and discuss why it is desirable to remove them. At many occasions the report will refer back to theses paragraphs. The succeeding sections 2.2.3-2.2.5 report on the works [A3-6] which aim at an understanding of how one can address deficiencies D1 and D2 mathematically in certain representatives of scalar field models of persistent charges. At the heart lies a powerful mathematical technique, which is usually referred to as *multi-scale analysis*, first introduced by Pizzo in [83], which shares great similarity with the renormalization group method. Finally, deficiency D3 is addressed in Section 2.3 that arises from the attempt of employing relativistic dispersion relations for the charges and leads to a class of non-persistent but varying charges. A report on the works [A7-8] on a simple model of varying charges, the external field quantum electrodynamics, serves as a conclusion of the main report and again contains two central paragraphs both labeled "Deficiency D3" reviewing the implications of D3.

Formal and informal parts. Since mathematical quantum field theory lives on the ridge between physics and mathematics, it is unavoidable to mix mathematical informal and formal discussions. Wherever possible, I will try to visually distinguish informal paragraphs from formal ones by indenting the latter by a vertical line on the left, such as in this paragraph.

2.2 Persistent charge models

2.2.1 Failure of introducing relativistic interaction by potentials

This section comprises a report on the following article:

A1. Consistency of multi-time Dirac equations with general interaction potentials, D.-A. Deckert, L. Nickel, Journal of Mathematical Physics 57:072301, 15 pages, 2016

The openly accessible version arXiv:1603.02538 is attached in Section A, page 67.

The birth hours of quantum field theory, alongside Heisenberg and Pauli's fundamental paper [65] of 1929, was certainly marked by Dirac's work [29] of 1932. There, Dirac opened with the observation that the typical wave function for a quantum system of N particles, $\psi(t, \mathbf{x}_1, \dots, \mathbf{x}_N)$ depending on a single time t and the position variables $\mathbf{x}_1, \dots, \mathbf{x}_N$ for the particles, is an intrinsically non-relativistic object. There is simply no unitary transformation that would allow ψ to transform, e.g., as a spinor field. He therefore introduced an object that has a better chance to describe a relativistic N-body system, namely a wave function $\psi(x_1, \ldots, x_N)$ that depends on space-time coordinates $x_1, \ldots, x_N$, i.e., on N time and N position coordinates for which the notation $x_k = (t_k, \mathbf{x}_k)$ will be used. This new so-called multi-time wave function raises two fundamental questions. First, how would one express the law of motion, and second, how does the multi-time wave function relate to the empirical relative frequencies of events measured, e.g., in a laboratory? Regarding the former question, Dirac proposed to replace the single-time Schrödinger equation by a system of N Schrödinger-type equations, one per time variable

$$i\partial_{t_k}\psi(x_1, \ldots, x_N) = H_k(x_1, \ldots, x_N)\psi(x_1, \ldots, x_N) \qquad \text{for} \qquad k = 1, \ldots, N, \tag{10}$$

for which an appropriate choice of Hamiltonian H_k governs the time evolution along the time coordinate t_k. Regarding the latter question, Dirac proposed to interpret the restriction of the multi-time wave function to an equal-time hyperplane, i.e., $\psi_t(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \psi(x_1, \ldots, x_N)\big|_{t_1=\cdots=t_N=t}$, as the usual single-time wave function which would then fulfill

$$i\partial_t\psi_t(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{k=1}^{N} H_{k,t}(\mathbf{x}_1, \ldots, \mathbf{x}_N)\psi_t(\mathbf{x}_1, \ldots, \mathbf{x}_N) \tag{11}$$

for single-time Hamiltonians $H_{k,t}(\mathbf{x}_1, \ldots, \mathbf{x}_N) = H_k(x_1, \ldots, x_N)\big|_{t_1=\cdots=t_N=t}$, which, thanks to the definition of the derivative, has the typical summation form common in non-relativistic quantum mechanics. The relation between multi-time wave functions and empirical frequencies of events was studied in more detail by Bloch in [15] and the notion of equal-time hyperplanes can of course be generalized to any Cauchy surfaces in space-time $\mathbb{R}^4$ which connects nicely to Schwinger's formalism on Cauchy surfaces [91, 92, 94, 93, 95, 96].

Rigorous results on the failure of relativistic pair-potentials. On the mathematical side, the most pressing question is whether the multi-time system of equations (10) gives rise to a well-posed problem of finding solutions in a relevant sense, for example in terms of an initial value problem on a Hilbert space. In the original paper, Dirac [29] already noticed that the additional condition

$$\left[i\partial_{x_k^0} - H_k, i\partial_{x_l^0} - H_l\right]\psi(x_1, \ldots, x_N) = 0 \qquad \text{for all} \qquad k \neq l \tag{12}$$

has to be imposed. In fact, it is only needed on the following domain of space-time configurations

$$\mathcal{S}^N := \left\{(x_1, \ldots, x_N) \in \mathbb{R}^{4N} \,\middle|\, \forall\, k \neq l : |x_k^0 - x_l^0| < |\mathbf{x}_k - \mathbf{x}_l|\right\} \tag{13}$$

which ensures that all N space-time points lie pairwise space-like to each other. Only then the value of ψ at the time configuration $(t_1, \ldots, t_N)$ can be given a well-defined meaning. This condition (12) can be recast into a more implicit but maybe geometrically more intuitive integral form, in which it states that the value of ψ at time configuration $(t_1, \ldots, t_N)$ is independent of the path of integration in $\mathcal{S}^N$ that connects it to an initial value, e.g., at time configuration $(t_1, \ldots, t_N) = 0$. Given the solution of (10) is sufficiently regular, the condition (12) then follows by Schwarz' theorem. Although surely observed by Dirac in 1932, a first rigorous understanding of how restrictive this integrability condition (12) is first appeared in [80] in 2014. Among several results on the system of equations (10) for general bounded and smooth Hamiltonians H_k, it was shown that multi-time systems with Hamiltonians of the form

$$H_k = H_k^0 + V_k(x_1, \ldots, x_N), \tag{14}$$

where H_k^0 and V_k for $k = 1, \ldots, N$ denote the unbounded free Dirac Hamiltonian for the k-th particle, see (170) below, and smooth $\mathbb{R}$-valued multiplication operators, respectively, do not admit smooth $\mathbb{C}^{4N}$-valued solutions ψ on $\mathbb{R}^{4N}$ or $\mathcal{S}^N$ obeying the integrability condition (12) unless there are smooth $\mathbb{R}$-valued functions $\theta(x_1, \ldots, x_N)$ and $\widetilde{V}_k(x_k)$ for $k = 1, \ldots, N$ such that

$$i\partial_{t_k}\widetilde{\psi}(x_1, \ldots, x_N) = \left(H_k^0 + \widetilde{V}(x_k)\right)\widetilde{\psi}(x_1, \ldots, x_N) \qquad \text{for} \qquad k = 1, \ldots, N, \tag{15}$$

given

$$\widetilde{\psi}(x_1, \ldots, x_N) := e^{i\theta(x_1,\ldots,x_N)}\psi(x_1, \ldots, x_N) \tag{16}$$

holds true. The class of such potentials V_k are referred to as *non-interacting* since the seeming interaction can be gauged away by means of θ. In other words, as the integrability condition (12) is essential for the solution sense, there exist at least no strong solutions to the multi-time equations (10) mediating an actual interaction between the particles, i.e., one that cannot be gauged away in the sense of (15)-(16).

In the article [A1], this study was extended to also treat potentials that allow for spin-coupling. Due to the fast growing dimensionality $K = 4^N$ in the spin degrees of freedom, the rigoros proof was only given for $N = 2$. As explained in [A1], with sufficient effort, the exploited mechanism seems to work for any number N, however, for a no-go-type result the case $N = 2$ may already be sufficiently convincing. The central theorem states:

Theorem 2.1 (No-go regarding relativistic pair-potentials [A1])**.** *Let $N = 2, K = 4^N$, $\Omega = \mathbb{R}^{4N}$ or $\Omega = \mathcal{S}^N$ with one-sided derivatives at the boundary, and potentials $V_k \in C^1(\Omega, \mathbb{C}^{K\times K})$. If for all $\psi^0 \in C_c^\infty(\mathbb{R}^{3N}, \mathbb{C}^K)$, there is a strong solution $\psi \in C^2(\Omega, \mathbb{C}^K)$ to the multi-time system* (10) *with initial value $\psi\big|_{t_1=\cdots=t_N=0} = \psi^0$, then the potentials V_k are either non-interacting or interacting but not Poincaré invariant.*

The common notation is used to denote the set of n-times continuous differentiable functions $V \to W$ by $C^n(V, W)$ while a subscript $_c$ restricts the set to functions to compact support. In this context, the term *non-interacting* refers to all interactions that can be gauged away in the sense discussed above. It should be noted that the integrability condition (12) is not assumed explicitly but it was observed that the existence of solutions ψ to the multi-time equations (10) in the above sense already implies the integrability condition (21) which enforces restrictions on the class of admissible potentials V_k, $k = 1, \ldots, N$. The entire class of such admissible potentials was identified explicitly in [A1] and it is interesting to note that this class does indeed comprise interacting ones. However, none of them are Poincaré invariant. More precisely, none of the admissible family of potentials fulfills

$$V_k(x_1, \ldots, x_N) = S(\Lambda)^{\otimes N} V_k\left(\Lambda^{-1}(x_1 - d), \ldots, \Lambda^{-1}(x_N - d)\right) \tag{17}$$

for all translations d^μ, Lorentz boosts Λ^μ_ν and corresponding unitary spin-transformation matrices $S(\Lambda)$ such that $S(\Lambda)\gamma^\mu S(\Lambda)^{-1} = \Lambda^\mu{}_\nu\gamma^\nu$ holds true.

Beside the required regularity, the results in [80] and [A1] only rule out multiplication operators in configuration space. This still leaves open the possibility for admissible classes of general operators V_k, e.g., ones that may also depend on the respective momentum operators $-i\nabla_{\mathbf{x}_1}, \ldots, -i\nabla_{\mathbf{x}_N}$ in a pseudo-differential operator sense, or are formed by integral kernels acting on ψ as in the case of the Bethe-Salpeter-type equations [76] which may be appealing from the perspective of Wheeler-Feynman electrodynamics; see also [25, Chapter 8]. Nevertheless, the observations in [A1] render the possibility to formulate relativistic quantum mechanics with pair-interaction potentials in the sense of an initial value problem as rather remote.

2.2.2 Relativistic interaction through quantum fields

This section comprises a report on the following article:

A2. *Multi-time dynamics of the Dirac-Fock-Podolsky model of QED*, D.-A. Deckert, L. Nickel, Journal of Mathematical Physics, 60:072301, 20 pages, 2019

The openly accessible version arXiv:1903.10362 is attached in Section A, page 85.

The failure of relativistic quantum mechanics must have already been known in 1932 when Dirac suggested to replace the $\mathbb{C}^K$-valued potentials V_k by one operator-valued field on space-time [29]. Together with Fock and Podolsky, this idea was worked out in [32] in the example of quantum electrodynamics of N persistent electrons in 1934, showing also the equivalence to the 1929's formulation by Heisenberg and Pauli [65]. This ground breaking article [32] would later become the input for Tomonaga's famous work [103] that shaped the foundation of modern quantum field theory.

The motivation behind the work [A2] was to understand the type and well-posedness of the initial value problem of the multi-time equations (10) in Dirac's setting in which the interaction is mediated by an operator-valued field. For the purpose of the mathematical study, it will be beneficial to discuss Dirac's ideas in the case of a more simplified model of quantum field theory as compared to quantum electrodynamics, the so-called *scalar field model*. The latter allows to study the mentioned deficiencies D1 and D2 in full detail but avoids the additional theoretical complexity of electron spin, photon polarization, and gauge invariance. The road map for the following paragraphs in this section is therefore to introduce the multi-time setting of [32] for the case of a scalar field, discuss the nature of the new operator-valued field that mediates the interaction, derive an effective class of single-time models for the further mathematical study, present the deficiencies D1 and D2 mathematically, and conclude with a report on [A2] which contains a result on the existence of the corresponding multi-time dynamics.

Relativistic interaction in multi-time systems. Dirac's new ansatz still employed a system of multi-time equations such as (10), but with only one field φ on $\mathbb{R}^4$ that is supposed to mediate the interaction between the N charges instead of N interaction potentials V_k as in (14):

$$i\partial_{t_k}\Psi(x_1,\dots,x_N) = H_k\Psi(x_1,\dots,x_N) = \left(H_k^0 + g\varphi(x_k)\right)\Psi(x_1,\dots,x_N) \qquad \text{for all} \qquad k = 1,\dots,N. \tag{18}$$

It should be noted that the evolution equation along time axis t_k evaluates φ at the k-th space-time point x_k. As before, H_k^0 denotes the free Dirac operator for the k-th particle, see (170) below, and furthermore, $g \in \mathbb{R}$ represents a coupling constant. Now, for the field φ, Dirac required it to satisfy the free wave, i.e., Klein-Gordon, equation

$$\left(\square_x + \mu^2\right)\varphi(x) = 0, \tag{19}$$

where $\square_x = \partial_t^2 - \Delta_{\mathbf{x}}$ denotes the d'Alembert operator, $\Delta_{\mathbf{x}}$ the Laplacian with respect to $\mathbf{x}$, and $\mu \geqslant 0$ a field mass parameter. In the following, units are always chosen such that the speed of light is set to $c = 1$. The complete set of $N+1$ equations (18)-(19) could then be regarded to describe a system of N Dirac electrons that interact with a free scalar field φ. In order to introduce an effective interaction between the electrons, Dirac imposed the additional constraint for the scalar field to fulfill the commutation relation

$$[\varphi(x),\varphi(y)] = \varphi(x)\varphi(y) - \varphi(y)\varphi(x) = i\Delta(x,y), \tag{20}$$

for $x, y \in \mathbb{R}^4$, where Δ denotes the Pauli-Jordan function. The latter can be expressed informally as $\Delta = \Delta^+ - \Delta^-$ by means of the advanced and retarded Green's functions Δ^+, Δ^- of the Klein-Gordon operator. It is important to note that the distributions Δ^+, Δ^- are only supported on the light-cone including its boundary and that Δ even vanishes at the origin. This guarantees the integrability condition (12) to hold true for sufficiently regular Ψ, as can be seen from

$$\left[i\partial_{x_k^0} - H_k, i\partial_{x_l^0} - H_l\right]\Psi = [\varphi(x_k),\varphi(x_l)]\Psi = i\Delta(x_k,x_l)\Psi = 0 \quad \text{for all} \quad k \neq l, (x_1,\dots,x_N) \in \mathcal{S}^N. \tag{21}$$

Hence, in view of the discussion of the integrability constraint (12) of the previous section, the set of $N+1$ evolution equations (18)-(19) together with the additional constraint (20) that enforces (21) has a viable chance to define a multi-time dynamics. Before rigorously answering to the question of existence of such multi-time solutions, which is the content of [A2] and will be discussed in the very end of this section, it is worthwhile to understand as to why the requirement (20) eventually gives rise to a sensible interaction between the charges.

For this purpose, the existence of dynamics is assumed in a form such that on an appropriate N-particle Hilbert space $\mathcal{H}$, there is a unitary map $U(t_1,\ldots,t_N)$ sufficiently regularly parametrized by times $t_1,\ldots,t_N\in\mathbb{R}$ such that a multi-time solution can be represented by means of

$$\Psi(t_1,\mathbf{x}_1,\ldots,t_N,\mathbf{x}_N)=\left(U(t_1,\ldots,t_N)\Psi^0\right)(\mathbf{x}_1,\ldots,\mathbf{x}_N), \tag{22}$$

provided a sufficiently regular initial value $\Psi^0\in\mathcal{H}$. The abbreviation $U(t)=U(t_1,\ldots,t_N)\big|_{t_1=\cdots=t_N=t}$ shall denote the evaluation on equal-time hyperplane $\{t\}\times\mathbb{R}^3$ at times $t\in\mathbb{R}$ which foliate space-time $\mathbb{R}^4$. In this notation, one finds that the interacting field operator

$$\varphi^{\mathrm{I}}(t,\mathbf{x})=U(t)^{-1}\varphi(t,\mathbf{x})U(t) \tag{23}$$

fulfills the inhomogeneous wave equation

$$\left(\square_{t,\mathbf{x}}+\mu^2\right)\varphi^{\mathrm{I}}(t,\mathbf{x})=-g\sum_{k=1}^{N}\delta^3\left(\mathbf{x}-\hat{\mathbf{x}}_k^{\mathrm{I}}(t)\right), \tag{24}$$

where $\hat{\mathbf{x}}_k^{\mathrm{I}}$ denotes the interacting position operator

$$\hat{\mathbf{x}}_k^{\mathrm{I}}(t)=U(t)^{-1}\hat{\mathbf{x}}_kU(t), \tag{25}$$

$\hat{\mathbf{x}}_k$ the position operator of the k-th particle, i.e., the multiplication operator $\hat{\mathbf{x}}_k\Psi(x_1,\ldots,x_N)=\mathbf{x}_k\Psi(x_1,\ldots,x_N)$, and δ^3 represents the three-dimensional Dirac delta distribution. Hence, according to (24), the sources of the interacting field are given by the N time evolved charges. To see that equation (24) is implied by the multi-time equations (18)-(19) and constraint (20), the following computations are helpful:

$$\partial_t\varphi^{\mathrm{I}}(t,\mathbf{x})=U(t)^{-1}\left(i\sum_{k=1}^{N}[H_k,\varphi(t,\mathbf{x})]+\partial_t\varphi(t,\mathbf{x})\right)U(t), \tag{26}$$

$$[H_k,\varphi(t,\mathbf{x})]=[\varphi(t,\mathbf{x}_k),\varphi(t,\mathbf{x})]=0, \tag{27}$$

$$\partial_t^2\varphi^{\mathrm{I}}(t,\mathbf{x})=U(t)^{-1}\left(i\sum_{k=1}^{N}[g\varphi(t,\mathbf{x}_k),\partial_t\varphi(t,\mathbf{x})]+(\Delta_{\mathbf{x}}-\mu^2)\varphi(t,\mathbf{x})\right)U(t), \tag{28}$$

$$[\varphi(t,\mathbf{x}_k),\partial_t\varphi(t,\mathbf{x})]=\partial_{x^0}[\varphi(x_k),\varphi(x)]\big|_{x_k^0=x^0=t}=i\partial_{x^0}\Delta(x_k,x)\big|_{x_k^0=x^0=t}=i\delta^3(\mathbf{x}_k-\mathbf{x}), \tag{29}$$

where the relations on the right-hand sides of (27) and (29) already appeared in [70] and are today the starting point for the canonical commutation relations in quantum field theory and sometimes referred to as “second quantization”.

It is important to note that the source terms on the right-hand side of (24) stem from an underlying interaction between the charges and the field as opposed to a direct interaction between the charges as it was the case for the previously considered pair-potentials in (10). This becomes particularly obvious for $N=1$. As it turns out, the charges act on its field as sources, and in turn, the field reacts back on the charges influencing their motion. Similarly to classical electrodynamics, this interaction turns out to have two kinetically rather distinct effects. First, the field modes created by charge i that reach charge $j\neq i$ mediate an effective interaction between those charges while, when reacting back on the same charge i, they effectively change its inertia. This will soon be illustrated in a toy model (54) below which requires a renormalization of the charges' rest energies due to this so-called self-interaction. In fact, for $N = 1$ the interaction between the charge and the field can be studied separately from the effective interaction between the charges, a further understanding of which is the main motivation behind the works [A3-6] that exclusively consider $N = 1$ and are reported on the in the later sections.

A representation for the quantum fields. At first sight, starting with an interaction mediated by a free field (19) and slipping in the interaction (24) through the commutation relation (20) may seem like a magic trick. However, it becomes more transparent when clarifying the nature of the field operator φ fulfilling the free wave equation (19) together with the commutation relation (20). This is reviewed next, first informally and later, in the paragraph 'Fock representation" below, formally. Nowadays, a commonly used representation of (20) is the one introduced by Fock, see [47, 48], which can be expressed in momentum space by introducing so-called creation and annihilation operators $a^*_{\mathbf{k}}, a_{\mathbf{k}}$ satisfying

$$[a_{\mathbf{k}}, a^*_{\mathbf{l}}] = \delta^3(\mathbf{k} - \mathbf{l}), \qquad [a_{\mathbf{k}}, a_{\mathbf{l}}] = 0 = [a^*_{\mathbf{k}}, a^*_{\mathbf{l}}]. \tag{30}$$

With their help, the free field operator φ in (19) can informally be assigned the expression

$$\varphi(x) = \int d^3k\, \gamma(\mathbf{k}) \left(a_{\mathbf{k}} e^{-ik_\mu x^\mu} + a^*_{\mathbf{k}} e^{ik_\mu x^\mu}\right), \tag{31}$$

where the Minkowski metric $g^{\mu\nu}$ is chosen such that $k_\mu x^\mu = k^0 x^0 - \mathbf{k} \cdot \mathbf{x}$. The requirement for φ to satisfy the free wave equation (19) dictates the dispersion

$$k^0 = \omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + \mu^2}. \tag{32}$$

Dirac's additional requirement to fulfill the commutation relation (20) for the given choice of Pauli-Jordan function Δ determines what physicists call the form factor

$$\gamma(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(\mathbf{k})}}. \tag{33}$$

It is essential for the later discussion of the deficiencies D1 and D2 that are encountered when trying to give φ, and eventually the Hamiltonians $H^0_k + g\varphi(x_k)$, a mathematical meaning that $\omega(\mathbf{k})$ and $\gamma(\mathbf{k})$ are already completely determined by the two requirements (19) and (20). This predetermination of (32) and (33) can at least on a symbolic level be checked by employing (30). Translated to the bigger context of quantum field theory, the same mechanism implies that Wigner's representation of the Poincaré group [104], which gives rise to all known families of fields, together with Tomonaga's general prescription of the commutation relations [103] in principle leave no freedom in adjusting the corresponding $\omega(\mathbf{k})$ and $\gamma(\mathbf{k})$, as it is nevertheless done later when introducing the mentioned cut-offs to regularize the models in order to avoid D1 and D2. In effective theories, however, it may of course be sensible to adjust the form factor $\gamma(\mathbf{k})$ by hand to encode the intended effective charge model. For example, an extended charge density in position space described by a density function $\rho(\mathbf{x})$ may be modeled by means of a form factor

$$\gamma^\rho(\mathbf{k}) = \widehat{\rho}(\mathbf{k})\gamma(\mathbf{k}) \tag{34}$$

where $\widehat{\rho}$ denotes the Fourier transform of ρ, or equivalently, by employing a spatial convolution between ρ and the field φ in (31) containing the original form factor (33), i.e.,

$$\varphi^\rho(t, \mathbf{x}) = \rho *_{\mathbf{x}} \varphi(t, \mathbf{x}) = \int d^3y\, \rho(\mathbf{x} - \mathbf{y})\varphi(t, \mathbf{y}). \tag{35}$$

This turns (24) into

$$\left(\square_{t,\mathbf{x}} + \mu^2\right) \varphi^{\rho,\mathrm{I}}(t, \mathbf{x}) = -g \sum_{k=1}^{N} \rho\left(\mathbf{x} - \hat{\mathbf{x}}^{\mathrm{I}}_k(t)\right), \qquad \text{for} \qquad \varphi^{\rho,\mathrm{I}}(t, \mathbf{x}) = U(t)^{-1} \varphi^\rho(t, \mathbf{x}) U(t). \tag{36}$$

The class of scalar field models. As a last preparatory step before discussing the deficiencies D1 and D2, it is helpful to make two observations and thereby reveal the form in which the set of N multi-time equations (18), the time evolution equation of the quantum field (19), and the commutation relation (20) gives rise to a single-time model in Fock's representation as it is commonly used in today's literature on mathematical quantum field theory. First, the restriction to equal-time hyperplanes, turns the set of equations (18) into one single-time Schrödinger equation

$$i\partial_t \Psi_t(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{k=1}^{N} \left(H_k^0 + \varphi(t, \mathbf{x}_k) \right) \Psi_t(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{37}$$

cf. (11), using the notation $\Psi_t(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \Psi(t, \mathbf{x}_1, \ldots, t, \mathbf{x}_N)$. The field φ is thus always evaluated at time t. Second, in the representation (31) and with the help of the commutation relations (30), the time evolution generated by the free wave equation (19) of the field operator $\varphi(t, \mathbf{x})$ can be expressed as

$$\varphi(t, \mathbf{x}) = e^{-itH_\omega^0} \varphi(0, \mathbf{x}) e^{itH_\omega^0} \tag{38}$$

given the free field Hamiltonian

$$H_\omega^0 = \int d^3k\, \omega(\mathbf{k}) a_\mathbf{k}^* a_\mathbf{k} \tag{39}$$

which implies

$$e^{-itH_\omega^0} a_\mathbf{k} e^{itH_\omega^0} = a_\mathbf{k} e^{it\omega(\mathbf{k})} \qquad \text{and} \qquad e^{-itH_\omega^0} a_\mathbf{k}^* e^{itH_\omega^0} = a_\mathbf{k}^* e^{-it\omega(\mathbf{k})}. \tag{40}$$

By implementing the transformation

$$\widetilde{\Psi}_t = e^{-itH_\omega^0} \Psi_t, \tag{41}$$

it is possible to recast the single-time Schrödinger equation (37) into the form

$$i\partial_t \widetilde{\Psi}_t(\mathbf{x}_1, \ldots, \mathbf{x}_N), = \left(\sum_{k=1}^{N} H_k^0 + H_\omega^0 + g \sum_{k=1}^{N} \varphi(0, \mathbf{x}_k) \right) \widetilde{\Psi}_t(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{42}$$

for which the resulting Hamiltonian on the right-hand side is time-independent. Thanks to the unitarity of the transformation, one can similarly recover (37) from (42) so that both equations can later be shown to be equivalent on a certain domain of solutions. Usually (37) is called the interaction picture and (42) the Schrödinger picture.

Nowadays, this model serves as first hand choice for mathematical studies of persistent quantum charges interacting with their quantum fields as long as spin degrees of freedom are not of interest. Depending on the type of the free Hamiltonian H_k^0, it is called *Nelson model* in case of a Schrödinger dispersion $H_k^0 = -\frac{\Delta_{\mathbf{x}_k}}{2M}$, *Yukawa model* in the case of a pseudo-relativistic dispersion $H_k^0 = \sqrt{-\Delta_{\mathbf{x}_k} + M^2}$, or simply *scalar field model* for charges of potentially any type that interact with a spinless field φ. Another at least equally important model of non-relativistic persistent charges for which many mathematical results can be found in the literature is the Pauli-Fierz model. The latter takes into account the polarization degrees of freedom of the electromagnetic field and models the interaction between the electrodynamic field in Coulomb gauge with non-relativistic charges by means of minimal coupling, which is why it is referred to as non-relativistic model of quantum electrodynamics. An extensive overview over these models can be found in [100].

After this informal discussion of the scalar field model, the next paragraphs are devoted to its mathematical structure.

Fock representation. Both mentioned mathematical difficulties D1 and D2 arise from the definition of the field operator φ which, independent of the approach, one would eventually like to define on the Fock space

$$\mathcal{F}[\mathfrak{h}] := \bigoplus_{n=0}^{\infty} \mathcal{F}_n[\mathfrak{h}], \qquad \mathcal{F}_n[\mathfrak{h}] := \mathfrak{h}^{\odot n}, \qquad \mathfrak{h} := L^2(\mathbb{R}^3, \mathbb{C}), \tag{43}$$

where $\mathfrak{h}$ is the Hilbert space of square-integrable and complex-valued functions that will often be omitted in the notation and $\odot$ denotes the symmetric tensor product in the Hilbert space sense employing the convention $\mathfrak{h}^{\odot n}\big|_{n=0} = \mathbb{C}$. This wish, more precisely, the requirement of square-integrability, is inherited from quantum mechanics in order to allow for its probabilistic interpretation. By virtue of its definition, $\mathcal{F}$ is again a Hilbert space, and an element $\Phi \in \mathcal{F}$ can be represented as a family of so-called n-mode wave functions

$$(\phi^{(n)})_{n\in\mathbb{N}_0}, \qquad \phi^{(n)} \in \mathcal{F}_n. \tag{44}$$

For all $f \in \mathfrak{h}$, the informal integral notation, e.g., as employed in the field operator (31),

$$a(f) = \int d^3k\, f^*(\mathbf{k}) a_{\mathbf{k}}, \qquad a^*(f) = \int d^3k\, f(\mathbf{k}) a^*_{\mathbf{k}}, \tag{45}$$

can then be given the following mathematical meaning on the level of n-mode wave functions. Given a $\Phi \in \mathcal{F}$, the expression involving the annihilation operator is defined by

$$\left(a(f)\Phi\right)^{(n)}(\mathbf{k}_1, \ldots, \mathbf{k}_n) := \sqrt{n+1} \int d^3k\, f^*(\mathbf{k}) \phi^{(n+1)}(\mathbf{k}, \mathbf{k}_1, \ldots, \mathbf{k}_n), \tag{46}$$

where the superscript * over f denotes complex conjugation, implying that $a(f)$ is anti-linear in f. The expression involving the creation operator is then the respective adjoint for which one finds

$$\left(a^*(f)\Phi\right)^{(n)}(\mathbf{k}_1, \ldots, \mathbf{k}_n) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} f(\mathbf{k}_i) \phi^{(n-1)}(\mathbf{k}_1, \ldots, \widehat{\mathbf{k}}_i, \ldots, \mathbf{k}_n), \tag{47}$$

where the $\widehat{\mathbf{k}}_i$ denotes the omission of the variable $\mathbf{k}_i$ from the function arguments in $\phi^{(n-1)}$. As regards domains of these operators on $\mathcal{F}$, it is convenient to first establish a meaning for the informal expression of the free field Hamiltonian H^0_ω in (39) when acting on the n-mode wave functions of $\Phi \in \mathcal{F}$ as

$$\left(H^0_\omega \Phi\right)^{(n)}(\mathbf{k}_1, \ldots, \mathbf{k}_n) = \sum_{j=1}^{n} \omega(\mathbf{k}_j) \phi^{(n)}(\mathbf{k}_1, \ldots, \mathbf{k}_n). \tag{48}$$

It is well-known [86] that H^0_ω is a positive, unbounded, and self-adjoint operator whose domain shall be denoted by $D(H^0_\omega)$. Finally, for $f \in \mathfrak{h}$, the domains of $a(f), a^*(f)$ can be seen [85] to be dense and to lie in the form domain of H^0_ω, i.e., $D(\sqrt{H^0_\omega})$. For $f \notin \mathfrak{h}$, the corresponding annihilation operator $a(f)$ may still be well-defined provided the integral of the right-hand side of (46) exists. However, the domain of the creation operator $a^*(f)$ then only contains zero. Finally, it can now be checked that for all $f, g \in \mathfrak{h}$, the algebraic commutation relations (30) take the form

$$[a(f), a^*(g)] = \langle f, g \rangle_{\mathfrak{h}}, \qquad [a(f), a(g)] = 0, \qquad [a^*(f), a^*(g)] = 0, \tag{49}$$

where the operators on the left-hand side are bounded and densely defined such that they have a unique meaning on entire $\mathcal{F}$. In addition, there is one distinguished non-zero Fock space $\mathcal{F}$ element, more precisely a ray, called the vacuum state

$$\Omega = (1, 0, 0, \dots), \tag{50}$$

which, independently of f, fulfills

$$a(f)\Omega = 0. \tag{51}$$

The tuple (a, a^*, Ω) of creation and annihilation operators (45) together with the vacuum (50) fulfilling (49) and (51) furthermore characterizes the Fock space $\mathcal{F}$ as the completion of all finite linear combinations of creation and annihilation operators acting on Ω. It must be emphasized that the explicit choice of (50) is not necessarily needed in computations of expectation values and the implicit relation (51) together with commutation relations (49) already suffice to define a Fock space. This allows to define Fock spaces for other choices of representations (a, a^*, Ω) obeying the relations (49) and (51). The explicit choice of Ω can be seen as a choice of a reference state with respect to which the corresponding creation and annihilation operators introduce or relax excitations relative to this reference. The Fock space resulting from the particular specification (50) is called the standard Fock space. It should be noted that, physically, the latter choice is somewhat artificial as charges always carry a non-zero near-fields which is already implied by (24) in the simple model at hand and discussed in the next paragraph. Although this jargon, which is also used in the following, may suggest that there are many Fock spaces, mathematically, one may rightfully argue that there is only one Hilbert space and it is only the interpretation of its elements that is a changing according to the choice of representation (a, a^*, Ω).

Deficiency D1. One may now be inclined to give the field operator φ that was informally defined in (31) a mathematical meaning for time $t = 0$ as

$$\varphi(0, \mathbf{x}) = a\left(\mathbf{k} \mapsto \gamma(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}\right) + a^*\left(\mathbf{k} \mapsto \gamma(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}\right). \tag{52}$$

However, due to the behavior of the form factor

$$\gamma(\mathbf{k}) = O_{|\mathbf{k}|\to\infty}\left(|\mathbf{k}|^{-1/2}\right), \tag{53}$$

the decay at high momenta, commonly referred to as the ultraviolet regime, is not sufficient to ensure square-integrability, and thus, $\gamma \notin \mathfrak{h}$. In turn, at least the creation operator in (52) is ill-defined on all Fock space elements except zero. It is important to emphasize once again that the form factor $\gamma(\mathbf{k})$ was predetermined by the Klein-Gordon equation (19) and the choice of Pauli-Jordan function Δ in the commutation relation (20) which later implies the types of source in (24) by means of (29).

This tension between the regularity of solutions of the inhomogeneous Klein-Gordon equation (24) and the requirement of square-integrability of the excitation wave functions relative to a vacuum in a Fock space representation can be seen as one origin of the deficiency D1, i.e., the *ultraviolet divergence* of bosonic fields mediating the interaction mentioned in the introduction in Section 2.1. One may therefore ask if this might just be a homemade problem due to the choice of standard Fock space representation of (a, a^*, Ω) in (50). As will be explained next by means of a toy model, the answer turns out to be partly yes but partly no. Yes, because in certain settings, there are better choices for the vacuum Ω swallowing those modes that are not square-integrable, but no, because these models inherently contain an ill-defined self-interaction much like the one in classical electrodynamics [100]. In other words, D1 presents itself as a two-faced problem, the first one directed towards the Fock representations, and the second one towards a much more fundamental issue in quantum field theory which questions the sanity of the proposed equation of motion (42).

In order to substantiate this partly yes-and-no-type answer, it suffices to regard the following simplified model Hamiltonian

$$H^\Lambda = H^0_\omega + g\sum_{i=1}^N \varphi^\Lambda(\mathbf{x}_i), \qquad H^0_\omega = \int d^3k\, \omega(\mathbf{k}) a^*_\mathbf{k} a_\mathbf{k}, \tag{54}$$

which is derived from (42) by setting the dispersion of the charges H^0_k to zero and, in view of (52), replacing the time-zero field $\varphi(0, \mathbf{x}_i)$ by

$$\varphi^\Lambda(\mathbf{x}) = a\left(\mathbf{k} \mapsto \gamma^\Lambda(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}\right) + a^*\left(\mathbf{k} \mapsto \gamma^\Lambda(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}\right), \tag{55}$$

for a Λ-parametrized choice of form factors obeying

$$\forall\, \Lambda < \infty: \quad \gamma^\Lambda \in \mathfrak{h}, \qquad \text{and} \qquad \forall\, \mathbf{k} \in \mathbb{R}^3: \quad \lim_{\Lambda\to\infty} \gamma^\Lambda(\mathbf{k}) = \gamma(\mathbf{k}). \tag{56}$$

The parameter $0 \leqslant \Lambda < \infty$ tunes the cut-off or suppression of the problematic ultraviolet momenta to ensure $\gamma^\Lambda \in \mathfrak{h}$ for $\Lambda < \infty$ and allows to reinstate the original form factor γ in the limit $\Lambda \to \infty$. As exemplified in (35), this can be achieved by introducing a smearing with an extended charge distribution $\rho^\Lambda \in C^\infty_c(\mathbb{R}^3, \mathbb{R})$ on the scale of Λ^{-1} in positions space that approaches Dirac's delta distribution in the limit $\Lambda \to \infty$, or alternatively, if geometry or smoothness does not play a role, simply by means of a hard cut-off of all momenta $|\mathbf{k}| > \Lambda$, i.e., $\gamma^\Lambda(\mathbf{k}) = \gamma(\mathbf{k})\, 1_{|\mathbf{k}|\leqslant\Lambda}$. For the following discussion, the particular choice is not relevant as long as the properties in (56) are fulfilled. As it is well-known from [79] or [86, 85], the unbounded operator $\varphi^\Lambda(\mathbf{x})$, and hence H^Λ in (54), can be given a meaning as essentially self-adjoint operators on $\mathcal{F}$ on domain $D(H^\Lambda) = D(H^0_\omega)$. Physically, this toy model describes a quantum scalar field for N charges at fixed classical positions $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^3$, or in view of (42), with infinitely heavy charges. This model is simple enough to be solved explicitly, see [90] in case $N = 1$, and thus, allows for a directly accessible heuristic interpretation. Nevertheless, it contains all the structure needed to comprehensively expose and discuss the deficiencies D1 and D2. Therefore, many remarks in the reports on the works [A3-6] of the later sections will refer back to this and the next paragraph.

As can be checked by direct computation, for $\Lambda < \infty$, the linear transformation T^Λ on Fock space

$$T^\Lambda a_\mathbf{k} T^{\Lambda *} = a_\mathbf{k} - g\sum_{j=1}^N \frac{\gamma^\Lambda(\mathbf{k})}{\omega(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{x}_j}, \tag{57}$$

$$T^\Lambda a^*_\mathbf{k} T^{\Lambda *} = a^*_\mathbf{k} - g\sum_{j=1}^N \frac{\gamma^\Lambda(\mathbf{k})}{\omega(\mathbf{k})} e^{+i\mathbf{k}\cdot\mathbf{x}_j}, \tag{58}$$

using the notation (45), is well-defined and unitary, and furthermore turns the Hamiltonian H^Λ in (54) into

$$\tilde{H}^\Lambda := T^\Lambda H^\Lambda T^{\Lambda *} = H^0_\omega - \frac{g^2}{2}\sum_{i,j=1}^N V^\Lambda(\mathbf{x}_i - \mathbf{x}_j), \quad \text{for} \quad V^\Lambda(\mathbf{x}) = 2\int d^3k\, \frac{\gamma^\Lambda(\mathbf{k})^2}{\omega(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{x}}. \tag{59}$$

Instead of transforming the Hamiltonian, one may also simply change the representation from standard Fock representation (a, a^*, Ω) to a new one $(\tilde{a}^\Lambda, \tilde{a}^{\Lambda *}, \tilde{\Omega}^\Lambda)$ defined by

$$\tilde{a}^\Lambda_\mathbf{k} := T^{\Lambda *} a_\mathbf{k} T^\Lambda, \qquad \tilde{a}^{\Lambda *}_\mathbf{k} := T^{\Lambda *} a^*_\mathbf{k} T^\Lambda, \qquad \tilde{\Omega}^\Lambda := T^{\Lambda *}\Omega. \tag{60}$$

In this representation, also the original Hamiltonian is of this particular simple form

$$H^\Lambda = \int d^3k\, \omega(\mathbf{k}) \tilde{a}_{\mathbf{k}}^{\Lambda *} \tilde{a}_{\mathbf{k}}^{\Lambda} - \frac{g^2}{2} \sum_{i,j=1}^{N} V^\Lambda(\mathbf{x}_i - \mathbf{x}_j) \tag{61}$$

which allows to readily read off its ground state. The latter is given by the new vacuum $\tilde{\Omega}^\Lambda$ whose representation back in standard Fock representation reads

$$\tilde{\Omega}^\Lambda = \sum_{n=0}^{\infty} \int d^3k_1 \dots \int d^3k_n\, \tilde{\Omega}^{\Lambda,(n)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \frac{1}{\sqrt{n!}} a^*_{\mathbf{k}_1} \dots a^*_{\mathbf{k}_n} \Omega \tag{62}$$

$$\tilde{\Omega}^{\Lambda,(n)}(\mathbf{k}_1, \dots, \mathbf{k}_n) = \frac{1}{\sqrt{Z^\Lambda}} \frac{(-g)^n}{\sqrt{n!}} \prod_{i=1}^{n} \sum_{j=1}^{N} \frac{\gamma^\Lambda(\mathbf{k}_i)}{\omega(\mathbf{k}_i)} e^{-i\mathbf{k}_i \cdot \mathbf{x}_j}, \tag{63}$$

where

$$Z^\Lambda = \exp\left(g^2 \left\| \mathbf{k} \mapsto \sum_{j=1}^{N} \frac{\gamma^\Lambda(\mathbf{k})}{\omega(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{x}_j} \right\|_{\mathfrak{h}}^2 \right) \tag{64}$$

is a normalization constant ensuring $\|\tilde{\Omega}^\Lambda\|_{\mathcal{F}} = 1$. The following observations can be made:

1. For $\Lambda \to \infty$, V^Λ converges to the Yukawa potential $V(\mathbf{x}) = \frac{\exp(-\mu|\mathbf{x}|)}{4\pi|\mathbf{x}|}$. Hence, the $i = j$ terms $V^\Lambda(0)$ in the sum of the Hamiltonian (59) obviously diverge. Returning to the discussion of the two rather distinct kinetic effects of the interaction (24) between the charges and the field, these problematic terms may be interpreted as the i-th particle acting back on itself by instantaneous emission and absorption of field modes – notably, much like in classical electrodynamics for which the divergence in total energy is also linear in Λ. However, for all $\Lambda < \infty$, the self-interaction terms $i = j$ are only constants in this simple toy model and dropping them from the transformed Hamiltonian (59) yields a renormalized one

$$\tilde{H}^{\text{ren},\Lambda} = H^0_\omega - g^2 \sum_{1 \leqslant i < j \leqslant N} V^\Lambda(\mathbf{x}_i - \mathbf{x}_j) \tag{65}$$

that changes the original dynamics only by a constant phase. The latter Hamiltonian (65) can obviously be given a mathematical sense as self-adjoint operator despite the limit $\Lambda \to \infty$. For $N > 1$, the only interaction left is contained in the effective Yukawa potentials between the charges. This separation of the two-fold kinetic nature of the interaction is not as cleanly possible once the charges are not fixed anymore but are allowed to disperse. While in the toy model above, the self-interaction terms only change the rest energy, in models with non-trivial dispersion relation for the charges, it turns out that they give rise to an effective inertia of the charges similarly as in classical electrodynamics; see report on the work [A4] in Section 2.2.4.

2. Looking more closely at the transformation T^Λ, which allowed to extract the divergent self-energies $V^\Lambda(0)$ and arrive at the renormalized transformed Hamiltonian (65), reveals that it is only well-defined for $\Lambda < \infty$ due to the fact that the amplitudes $\frac{\gamma^\Lambda}{\omega}$ on the right-hand side of (57) are only square integrable for $\Lambda < \infty$. For the same reason, the ground state $\tilde{\Omega}^\Lambda$ in (63) also leaves the standard Fock space $\mathcal{F}$ as $\Lambda \to \infty$. However, this problem can be swept under the rug by the mentioned change to Fock representation $(\tilde{a}^\Lambda, \tilde{a}^{\Lambda *}, \tilde{\Omega}^\Lambda)$. Though

this representation is Λ dependent, all respective computations of expectation values will be independent of Λ as can be seen from the right-hand sides of the relations

$$\left[\tilde{a}^{\Lambda}(f), \tilde{a}^{\Lambda *}(g)\right] = \langle f, g\rangle_{\mathfrak{h}}, \quad \left[\tilde{a}^{\Lambda}(f), \tilde{a}^{\Lambda}(g)\right] = 0, \quad \left[\tilde{a}^{\Lambda *}(f), \tilde{a}^{\Lambda *}(g)\right] = 0, \quad \tilde{a}^{\Lambda}\tilde{\Omega}^{\Lambda} = 0. \tag{66}$$

In this new representation, the self-energy terms can again be dropped from the original Hamiltonian (61), analogously to what was done for (65), to find the renormalized version

$$H^{\text{ren},\Lambda} = H^{\Lambda} - \frac{g^2}{2}\sum_{i=1}^{N} V^{\Lambda}(0) = \int d^3k\, \omega(\mathbf{k})\tilde{a}_{\mathbf{k}}^{\Lambda *}\tilde{a}_{\mathbf{k}}^{\Lambda} - g^2 \sum_{1\leqslant i<j\leqslant N} V^{\Lambda}(\mathbf{x}_i - \mathbf{x}_j). \tag{67}$$

Again, due to the Λ independence of the relations (66), this Hamiltonian can be given a meaning as self-adjoint operator even for $\Lambda \to \infty$. However, one needs to note that the representations (a, a^*, Ω) and $(\tilde{a}^{\Lambda}, \tilde{a}^{\Lambda *}, \tilde{\Omega}^{\Lambda})$ are not related by a unitarily transformation in the limit $\Lambda \to \infty$ and their vacua have different physical interpretations. While Ω represents an unphysical state containing no field modes at all, $\tilde{\Omega}^{\Lambda}$ represents the ground state containing the Yukawa near-field modes that are attached to the charges.

This shows the two faces of deficiency D1 more clearly and explains the partly yes-and-no-type of answer to the question, whether D1 is only a homemade problem of the particular choice of representation. While observation 2 above gives a positive answer by showing that the non-square-integrable field modes of the ground state can successfully be hidden in the vacuum of the new representation, observation 1 shows that the self-interaction causes a more fundamental problem, namely the presence of the divergent self-interaction terms which are unaffected by a change of representation and have to be removed by hand. As it turns out, these self-interaction terms are inherent in all scalar field models in a similar way as in their classical analogues.

As mentioned before, it should again be noted that the annihilation operator $a(f)$ is a bit better behaved than its adjoint. It can be given a meaning as densely defined operator even for $f \notin \mathfrak{h}$ as long as the corresponding integral (46) exists. On the contrary, $a^*(f)$ for $f \notin \mathfrak{h}$ simply has domain $\{0\}$. One may exploit this fact and attempt to define the generator of the time evolution by means of a quadratic form in which the creation operator is to be interpreted as annihilation operator acting to the left, thus, avoiding the problem of defining φ in (52) as an operator on Fock space in the first place. Such a strategy was successfully pursued in Nelson's famous work [79], in which the more complicated model (42) with H_k^0 comprising the Schrödinger dispersion was studied. In particular, the dynamics was shown to exist after an energy renormalization even when removing the cut-off Λ, which will be reviewed in the report on work [A3] in Section 2.2.3. Unfortunately, this strategy does not work for relativistic dispersion of the charges, which will be discussed in detail in the report on work [A4] in Section 2.2.4.

Deficiency D2. In the case of a massless scalar field, i.e., $\mu = 0$, one observes another representational problem. Even with an ultraviolet cut-off $\Lambda < \infty$ in place, the ground state $\tilde{\Omega}^{\Lambda}$ in (63) leaves the standard Fock space for $\mu \to 0$. This is caused by the singular behavior of its amplitudes

$$\left.\frac{\gamma^{\Lambda}(\mathbf{k})}{\omega(\mathbf{k})}\right|_{\mu=0} = O_{|\mathbf{k}|\to 0}\left(|\mathbf{k}|^{-3/2}\right), \tag{68}$$

which are not square-integrable. This behavior does not affect the finite time dynamics. In fact, the self-adjointness result of the Hamiltonian H^{Λ} holds for all $\mu \geqslant 0$. However, in the long-time limit $t \to \infty$ of scattering theory, an initial state, e.g., in standard Fock space, would decay into the ground state $\tilde{\Omega}^{\Lambda}$ in (63) with additional asymptotically outgoing field modes, a state that due to

(68) is not anymore in standard Fock space for $\mu = 0$. This behavior is referred to as the *infrared catastrophe* of massless bosonic fields mediating the interaction, i.e., deficiency D2 as mentioned in the introduction in Section 2.1. Unlike the two-faced deficiency D1, at least in principle, D2 can always be remedied by a change of representation. In the simple toy model of fixed charges (54), one may simply employ the same transformation T^Λ as described in observation 2 of D1 above and change the representation to $(\tilde{a}^\Lambda, \tilde{a}^{\Lambda *}, \tilde{\Omega}^\Lambda)$ in (60) in order to hide the non-square-integrable amplitudes. However, in settings in which also the charges take part in the dynamics, it turns out to be rather difficult to identify such convenient representations since they directly depend on the dynamics of the charges. To illustrate this behavior, let us consider a single classical charge moving with constant velocity $\mathbf{v} \in \mathbb{R}^3$ and interacting with its quantized field as described by the time-dependent interaction picture Hamiltonian

$$H^\Lambda_{\mathbf{v}} = g\varphi^\Lambda(t, \mathbf{v}t). \tag{69}$$

This model was considered in [68] where the following scattering state with n-mode wave functions

$$\tilde{\Omega}^{\Lambda,(n)}_{\mathbf{v}}(\mathbf{k}_1, \ldots, \mathbf{k}_n) = \frac{1}{\sqrt{Z^\Lambda}} \frac{(-g)^n}{\sqrt{n!}} \prod_{i=1}^{n} \frac{\gamma^\Lambda(\mathbf{k}_i)}{\omega(\mathbf{k}_i) - \mathbf{k} \cdot \mathbf{v}}, \qquad n \in \mathbb{N}_0, \tag{70}$$

was computed, again for Z^Λ denoting the normalization constant such that $\|\tilde{\Omega}^\Lambda_{\mathbf{v}}\|_{\mathcal{F}} = 1$. Despite the simplicity of the model, one readily observes a dependence on the dynamics of the charges and the implications on the corresponding Fock representations. Not only do the states $\tilde{\Omega}^\Lambda_{\mathbf{v}}$ leave the standard Fock space for $\mu \to 0$, neither two states $\tilde{\Omega}^\Lambda_{\mathbf{v}}$ and $\tilde{\Omega}^\Lambda_{\mathbf{v}'}$ for $\mathbf{v}, \mathbf{v}' \in \mathbb{R}^3$ are Fock states with respect to the same representation unless $\mathbf{v} = \mathbf{v}'$. Although, for $\mu > 0$, there are unitary transformations $T^\Lambda_{\mathbf{v}}$, $\mathbf{v} \in \mathbb{R}^3$, much like (57) above, such that $\tilde{\Omega}^\Lambda_{\mathbf{v}} = T^\Lambda_{\mathbf{v}}\Omega$ holds true and the anticipated singularities in (70) arising from $\mu \to 0$ are absorbed in the corresponding representation $(\tilde{a}^\Lambda_{\mathbf{v}}, \tilde{a}^{\Lambda *}_{\mathbf{v}}, \tilde{\Omega}^\Lambda_{\mathbf{v}})$ given by

$$\tilde{a}^\Lambda_{\mathbf{v},\mathbf{k}} := T^{\Lambda *}_{\mathbf{v}} a_{\mathbf{k}} T^\Lambda_{\mathbf{v}}, \qquad \tilde{a}^{\Lambda *}_{\mathbf{v},\mathbf{k}} := T^{\Lambda *}_{\mathbf{v}} a^*_{\mathbf{k}} T^\Lambda_{\mathbf{v}}, \tag{71}$$

the map $T^{\Lambda *}_{\mathbf{v}'} T^\Lambda_{\mathbf{v}}$ survives the limit $\mu \to 0$ only for $\mathbf{v} = \mathbf{v}'$. Hence, for different velocities $\mathbf{v} \in \mathbb{R}^3$, the representations $(\tilde{a}^\Lambda_{\mathbf{v}}, \tilde{a}^{\Lambda *}_{\mathbf{v}}, \tilde{\Omega}^\Lambda_{\mathbf{v}})$ are not unitarily equivalent. For more general models in which the charges are allowed to disperse and interact with their field, this behavior becomes much more complicated to track. In order to build a scattering theory, usually a sophisticated technology has to be developed, e.g., [84, 20], in order to identify the so-called super-selection rules that allow to discern convenient representations.

Mathematically, at least in the class of Hamiltonians considered in (42), such studies are accompanied by another difficulty as the limit $\mu \to 0$ implies the closure of the spectral gap between the ground state energy and the continuous spectrum above it. Since the spectral gap is an essential ingredient for analytic perturbation theory usually employed to analyze these models, substantial efforts are needed to control the model for $\mu \to 0$, see in particular [83]. In Section 2.2.3, the work [A3] will be discussed which allows to control the mass shell of the Nelson model under simultaneous removal of the infrared and ultraviolet cut-offs. Furthermore, in Section 2.2.5, the works [A5-6] are discussed in which, despite the infrared divergent behavior, a technique to control the long-time limits in the Spin-Boson model is demonstrated.

After this introduction to the class of scalar field models and their immanent deficiencies D1 and D2, the rest of this report turns to their rigoros study. The typical approach is, in a first step, to introduce some kind of ultraviolet and infrared regularization that remedies D1 and D2, respectively, and to investigate the well-posedness of the corresponding initial value problem. In a second step, one studies the behavior of the model when the cut-offs are attempted to be removed in order to identify a suitable renormalization procedure. Therefore, this section closes with a report on work [A2] in which the existence of the dynamics of the original multi-time model (18), (19), and (21) featuring an ultraviolet regularization is proven. This complements the classical literature that predominantly studied the derived single-time models (42).

Existence of dynamics of the multi-time system. Turning to the question of existence of the dynamics for (18), (19), and (21), the first task is to give the right-hand side of (18) a mathematical meaning. For this purpose, it will be convenient to regard smooth maps of the type

$$\psi : \mathbb{R}^N \to \mathcal{H}, \qquad (t_1, \ldots, t_N) \mapsto \psi(t_1, \ldots, t_N) \tag{72}$$

for a target domain

$$\mathcal{H} = L^2(\mathbb{R}^{3N}, \mathcal{F}^K) \cong L^2(\mathbb{R}^{3N}, \mathbb{C}) \otimes \mathcal{F}^K \cong L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathcal{F} \tag{73}$$

as solution candidates. The constant $K = 4^N$ counts the number of spin degrees of freedom for N spin $1/2$ charges. The three tensor product spaces on the right-hand side of (73) are isomorphic and isometric and will all be identified with the same symbol $\mathcal{H}$ and used interchangeably in the notation. In particular, the one on the right allows to easily carry over the Fock space formalism as introduced previously while the one on the left allows to focus on the properties of the multi-time wave functions and temporarily forget about the Fock degrees of freedom in computations. An element $\phi \in \mathcal{H}$ can thus be thought of as an N-particle wave function taking values in the Fock space $\mathcal{F}$, i.e., for a.e. $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^3$, the element ϕ may be evaluated to give a sequence of n-mode wave functions $(\phi^{(n)}(\mathbf{x}_1, \ldots, \mathbf{x}_N))_{n \in \mathbb{N}_0}$, each of which may in turn be evaluated at a.e. $\mathbf{k}_1, \ldots, \mathbf{k}_n \in \mathbb{R}^3$ to give a value $\phi^{(n)}(\mathbf{x}_1, \ldots, \mathbf{x}_N; \mathbf{k}_1, \ldots, \mathbf{k}_n)$ in $\mathbb{C}^K$.

In this setting, the definition of the annihilation and creation operators as given in (46) and (47) can readily be implemented as follows

$$a(f) \equiv 1_{L^2(\mathbb{R}^3, \mathbb{C}^K)} \otimes a(f), \qquad a^*(f) \equiv 1_{L^2(\mathbb{R}^3, \mathbb{C}^K)} \otimes a^*(f), \qquad H^0_\omega \equiv 1_{L^2(\mathbb{R}^3, \mathbb{C}^K)} \otimes H^0_\omega \tag{74}$$

for $f \in \mathfrak{h}$. Those can now be employed to give φ on the right-hand side of the multi-time equations (18) a mathematical meaning. However, as discussed previously, this requires the introduction of a regularization. Unfortunately, this introduces a further complication as it also impacts the integrability condition (21). The geometric nature of this complication can best be made apparent using a regularization by means of an extended charge density ρ, as exemplified in (35), that is smooth and compactly supported in a ball of diameter $\delta > 0$ around the origin, i.e.,

$$\rho \in C^\infty_c(\mathbb{R}^3, \mathbb{R}), \qquad \operatorname{supp} \rho \subseteq B_\delta(0). \tag{75}$$

As this regularization will be kept fixed, the notation can be simplified by introducing an abbreviation for the action of the resulting field operator φ comprising both the regularization and the evaluation at the respective particle position $\mathbf{x}_j$ as follows

$$\left(\varphi_j(t)\phi\right)(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \varphi(t, \mathbf{x}_j)\phi(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{76}$$

at least for ϕ in the respective domain. In the notation of (45), the field operator then takes the form

$$\varphi(t, \mathbf{x}_j) = \int d^3k \, \frac{1}{(2\pi)^{3/2}} \frac{\widehat{\rho}(\mathbf{k})}{\sqrt{2\omega(\mathbf{k})}} \left(a_{\mathbf{k}} e^{-i\omega(\mathbf{k})t + i\mathbf{k}\cdot\mathbf{x}_j} + a^*_{\mathbf{k}} e^{i\omega(\mathbf{k})t - i\mathbf{k}\cdot\mathbf{x}_j} \right). \tag{77}$$

The geometric impact on Dirac's integrability constraint (21) can be read off the following relation

$$[\varphi(x), \varphi(y)] = i\rho *_{\mathbf{x}} \rho_{\mathbf{y}} * \Delta(x - y), \tag{78}$$

where $*_{\mathbf{x}}$ and $*_{\mathbf{y}}$ again denote convolutions in the $\mathbf{x}$ and $\mathbf{y}$ coordinates, respectively. Hence, after regularization, Dirac's integrability constraint cannot be fulfilled anymore on entire $\mathcal{S}^N$, as defined in (13). In order to allow for a path-independent integration of the multi-time evolution (18), and thus, an unambiguous definition of the values of a potential solution ψ for certain space-time configurations, the set of admissible configurations needs to be restricted as follows

$$\mathcal{S}_\delta^N := \left\{(x_1, \ldots, x_N) \in \mathbb{R}^{4N} \,\middle|\, \forall\, k \neq l : t_k = t_l \vee |x_k^0 - x_l^0| + \delta < |\mathbf{x}_k - \mathbf{x}_l|\right\}, \tag{79}$$

for $\delta > 0$. It should be noted that this definition coincides with the previously defined $\mathcal{S}^N$ in (13) in the limit $\delta \to 0$.

Opposed to the introduced notion of maps of the type (72) as suggested above, a seemingly more natural notion for strong solutions to the multi-time system (18), (19), and (78) may now appear to be smooth maps of the type

$$\psi : \mathcal{S}_\delta^N \to \mathcal{F}^K. \tag{80}$$

At least, this would avoid regions in the set of space-time configurations $\mathbb{R}^{4N}$ for which the value of ψ cannot be defined unambiguously due to the violation of the integrability constraint (78). But this advantage comes with two drawbacks.

As first drawback, $\mathcal{S}_\delta^N$ is not an open set in $\mathbb{R}^4$ so that partial time derivatives cannot always be straightforwardly defined. Therefore, the following notion of partial derivatives was adopted from [80]: Each point $x \in \mathcal{S}_\delta^N$ defines a partition of the set of $\{1, \ldots, N\}$ into non-empty disjoint subsets $P_1, \ldots, P_L$ by means of the equivalence relation given by the transitive closure of the relation that holds between k and l if and only if $|t_k - t_l| + \delta \geqslant |\mathbf{x}_k - \mathbf{x}_l|$. All points x_k, x_l for k, l in a partition P_i necessarily fulfill $t_k = t_l$ and this common time coordinate is denoted by t_{P_i}. The partial derivative with respect to t_{P_i} can hence be defined for $\psi : \mathbb{R}^N \to \mathcal{H}$ a.e. as follows

$$\left(\frac{\partial}{\partial t_{P_i}} \psi(t_1, \ldots, t_N)\right)(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{j \in P_i} \left(\frac{\partial}{\partial t_j} \psi(t_1, \ldots, t_N)\right)(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{81}$$

provided the partial derivatives on the right-hand side exist. In the following, a ψ as given in (80) is called smooth if for all configurations in $\mathcal{S}_\delta^N$ all corresponding derivatives ∂_{P_i} are well-defined.

The second drawback of the notion (80) is that it does not allow to easily exploit the classical results of functional analysis. Luckily, by definition, only sequences of configurations in $\mathcal{S}_\delta^N$ are required to obtain the corresponding limits involved in the derivatives ∂_{P_i}. Hence, the value of a potential solution ψ on $\mathcal{S}_\delta^N$ and its relevant derivatives does not depend on configurations outside of $\mathcal{S}_\delta^N$. But such values are anyhow the only ones that have a chance to be unambiguously defined thanks to the path-independence of the integration of the multi-time equations (18) that is shown to be enforced by the integrability constraint (78) in [A2]. Hence, with sufficient regularity, it is possible to extract from potential solutions ψ, in the sense of notion (72), potential solutions in the sense of (80) by restricting the former to $\mathcal{S}_\delta^N$. Vice versa, potential solutions of type (80) can be extended to type (72) by specifying arbitrary values outside of $\mathcal{S}_\delta^N$ because, as also shown in [A2], the values outside $\mathcal{S}_\delta^N$ do not influence the evolution on $\mathcal{S}_\delta^N$. This observation is one of the main technical ingredients in [A2] that allows to exploit functional analysis results of the classical literature.

With the introduced notation, it is possible to state the solution sense and the existence of dynamics result of [A2] for the regularized version of Dirac's original multi-time system (18), (19), and (21) for the following N Hamiltonians

$$H_k(t) = H_k^0 + g\varphi_k(t), \qquad k = 1, \ldots, N, \tag{82}$$

where H_k^0 denotes the free Dirac Hamiltonian of the kth particle, see (170) below, and $\varphi_k(t)$ is given in (76)-(77). One should note that, thanks to the Fock representation by means of creation and annihilation operators and by definitions of $\omega(\mathbf{k})$ and $\gamma(\mathbf{k})$, the regularized field φ in (77) automatically fulfills the free field equation (19) and the regularized version of Dirac's integrability constraint (78).

Due to the described complications that are introduced by the regularization, the solution sense will be defined as follows:

Definition 2.2 (Multi-time solution sense)**.** *A map $\psi : \mathbb{R}^N \to \mathcal{H}, (t_1, \ldots, t_N) \mapsto \psi(t_1, \ldots, t_N)$ is called a solution of the regularized multi-time solution if the following properties are fulfilled:*

1. *(Time regularity) ψ is differentiable.*
2. *(Point-wise evaluation) For all configurations $(x_1, \ldots, x_N) \in \mathcal{S}_\delta^N$ and $k = 1, \ldots, N$, the following point-wise evaluations are well-defined:*

$$(\psi(t_1, \ldots, t_N))\,(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{83}$$
$$(\partial_{t_k}\psi(t_1, \ldots, t_N))\,(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{84}$$
$$\big(H_j(t_k)\psi(t_1, \ldots, t_N)\big)\,(\mathbf{x}_1, \ldots, \mathbf{x}_N). \tag{85}$$

3. *(Evolution equations) For all $(x_1, \ldots, x_N) \in \mathcal{S}_\delta^N$ with corresponding partitions $P_1, \ldots, P_L$, for an $L \in \{1, \ldots, N\}$, the following equations hold true:*

$$\left(\partial_{t_{P_k}}\psi(t_1, \ldots, t_N)\right)(\mathbf{x}_1, \ldots, \mathbf{x}_N) = (H_{P_k}\psi(t_1, \ldots, t_N))\,(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{86}$$

where the partial Hamiltonians are given by

$$H_{P_k} = \sum_{j \in P_k} H_j(t_{P_k}). \tag{87}$$

Compared to classical existence results for single-time quantum systems, one notes the prominent regularity requirement. This additional requirement allows to restrict the solutions sense conveniently to the relevant domain $\mathcal{S}_\delta^N$ of space-time configuration space $\mathbb{R}^{4N}$. In the future, this condition may be relaxed by regarding solutions as distributions acting on test functions supported in $\mathcal{S}_\delta^N$ only, but this generalization was not thematized in [A2]. The main results of [A2] are summarized in the following theorem:

Theorem 2.3 (Dirac-Fock-Podolsky multi-time dynamics [A2])**.** *Let*

$$\psi^0 \in \mathcal{D} := C_c^\infty(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathcal{F} \bigcap L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \left(\bigcap_{n \in \mathbb{N}} D\left((H_\omega^0)^n\right) \right). \tag{88}$$

1. *(Existence) There exists a multi-time solution ψ in the sense of Definition 2.2 with initial value ψ_0, i.e.,*

$$\psi(t_1, \ldots, t_N)\big|_{t_1, \ldots, t_N = 0} = \psi^0. \tag{89}$$

2. *(Uniqueness) Furthermore, if $\widetilde{\psi}$ is another multi-time solution with initial value ψ^0, then $\widetilde{\psi}$ and ψ coincide on S_δ^N, i.e., for all $(x_1, \ldots, x_N) \in \mathcal{S}_\delta^N$, the following equality holds*

$$\big(\widetilde{\psi}(t_1, \ldots, t_N)\big)\,(\mathbf{x}_1, \ldots, \mathbf{x}_N) = (\psi(t_1, \ldots, t_N))\,(\mathbf{x}_1, \ldots, \mathbf{x}_N). \tag{90}$$

3. *(Regularity) For $t_1, \ldots, t_N \in \mathbb{R}$, the multi-time solution ψ fulfills*

$$\psi(t_1, \ldots, t_N) \in \mathcal{D}. \tag{91}$$

There are several technical inconveniences to be accounted for in the strategy of proof. Due to the fact that the free Dirac Hamiltonians H_k^0 are not bounded from below, the time-zero fields $\varphi(0, \mathbf{x}_k)$ cannot directly be controlled as perturbations of $H_k^0 + H_\omega^0$ in the Schrödinger picture. For this purpose, a self-adjointness result by Arai [2] was employed as main ingredient to define single-time evolutions $(U_{P_k}(t))_{t\in\mathbb{R}}$ generated by the partial Hamiltonians H_{P_k} for relevant partitions P_k. Candidate solutions of the type (72) are then generated by means of concatenation of partial time evolutions (86). For example, for the special case of only two charges $N = 2$ and times $t_2 > t_1$, a candidate solution may be constructed by

$$\psi(t_1, t_2) = U_{\{1\}}(t_1, t_2) U_{\{1,2\}}(t_2, 0)\psi^0, \tag{92}$$

which, loosely speaking, comprises a single-time evolution for both charges from initial value ψ^0 at times zero forward to the largest time t_2 and afterwards a backwards evolution in the tensor component of the first charge to time t_1. Thanks to initial regularity, the candidate ψ readily fulfills (86) for $k = 1$, however, for $k = 2$ one needs to show that H_2 commutes with $U_{\{1,2\}}$, at least when acting on sufficient regular functions evaluated on admissible configurations $\mathcal{S}_\delta^N$. In order to show the respective commutator relation, one has to exploit Dirac's regularized constraint (78) and the fact that the evolutions generated by H_k are causal, and thus, affect respective supports only within light-cones. For those arguments, point-wise evaluation is very helpful for which the invariance of the domain $\mathcal{D}$ over time is controlled with the help of a powerful commutator technique similar to the one described in [67].

Furthermore, in [A2] the question whether such solutions entail a relativistic interaction between the charges mediated by the field φ, cf. (24), is addressed by:

Theorem 2.4 (Dirac-Fock-Podolsky interaction [A2]). *Let $\psi^0 \in \mathcal{D}$, ψ the corresponding multi-time solution, and $\psi_t = \psi_{t_1,\ldots,t_N=t}$ for $t \in \mathbb{R}$, then*

$$(\square_{t,\mathbf{x}} + \mu^2) \langle \psi_t, \varphi(t,\mathbf{x})\psi_t \rangle_{\mathcal{H}} = -g \sum_{k=1}^{N} \left\langle \psi_t, \rho *_{\mathbf{x}} \rho *_{\mathbf{y}} \delta^3(\mathbf{x}-\mathbf{y})\big|_{\mathbf{y}=\hat{\mathbf{x}}_k} \psi_t \right\rangle \tag{93}$$

holds for all $t \in \mathbb{R}, \mathbf{x} \in \mathbb{R}^3$, where $\hat{\mathbf{x}}_k$ denotes the position multiplication operator of the k-th charge.

This concludes the discussion of regularized multi-time systems which set the stage for the corresponding single-time models of quantum field theory of Schrödinger-type (42). The next sections focus on the interaction between only $N = 1$ charge and its field and report on studies of the model properties while the corresponding regularizations in the ultraviolet and, for $\mu = 0$, also in the infrared are attempted to be removed.

2.2.3 Removal of the cut-offs for non-relativistic charges

This section comprises a report on the following article:

A3. *The Mass Shell of the Nelson Model without Cut-offs*, S. Bachmann, D.-A. Deckert, A. Pizzo, Journal of Functional Analysis, 263(5):1224, 58 pages, 2012

The openly accessible version arXiv:1104.3271 is attached in Section A, page 111.

In [A3], the single-time model introduced in (42) is studied for the case of a single, i.e., $N = 1$, non-relativistic, persistent, and spinless charge that interacts with its scalar field. In this case, the corresponding Hamiltonian takes the form

$$i\partial_t \Psi_t(\mathbf{x}) = \left(-\frac{\Delta_{\mathbf{x}}}{2M} + H_\omega^0 + g\varphi(0,\mathbf{x}) \right) \Psi_t(\mathbf{x}). \tag{94}$$

This model is commonly known as the Nelson model since its first rigorous study was conducted by Nelson [79] in 1964. As discussed in the previous section, due to the ill-defined nature of the field operator φ, the Hamiltonian expression in the parentheses on the right-hand side of (94) cannot be given a ready meaning unless a regularization such as (56) is introduced. Contrary to the setting of the work [A2] discussed in the previous section, the particular geometry of this regularization is of no importance here and one may employ the following simple choice by replacing $\varphi(0,\mathbf{x})$ in (94) with the expression

$$\varphi(\mathbf{x})|_\kappa^\Lambda = \int d^3k\, \gamma_\kappa^\Lambda(\mathbf{k}) \left(a_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} + a_\mathbf{k}^* e^{-i\mathbf{k}\cdot\mathbf{x}}\right), \qquad \gamma_\kappa^\Lambda(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \frac{1_{\kappa\leqslant|\mathbf{k}|\leqslant\Lambda}}{\sqrt{2\omega(\mathbf{k})}}, \qquad \omega(\mathbf{k}) = \sqrt{\mathbf{k}^2+\mu^2}, \tag{95}$$

for boson mass $\mu \geqslant 0$ and infrared and ultraviolet cut-off parameters $0 \leqslant \kappa \leqslant \Lambda < \infty$. As shown in [79], for this range of cut-offs, the regularized Hamiltonians

$$H|_\kappa^\Lambda = H^0 + g\varphi(\mathbf{x})|_\kappa^\Lambda, \qquad H^0 = -\frac{\Delta_\mathbf{x}}{2M} + H_\omega^0, \qquad H_\omega^0 = \int d^3k\, \omega(\mathbf{k}) a_\mathbf{k}^* a_\mathbf{k} \tag{96}$$

on Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}) \otimes \mathcal{F} \tag{97}$$

are essentially self-adjoint with domain $D(H|_\kappa^\Lambda) = D(H^0)$. It should be noted that this result includes the complete removal of the infrared cut-off, i.e., $\kappa = 0$, even for zero boson mass $\mu = 0$. As remarked in the discussion of deficiency D2 in Section 2.2.2, the infrared catastrophe is not an obstacle to the existence of dynamics. It can only lead to a representation problem of certain states in standard Fock spaces and introduces the technical difficulty of an absence of a spectral gap.

The remarkable main result of [79] ensures the existence of dynamics in the limit $\Lambda \to \infty$ after a so-called Gross transformation

$$T|_\kappa^\Lambda a_\mathbf{k} T|_\kappa^{\Lambda *} = a_\mathbf{k} - g\frac{\gamma_\kappa^\Lambda(\mathbf{k})}{\frac{\mathbf{k}^2}{2M} + \omega(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{98}$$

$$T|_\kappa^\Lambda a_\mathbf{k}^* T|_\kappa^{\Lambda *} = a_\mathbf{k}^* - g\frac{\gamma_\kappa^\Lambda(\mathbf{k})}{\frac{\mathbf{k}^2}{2M} + \omega(\mathbf{k})} e^{+i\mathbf{k}\cdot\mathbf{x}}, \tag{99}$$

using notation (45), is applied to the Hamiltonian $H|_\kappa^\Lambda$, see [59], and from it, a logarithmically divergent energy

$$V_{\text{self}}|_\kappa^\Lambda = -\frac{g^2}{2(2\pi)^3} \int_{\kappa\leqslant|\mathbf{k}|\leqslant\Lambda} d^3k \frac{1}{\omega(\mathbf{k})\left[\frac{|\mathbf{k}|^2}{2M} + \omega(\mathbf{k})\right]} \tag{100}$$

is subtracted. More precisely, for fixed infrared cut-offs $0 \leqslant \kappa$, it is shown that for the family of energy renormalized Hamiltonians

$$H'|_\kappa^\Lambda = T|_\kappa^\Lambda H|_\kappa^\Lambda T|_\kappa^{\Lambda *} - V_{\text{self}}|_\kappa^\Lambda, \qquad \Lambda < \infty, \tag{101}$$

there is a unique self-adjoint operator $H'|_\kappa^\infty$ with a domain being a subset of the form domain of H^0, i.e., $D(H'|_\kappa^\infty) \subset D\left(\sqrt{H^0}\right)$, such that for all $t \in \mathbb{R}$ and $\Psi \in \mathcal{H}$

$$\lim_{\Lambda\to\infty} e^{itH'|_\kappa^\Lambda}\Psi = e^{itH'|_\kappa^\infty}\Psi \tag{102}$$

holds true. Thanks to this result, the Nelson model has been one of the standard toy models in mathematical quantum field theory to study the deficiency D1.

It is interesting to observe the similarity to the energy renormalization that was employed in the toy model (54), cf. (59) and (65), of the previous section. The crucial difference between the Gross transformation and the one used in the toy model in (57) is the additional $\frac{\mathbf{k}^2}{2M}$ summand in the denominator of the amplitude on the right-hand side of (98) which originates from the Schrödinger dispersion relation $-\frac{\Delta_{\mathbf{x}}}{2M}$ of the charges. This additional term guarantees the square-integrability of these amplitude even in the limit $\Lambda \to \infty$. In turn, and contrary to the toy model case (57), the implied Gross transformation (98) remains well-defined in the limit $\Lambda \to \infty$. All corresponding representations of the commutation algebra (30) are therefore unitarily equivalent to the one on standard Fock space. Loosely speaking, in the Nelson model, the deficiency D1 is not two-faced as in the toy model (59). It resides exclusively in self-interaction and not in the choice of Fock representation. Furthermore, it should be noted that the self-energy term $V_{\text{self}}|_\kappa^\Lambda$ in (100) only diverges logarithmically as opposed to linearly in the case of $V^\Lambda(0)$ in (59) or in the energy of the classical analogue. Such observations were the source of hope that the quantum dispersion of the charges, and in non-persistent models also their fluctuations, would render the models sufficiently regular even though their classical analogues are ill-defined. The work [A4] presented in the next section, however, shows that this hope cannot be substantiated when considering more relativistic dispersions such as $\sqrt{-\Delta_{\mathbf{x}} + M^2}$.

Despite the success of removing the ultraviolet cut-off, it turns out that the underlying technique that controls the limit of the Hamiltonians $H'|_\kappa^\Lambda$, $\kappa \leqslant \Lambda < \infty$, in the spirit of the KLMN theorem on quadratic forms is rather abstract and provides little information on the particular expression and domain of the limiting Hamiltonian $H'|_\kappa^\infty$; for recent progress in characterization of its domain, see [72]. Shortly after Nelson's result [79], Cannon [17] was able to construct the mass shell $(E'_{\mathbf{P}}|_\kappa^\Lambda, \mathbf{P})_{|\mathbf{P}|<1}$ in the limit $\Lambda \to \infty$, where $E'_{\mathbf{P}}|_\kappa^\Lambda \in \mathbb{R}$ and $\mathbf{P} \in \mathbf{R}^3$ denote the spectral variables of the Hamiltonian $H'|_\kappa^\Lambda$ and the total momentum operator

$$\mathbf{P}_{\text{total}} = -i\nabla_{\mathbf{x}} + \mathbf{P}_{\text{field}}, \qquad \mathbf{P}_{\text{field}} = \int d^3k\, \mathbf{k}\, a^*_{\mathbf{k}} a_{\mathbf{k}}, \tag{103}$$

respectively. The field moment operator $\mathbf{P}_{\text{field}}$ is defined analogously to (48). Since the model is translation invariant, $H'|_\kappa^\Lambda$ and $\mathbf{P}_{\text{total}}$ commute. In order to compute the mass shell, one may therefore regard the natural decomposition of the Hamiltonian $H|_\kappa^\Lambda$ in terms of the total momentum fibers $\mathbf{P} \in \mathbb{R}^3$, i.e.,

$$H|_\kappa^\Lambda = \int_{\mathbb{R}^3}^{\oplus} d^3p\, H_{\mathbf{P}}|_\kappa^\Lambda, \tag{104}$$

and attempt to construct the corresponding spectral infima $E_{\mathbf{P}}|_\kappa^\Lambda$ of $H'_{\mathbf{P}}|_\kappa^\Lambda$ in the momentum fibers $\mathbf{P}$ of interest. Cannon succeeded in this construction for positive but sufficiently small coupling constants $|g|$ by employing analytic perturbation theory of quadratic forms with respect to the free Hamiltonian H^0. This technique moreover relies on the existence of a spectral gap which requires boson masses $\mu > 0$ and/or infrared cut-offs $\kappa > 0$. Only shortly after Cannon's result, Fröhlich [69] succeeded in a construction of the mass shell without a κ-dependence in the coupling constant and for arbitrarily small but positive infrared cut-offs $\kappa > 0$, even in the case of zero boson mass $\mu = 0$, which relied on a lattice approximation technique that was inspired by earlier works of Glimm and Jaffe.

However, both approaches in constructing the mass shell only provided rather implicit formulas for perturbative expansions of the energies $E'_{\mathbf{P}}|_\kappa^\Lambda$ making computations of approximations and respective errors rather intractable. These results were furthermore extended by a major advance by Pizzo [83] that allows to control the mass shell of the Nelson model for the range of cut-offs $0 \leqslant \kappa < \Lambda < \infty$, i.e., a fixed and finite ultraviolet cut-off, but now including the case of complete removal of the infrared cut-off $\kappa \to 0$. Contrary to the analytic perturbation of quadratic forms, the employed technique comprises a multi-scale perturbation analysis that can be applied on the level of operators, in particular, for the corresponding spectral projections of $H'_{\mathbf{P}}|_\kappa^\Lambda$, for sufficiently small positive Λ-dependent but otherwise uniform coupling constants $|g|$.

Construction of the mass shell while removing all cut-offs. With respect to the preceding results, the main advance of [A3] is a construction of the mass shell in the limit of complete removal of both the ultraviolet and infrared regularizations, including the case of zero boson mass $\mu = 0$.

Furthermore, tractable expansion formulas are provided similar to those in [83] but now for a sufficiently small range of positive coupling constants $|g|$ that is uniform in both cut-off parameters Λ and κ.

To put this result in perspective, it should be notated that already by means of standard analytic perturbation theory, one can show that the family of restricted fiber Hamiltonians

$$H'_{\mathbf{P}}|_{\kappa}^{\Lambda} \upharpoonright \mathcal{F}|_{\kappa}^{\Lambda}, \qquad \mathcal{F}|_{\kappa}^{\Lambda} = \mathcal{F}(L^2(B_\Lambda \backslash B_\kappa)), \tag{105}$$

where $B_r \subset \mathbb{R}^3$ denotes the ball for radius $r \geqslant 0$ around the origin and the symbol $\upharpoonright$ indicates the restriction of the domain, in this case to the corresponding momentum shell $\kappa \leqslant |\mathbf{k}| < \Lambda$ of the Fock space $\mathcal{F}|_{\kappa}^{\Lambda}$, admit isolated and non-degenerate ground state energies

$$E_{\mathbf{P}}|_{\kappa}^{\Lambda} := \inf \sigma(H_{\mathbf{P}}|_{\kappa}^{\Lambda} \upharpoonright \mathcal{F}|_{\kappa}^{\Lambda}), \tag{106}$$

for $0 < \kappa \leqslant \Lambda < \infty$. Here, $\sigma(\cdot)$ denotes the spectrum of the corresponding self-adjoint operator. However, adding the interaction $g\varphi(\mathbf{x})$ to the free Hamiltonian H^0 in one shot comes at the cost of a cut-off dependent smallness restriction on the coupling constant $|g|$. Ultimately, it only allows for the trivial case $g = 0$ in the limit of complete cut-off removal due to the logarithmic divergence of the interaction for $\Lambda \to \infty$ and, in case of $\mu = 0$, the closure of the spectral gap for $\kappa \to 0$. To overcome this restriction and gain control of the mass shell for a positive range of coupling constants $|g|$ uniformly in the cut-offs Λ and κ, a multi-scale perturbation analysis similar to [83] was adopted and extended to include the ultraviolet regime. Contrary to the one-shot perturbation expansion, one considers an iterative expansion in which one adds smaller momentum slices of the interaction by repetitive application of analytic perturbation theory until the desired range of allowed interaction momenta is reached. In this process, the motion of the non-degenerate ground state $E_{\mathbf{P}}|_{\kappa}^{\Lambda}$ and the continuous spectrum of $H_{\mathbf{P}}|_{\kappa}^{\Lambda}$ that starts at the energy $\max\{\kappa, \mu\}$ must be carefully monitored during each addition of a new slice of interaction. Two main types of spectral motion occur. First, when increasing the ultraviolet cut-off Λ, the spectrum of $H_{\mathbf{P}}|_{\kappa}^{\Lambda}$ is shifted towards the left on the real axis, a behavior that is already indicated by the negatively divergent energy $V_{\text{self}}|_{\kappa}^{\Lambda}$ in (100). Second, when decreasing the infrared cutoff κ, the spectral gap between the ground state energy and the continuous spectrum decreases with a certain velocity, and in case of zero boson mass $\mu = 0$, it finally closes. As already discussed in Section 2.2.2 with regards to deficiency D2, in addition to this technical difficulty for $\mu = 0$, the family of corresponding ground states will not converge in standard Fock space for $\kappa \to 0$ and the Fock space representation will have to be adapted. In order to focus on the two types of spectral motion and the necessary change of representation in case of $\mu = 0$ separately, the construction of the mass shell was carried out in the following three main steps.

Step 1: The ultraviolet regime. To counteract the shift of the spectrum towards the left, one regards the transformed fiber Hamiltonians $H'_{\mathbf{P}}|_{\kappa}^{\Lambda}$ of the renormalized Hamiltonian as given in (101) and the corresponding renormalized ground state energies

$$E'_{\mathbf{P}}|_{\kappa}^{\Lambda} = E_{\mathbf{P}}|_{\kappa}^{\Lambda} - V_{\text{self}}|_{\kappa}^{\Lambda}, \tag{107}$$

which are implied by the unitarity of the Gross transformation (98). In this first main step of [A3], the infrared cut-off $\kappa > 0$ is kept fixed and slices of interaction momenta of the form

$$[\sigma_n, \sigma_{n-1}), \qquad \sigma_n := \kappa \beta_{\text{UV}}^n, \qquad 1 < \beta_{\text{UV}}, \qquad n \in \mathbb{N}, \tag{108}$$

are added in an inductive scheme. When stepping from scale $(n-1)$ to scale n, one regards $H'_{\mathbf{P}}|_{\kappa}^{\sigma_n}$ as an analytic perturbation of $H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}}$ by

$$\Delta H'_{\mathbf{P}}|_{\sigma_{n-1}}^{\sigma_n} = H'(\mathbf{P})|_{\kappa}^{\sigma_n} - H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}}. \tag{109}$$

For a carefully chosen sequence $(\xi_n)_{n\in\mathbb{N}}$ of decreasing positive gap estimates, the inductive hypotheses

1. $\Psi'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}}$ is the unique ground state of $H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}}$ with energy $E'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}}$;
2. The spectral gap of $H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}} \restriction \mathcal{F}|_{\kappa}^{\sigma_{n-1}}$ is bounded from below by ξ_{n-1};

allow to estimate the spectral gap $H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}} \otimes 1_{\mathcal{F}|_{\sigma_{n-1}}^{\sigma_n}}$ restricted to $\mathcal{F}|_{\kappa}^{\sigma_n}$ from below also by ξ_{n-1}. At the cost of decreasing the gap estimate form ξ_{n-1} to ξ_n, it is possible to apply analytic perturbation theory once again to construct the new ground state $\Psi'_{\mathbf{P}}|_{\kappa}^{\sigma_n}$ and show that is has a non-degenerate ground state energy $E'_{\mathbf{P}}|_{\kappa}^{\sigma_n}$. Moreover, the Neumann series of the resolvent

$$\frac{1}{H'_{\mathbf{P}}|_{\kappa}^{\sigma_n} - z} = \frac{1}{H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}} - z} \sum_{j=0}^{\infty} \left[-\Delta H'_{\mathbf{P}}|_{\sigma_{n-1}}^{\sigma_n} \frac{1}{H'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}} - z} \right]^j \tag{110}$$

can be shown to be well-defined for all complex z in the domain

$$\frac{1}{2}\xi_n \leqslant |E'_{\mathbf{P}}|_0^{n-1} - z| \leqslant \xi_n < \xi_{n-1}, \tag{111}$$

and an a priori variational argument ensures $E'_{\mathbf{P}}|_{\kappa}^{\sigma_n} \leqslant E'_{\mathbf{P}}|_{\kappa}^{\sigma_{n-1}}$ such that the new spectral gap can be bounded from below by ξ_n. Tuning β_{UV} sufficiently close to 1 and adapting the choice of spectral gap bounds $(\xi_n)_{n\in\mathbb{N}}$ ensures the convergence of the Neumann series for a range of sufficiently small but positive $|g|$ that is uniform in the scale parameter n. This allows to close the induction and derive the following result for the limit $n \to \infty$, i.e., the limit of removal of the ultraviolet cut-off $\Lambda \to \infty$:

Theorem 2.5 (Ultraviolet construction [A3])**.** *Let $|\mathbf{P}| \leqslant \frac{1}{4}$. There is a constant $g_{max} > 0$ such that for all $|g| < g_{max}$ the following holds true:*

1. *The sequence of operators $(H'_{\mathbf{P}}|_{\kappa}^{\sigma_n})_{n\in\mathbb{N}}$ converges in the norm resolvent sense to a self-adjoint operator $H'_{\mathbf{P}}|_{\kappa}^{\infty}$ acting on $\mathcal{F}$.*
2. *The limit $\Psi'_{\mathbf{P}}|_{\kappa}^{\infty} := \lim_{n\to\infty} \Psi'_{\mathbf{P}}|_{\kappa}^{\sigma_n}$ exists in $\mathcal{F}$ and is non-zero.*
3. *$E'_{\mathbf{P}}|_{\kappa}^{\infty} := \lim_{n\to\infty}(E'_{\mathbf{P}}|_{\kappa}^{\sigma_n})$ exists.*
4. *$E'_{\mathbf{P}}|_{\kappa}^{\infty}$ is the non-degenerate ground state energy of the Hamiltonian $H'_{\mathbf{P}}|_{\kappa}^{\infty}$ with corresponding ground state $\Psi'_{\mathbf{P}}|_{\kappa}^{\infty}$. Moreover, the spectral gap of $H'_{\mathbf{P}}|_{\kappa}^{\infty} \restriction \mathcal{F}|_{\kappa}^{\infty}$ is bounded from below by a fraction of κ.*

Step 2: The infrared regime. In the second main step of [A3], another scaling is introduced in order to add slices of momenta of the interaction

$$(\tau_m, \tau_{m-1}], \qquad \tau_m := \kappa\beta_{\mathrm{IR}}^m, \qquad 0 < \beta_{\mathrm{IR}} < \frac{1}{2}, \qquad m \in \mathbb{N}, \tag{112}$$

below the original infrared cut-off κ. In a similar inductive scheme as applied for the ultraviolet regime, it is shown that $H'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}$ admits non-degenerate ground state energies $E'_{\mathbf{P}}|^{\sigma_n}_{\tau-m}$ with corresponding ground states $\Psi'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}$ while the spectral gap is bounded from below by a fraction of τ_m. Also, these results hold for a sufficiently small range of positive coupling constants $|g|$, however, uniformly in $n, m \in \mathbb{N}$.

Step 3: The removal of both cut-offs. In the third and final main step of [A3], the representational problem for $\mu = 0$ is addressed based on the previous results. Recall the discussion of deficiency D2 in the case of the toy model presented in the Section 2.2.2 where it was shown that the corresponding ground sate (63) leaves the standard Fock space when removing the infrared cut-off $\kappa \to 0$. The same problem occurs in the Nelson model and it was already shown in [69] that the normalized versions of the ground states $\Psi'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}$ weakly converge to zero as $m \to \infty$, i.e., in the limit of removal of the infrared cut-off $\kappa \to 0$. In order to counteract this behavior, in [69] yet another Bogolyubov transformation is introduced

$$W_{\tau_m}(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m})\, a_{\mathbf{k}}\, W_{\tau_m}(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m})^* = a_{\mathbf{k}} - g\frac{\gamma^{\sigma_n}_{\tau_m}(\mathbf{k})}{\omega(\mathbf{k}) - \mathbf{k}\cdot\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}} e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{113}$$

$$W_{\tau_m}(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m})\, a^*_{\mathbf{k}}\, W_{\tau_m}(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m})^* = a^*_{\mathbf{k}} - g\frac{\gamma^{\sigma_n}_{\tau_m}(\mathbf{k})}{\omega(\mathbf{k}) - \mathbf{k}\cdot\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}} e^{+i\mathbf{k}\cdot\mathbf{x}}, \tag{114}$$

using notation (45), and one may regard the family of transformed Hamiltonians

$$H^{W'}_{\mathbf{P}}|^{\sigma_n}_{\tau_m} := W_{\tau_m}(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m})\, H'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}\, W_{\tau_m}(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m})^*. \tag{115}$$

Heuristically, this transformation dresses each naked total momentum fiber state $e^{-i\mathbf{P}\cdot x} \otimes \Omega$ with its natural field modes, cf. (24), much like the ones in (70) as observed in the simple model of a classical charge moving along a straight line with velocity $\mathbf{v} = \nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\Lambda}_{\kappa}$. In the same way, the amplitudes on the right-hand side of (113) are tuned to absorb the non-square-integrable field modes attached to the charge in order to circumvent deficiency D2 by carefully adapting the representation. This transformation (113) was the key ingredient in the construction of scattering states without infrared regularization [83, 19].

Following closely [83], which however assumed a fixed ultraviolet cut-off $\Lambda < 0$ and did not allow to study $\Lambda \to \infty$, another inductive scheme is employed in [A4] in order to construct the sequence of transformed ground states

$$H^{W'}_{\mathbf{P}}|^{\sigma_n}_{\tau_m} \Phi_{\mathbf{P}}|^{\sigma_n}_{\tau_m} = E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m} \Phi_{\mathbf{P}}|^{\sigma_n}_{\tau_m}, \tag{116}$$

maintaining the uniformity in the smallness restriction of the coupling constant $|g|$ in n and m. Many techniques from [69, 83] were recycled in order to treat the many summands in the expression of the transformed Hamiltonian (115). Since the Bogolyubov transformation depends explicitly on the effective velocity $\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\sigma_n}_{\tau_m}$, the induction faces a further complication as those entities have to be constructed and controlled simultaneously in each step. Furthermore, to conduct the removal of both cut-offs, it turns out that, as the spectral gap closes due to the removal of the infrared limit, the ultraviolet limit must be approached at a comparatively sufficient fast rate:

Theorem 2.6 (Removal of both cut-offs [A3]). *Let $|P| \leqslant \frac{1}{4}$. There is a constant $g_{max} > 0$ such that for all $|g| < g_{max}$ the following holds true:*

1. *There exists an* $\alpha_{min} > 0$ *such that for any integer* $\alpha > \alpha_{min}$ *and* $n(m) = \alpha m$*, the limit*

$$\Phi_{\mathbf{P}}|_0^\infty := \lim_{m\to\infty} \Phi_{\mathbf{P}}|_{\tau_m}^{\sigma_{n(m)}} \tag{117}$$

exists in $\mathcal{F}$ *and is non-zero.*

2. $E'_{\mathbf{P}}|_0^\infty := \lim_{m\to\infty} E'_{\mathbf{P}}|_{\tau_m}^\infty$ *exists and is the ground state energy corresponding to the eigenvector* $\phi_{\mathbf{P}}|_0^\infty$ *of the self-adjoint operator*

$$H_{\mathbf{P}}^{W'}|_0^\infty := \lim_{m\to\infty} H_{\mathbf{P}}^{W'}|_{\tau_m}^{\sigma_{n(m)}}, \tag{118}$$

where the limit is understood in the norm resolvent sense.

2.2.4 Ultraviolet behavior of relativistic charges

This section comprises a report on the following article:

A4. *Ultraviolet Properties of the Spinless, One-Particle Yukawa Model*, D.-A. Deckert, A. Pizzo, Communications in Mathematical Physics, 327(3):887, 33 pages, 2014

The openly accessible version arXiv:1208.2646 is attached in Section A, page 167.

Regarding the Nelson model, in [A3], all cut-offs were successfully removed during the construction of the mass shell, but although tractable expansion formulas were provided, tools to conduct a rigoros study of the mass shell properties were still missing in the limiting regime of the cut-off removal. Furthermore, as also discussed in the previous section, the achieved results strongly relied on the nature of the non-relativistic dispersion relation of the charge in the model Hamiltonian (94). The latter implied the $\frac{\mathbf{k}^2}{2M}$ summand in the denominator of the Gross transformation amplitude (98), and hence, guaranteed the unitarity of this transformation even in the limit of removing the ultraviolet cut-off $\Lambda \to \infty$. Two next natural questions are whether the successful construction of the mass shell can be repeated for a "more" relativistic, and therefore, less regularizing dispersion relation, and how the provided expansion formulas can be exploited to study the mass shell's behavior when varying the cut-offs. Therefore, in [A4] the non-relativistic dispersion relation of the charge was replaced by the so-called Klein-Gordon one, which results in a model Hamiltonian of the form

$$H = \sqrt{-\Delta_{\mathbf{x}} + M^2} + H_\omega^0 + g\varphi(\mathbf{x}) \tag{119}$$

This model is usually referred to as Yukawa model and can be seen to effectively describe the strong nuclear force between heavy nucleons interacting with chargeless mesons. Again, as it stands, the Hamiltonian (119) cannot be given a mathematical meaning and an ultraviolet regularization has to be imposed in the field operator φ. The same cut-off as introduced in (95) was also used in [A4] and the same notation as in the previous section is adopted here to prescribe the regularized version of the model Hamiltonian (119), i.e.,

$$H|_\kappa^\Lambda = \sqrt{-\Delta_{\mathbf{x}} + M^2} + H_\omega^0 + g\varphi(\mathbf{x})|_\kappa^\Lambda. \tag{120}$$

Already in 1970, a similar model to (120) appeared in the mathematical physics literature in the work of Eckmann [35] in which the interaction term φ was replaced by the slightly more regular version

$$\int\limits_{|\mathbf{p}|,|\mathbf{k}|,|\mathbf{p}-\mathbf{k}|\leqslant\Lambda} d^3p \int d^3k \frac{n^*_{\mathbf{p}-\mathbf{k}}\, a^*_{\mathbf{k}}\, n_{\mathbf{p}}}{\sqrt{((\mathbf{p}-\mathbf{k})^2 + M^2)^{1/2}(\mathbf{k}^2+\mu^2)^{1/2}(\mathbf{p}^2+M^2)^{1/2}}} + h.c, \tag{121}$$

where $n^*_{\mathbf{p}}$ and $n_{\mathbf{p}}$ denote the creation and annihilation operator for the charges. The additional regularity as compared to φ alone, cf. (95), is due to the form factor of the corresponding charge field

$$\psi(\mathbf{x}) = \int d^3p \frac{1}{\left(2(2\pi)^3\sqrt{\mathbf{p}^2+M^2}\right)^{1/2}} \left(n_{\mathbf{p}} e^{+i\mathbf{p}\cdot x} + n^*_{\mathbf{p}} e^{-i\mathbf{p}\cdot x}\right) \tag{122}$$

from which the factors involving the charge mass M in the denominator of the integrand in (121) originate. These are not present in the original persistent charge model (42) since the charges were represented by quantum particles and not by quantized fields as it is the case in full quantum field theory. It should be noted that Eckmann's model nevertheless preserves the total number of charges. Similar to the result of [A3] in the Nelson model, it was shown that a logarithmically divergent energy renormalization of the family of Hamiltonians (120) in Λ suffices to ensure convergence in the norm resolvent sense. The Yukawa model was also treated in the extensive studies of [69, 49] which contain another existence result for a renormalized Hamiltonian, again, for a slightly more regular form factor compared to $\gamma_\kappa^\Lambda(\mathbf{k})$ in (95) and at the cost of a logarithmically divergent energy renormalization. Moreover, in [101], the existence of ground states are proven for a more relativistic version of the model in which a Dirac dispersion relation is employed for the charges and the type of interaction (121) was used for a fixed finite ultraviolet cut-off.

Ultraviolet behavior of the mass shell of the Yukawa model. As mentioned above, the natural questions are how to construct and also investigate the properties of the mass shell as the ultraviolet cut-off Λ approaches infinity. This is the content of the work [A4], in which the less regular interaction term as given in (120), and as originally imposed by the form of the commutation relation (20), is considered. The exact restrictions of the model parameters are given as follows

$$M > 0, \qquad \mu > 1, \qquad 0 < |g| \leqslant 1, \qquad \kappa = 1 \leqslant \Lambda < \infty. \tag{123}$$

Thanks to translation invariance, it is again possible to study the corresponding Hamiltonians (120) in terms of its total momentum fibers $H_{\mathbf{P}}|_\kappa^\Lambda$ for $\mathbf{P} \in \mathbb{R}^3$, cf. (104). As well-known from the classical literature, for $0 \leqslant \kappa \leqslant \Lambda < \infty$, these Hamiltonians are essentially self-adjoint on the domain $D(H_\omega^0)$ and bounded from below. The latter allows again to define the ground state energies as follows

$$E_{\mathbf{P}}|_\kappa^\Lambda := \inf \sigma(H_{\mathbf{P}}|_\kappa^\Lambda \upharpoonright \mathcal{F}|_\kappa^\Lambda). \tag{124}$$

It should be noted that a non-zero boson mass $\mu > 0$ renders the infrared cut-off κ redundant since the spectral gap is bounded from below by $\min\{\kappa, \mu\}$, and in [A4], κ is only kept for computational convenience.

The main part of the work in [A4] is again to set up a multi-scale technique similar to the ones discussed in the previous section in order to construct the mass shell in a certain spectral range $(E_{\mathbf{P}}|_\kappa^\Lambda, \mathbf{P})_{\mathbf{P}\in\mathbb{R}^3}$ and infer expansion formulas that are uniform in Λ, at least for a fixed range of coupling constants g. Besides the results on the Nelson model in [A3], which behaves much better in the ultraviolet regime, [A4] is the first work that features an application of such a multi-scale technique to study the ultraviolet behavior in quantum field theory. Similar to the technique applied in [A3], the two key ingredients for this purpose are, first, a suitable scaling in which slices of momenta of the interaction are added iteratively using analytic perturbation theory, and second, sufficient external information on the spectral motion that occurs during the iteration and ultimately allows to close the corresponding inductive scheme. In [A4], the following scaling

$$(\Lambda\beta^n, \Lambda], \qquad \frac{1}{2} < \beta < 1 \tag{125}$$

was employed which results in a number of scales

$$N = \frac{\log \Lambda}{-\log \beta}, \tag{126}$$

assuming the fineness parameter β is chosen such that N is a natural number. In order to gain control on the Neumann expansion of Hamiltonian $H_{\mathbf{P}}|^{\Lambda}_{\Lambda\beta^n}$ with respect to perturbation

$$\Delta H_{\mathbf{P}}|^{\Lambda\beta^{n-1}}_{\Lambda\beta^n} := H_{\mathbf{P}}|^{\Lambda}_{\Lambda\beta^{n-1}} - H_{\mathbf{P}}|^{\Lambda}_{\Lambda\beta^n}, \tag{127}$$

similar to (110), it turned out to be crucial to fill in the slices of momenta of the interaction starting from the ultraviolet cut-off Λ down to the infrared cutoff $1 = \kappa = \Lambda\beta^N$. In such a scaling, one can exploit the spectral gap implied by the lower cut-off $\Lambda\beta^n$ of $H_{\mathbf{P}}|^{\Lambda}_{\Lambda\beta^n}$ in the required norm estimates of the corresponding resolvent to compensate the contributions of the interaction momenta of the perturbation $\Delta H_{\mathbf{P}}|^{\Lambda\beta^{n-1}}_{\Lambda\beta^n}$ up to $\Lambda\beta^{n-1}$. This strategy allows to control the expansions on all scales for a sufficiently small range of couplings constants g that is uniform in Λ. In turn, the mass shell can be studied for varying Λ. Furthermore, a fine-tuning of $\beta \to 1$ allows to control error terms in the multi-scale expansions of the type $O(N(1-\beta)^{1+\epsilon})$ for any $\epsilon > 0$ and ultimately enables a study of the model behavior for $\Lambda \to \infty$. After carrying out the multi-scale construction in [A4], the resulting multi-scale expansion formulas allowed to show the following result, which basically states that independent of the choice of a possible energy or mass renormalization, the mass shell collapses.

Theorem 2.7 (Ultraviolet properties of the mass shell [A4])**.** *Let $|g| > 0$ be sufficiently small and $|\mathbf{P}| < \frac{1}{2}$.*

1. *There exist universal constants $a, b > 0$ such that for all $1 = \kappa < \Lambda < \infty$ it holds*

$$\sqrt{P^2 + M^2} - g^2 b\Lambda \leqslant E_{\mathbf{P}}|^{\Lambda}_{\kappa} \leqslant \sqrt{P^2 + M^2} - g^2 a\Lambda \tag{128}$$

2. *There exist universal constants $c, C > 0$ such that the following estimate holds true*

$$\limsup_{\beta\to 1} \left|\nabla_{\mathbf{P}} E_{\mathbf{P}}|^{\Lambda}_{\kappa}\right| \leqslant \Lambda^{-g^2 c} \frac{|\mathbf{P}|}{[\mathbf{P}^2 + M^2]^{1/2}} + C|g|^{1/2}, \qquad i = 1,2,3. \tag{129}$$

The first observation states that the divergence of the ground state energies is linear in Λ. This behavior is due to the slightly less regular form factor $\gamma^{\Lambda}_{\kappa}(\mathbf{k})$ as compared to the works [35, 49] which found only a logarithmic divergence. Furthermore, a direct consequence of the bound in (129) is the flatness of the mass shell up to a remaining error term as the ultraviolet cut-off is removed:

$$\limsup_{\Lambda\to\infty} \left|\nabla_{\mathbf{P}} E_{\mathbf{P}}|^{\Lambda}_{\kappa}\right| \leqslant C|g|^{1/2}. \tag{130}$$

In order to interpret the latter observation, it is helpful to note that $\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\Lambda}_{\kappa}$ encodes the effective velocities of the charges. In the free case $g = 0$, one finds

$$\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\Lambda}_{\kappa} = \frac{\mathbf{P}}{\sqrt{\mathbf{P}^2 + M^2}}, \tag{131}$$

i.e., the velocity of a free relativistic particle. For $|g| > 0$, the study of the effective velocities $\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\Lambda}_{\kappa}$ thus allows to gain inside in the effect of the self-interaction on the kinetics of the charge; recall the discussion of the two-fold kinetic nature of the interaction implied by a scalar field φ contrary to the one of direct interaction potentials in Section 2.2.2. According to (130), the effective velocity decreases with increasing Λ and eventually, upon complete removal of the ultraviolet cut-off, the mass shell becomes flat up to a remaining error of the order $|g|^{1/2}$. This remaining error in (130) is very likely only of technical nature as suggested by a comparison of the free mass shell for $g = 0$, i.e., (131), with the one of an arbitrarily small $|g| > 0$, i.e., (130). The latter is flat no matter how small $|g|$ is chosen.

Furthermore, in the total momentum fiber $\mathbf{P} = 0$, the inverse of the effective velocity can be seen as the effective inertia of the charge

$$m_{\text{effective}} = \left(\nabla_{\mathbf{P}} E'_{\mathbf{P}}|^{\Lambda}_{\kappa}\right)^{-1}\Big|_{\mathbf{P}=0}. \tag{132}$$

Since the theorem above states that this quantity diverges for $\Lambda \to \infty$, one may be inclined to counteract such an behavior by a Λ-dependent renormalization of the bare mass parameter, more precisely, to arrange a scaling $m = m(\Lambda)$ in such a way that the effective inertia (132) is kept constant and equal to, e.g., an experimentally measured value. Unfortunately, in the Yukawa model such a rescaling of the mass has no effect, as can be understood from the right-hand side of (129), and a successful renormalization scheme model will require a more sophisticated method than energy or mass renormalization, for instance, wave function renormalization. It is interesting to note that this behavior seems to be characteristic to the more relativistic dispersion relations. In the case of non-relativistic charges, in which the free mass shell takes the form of $\frac{\mathbf{P}^2}{2M}$ instead of (131), there is a viable chance that the increase of the effective mass can be counteracted by a conveniently chosen scaling $\lim_{\Lambda\to 0} m(\Lambda) = 0$. In the case of the Pauli-Fierz model, there already exists a conjecture about a potentially successful scaling rate [66]; see [100] for an overview. It must however be emphasized that variational lower and upper bounds on the minimum of the mass shell as first found in [75] and recently proved in [10] suggest that one may not trust regular one-shot perturbation theory in the limit $\Lambda \to \infty$, so that this issue remains a challenge for the future. In this respect, it is interesting to note that the first instance of a mass renormalization procedure appeared in classical electrodynamics in [31], where it turned out convenient to consider a bare mass $m(\Lambda)$ that diverges to negative infinity; see overview [100]. These three rather distinct behaviors may provoke the question whether mass renormalization is a general theme of the classical and quantum field theory that is to be applied as a standard procedure in order to make dedicated models interpretable in the relativistic regime or whether it is simply a loose patch work to fix the implications of a broken equation of motion (42). Finally, beyond the change of the inertia of the charge, the self-interaction term seems to have another interesting effect that cannot be observed in the above models, namely the phenomenon of enhancement binding which has been proven for a single charge in external potentials in the setting of non-relativistic quantum electrodynamics, see [64, 60, 18].

2.2.5 Coping with the absence of a spectral gap

This section comprises a report on the following two articles:

A5. *Relation Between the Resonance and the Scattering Matrix in the Massless Spin-Boson Model*, M. Ballesteros, D.-A. Deckert, F. Hänle, Communications in Mathematical Physics, 370, 41 pages, 2019

The openly accessible version arXiv:1801.04843 is attached in Section A, page 197.

A6. *One-boson scattering processes in the massless Spin-Boson model – A non-perturbative formula*, M. Ballesteros, D.-A. Deckert, F. Hänle, Advances in Mathematics, 371:107248, 26 pages, 2020

The openly accessible version arXiv:1907.03013 is attached in Section A, page 243.

The works [A5-6] comprise a study of the so-called massless Spin-Boson model which describes the interaction of a two-level atom with its scalar field. In terms of complexity, this model lies in between the simple toy model of fixed charges (54) considered in Section 2.2.2 and models with a continuous dispersion relations for the charges such as the Nelson and Yukawa model (94) and (119) considered in Sections 2.2.3 and 2.2.4, respectively. The atom is considered fixed at the origin of position space and its only degree of freedom is the transition between its ground and excited states. On the Hilbert space

$$\mathcal{H} = \mathcal{K} \otimes \mathcal{F}, \qquad \mathcal{K} = \mathbb{C}^2, \tag{133}$$

the model Hamiltonian is of the form

$$H = H_0 + gV. \tag{134}$$

Here, $g \in \mathbb{R}$ is again a coupling constant, and the free Hamiltonian

$$H_0 = K + H_\omega^0, \qquad K := \begin{pmatrix} e_1 & 0 \\ 0 & e_0 \end{pmatrix}, \qquad H_\omega^0 := \int d^3k\, \omega(\mathbf{k}) a_\mathbf{k}^* a_\mathbf{k}, \tag{135}$$

consists of the idealized free Hamiltonian of a two-level atom K that encodes two energy levels denoted by the real numbers $0 = e_0 < e_1$ and the corresponding free Hamiltonian H_ω^0 of the scalar field, see (48). The interaction of the two-level atom with its scalar field is encoded in the expression

$$V = \sigma_1 \otimes (a(f) + a^*(f)), \qquad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{136}$$

given a form factor f of the type

$$f : \mathbb{R}^3 \backslash \{0\} \to \mathbb{R}, \qquad \mathbf{k} \mapsto e^{-\frac{\mathbf{k}^2}{\Lambda^2}} |\mathbf{k}|^{-\frac{1}{2}+\kappa}. \tag{137}$$

It should be noted that despite the matrix σ_1 that may induce atomic state transitions, the expression (136) resembles the scalar field of the form (52), where the position was fixed to $\mathbf{x} = 0$ and the form factor γ was replaced by f. The special choice of f in (137) is derived from the relativistic γ in (33) by setting the boson mass to zero, decorating the resulting expression with a Gaussian suppression of the ultraviolet frequencies that can be tuned with the help of the cut-off parameter Λ, and adding a regularization parameter $\kappa > 0$ that tempers the singular behavior for $|\mathbf{k}| \to 0$. The reason to use a Gaussian ultraviolet regularization instead of a hard cut-off in this model is to preserve certain analyticity properties that will be crucial for the applied strategy. Both parameters the ultraviolet cut-off $\Lambda < \infty$ and also $\kappa \in (0, 1/2)$ are kept fixed. All remaining constant factors are thought to be absorbed in the coupling constant g in this notation.

Despite the simple kinetic term of the atom, this model is physically quite interesting as the interaction with the scalar field may induce transitions between the atom levels. For this reason, it is frequently employed in quantum optics to investigate scattering processes between bosons and atoms. Likewise, the underlying mechanism is also mathematically quite rich as the ground state energy e_0 in the non-interacting case, i.e., $g = 0$, is shifted on the real line to the interacting ground state energy λ_0 while the free excited state with energy e_1 turns into a resonance with complex "energy" λ_1 when the interaction is switched on for $g > 0$; see, e.g., [13]. However, in view of the discussed deficiencies D1 and D2, D1 is entirely avoided due to the fixed ultraviolet cut-off $\Lambda < 0$ and also the representation problem of D2 is not present thanks to the choice $\kappa \in (0, 1/2)$. It turns out that the only remaining difficulty in the control of this model in the prescribed range of parameters is the absence of a spectral gap. The spectrum of H_ω^0 is absolutely continuous and supported on $[0, \infty)$; see [86]. Consequently, the spectrum of H_0 is given by $[e_0, \infty)$ and e_0 and e_1 are eigenvalues embedded in the absolutely continuous spectrum; see [85]. The latter difficulty is entirely of mathematical nature as it does not allow a ready application of analytic perturbation theory but requires a more subtle approach. The first objective of the works [A5-6] is therefore to enable the rigorous investigation of the atomic state transitions due to the interaction with the scalar field. As also partly outlined in the previous sections, a lot of technology has already been developed to overcome this mathematical obstacle, which can be categorized into two principal approaches: The so-called renormalization group approach, see, e.g., [6, 8, 7, 5, 9, 3, 52, 58, 98, 37, 14], which was the first one applied successfully to construct resonances in models of quantum field theory, and furthermore, the so-called multi-scale approach also discussed in Sections 2.2.3 and 2.2.4 that was originally developed in [83, 84, 4] and also successfully applied in various models of quantum field theory – e.g., in the discussed works [A3-4] which first extended the multi-scale method to the ultraviolet regime. In order to study the interacting ground state λ_0 and resonance λ_1, in both approaches, one ultimately analyzes a family of complex-dilated Hamiltonians which allow to regard the resonance λ_1 as a complex eigenvalue. The construction of the ground state and resonance, its analyticity properties, and crucial spectral estimates on which the works [A5-6] are crucially based on were obtained in a preceding article [13], which employs a multi-scale technique.

After the development of the necessary tools to study the Spin-Boson model despite the absence of a spectral gap, the second objective of [A5-6] is to establish a link between resonance and scattering theory in a similar manner as it was done for non-relativistic N-body quantum mechanics, see Simon's review in [99]. One of the main results of the latter article shows that the integral kernel of the scattering matrix elements are related to the resolvent of the corresponding N-body Schrödinger operator. Furthermore, it was proven that the singularities of a meromorphic continuation of the integral kernel of the scattering matrix are located precisely at the resonance energies. Similar to resonance theory, also scattering theory is well-established in various models of quantum field theory, e.g., in [39, 38, 16, 51, 50], and in particular in the massless Spin-Boson model, e.g., in [22, 23, 24, 28, 11]. However, most results aim at more abstract properties such as the existence of the scattering operator and asymptotic completeness, and further strategies had to be developed for the works [A5-6] to live up to its objectives. The work [A5] provides a formula for the leading order of the scattering matrix elements for one-boson processes together with an estimate of the error term. This formula already displays the dependence on the resonance λ_1 explicitly. The succeeding work [A6] provides a major improvement by establishing an exact formula for the integral kernel of the scattering matrix elements for one-boson processes in terms of the dilated resolvent. Both results are the first of their kind for a maybe simple, nevertheless non-trivial model of quantum field theory. In order to state these main results, it will be helpful to briefly review a few of the employed tools from resonance and scattering theory.

Complex dilation. As mentioned above, a complex dilation is employed in order to study the resonance λ_1 as complex eigenvalue, which is a standard strategy of resonance theory, see, e.g., [13] and [A3] for a self-comprehensive introduction regarding the particular model at hand. The basic tool to conduct this dilation is a family of unitary operators on $\mathcal{H}$ indexed by $\theta \in \mathbb{R}$:

$$u_\theta : \mathfrak{h} \to \mathfrak{h}, \qquad \psi \mapsto \left(\mathbf{k} \mapsto e^{-\frac{3\theta}{2}} \psi(e^{-\theta}\mathbf{k})\right). \tag{138}$$

Its canonical lift $U_\theta : \mathcal{F} \circlearrowleft$ to standard Fock space $\mathcal{F}$ can be established by means of the lift condition

$$U_\theta\, a^*(h)\, U_\theta^{-1} = a^*(u_\theta h), \qquad h \in \mathfrak{h}. \tag{139}$$

The latter defines U_θ uniquely up to a phase which, in the following, is simply set to equal one. As done in the previous sections, all tensored identities are absorbed in the notation. For instance, U_θ on $\mathcal{F}$ and $1_{\mathcal{K}} \otimes U_\theta$ on $\mathcal{H}$ are identified by the same symbol U_θ. Furthermore, a state $\Psi \in \mathcal{F}$ is called an analytic vector if the map $\theta \mapsto \Psi^\theta := U_\theta \Psi$ has an analytic continuation from an open connected set in the real line to a connected domain in the complex plane. This unitary group $(U_\theta)_{\theta\in\mathbb{R}}$ allows to define a family of transformed Hamiltonians, for $\theta \in \mathbb{R}$,

$$H^\theta := U_\theta H U_\theta^{-1} = K + H_f^\theta + gV^\theta, \tag{140}$$

where

$$H_f^\theta := \int d^3k\, \omega^\theta(\mathbf{k}) a_{\mathbf{k}}^* a_{\mathbf{k}}, \qquad V^\theta := \sigma_1 \otimes \left(a(f^{\bar\theta}) + a^*(f^\theta)\right) \tag{141}$$

and

$$\omega^\theta(\mathbf{k}) := e^{-\theta}|\mathbf{k}|, \qquad f^\theta : \mathbb{R}^3\backslash\{0\} \to \mathbb{R}, \quad \mathbf{k} \mapsto e^{-\theta(1+\kappa)} e^{-e^{2\theta}\frac{\mathbf{k}^2}{\Lambda^2}} |\mathbf{k}|^{-\frac{1}{2}+\kappa}. \tag{142}$$

Next, it is crucial to note that the mathematical meaning of (142), (141), and (140) can be extended to complex θ. In fact, if $|\theta|$ is small enough, H^θ is a closed, though non-self-adjoint, operator and it can be shown that the family $(H^\theta)_{\theta\in\mathbb{R}}$ of unitary equivalent, self-adjoint operators with domains $D(H^\theta) = D(H)$ extends to an analytic family of type A for θ in a suitable neighborhood of 0, see

[A4] for details. For sufficiently small coupling constants and a suitable range of complex θ, it has also been shown that H^θ has two non-degenerate eigenvalues λ_0^θ and λ_1^θ with corresponding rank-one projectors denoted by P_0^θ and P_1^θ, respectively; see, e.g., [13, Proposition 2.1]. In this case, the corresponding dilated eigenstates can be expressed as

$$\Psi_i^\theta := P_i^\theta \varphi_i \otimes \Omega, \qquad i = 0, 1, \tag{143}$$

where the eigenstates φ_i of the free atomic Hamiltonian K are given by

$$\varphi_0 = (0,1)^T \qquad \text{and} \qquad \varphi_1 = (1,0)^T \qquad \text{with} \qquad K\varphi_i = e_i\varphi_i, \quad i = 0, 1. \tag{144}$$

The resulting eigenstates Ψ_i^θ are not necessarily normalized and, as known from [13, Theorem 2.3], the eigenvalues λ_i^θ are independent of the dilation parameter θ, which is why in the following the reference to it is suppressed in the notation. It must be emphasized, however, that for real θ the eigenstate Ψ_1^θ does not exist as it would contradict self-adjointness. Only the construction of the ground state Ψ_0^θ can also be carried out for real θ in which $\Psi_0^{\theta=0} = \Psi_0^\theta$, see [13, Remark 2.4].

Scattering matrix. The second tool needed is a working definition of the scattering matrix, which is briefly reviewed in the following; for details, see Section 1.3 of [A5]. With the following dense subspace of compactly supported, smooth, and complex-valued functions on $\mathbb{R}^3\backslash\{0\}$

$$\mathfrak{h}_0 := C_c^\infty(\mathbb{R}^3\backslash\{0\}, \mathbb{C}) \subset \mathfrak{h} \tag{145}$$

at hand, the basic components of scattering theory are comprised by:

1. For $h \in \mathfrak{h}_0$, the limit operators

$$a_\pm(h)\Psi := \lim_{t\to\pm\infty} a_t(h)\Psi, \quad a_t(h) := e^{itH}a(h_t)e^{-itH}, \quad h_t(\mathbf{k}) := h(\mathbf{k})e^{-it\omega(\mathbf{k})}, \tag{146}$$

   for all $\Psi \in \mathcal{H}$ such that the limit exists, and analogously the respective adjoints $a_\pm^*(h)$.

2. The asymptotic Hilbert spaces

$$\mathcal{H}^\pm := \mathcal{K}^\pm \otimes \mathcal{F}[\mathfrak{h}] \quad \text{where} \quad \mathcal{K}^\pm := \{\Psi \in \mathcal{H} \,|\, \forall\, h \in \mathfrak{h}_0 : a_\pm(h)\Psi = 0\}. \tag{147}$$

3. The wave operators

$$\Omega_\pm : \mathcal{H}^\pm \to \mathcal{H} \tag{148}$$
$$\Omega_\pm \Psi \otimes a^*(h_1)...a^*(h_n)\Omega := a_\pm^*(h_1)...a_\pm^*(h_n)\Psi, \quad h_1, ..., h_n \in \mathfrak{h}_0, \quad \Psi \in \mathcal{K}^\pm. \tag{149}$$

4. The scattering operator $S := \Omega_+^*\Omega_-$.

The limiting operators $a_\pm$ and $a_\pm^*$ are called asymptotic outgoing/ingoing annihilation and creation operators. The existence of the limits in (146), e.g., for $\Psi \in D(\sqrt{H_0})$, their properties, in particular $\Psi_0 \in \mathcal{K}^\pm$, and the well-definedness of $\Omega_\pm$ are well-known for various models from the classic literature; see, e.g., [39, 38, 16, 51, 50, 22, 23, 24, 28, 11]. A self-comprehensive proof of these properties for the model at hand is given in Lemma 4.1 of [A5]. The scattering matrix coefficients for one-boson processes are thus given by

$$S(h,l) = \|\Psi_0\|^{-2}\left\langle a_+^*(h)\Psi_0, a_-^*(l)\Psi_0\right\rangle, \qquad \forall\, h, l \in \mathfrak{h}_0, \tag{150}$$

In addition to the scattering matrix coefficients, it will be convenient to work with the corresponding transition matrix coefficients for one-boson processes given by

$$T(h,l) = S(h,l) - \langle h,l\rangle_2, \qquad \forall\, h,l \in \mathfrak{h}_0, \tag{151}$$

as those carry a ready physical interpretation as transition amplitudes for a process in which an incoming boson with wave function l is scattered at the two-level atom into an outgoing boson with wave function h.

Leading term of the one-boson scattering kernel. The first link between resonance and scattering theory is established in form of a perturbative result, however, with full control on the remaining error.

Theorem 2.8 (Leading order of the scattering kernel [A5])**.** *For sufficiently small g, θ in the set*

$$\mathcal{S} = \{\theta \in \mathbb{C} \mid -10^{-3} < \operatorname{Re}\theta < 10^3 \ \wedge\ 0 < \operatorname{Im}\theta < \pi/16\} \tag{152}$$

and for all $h,l \in \mathfrak{h}_0$, the two-body transition matrix coefficients are given by

$$T(h,l) = T_P(h,l) + R(h,l), \tag{153}$$

where

$$T_P(h,l) := 4\pi i g^2 \,\|\Psi_0\|^{-2} \int dr\, G(r) \left(\frac{\operatorname{Re}\lambda_1 - \lambda_0}{\left(r + \lambda_0 - \lambda_1\right)\left(r - \lambda_0 + \overline{\lambda_1}\right)} \right) \tag{154}$$

$$= A \int dr\, G(r) \left(\frac{E_1 g^2}{\left(r + \lambda_0 - \operatorname{Re}\lambda_1 - i g^2 E_1\right)\left(r - \lambda_0 + \overline{\lambda_1}\right)} \right). \tag{155}$$

Here, the abbreviations

$$E_1 := g^{-2} \operatorname{Im}\lambda_1, \tag{156}$$

$$A := 4\pi i (\operatorname{Re}\lambda_1 - \lambda_0) E_1^{-1} \,\|\Psi_0\|^{-2}. \tag{157}$$

and, for solid angles $\mathrm{d}\Sigma, \mathrm{d}\Sigma'$ in $\mathbb{R}^3$ and $h,l \in \mathfrak{h}_0$, the notation

$$G : \mathbb{R} \to \mathbb{C}, \qquad r \mapsto G(r) := \begin{cases} \int d\Sigma \int d\Sigma'\, r^4 \overline{h(r,\Sigma)} l(r,\Sigma') f(r,\Sigma)^2 & \textit{for} \quad r \geqslant 0 \\ 0 & \textit{for} \quad r < 0 \end{cases} \tag{158}$$

were used. Furthermore, there are explicitly determined constants $C(h,l)$ such that the error term satisfies

$$|R(h,l)| \leqslant C(h,l) g^3 |\log(g)|. \tag{159}$$

This property separates the error term from the principal one $T_P(h,l)$ which is of order g^2.

With regards to physics, the principal term $T_P(h,l)$ may be rewritten as

$$T_P(h,l) = \int d^3k \int d^3k'\, \overline{h(\mathbf{k})} l(\mathbf{k}') \delta(|\mathbf{k}| - |\mathbf{k}'|) T_P(\mathbf{k},\mathbf{k}'), \tag{160}$$

for

$$T_P(\mathbf{k},\mathbf{k}') = Af(\mathbf{k})f(\mathbf{k}')\left(\frac{E_1 g^2}{\left(|\mathbf{k}'| + \lambda_0 - \operatorname{Re}\lambda_1 - ig^2E_1\right)\left(|\mathbf{k}'| - \lambda_0 + \overline{\lambda_1}\right)}\right). \tag{161}$$

This allows to identify the leading order of the scattering cross section as proportional to

$$|T_P(\mathbf{k},\mathbf{k}')|^2 = \left(\frac{|A|^2|f(\mathbf{k})|^2|f(\mathbf{k}')|^2}{||\mathbf{k}'| - \lambda_0 + \overline{\lambda_1}|^2}\right)\frac{E_1^2 g^4}{(|\mathbf{k}'| + \lambda_0 - \operatorname{Re}\lambda_1)^2 + g^4E_1^2}. \tag{162}$$

For incoming momenta $|\mathbf{k}'|$ in a neighborhood of $\operatorname{Re}\lambda_1 - \lambda_0$, this formula is dominated by the Lorentzian envelope known from physics text-books. As expected, there is a maximum when the energy of the incoming photons is close to the real value difference of the resonance λ_1 and the ground state energy λ_0, and the width of this peak is controlled by the imaginary part of the resonance $\operatorname{Im}\lambda_1$.

Exact formula for the one-boson scattering kernel. Though the above result is explicit in the first relevant order of perturbation in g, and therefore useful in computations, the next result is more implicit but reveals the link between the resonance and scattering theory more clearly by means of an exact dependence of the integral kernel of the scattering matrix on the resolvent of the dilated Hamiltonians:

Theorem 2.9 (Non-perturbative scattering kernel [A5])**.** *For sufficiently small g, $\theta \in \mathcal{S} \subset \mathbb{C}$ and all $h, l \in \mathfrak{h}_0$, the transition matrix coefficients for one-boson processes are given by*

$$T(h,l) = \int d^3k \int d^3k'\, \overline{h(\mathbf{k})} l(k')\delta(|\mathbf{k}| - |\mathbf{k}'|)T(\mathbf{k},\mathbf{k}'), \tag{163}$$

where

$$T(\mathbf{k},\mathbf{k}') = 2\pi i g^2 f(\mathbf{k})f(\mathbf{k}')\,\|\Psi_0\|^{-2}\left(\left\langle \sigma_1\Psi_0^{\overline{\theta}}, \left(H^\theta - \lambda_0 - |\mathbf{k}'|\right)^{-1}\sigma_1\Psi_0^\theta\right\rangle\right. \tag{164}$$

$$\left. + \left\langle \sigma_1\Psi_0^\theta, \left(H^{\overline{\theta}} - \lambda_0 + |\mathbf{k}'|\right)^{-1}\sigma_1\Psi_0^{\overline{\theta}}\right\rangle\right). \tag{165}$$

As before, the integral with respect to the Dirac delta distribution δ in (163) is to be understood as

$$T(h,l) = \int_0^\infty d|\mathbf{k}| \int d\Sigma \int d\Sigma'\, \overline{h(|\mathbf{k}|,\Sigma)} l(|\mathbf{k}|,\Sigma')T(|\mathbf{k}|,\Sigma,|\mathbf{k}|,\Sigma'), \tag{166}$$

where again spherical coordinates $\mathbf{k} = (|\mathbf{k}|,\Sigma)$ with Σ being the solid angle in $\mathbb{R}^3$ are used, and $T(\mathbf{k},\mathbf{k}') \equiv T(|\mathbf{k}|,\Sigma,|\mathbf{k}|,\Sigma')$ is given by (164). Finally, one may now apply perturbation theory again to recover the result (162) and make its Lorentzian shape more apparent.

Beside several Spin-Boson model specific computations that allowed to rewrite the scattering coefficients in a more explicit form, a crucial tool employed in gaining the required control on the long-time evolution was the following representation of the unitary time evolution generated by the model Hamiltonian H in (134) for analytic vectors $\phi,\psi \in \mathcal{H}$:

$$\left\langle \phi, e^{-itH}\psi\right\rangle = \lim_{\epsilon\downarrow 0}\frac{1}{2\pi i}\int_{\mathbb{R}+i\epsilon} dz\, e^{-itz}\left\langle \phi, (H-z)^{-1}\psi\right\rangle. \tag{167}$$

In the considered model, the justification of this identity was possible, first, due to the rather precise resolvent estimates close to the real axis provided in the preceding work [13], and second, due to the fact that, after implementing the complex dilation U_θ, the continuous spectrum of the original Hamiltonian

(134) is tilted to the lower complex plane and localized in cones attached to eigenvalues λ_0 and λ_1. Thanks to this fact, it is possible to give (167) a meaning by deforming the integration path $\mathbb{R} + i\epsilon$ at $-\infty$ and $+\infty$ towards the lower complex plane. It is interesting to note that in the massive version of this model, though it features a spectral gap that makes the construction of the ground state and resonance much easier, this strategy fails. This is to be attributed to the corresponding unperturbed Hamiltonian exhibiting the spectrum

$$\{e_0, e_1\} \cup \bigcup_{k=1}^{\infty} \Big(\{e_0, e_1\} + [k\mu, +\infty)\Big), \tag{168}$$

i.e., a spectrum consisting of the ground state energy e_0, excited state energy e_1, and in addition continuous spectra attached to every multiple of m starting from e_0 and e_1 with a gap of the magnitude of the boson mass μ. This leads to an absence of decay of the corresponding complex-dilated resolvent of the model Hamiltonian close to the real line. Therefore, a different strategy had to be employed in a successive work [12] to control the time evolution and obtain an analogous result to Theorem 2.8 above. Despite the different strategy of proof, it turns out that the formula of the integral kernel of the scattering matrix differs only in terms of replacing the bosonic dispersion $\omega(\mathbf{k}) = |\mathbf{k}|$ by $\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + \mu^2}$ and including the respective Jacobi determinant resulting from the argument of the delta distribution. A posteriori, the scattering kernel of the massless model can thus be retrieved from the massive one by considering $\mu \to 0$. This may also have been the physical expectation as, contrary to deficiency D1, D2 does not seem to imply any fundamental problem with the equations of motion of a particular model of quantum field theory. Switching from $\mu > 0$ to $\mu = 0$ may rather be regarded as a tuning of the underlying wave equation (24) which introduces several mathematical subtleties that have to be addressed.

2.3 Models of varying charges

This concluding section provides selected adoptions from the review article

A7. *A Perspective on External Field QED.*, D.-A. Deckert, F. Merkl, book edition Quantum Mathematical Physics, Birkhäuser, 381-399, 18 pages, 2016

The openly accessible version arXiv:1510.03890 is attached in Section A, page 269.

and furthermore a report on the work:

A8. *External Field QED on Cauchy Surfaces for Varying Electromagnetic Fields*, D.-A. Deckert, F. Merkl, Communications in Mathematical Physics, 345(3):973–1017, 44 pages, 2016

The openly accessible version arXiv:1505.06039 is attached in Section A, page 287.

The models discussed so far were motivated in Section 2.2.2 with the objective to introduce a relativistic interaction between the N quantum charges. The described route taken by the founding pioneers to introduce such an interaction by means of a quantized field of type (20) is the first stepping stone to quantum field theory. Nowadays, there is good hope that the deficiency D2 entirely as well as the representation problem caused by the two-faced deficiency D1 can be addressed by sufficiently advanced mathematical tools. Furthermore, the self-interaction problem caused by D1 does at least not seem to be worse than its analogue in classical field theory. However, relativistic interaction between persistent charges is only half of the story of quantum field theory and this section concludes with a brief overview on the other half, the relativistic nature of the charges themselves. As regards this report, it is to be emphasized that, except for the works on the existence of dynamics [A1-2] reported on in Section 2.2.1 and 2.2.2, none of the considered models so far feature a relativistic dispersion for the charges. Even the Yukawa model (119) only caricatures a relativistic dispersion by $\sqrt{-\Delta_{\mathbf{x}} + M^2}$ in the sense that its Fourier multiplication operator is linear and not quadratic in the momentum variable, nevertheless its resulting propagator is not causal. The reason why many works in the recent and also classical mathematical physics literature do not address relativistic candidates of dispersion relations for the charges, e.g., as the ones derived from the Klein-Gordon or Dirac equation, is that the latter have rather peculiar properties which may not allow for a ready interpretation in terms of quantum particles. The free one-particle Dirac equation, for example,

$$(i\partial\!\!\!/ - M)\psi(x) = 0, \qquad \text{for } \psi \in \mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4), \tag{169}$$

was originally suggested to describe the free motion of single electrons. Here, $\gamma^\mu, \mu = 0, \ldots, 3$ denote the Dirac matrices fulfilling the anti-commutator relation $\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$, and furthermore, Feynman's slash notation $\partial\!\!\!/ = \gamma^\mu \partial_\mu$ is used. Curiously enough, (169) allows for solutions with arbitrarily negative kinetic energies as the corresponding Hamiltonian

$$H^0 = \gamma^0(-i\boldsymbol{\gamma} \cdot \nabla_{\mathbf{x}} + M) \tag{170}$$

exhibits an absolutely continuous spectrum $\sigma(H^0) = (-\infty, -m] \cup [+m, \infty)$. Due to this fact, physicists rightfully argue [57] that a Dirac electron coupled to the electromagnetic field may cascade to ever lower and lower energies by emission of radiation that is transported to spatial infinity. Other peculiarities stemming from the presence of a negative energy spectrum are the so-called *Zitterbewegung*, first observed by Schrödinger [89], and *Klein's paradox* [71]. In 1934, Dirac demonstrated [30] how those peculiarities can be reconciled and brought into a coherent description when switching from the one-particle Dirac equation (169) to a many, in the mathematical idealization even infinitely many, particle description known as the *Dirac sea* or the *second quantization* of the Dirac equation. Perhaps the most striking consequence of this description is the phenomenon of electron-positron pair creation, which only little later was observed experimentally by Anderson [1]. Though models of persistent charges remain meaningful in physically interesting regimes, as for instance, in non-relativistic quantum electrodynamics or heavy-ion physics, it became clear that a complete quantum field theory will have to describe also the charges in terms of a relativistic quantum field. In the following, a brief historic introduction is provided in order to emphasize some basic aspects of this approach, which specialists can of course safely skip, at least until the paragraph "Time evolution of Dirac seas".

In order to rid relativistic quantum theory from peculiarities arising from the negative energy states, Dirac proposed to introduce a "sea" of electrons occupying all negative energy states. The Pauli exclusion principle then acts to prevent any of the electrons that may be dragged to the positive energy part of the spectrum by, e.g., a temporary binding potential, to dive back unboundedly into the negative part. For P^+ and P^- denoting the orthogonal projectors onto the positive and negative energy subspaces $\mathcal{H}^+ = P^+\mathcal{H}$ and $\mathcal{H}^- = P^-\mathcal{H}$ of the Hamiltonian H^0 in (170), respectively, Dirac's heuristic picture may amount to an antisymmetric infinitely-particle wave function, usually called a Dirac sea, such as

$$\Omega = \varphi_1 \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots, \qquad (\varphi_n)_{n\in\mathbb{N}} \text{ being an orthonormal basis of } \mathcal{H}^-, \tag{171}$$

where $\wedge$ denotes the antisymmetric tensor product with respect to the Hilbert space $\mathcal{H}$. According to Dirac, the state in (171), though full of particles, is to be interpreted as an effective vacuum due to the uniform distribution of the particles so that only excitations from this vacuum may become observable:

> *Admettons que dans l'Univers tel que nous le connaissons, les états d'energie négative soient presque tous occupés par des électrons, et que la distribution ainsi obtenue ne soit pas accessible à notre observation à cause de son uniformité dans toute l'etendue de l'espace. Dans ces conditions, tout état d'energie négative non occupé représentant une rupture de cette uniformité, doit se révévler à observation comme une sorte de lacune. Il es possible d'admettre que ces lacunes constituent les positrons.*
>
> P.A.M. Dirac, 1934 in Théorie du Positron

Although, such a conjecture would eventually have to be justified by showing that, e.g., thanks to the Fermi and perhaps also the Coulomb repulsion, the respective density matrices of the actual entangled ground state of a model of interacting quantum electrodynamics and the product state ansatz (171) are in some sense close and resemble such a uniform distribution, Dirac's heuristic picture serves already well as a working prescription, and at least in the regime of scattering theory, it has proven its empirical adequacy. As described in [30], a first attempt to study such a system is to introduce an external disturbance that may provoke the described excitations. The natural candidate is an electromagnetic field

$$A : \mathbb{R}^4 \to \mathbb{R}^4, \qquad x \mapsto (A_\mu(x))_{\mu=0,1,2,3} = (A^0(x), \mathbf{A}(x)) \tag{172}$$

which turns the free Dirac equation in (170) into the following version, featuring an external potential

$$(i\partial\!\!\!/ - M)\psi(x) = eA\!\!\!/(x)\psi(x), \tag{173}$$

where e represents the electron charge in this notation. The external potential $A_\mu(x)$ may now allow for transitions of states between the subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$. Provided sufficient regularity, (173) gives rise to a one-particle evolution operator $U^A(t_1, t_0) : \mathcal{H} \circlearrowleft$ for times $t_1, t_0 \in \mathbb{R}$, see [102]. A natural candidate for a time evolution of (171) may thus be given by an operator $\mathcal{L}_U$ acting as

$$\mathcal{L}_U \Omega = U\varphi_1 \wedge U\varphi_2 \wedge U\varphi_3 \wedge \ldots \qquad \text{for} \qquad U = U(t_1, t_0). \tag{174}$$

Heuristically speaking, an excitation may then be created as follows. A state $\varphi_1 \in \mathcal{H}$ in the Dirac sea Ω may be bound by the potential $A_\mu(x)$ and over time dragged into the positive energy subspace to become $\chi \in \mathcal{H}^+$. As an oversimplified but illustrative example, a resulting excited state could therefore be of the form

$$\Psi = \chi \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots \tag{175}$$

in which φ_1 is missing. Due to (173), states in $\mathcal{H}^+$ disperse rather differently as compared to the ones in $\mathcal{H}^-$. Hence, an electron described by $\chi \in \mathcal{H}^+$ may emerge from the "vacuum" and so does the "hole" in the sea described by the missing $\varphi_1 \in \mathcal{H}^-$ the state (175), which is left behind. Following Dirac, the *hole* itself can be interpreted as a particle, which is referred to as *positron*, and both names can be used as synonyms. It turns out that the dispersion of a positron is given by the one of an electron except for an opposite sign of its charge e. The state (175) is therefore referred to as electron-positron pair. This heuristic picture can be developed into an economic Fock space formalism to describe Dirac seas and their excitations which, first, is introduced informally, and later, formally.

Fock space description. Instead of tracking all infinitely many particles individually, one may equivalently describe the motion of the electron χ, the corresponding hole φ_1, and the net evolution of Ω. Since the number of electron-hole pairs may vary over time, a formalism for variable particle numbers is needed. This is provided by the Fock space formalism associated to the second quantization of the Dirac equation. One introduces a so-called creation operator a^* that algebraically acts as

$$a^*(\chi)\varphi_1 \wedge \varphi_2 \wedge \ldots = \chi \wedge \varphi_1 \wedge \varphi_2 \wedge \ldots, \tag{176}$$

and also its corresponding adjoint a, which is called annihilation operator. The state Ψ from the example in (175) can then be written as $\Psi = a^*(\chi)a(\varphi_1)\Omega$. Moreover, as the operator $a^*(f)$ is linear in its argument $f \in \mathcal{H}$, it is commonly split into the sum

$$a^*(f) = b^*(f) + c^*(f) \qquad \text{with} \qquad b^*(f) := a^*(P^+ f), \quad c^*(f) := a^*(P^- f). \tag{177}$$

Hence, b^* and c^* and their adjoints are creation and annihilation operators of electrons having positive and negative energy, respectively. In order to focus on the excitations with respect to the infinitely many-particle state Ω, in the notation, one introduces the following change in language. First, the space generated by the completion of all finite linear combinations of states $b^*(f_1)b^*(f_2)\ldots b^*(f_n)\Omega$ for $f_k \in \mathcal{H}^+, n \in \mathbb{N}$, is identified with the *electron Fock space*

$$\mathcal{F}_e = \bigoplus_{n \in \mathbb{N}_0} (\mathcal{H}^+)^{\wedge n}. \tag{178}$$

Second, the space generated by the completion of all finite linear combinations of states of the form $c(g_1)c(g_2)\dots c(g_n)\Omega$ for $g_k \in \mathcal{H}^-, n \in \mathbb{N}$, is identified with the *hole Fock space*

$$\mathcal{F}_h = \bigoplus_{n\in\mathbb{N}_0} (\mathcal{H}^-)^{\wedge n}. \tag{179}$$

Note that this time it is the annihilation operator of negative energy states that generates the Fock space. To make the notation more coherent, one furthermore replaces the annihilation operator of negative energy states $c(g)$ by the symbol $d^*(g)$, which reminds of a creation operator. However, unlike creation operators, $d^*(g)$ would still be anti-linear in its argument $g \in \mathcal{H}^-$. Thus, in a third step, one replaces $\mathcal{H}^-$ by its complex conjugate $\overline{\mathcal{H}^-}$, i.e., the set $\mathcal{H}^-$ equipped with the usual $\mathbb{C}$-vector space structure except for the scalar multiplication $\cdot^\star : \mathbb{C} \times \overline{\mathcal{H}^-} \to \overline{\mathcal{H}^-}$ which is redefined by $\lambda \cdot^\star g = \lambda^* g$ for all $\lambda \in \mathbb{C}$ and $g \in \overline{\mathcal{H}^-}$. This turns $\mathcal{F}_h$ into

$$\overline{\mathcal{F}_h} = \bigoplus_{n\in\mathbb{N}_0} (\overline{\mathcal{H}^-})^{\wedge n}, \tag{180}$$

and $d^*(g) = c(g)$ becomes linear in its argument $g \in \overline{\mathcal{H}^-}$ and may be referred to as a hole creation operator. To treat electrons and holes more symmetrically, one also introduces the anti-linear charge conjugation operator $C : \mathcal{H} \to \mathcal{H}$, $C\psi = i\gamma^2\psi^*$. This operator exchanges $\mathcal{H}^+$ and $\mathcal{H}^-$, i.e., $C\mathcal{H}^\pm = \mathcal{H}^\mp$, and thus, gives rise to a linear map $C : \overline{\mathcal{H}^-} \to \mathcal{H}^+$. A hole wave function $g \in \overline{\mathcal{H}^-}$ living in the space negative states can then be represented by a wave function $Cg \in \mathcal{H}^+$ living in the positive energy space.

By definition (176), at least informally, it can be seen that b, b^* and d, d^* fulfill the well-known anti-commutator relations

$$\begin{aligned} \{b(g), b(h)\} &= 0 = \{b^*(g), b^*(h)\}, &\quad \{b^*(g), b(h)\} &= \langle g, P^+h\rangle_{\mathcal{H}}\, 1_{\mathcal{F}_e}, \\ \{d(g), d(h)\} &= 0 = \{d^*(g), d^*(h)\}, &\quad \{d^*(g), d(h)\} &= \langle g, P^-h\rangle_{\mathcal{H}}\, 1_{\overline{\mathcal{F}_h}} \end{aligned} \tag{181}$$

for $g, h \in \mathcal{H}$ and the full Fock space for the electrons and positrons is then given by

$$\mathcal{F} = \mathcal{F}_e \otimes \overline{\mathcal{F}_h}. \tag{182}$$

In this space, the vacuum (171) is represented by $\Omega = 1 \otimes 1$ instead of an infinite antisymmetric product state as in (171) and the example electron-positron pair state Ψ in (175) by $a^*(\chi)d^*(\varphi_1)\Omega$. Two goals are achieved with this formalism. First, the description focuses on the excitation above the vacuum while the infinity many sea particles are implicitly encoded in the choice of $\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-$ by means of

$$b(f)\Omega = 0 = d(f)\Omega \qquad \text{for all } f \in \mathcal{H}. \tag{183}$$

And second, the wave functions in the arguments of the creation operators turn out to have positive kinetic energy.

Time evolution of Dirac seas. In this Fock space formalism, one-particle operators U on $\mathcal{H}$, as for instance the evolution operator $U^A : \mathcal{H} \circlearrowleft$ generated by (173), can be lifted to unitary operators $\widetilde{U}$ on $\mathcal{F}$ by requiring the following lift condition to hold

$$\widetilde{U} a^*(f) \widetilde{U}^* = a^*(Uf). \tag{184}$$

This condition determines a lift $\widetilde{U} : \mathcal{F} \circlearrowleft$ up to a phase as can be seen from the left-hand side of (184). For a prescribed external potential $A_\mu(x)$, one would be inclined to readily compute transition probabilities for the creation of pairs, as for example for a transition from Ω to Ψ as given in (171) and (175), respectively. Given orthonormal bases $(\varphi_n)_n$ and $(\chi_n)_n$ of $\mathcal{H}^-$ and $\mathcal{H}^+$, respectively, the leading order of such a transition is given by

$$1 - |\langle \Omega, \widetilde{U}^A(t_1, t_0)\Omega\rangle_{\mathcal{F}}|^2 \approx \sum_{nm} \left|\langle \chi_n, U^A(t_1, t_0)\varphi_m\rangle_{\mathcal{H}}\right|^2 = \|U^A_{+-}(t_1, t_0)\|_{I_2}, \tag{185}$$

where the notation $U^A_{\pm\mp} = P^\pm U^A P^\mp$ was used and the space of bounded operators with finite Hilbert-Schmidt norm $\|\cdot\|_{I_2}$ is denoted by $I_2(\mathcal{H})$. This is where the otherwise smooth story of the second quantization of the Dirac equations comes to an abrupt ending:

Deficiency D3: Another representation problem. For quite general yet sufficiently regular potentials A that ensure the existence of the one-particle time evolution operator U^A, and whose time evolution shall be abbreviated by $t \mapsto A(t)$, it turns out that:

Theorem 2.10 (Ruijsenaars [87]). *The right-hand side of* (185) $< \infty \Leftrightarrow \mathbf{A}(t_0) = 0 = \mathbf{A}(t_1)$.

In view of (185), the transition probability is thus only defined for external potentials A that, at the times of interest t_0, t_1, have zero spatial components $\mathbf{A}$. Even worse, the criterion for the well-definedness of a possible lift $\widetilde{U} : \mathcal{F} \circlearrowleft$ of any unitary one-particle operator $U : \mathcal{H} \circlearrowleft$ according to (184) is given by:

Theorem 2.11 (Shale-Stinespring [97]). *There is a unitary operator* $\widetilde{U} : \mathcal{F} \circlearrowleft$ *that fulfills* (184) $\Leftrightarrow U_{+-}, U_{-+} \in I_2(\mathcal{H})$.

Hence, Theorem 2.10 together with Theorem 2.11 imply that a lift $\widetilde{U}^A$ of the one-particle time evolution U^A is well-defined if and only if the spatial components $\mathbf{A}$ are zero at the relevant times t_0, t_1. The mechanism behind this effect is that the Hamiltonian for Dirac electrons in an external field

$$H^A = \gamma^0 \left(\boldsymbol{\gamma} \cdot (-i\nabla_{\mathbf{x}} - e\boldsymbol{A}) + M \right) + eA^0 \tag{186}$$

features a $\gamma^0\boldsymbol{\gamma}$ matrix in front of $\boldsymbol{A}$ which, when applied to (171), instantly develops components in the positive energy spectrum in each of the infinite tensor components and renders the corresponding Fock norm infinite. Loosely speaking, infinite many electron-positron pairs are already produced by the action of the Hamiltonian only. If $\boldsymbol{A}$ eventually becomes zero again, these positive energy components relax back to the negative spectrum and the corresponding pairs disappear. Therefore, the scattering matrix for an external field localized in a finite domain of space-time is unaffected, which is why physicists refer to those pairs at intermediate times as *virtual pairs*. The time evolution operators $\widetilde{U}^A$ for intermediate times that lie in the support of the spatial components of the external field $\mathbf{A}$ are however ill-defined and cause divergences such as in (185). This ill-definedness of the evolution operator, and likewise of its generator, for general potentials A can be addressed by yet another ultraviolet cut-off of large momenta that ensures the finiteness of (185), which is why deficiency D3 was coined *ultraviolet divergence of fermionic fields modeling matter and charges* in the introduction in Section 2.1. The fundamental problem, however, turns out to be yet another problem of the fixed representation of standard Fock space which is defined by the choice of splitting $\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-$ employed in (178) and (179). In fact, one way to construct a well-defined second-quantized time evolution operator, as sketched in [41], is to implement it between time-varying Fock spaces instead of on the single fixed standard Fock space $\mathcal{F}$. Such constructions have successfully been carried out for general potentials in [73, 77, 26]. With regards to deficiency D2, and in parts also D1, the necessity to adapt the Fock space representations is not unfamiliar. Especially in a relativistic setting, a change of Fock spaces should be expected, as for instance any Lorentz boost may tilt an equal-time hyperplane $\{t\} \times \mathbb{R}^3$ to a space-like hyperplane Σ in space-time $\mathbb{R}^4$, which would require a change from standard Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^4)$ to $L^2(\Sigma, \mathbb{C}^4)$ attached to Σ, and likewise, the corresponding Fock spaces are bound to change.

Despite the fact that there are solutions for this part of deficiency D3, the fact that remained particularly strange in view of Lorentz and gauge invariance was the explicit reference to the spatial components of A. This gave rise to the work [A8] in which the underlying geometry of Ruijsenaars' criterion was investigated and the existing constructions in [73, 77, 26] based on equal-time hyperplanes were generalized by implementing the second-quantized Dirac evolution from one Cauchy surface to another. The resulting formulation of external field QED has several advantages. First, its Lorentz and gauge covariance can be made explicit. Second, it treats the initial value problem for general Cauchy surfaces, and therefore, allows to study the evolution in the form of local deformations of Cauchy surfaces in the spirit of Tomonaga and Schwinger, e.g., [103, 91, 92, 94, 93, 95, 96]. And third, it gives a geometric and more general version of the implementability criterion $\mathbf{A} = 0$ that is formalized by the above theorems by Ruijsenaars and Shale-Stinespring in the special case of equal-time hyperplanes. These main results of work [A8] are described in the following.

Evolution on varying Fock spaces. The central geometric objects to formulate the well-posedness result of the initial value problems of (173), see [27], are Cauchy surfaces Σ in $\mathbb{R}^4$, which are understood as smooth, three-dimensional submanifolds of $\mathbb{R}^4$ that fulfill the following three conditions:

1. Every inextensible, two-sided, time- or light-like, continuous path in $\mathbb{R}^4$ intersects Σ in a unique point.
2. For every $x \in \Sigma$, the tangential space $T_x\Sigma$ is space-like.
3. The tangential spaces to Σ are bounded away from light-like directions in the following sense: The only light-like accumulation point of $\bigcup_{x\in\Sigma} T_x\Sigma$ is zero.

The one-particle Hilbert space attached to a Cauchy surface Σ is given by the space of $\mathbb{C}^4$-valued square-integrable functions $\mathcal{H}_\Sigma = L^2(\Sigma, \mathbb{C}^4)$. In the same way $\mathcal{H}$ was split into the polarizations $\mathcal{H}^\pm$ by $\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-$, one may proceed with $\mathcal{H}_\Sigma$. All admissible polarizations $\mathtt{Pol}(\mathcal{H}_\Sigma)$ are given by the set of all closed, linear subspaces $V \subset \mathcal{H}_\Sigma$ such that V and $V^\perp$ are both infinite dimensional. For $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ the corresponding orthogonal projector on $\mathcal{H}_\Sigma$ is denoted by $P_\Sigma^V : \mathcal{H}_\Sigma \to V$. Each polarization $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ then splits the Hilbert space $\mathcal{H}_\Sigma$ into a direct sum, i.e., $\mathcal{H}_\Sigma = V^\perp \oplus V$. The so-called standard polarizations $\mathcal{H}_\Sigma^+$ and $\mathcal{H}_\Sigma^-$ are determined by the orthogonal projectors P_Σ^+ and P_Σ^- onto the free positive and negative energy Dirac solutions, respectively, restricted to Σ:

$$\mathcal{H}_\Sigma^+ := P_\Sigma^+ \mathcal{H}_\Sigma = (1 - P_\Sigma^-)\mathcal{H}_\Sigma, \qquad \mathcal{H}_\Sigma^- := P_\Sigma^- \mathcal{H}_\Sigma. \tag{187}$$

Loosely speaking, in terms of Dirac's hole theory, the polarization $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ indicates the "sea level" of the Dirac sea, and the electron wave functions in $V^\perp$ and V are considered to be "above" and "below" sea level, respectively. Finally, given a Cauchy surface Σ and a polarization $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, one can define the corresponding Fock space

$$\mathcal{F}(V, \mathcal{H}_\Sigma) := \bigoplus_{c\in\mathbb{Z}} \mathcal{F}_c(V, \mathcal{H}_\Sigma), \qquad \mathcal{F}_c(V, \mathcal{H}_\Sigma) := \bigoplus_{\substack{n,m\in\mathbb{N}_0 \\ c=m-n}} (V^\perp)^{\wedge n} \otimes \overline{V}^{\wedge m}, \tag{188}$$

whose creation and annihilation operators are denoted by a_Σ^* and a_Σ.

For the sake of simplicity, in order to investigate the lift of the one-particle Dirac evolution $U_{\Sigma'\Sigma}^A : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$ from Cauchy surface Σ to Σ' that is generated by (173), see [27], the following external potential

$$A = (A_\mu)_{\mu=0,1,2,3} = (A_0, \mathbf{A}) \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4), \tag{189}$$

that is smooth and compactly supported is assumed, although this condition is unnecessarily strong and can be generalized. The first question is whether there are polarizations $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ and $W \in \mathtt{Pol}(\mathcal{H}_{\Sigma'})$ such that a potential lift

$$\widetilde{U}_{\Sigma'\Sigma}^A : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'}) \tag{190}$$

fulfilling the generalized lift condition

$$\widetilde{U}^A_{\Sigma'\Sigma}\, \psi_{V,\Sigma}(f)\, \widetilde{U}^A_{\Sigma\Sigma'} = \psi_{W,\Sigma'}(U^A_{\Sigma'\Sigma} f), \qquad \text{for } f \in \mathcal{H}_\Sigma \tag{191}$$

exists, where $\psi_{V,\Sigma}$ denotes the Dirac field operator corresponding to Fock space $\mathcal{F}(V,\Sigma)$, i.e.,

$$\psi_{V,\Sigma}(f) := a_\Sigma(P^{V^\perp}_\Sigma f) + a^*_\Sigma(P^V_\Sigma f), \qquad \text{for all } f \in \mathcal{H}_\Sigma. \tag{192}$$

The condition under which such a lift $\widetilde{U}^A_{\Sigma'\Sigma}$ exists can be inferred from an application of Shale and Stinespring's well-known theorem [97]:

Theorem 2.12 (Generalized Shale-Stinespring)**.** *The following statements are equivalent:*

1. *There is a unitary operator* $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V,\mathcal{H}_\Sigma) \to \mathcal{F}(W,\mathcal{H}_{\Sigma'})$ *which fulfills* (191).
2. *The off-diagonals* $P^{W^\perp}_{\Sigma'} U^A_{\Sigma'\Sigma} P^V_\Sigma$ *and* $P^W_{\Sigma'} U^A_{\Sigma'\Sigma} P^{V^\perp}_\Sigma$ *are Hilbert-Schmidt operators.*

Again, it is important to emphasize that the phase of the lift is not fixed by condition (191) and, depending on the external field A, this condition is not always satisfied as Ruijsenaars' theorem above shows. On the other hand, the choices of polarizations V and W are at one's expense in order to arrange for well-definedness. There is a trivial but little useful choice: Pick a Cauchy surface Σ_{in} in the remote past of the support of A fulfilling

$$\Sigma_{\text{in}} \text{ is a Cauchy surface such that } \operatorname{supp} A \cap \Sigma_{\text{in}} = \emptyset \tag{193}$$

to define $V = U^A_{\Sigma\Sigma_{\text{in}}} \mathcal{H}^-_{\Sigma_{\text{in}}}$ and $W = U^A_{\Sigma'\Sigma_{\text{in}}} \mathcal{H}^-_{\Sigma_{\text{in}}}$ which trivially fulfill point 2 of Theorem 2.12 as the off-diagonals are zero. The drawback of these choices is that the resulting lifts depend on the whole history of A between Σ_{in} and Σ, Σ'. Moreover, such V and W are rather implicit. But the statement in point 2 in Theorem 2.12 also allows to differ from the projectors P^V_Σ and $P^W_{\Sigma'}$ by a Hilbert-Schmidt operator. It is therefore interesting to study the corresponding classes of admissible polarizations and their dependence on A, which turn out to be rather canonical objects.

Classes of admissible polarizations. The preceding observations suggest to characterize admissible classes of polarizations as follows:

Definition 2.13 (Physical polarization classes [A8])**.** *For a Cauchy surface* Σ*, one defines the equivalence classes*

$$C_\Sigma(A) := \left[U^A_{\Sigma\Sigma_{\text{in}}} \mathcal{H}^-_{\Sigma_{\text{in}}} \right]_\approx, \tag{194}$$

where for $V, V' \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, $V \approx V'$ *means that the difference* $P^V_\Sigma - P^{V'}_\Sigma$ *is a Hilbert-Schmidt operator* $\mathcal{H}_\Sigma \circlearrowleft$ *in* $I_2(\mathcal{H}_\Sigma)$.

This definition immediately implies:

Corollary 2.14 (Dirac sea evolution)**.** *Let* Σ, Σ' *be Cauchy surfaces. Then any choice* $V \in C_\Sigma(A)$ *and* $W \in C_{\Sigma'}(A)$ *implies condition 2 of Theorem* 2.12*, and therefore, the existence of a lift* $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V,\mathcal{H}_\Sigma) \to \mathcal{F}(W,\mathcal{H}_{\Sigma'})$ *obeying* (191).

Consequently, any choice $V \in C_\Sigma(A)$ and $W \in C_{\Sigma'}(A)$ gives rise to a lift of the one-particle Dirac evolution between the corresponding $\mathcal{F}(V,\mathcal{H}_\Sigma)$ and $\mathcal{F}(W,\mathcal{H}_{\Sigma'})$ that is unique up to a phase. Two natural questions are therefore: On which properties of A and Σ do these polarization classes depend? And how do they behave under Lorentz and gauge transformations? Beside the above framework, the main import of the work [A8] are answers to these questions which are reported on next.

Properties of polarization classes. The first result ensures that the classes $C_\Sigma(A)$ are independent of the history of A. Instead, it is shown that they only depend on the tangential components of A on Σ.

Theorem 2.15 (Identification of polarization classes [A8])**.** *Let Σ be a Cauchy surface and let A and $\widetilde{A}$ be two smooth and compactly supported external fields. Then*

$$C_\Sigma(A) = C_\Sigma(\widetilde{A}) \qquad \Leftrightarrow \qquad A|_{T\Sigma} = \widetilde{A}|_{T\Sigma} \tag{195}$$

where $A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}$ means that for all $x \in \Sigma$ and $y \in T_x\Sigma$ the equality $A_\mu(x)y^\mu = \widetilde{A}_\mu(x)y^\mu$ holds true.

Ruijsenaar's no-go result as stated above may now be viewed as the special case of $\Sigma = \Sigma_t = \{x \in \mathbb{R}^4 |\ x^0 = t\}$ being an equal-time hyperplane.

The second main result furthermore shows that the polarization classes transform naturally under Lorentz and gauge transformations:

Theorem 2.16 (Lorentz and Gauge transformations [A8])**.** *Let $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ be a polarization.*

1. *Consider a* Lorentz transformation *given by $L_\Sigma^{(S,\Lambda)} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Lambda\Sigma}$ for a spinor transformation matrix $S \in \mathbb{C}^{4\times 4}$ and an associated proper orthochronous Lorentz transformation matrix $\Lambda \in \mathrm{SO}^\uparrow(1,3)$, cf. [27, Section 2.3]. Then:*

$$V \in C_\Sigma(A) \qquad \Leftrightarrow \qquad L_\Sigma^{(S,\Lambda)} V \in C_{\Lambda\Sigma}(\Lambda A(\Lambda^{-1}\cdot)). \tag{196}$$

2. *Consider a* gauge transformation $A \mapsto A + \partial\Gamma$ *for some $\Gamma \in C_c^\infty(\mathbb{R}^4, \mathbb{R})$ given by the multiplication operator $e^{-i\Gamma} : \mathcal{H}_\Sigma \to \mathcal{H}_\Sigma$, $\psi \mapsto \psi' = e^{-i\Gamma}\psi$. Then:*

$$V \in C_\Sigma(A) \qquad \Leftrightarrow \qquad e^{-i\Gamma} V \in C_\Sigma(A + \partial\Gamma). \tag{197}$$

Similarly to the unnecessarily strong restriction of $A \in C_c^\infty(\mathbb{R}^4, \mathbb{R})$, it is also possible to relax the condition of Γ, but this was not the focus of the work [A8].

These results render a geometric explanation for the peculiar no-go results on the existence of dynamics by Ruijsenaars and Shale-Stinespring in the special case of equal-time hyperplanes and fixed standard Fock space. In all generality, to construct the evolution for Dirac seas between Cauchy surfaces Σ and Σ', the initial step is to define Fock spaces $\mathcal{F}(V, \mathcal{H}_\Sigma)$ and $\mathcal{F}(W, \mathcal{H}_{\Sigma'})$ attached to Σ and Σ' by selecting polarizations V and W, respectively. The reported results of work [A8] now state that those polarizations V and W must be chosen from the polarization classes $C_\Sigma(A)$ and $C_{\Sigma'}(A)$, respectively. Only then there is a lift of the unitary one-particle Dirac evolution operator $U^A_{\Sigma'\Sigma} : \mathcal{H} \circlearrowleft$ to a unitary second-quantized evolution $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ fulfilling the lift condition (191). While the particular choice of V and W can be regarded as a "choice of coordinates" in the admissible Fock representations of the Dirac seas, the classes from which these polarizations are chosen are canonical objects in the sense that they behave covariantly under Lorentz and gauge transformations and are uniquely characterized only by the tangential components of the external potential A on the respective Cauchy surface. The resulting transition probabilities $|\langle\Psi, \widetilde{U}^A_{\Sigma'\Sigma}\Phi\rangle|^2$ are thus well-defined for all $\Psi \in \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ and $\Phi \in \mathcal{F}(V, \mathcal{H}_\Sigma)$, and furthermore, also unique because the potential phase that is left unspecified by the lift condition (191) drops out.

Finally, given a Cauchy surface Σ, the work [A8] provides another explicit representative $e^{Q^A_\Sigma}\mathcal{H}^-_\Sigma$ of the equivalence class of polarizations $C_\Sigma(A)$ in the form of a compact, skew-adjoint, linear operator $Q^A_\Sigma : \mathcal{H}_\Sigma \circlearrowleft$ that only depends on local information of A at Σ as opposed to the history of A such as, e.g., the trivial representative employed in (194), which is called "interpolating representation", and also those directly derived from global constructions of the fermionic projector [42, 45, 46, 43]. Given a family of Cauchy surfaces $(\Sigma_t)_{t\in\mathbb{R}}$ that interpolates smoothly between Σ and Σ', the work [A8] furthermore provides an infinitesimal version of how the external potential A changes the polarization in terms of the flow parameter t. Other representatives of the polarization class $C_\Sigma(A)$ can be inferred from the so-called Furry picture, which were worked out for equal-time hyperplanes in [41]. This choice amounts to the polarization obtained by a splitting into the positive and negative spectral subspaces of the Dirac Hamiltonian (173) with respect to an external field that is frozen at time t. However, as also concluded in [41], the resulting number operators of electrons and positrons for this choice of polarization are not Lorentz invariant and a vacuum state in one reference frame may look as a many-particle state in another. In fact, the mathematical structure of the external field problem in QED does not seem to discriminate between particular choices of polarizations within a class $C_\Sigma(A)$. Such a discrimination must therefore be introduced ad-hoc on physical grounds or inferred from a model of quantum electrodynamics that features an interaction between the charges, e.g., in order to devise a simple detector model. In scattering situations, one usually relies on Dirac's prescription that, whenever the external field A is switched off, in the long-time limits of scattering theory, the vacuum state (171) can be considered close to the actual ground state, and furthermore, excitations above it, i.e., with respect to polarizations $\mathcal{H}^+_\Sigma$ and $\mathcal{H}^-_\Sigma$, should be considered asymptotic electron-positron pairs. A similar prescription is given by the Furry picture in which the external fields are static. In such settings and for adiabatically tuned external fields, the effect of electron-positron pair creation was proven in [82]; see also [81].

Much more interesting than the external field model above are of course models that feature an electromagnetic interaction between the charges. While currently, a rigoros study of a complete model of quantum electrodynamics beyond individual perturbative corrections may yet be out of reach, in a long series of works Gravejat, Hainzl, Séré, and Solovej studied the stationary solutions of a non-linear model of quantum electrodynamics, among them [61, 62, 63, 54, 55] and, in particular, the overview in [74]. This model treats the Dirac sea in a Hartree-Fock approximation and features a self-consistent coupling to a classical electromagnetic field that is composed out of a prescribed external part, and most interestingly, another one that fulfills the time-independent Gauss laws given the expectation value of the charge current density generated by the Furry picture representation as input. Those models are not only able to describe the polarization of the vacuum by an external field but also the back reaction of its quantum expectation and establish the contact to effective models such as the Heisenberg-Euler Lagrangian [56] that are used in high-energy physics to describe the so-called non-linear properties of the quantum vacuum such as light-light scattering.

In general, models that couple to the charge current of the Dirac sea have to deal with yet another deficiency of type D3 that is more severe than the representational one described above. This section, and therefore this report, concludes with a short informal description of it:

Deficiency D3: The ill-defined charge current. As it is well-known [34], without a regularization of the momenta in the ultraviolet regime by another cut-off Λ, expectation values of the straight-forward charge current in quantum electrodynamics, as suggested by Noether's theorem, diverge logarithmically in Λ. In the external field model above, this behavior can be understood by means of Bogolyubov's formula

$$\widetilde{j}^\mu(x) = ie\widetilde{U}^A_{\Sigma_{\text{in}}\Sigma_{\text{out}}} \frac{\delta \widetilde{U}^A_{\Sigma_{\text{out}}\Sigma_{\text{in}}}}{\delta A_\mu(x)} \tag{198}$$

where, similar to Σ_{in} characterized in (193), Σ_{out} is a Cauchy surface in the remote future of the support of A such that $\Sigma_{\text{out}} \cap \operatorname{supp} A = \varnothing$. Moreover, $\frac{\delta}{\delta A_\mu(x)}$ denotes the functional derivative with respect to $A_\mu(x)$ in the sense of

$$\langle \Omega, \int d^4x\, F_\mu(x) \widetilde{j}^\mu(x) \Omega \rangle_{\mathcal{F}} = \frac{d}{d\epsilon} \langle \Omega, ie\widetilde{U}^A_{\Sigma_{\text{in}}\Sigma_{\text{out}}} \widetilde{U}^{A+eF}_{\Sigma_{\text{out}}\Sigma_{\text{in}}} \Omega \rangle_{\mathcal{F}} \Big|_{\epsilon=0} \tag{199}$$

for test functions $F \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4)$. While for each lift $\widetilde{U}^A_{\Sigma'\Sigma}$ the expression (199) is well-defined, it depends explicitly on the choice of phase that was left unspecified by the lift condition (191). Let for example $\varphi_A \in \mathbb{R}$ be a functional of A. Then

$$\overline{U}^A_{\Sigma'\Sigma} = e^{-i\varphi_A}\widetilde{U}^A_{\Sigma'\Sigma} \tag{200}$$

specifies another lift. By means of Bogolyubov's formula (198), the associated current is given by

$$\overline{j}^\mu(x) = \widetilde{j}^\mu(x) + e\frac{\delta\varphi_A}{\delta A_\mu(x)}. \tag{201}$$

Loosely speaking, the divergence of the expectation of the straight-forward charge current operator mentioned above is reflected in Bogolyubov's formula as the dependence of $\overline{j}^\mu$ on an arbitrarily chosen quantity, namely the phase φ_A. Hence, now it is the task to select a physically relevant one. A possible route, maybe most prominently investigated in [36, 88, 77, 53], is to impose extra conditions on the unidentified phase φ_A, such as causality and Lorentz and gauge invariance of the implied current (201), so that together with the groupoid property

$$\overline{U}^A_{\Sigma'\Sigma} = \overline{U}^A_{\Sigma'\Sigma''}\,\overline{U}^A_{\Sigma''\Sigma}, \tag{202}$$

for all Cauchy surfaces $\Sigma, \Sigma', \Sigma''$, the degrees of freedom in finding such a physically relevant vacuum expectation value for the current operator (201) are reduced to the known freedom of choice of a real number, i.e., the experimentally measured charge e_{exp}. While there is a suggestion of a phase motivated by parallel transport in [78], which also reproduces the second order of perturbation of the vacuum expectation value of the charge current, the program to arrive at a well-defined current was yet only carried out for individual orders of perturbation.

Furthermore, even if this program succeeds, there might be another difficulty to face when coupling self-consistently to the fields created by the potentially induced electron-positron pair excitations of the vacuum, which has been mentioned as the Landau pole problem in the introduction to this report in Section 2.1. While there is a lot of sophisticated physics literature on this topic, the mechanism is demonstrated particularly clear for the time component of the charge current vacuum expectation value in [63, Section 7 and 8] in the afore mentioned non-linearly coupled Hartree-Fock model of the quantum vacuum. On a very informal level, the general mechanism may be sketched as follows. According to [34], the Fourier modes in the momentum variable $q \in \mathbb{R}^4$ of the vacuum expectation value of the charge current operator under the influence of an external field A takes the form

$$\widehat{j}^\mu(q) = -\alpha\widehat{j}^\mu_A(q)(R_\Lambda - \Delta(q)) + O\left((\alpha\widehat{j}_A)^3\right), \tag{203}$$

where, in the employed system of units, the fine structure constant is given by $\alpha = \frac{e^2}{4\pi}$ and $\widehat{j}^\mu_A(q)$ denotes the Fourier modes of the external current that produces the external field A by means of the Maxwell equations. The term R_Λ is a constant that diverges logarithmically upon removal of the ultraviolet cut-off $\Lambda \to \infty$. Moreover, $\Delta(q)$ is a well-defined term that comprises two summands

$$\Delta(q) = \frac{1}{4\pi}\int_0^1 dx \frac{x}{\sqrt{1-x}} \log\left|1 - x\frac{q^2}{4M^2}\right| - \frac{i}{4}\operatorname{sign}(q^0)\int_0^1 dx\frac{x}{\sqrt{1-x}} 1_{x>\frac{4M^2}{q^2}} \tag{204}$$

describing the vacuum polarization and pair-creation, respectively, and $O\left((\alpha\widehat{j}_A)^2\right)$ denotes the remaining orders of perturbation theory. However, the expression (203) only reflects the "answer" of the Dirac sea when exposed to the external field. In addition, in a non-linear approximation, the vacuum expectation value of the polarization current (203) again produces an electromagnetic field and couples back to the Dirac sea. In order to make the computation self-consistent on the level of perturbation theory, a total current

$$\widehat{j}^\mu_{\text{tot}} = \widehat{j}^\mu + \widehat{j}^\mu_A \tag{205}$$

should be introduced and the equation (203) should be iterated to read

$$\alpha\widehat{j}_{\mathrm{tot}} = \alpha\widehat{j}_A - \alpha^2\widehat{j}_{\mathrm{tot}}(R_\Lambda - \Delta) + \alpha O\left((\alpha\widehat{j}_{\mathrm{tot}})^3\right) \tag{206}$$

$$= \frac{\alpha}{1+\alpha R_\Lambda}\widehat{j}_A + \frac{\alpha}{1+\alpha R_\Lambda}\alpha\widehat{j}_{\mathrm{tot}}\Delta + \frac{\alpha}{1+\alpha R_\Lambda}O\left((\alpha\widehat{j}_{\mathrm{tot}})^3\right) \tag{207}$$

Here, the tensor indices and the q-dependence were dropped for the sake of readability. In an attempt to remove the Λ dependence, one regards this equation for $q = 0$ in the time component of the current

$$\alpha\widehat{j}^0_{\mathrm{tot}}(q=0) = \frac{\alpha}{1+\alpha R_\Lambda}\widehat{j}^0_A(q=0), \tag{208}$$

for which all higher orders vanish in case the Dirac sea remains neutral. Thanks to the Fourier transform being evaluated at $q = 0$, the right-hand side of (208) equals the total external charge which suggests a scaling of the bare fine structure constant $\alpha = \alpha(\Lambda)$ such that

$$\frac{\alpha}{1+\alpha R_\Lambda} \xrightarrow{\Lambda\to\infty} \alpha_{\mathrm{exp}} \qquad \text{and} \qquad \alpha\widehat{j}_{\mathrm{tot}} \xrightarrow{\Lambda\to\infty} \alpha_{\mathrm{exp}}\widehat{j}_{\mathrm{exp}} \tag{209}$$

in order to swallow the Λ dependence and gauge the fine structure constant to the experimentally measured value α_{exp}. Implementing this scaling results in

$$\alpha_{\mathrm{exp}}\widehat{j}_{\mathrm{exp}} = \alpha_{\mathrm{exp}}\widehat{j}_A + \alpha^2_{\mathrm{exp}}\widehat{j}_{\mathrm{exp}}\Delta + \alpha_{\mathrm{exp}}O\left((\alpha_{\mathrm{exp}}\widehat{j}_{\mathrm{exp}})^3\right) \tag{210}$$

which looks good at first sight but it requires

$$\alpha(\Lambda) = \frac{\alpha_{\mathrm{exp}}}{1-\alpha_{\mathrm{exp}}R_\Lambda}. \tag{211}$$

The latter implies that the bare fine structure constant α grows with Λ and diverges already at a finite value, the so-called Landau pole. By virtue of the smallness of α_{exp}, this pole luckily occurs only at an extremely large momentum scale. Nevertheless, the introduction of the ultraviolet cut-off that breaks the Lorentz invariance of the model is already undesirable in the first place. In this respect, it is important to note that the scaling above stands on no grounds as a perturbation theoretic treatment is anyhow questionable for growing coupling parameters α. Finally, whether a well-defined and well-chosen definition of the non-perturbative charge current (198) even leads to this Landau pole problem after a self-consistent coupling is introduced is unclear at this point in time. In fact, e.g., in a more fundamental approach to quantum field theory dubbed the “Theory of Causal Fermion Systems” [42, 44, 43], this problem seems to be absent even for the sector of quantum electrodynamics.

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A Electronic reprints

Table of electronic reprints

Consistency of multi-time Dirac equations with general interaction potentials

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Abstract

In 1932, Dirac proposed a formulation in terms of multi-time wave functions as candidate for relativistic many-particle quantum mechanics. A well-known consistency condition that is necessary for existence of solutions strongly restricts the possible interaction types between the particles. It was conjectured by Petrat and Tumulka that interactions described by multiplication operators are generally excluded by this condition, and they gave a proof of this claim for potentials without spin-coupling. Under smoothness assumptions of possible solutions we show that there are potentials which are admissible, give an explicit example, however, show that none of them fulfills the physically desirable Poincaré invariance. We conclude that in this sense Dirac's multi-time formalism does not allow to model interaction by multiplication operators, and briefly point out several promising approaches to interacting models one can instead pursue.

Keywords: multi-time wave functions, relativistic quantum mechanics, Dirac equation, consistency condition, interaction potentials, spin-coupling, solution theory of multi-time systems

1 Introduction

The absence of absolute simultaneity in the theory of relativity has consequences for the formulation of relativistic quantum mechanics. Very elementarily, this can already be observed when considering the Lorentz transformation of a simultaneous configuration of N particles, $(t, \mathbf{x}_1), ..., (t, \mathbf{x}_N)$, which yields a configuration $(t'_1, \mathbf{x}'_1), ..., (t'_N, \mathbf{x}'_N)$ with N different times. This fact immediately poses the question of how a wave function or quantum state $\psi(t, \mathbf{x}_1, ..., \mathbf{x}_N)$, which is usually described as dependent on one time t and Euclidean positions $\mathbf{x}_1, \ldots, \mathbf{x}_N$, behaves under such a transformation. Dirac addressed this issue already in 1932 and suggested to generalize the concept of the familiar wave function $\psi(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ to a *multi-time* wave function $\psi(x_1, ..., x_N)$, where now $x_j = (t_j, \mathbf{x}_j)$ denote N space-time points in Minkowski space; see [1]. This idea led to the fundamental works [2, 3] which provided the basis for the relativistic formulation of quantum field theory. In his approach, Dirac defined the evolution of the multi-time state ψ by requiring it to fulfill N Dirac equations, one for each each time variable t_j. Although this concept seems natural, it is very restrictive in admission of solutions because it is a necessary condition for the existence of solutions, already discussed in [4] and henceforth called *consistency condition*, that the N single-time evolutions commute. This condition

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becomes subtle when the N particles are allowed to interact. In this respect, Dirac's approach calls for a mathematical study of the corresponding solution theory, which was initiated recently in a series of works by Petrat and Tumulka [5, 6, 7] and by Lienert [8, 9, 10] and Lienert and Nickel [11]. As shown in [5], the consistency condition basically rules out any interaction mediated by potentials without spin-coupling. In the following we extend the results of [5] and prove that the consistency condition is also violated for Poincaré invariant interaction potentials including spin-coupling.

This raises the question of how to introduce a sensible interaction in the multi-time formalism, which led Dirac et al. [2] to consider second-quantized fields that mediate the interaction; see also the recently studied multi-time models of quantum field theory in [6, 7]. In one dimension, another way of introducing a consistent interaction between the N particles was presented in [9, 11]. There, rigorous models of interaction by boundary conditions have been constructed. There is some connection to the new concept of interior-boundary conditions by Teufel and Tumulka, which has so far been used to formulate certain non-relativistic QFT models without divergences [12, 13, 14]. It is an open but very interesting question if the method of interior-boundary conditions can help to formulate mathematically well-defined models of particle creation and annihilation in the multi-time formalism.

A further strategy that has been pursued is to generalize the concept of a potential to terms of the form $V(x_1, \dots, x_N, p_1, \dots, p_n)$ that are no multiplication operators, but also depend on the momenta, i.e. derivatives [15, 16]. Lastly, we consider the idea of multi-time integral equations to be very promising. Instead of a system of differential equations such as (1), one can impose a single integral equation for $\psi(x_1, ...x_N)$. This avoids the problem of the consistency condition and makes a more general class of models possible. A prominent example known from QED is the Bethe-Salpeter equation [17, 18], whose mathematical features are not well-understood and would deserve further study (see also [19]).

Definition of the model. The model for our investigation is given by the system of evolution equations

$$i\frac{\partial}{\partial t_k}\psi(x_1, ..., x_N) = H_k(x_1, ..., x_N)\psi(x_1, ..., x_N), \quad k = 1, ..., N, \tag{1}$$

where the *partial Hamiltonians* H_k are given by

$$H_k = H_k^0 + V_k, \tag{2}$$

with H_k^0 being the free Dirac Hamiltonian of the k-th particle (see (6)) below). The interaction shall be described by the operator V_k which is given in terms of a (self-adjoint) spin-matrix valued multiplication operator $V_k(x_1, ...x_N)$ that depends on the space-time coordinates $x_1, \dots, x_N$. For this model, as was first recognized by Bloch [4] and further investigated by Petrat and Tumulka [5], a necessary condition for existence of solutions to (1) is the aforementioned *consistency condition*

$$\left([H_j, H_k] - i\frac{\partial V_k}{\partial t_j} + i\frac{\partial V_j}{\partial t_k}\right)\psi = 0, \qquad \forall k \neq j. \tag{3}$$

In [5], Petrat und Tumulka conjectured that interacting systems of the form (1) with general non-vanishing potentials that lead to interaction between the particles are excluded as they would violate the consistency condition (3). They gave a proof of this claim under the assumption that the potentials V_k depend on the spin-index of the k-th particle only. This rules out a number of conceivable potentials, but not all of them:

Potentials such as the one of the Breit equation [20, 21], which can be derived as an approximation to the Bethe-Salpeter equation of QED (see [22]), contain a more complicated spin-coupling, which poses the question whether more general potentials may indeed comply with condition (3) and thereby to well-posedness of (1) in terms of an initial value problem.

As main results of this paper, we present a concrete example of a spin-coupling interaction potential which satisfies the consistency condition. However, we will also show that the class of potentials admitted by the consistency condition is rather small. In particular, under certain smoothness conditions on possible solutions ψ, we identify this class completely and show that it does not contain Poincaré invariant potentials. Therefore, combining the mathematical consistency condition with the physical requirement of Poincaré invariance, our results show that any type of potential acting as a multiplication operator must be excluded as possible candidates for modeling the interaction between the N particles.

After the following paragraph about the employed notation and conventions, we present our results in Section 2 and the proofs and more detailed derivations in Sections 3 and 4.

Notations and conventions. We consider 4-dimensional Minkowski space-time with metric $g = \mathrm{diag}(1, -1, -1, -1)$, with the usual notation that Greek indices run from 0 to 3 and Latin indices $a, b, ...$ only over the spatial components $1, 2, 3$. The Einstein summation convention is employed for Greek indices only. Particle labels are denoted also by Latin indices, $j, k, ...$ and run from 1 to the total particle number N. Space-time points are denoted by $x = (t, \mathbf{x})$. Throughout, the abbreviation $\partial_{k,\mu} := \frac{\partial}{\partial x_k^\mu}$ will be used. The gamma matrices are arbitrary 4×4-matrices that form a representation of the Clifford algebra, i.e. fulfill the anti-commutation relation

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\mathbb{1}, \quad \mu, \nu = 0, 1, 2, 3. \tag{4}$$

Moreover, the matrix γ^0 is hermitian, γ^k anti-hermitian, and a fifth gamma matrix is defined as

$$\gamma^5 := i\gamma^0\gamma^1\gamma^2\gamma^3. \tag{5}$$

The free Dirac Hamiltonian for the k-th particle is given by

$$H_k^0 = -i\sum_{a=1}^{3} \gamma_k^0 \, \gamma_k^a \partial_{k,a} + \gamma_k^0 m_k, \tag{6}$$

where m_k is the mass of the k-th particle and we use the following convention for the matrices: Since we are always working in the N-fold tensor product of $\mathbb{C}^4$, we write for some 4×4-matrix M:

$$M_k := \mathbb{1} \otimes \cdots \otimes \mathbb{1} \underbrace{\otimes\, M \otimes}_{\text{k-th place}} \mathbb{1} \otimes \cdots \otimes \mathbb{1}. \tag{7}$$

It is well-known that the Dirac operator (6) is self-adjoint on $\mathrm{dom}(H_k^0) = H^1(\mathbb{R}^3, \mathbb{C}^4)$; see [23]. Furthermore, it will be convenient to use the notation $\alpha_k^\mu := \gamma_k^0\gamma_k^\mu$ so that we may write the multi-time system (1) as

$$(i\alpha_k^\mu\partial_{k,\mu} - \gamma_k^0 m_k)\psi(x_1, ..., x_N) = V_k(x_1, ...x_N)\psi(x_1, ..., x_N), \quad k = 1, ..., N. \tag{8}$$

Hence, the wave function $\psi(x_1, ..., x_N)$ takes values in $(\mathbb{C}^4)^{\otimes N} \cong \mathbb{C}^K$, $K := 4^N$.

2 Results

In order to present the results two remarks are in order. First, we need to make precise what is meant by the notion *interaction potential.* External potentials of the form $V_k(x_k)$ that do not generate entanglement must be excluded, and also potentials that seemingly depend on different coordinates, but that actually only arise from external potentials by a change of coordinates in the spinor space $\mathbb{C}^K$. Therefore we define:

Definition 2.1 *A collection of potentials V_k, $k = 1, ..., N$, given as spin-matrix valued multiplication operators $V_k(x_1, ..., x_N)$ is called non-interacting iff there is a unitary map $U(x_1, ..., x_N) : \mathbb{C}^K \to \mathbb{C}^K$ such that for all $k = 1, \ldots, N$, $\tilde{\psi} := U(x_1, ...x_N)(\psi(x_1, ...x_N))$ satisfies a system of the form (1) where for each k, the potential $V_k(x_k)$ is independent of all other coordinates $x_1, ...x_{k-1}, x_{k+1}, ...x_N$. In the other case, we call the collection of potentials interacting.*

Petrat and Tumulka called potentials that are connected via a unitary map U *gauge-equivalent* [5], which means that interacting potentials in the sense of our definition are exactly those that are not gauge-equivalent to external potentials.
Second, it has to be emphasized that the natural domain of a multi-time wave function is not the whole configuration space-time $\mathbb{R}^{4N}$, but the subset

$$\mathscr{S}^{(N)} := \left\{ (t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathbb{R}^{4N} \middle| \forall k \neq j : (t_j - t_k)^2 < |\mathbf{x}_j - \mathbf{x}_k|^2 \right\}, \tag{9}$$

which contains the configurations where the N particles are space-like separated. A detailed explanation of this fact is found in [9]. Here, we only state that there are at least two reasons to consider a multi-time wave function only on $\mathscr{S}^{(N)}$:

- *Sufficiency*: In order to interpret Born's rule on any space-like hypersurface, it is sufficient for ψ to have domain $\mathscr{S}^{(N)}$. A Lorentz transformation of a simultaneous configuration as presented above always yields a space-like configuration. Indeed, the mere concept of "N-particle configuration" implies the use of $\mathscr{S}^{(N)}$ because the presence of N particles is always understood with respect to a frame, e.g. a laboratory frame, which is represented by a space-like hypersurface.

- *Necessity*: In quantum field theory the left-hand side of the consistency condition (3) generically contains commutators of field operators, such as $[\phi(x_j), \phi(x_k)]$, which are given in terms of the Pauli-Jordan distribution [3]. However, the latter has only support for $(x_j - x_k)^2 \geq 0$, and hence, outside of $\mathscr{S}^{(N)}$. This is the reason why multi-time formulations of quantum field theory such as [2] as well as [6, 7] are consistent on $\mathscr{S}^{(N)}$, but not on $\mathbb{R}^{4N}$.

Therefore, all results will be proven mainly on $\mathscr{S}^{(N)}$ and only besides on $\mathbb{R}^{4N}$. Lastly, we have to make precise what is meant by Poincaré invariance of potentials. For Λ in the proper Lorentz group and $a \in \mathbb{R}^4$, the Poincaré transformation maps $x \mapsto x' = \Lambda x + a$ and the multi-time wave function transforms as

$$\psi'(x_1, ...x_N) = S(\Lambda)^{\otimes N} \psi\left(\Lambda^{-1}(x_1 - a), ..., \Lambda^{-1}(x_N - a)\right), \tag{10}$$

with the spin transformation matrix $S(\Lambda)$ that fulfills $S(\Lambda)\gamma S^{-1}(\Lambda) = \Lambda\gamma$. We call a potential V_k Poincaré invariant if it satisfies

$$V_k(x_1, ...x_N) = S(\Lambda)^{\otimes N} V_k\left(\Lambda^{-1}(x_1 - a), ...\Lambda^{-1}(x_N - a)\right) S^{-1}(\Lambda)^{\otimes N}, \tag{11}$$

which is the condition for (1) to be Poincaré invariant. Our main result can then be stated as follows:

Theorem 2.2 *Let* $N = 2$, $\Omega = \mathbb{R}^{4N}$ *or* $\Omega = \mathscr{S}^{(N)}$. *If* $V_k(x_1, \cdots, x_N)$ *are interacting potentials in* $C^1(\Omega, \mathbb{C}^{K\times K})$ *and for all initial values* $\varphi \in C_c^\infty(\mathbb{R}^{3N} \cap \Omega, \mathbb{C}^K)$, *there is a solution* $\psi \in C^2(\Omega, \mathbb{C}^K)$ *to the multi-time system of Dirac equations* (1), *then the potentials* V_k *are not Poincaré invariant.*

We only formulate the theorem for the case $N = 2$, although we expect it to hold for general N and we prove several intermediate results for any N. For larger numbers of particles, however, some parts in the proofs which are based on a direct computation in terms of gamma matrices quickly become very complex and hardly traceable. In several partial results, we will also not restrict to $\Omega = \mathbb{R}^{4N}$ or $\Omega = \mathscr{S}^{(N)}$, but consider any open set $\Omega \subset \mathbb{R}^{4N}$. The strategy of proof is illustrated as follows:

(a) **Existence** $\Longrightarrow$ **Consistency:** If a solution to (1) exists, then the consistency condition (3) has to hold.

(b) **Consistency** $\Longrightarrow$ **Restrictions on potentials:** If the consistency condition (3) holds, then the admissible potentials are restricted and no Poincaré invariant ones are possible.

Step (a): The consistency condition.

Let us first discuss why one expects the consistency condition (3) to be necessary for existence of solutions. The condition can heuristically be understood as path independence of the integration of the system of evolution equations (1): E.g. prescribing initial values $\psi(0, \mathbf{x}_1, ...0, \mathbf{x}_N)$ at $t_1 = ... = t_N = 0$, it makes no difference if one decides to evolve first in t_j-direction and then in t_k-direction or the other way around, one always has to arrive at the same well-defined $\psi(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N)$. Therefore, the actions of the respective equations in our system (1) on the possible initial values have to commute.
Petrat and Tumulka have proven that the existence of a solution for every initial datum in the Hilbert space necessitates the consistency condition (3) in two different cases [5, Theorems 1 and 2]:

- for time-independent, possibly unbounded partial Hamiltonians H_k,
- for time-dependent, but smooth and bounded partial Hamiltonians H_k.

Here, we generalize the results of Petrat and Tumulka to the relevant case of unbounded Hamiltonians that may include a time-dependence in the potentials. Our proposition is a rather direct consequence of the differentiability of solutions and makes the idea of Bloch [4, p. 304] mathematically precise.

Proposition 2.3 *Let* $\Omega \subset \mathbb{R}^{4N}$ *be open. Suppose the multi-time system* (1), *with* V_k *being a function in* $C^1(\Omega, \mathbb{C}^{K\times K})$, *possesses a solution* $\psi \in C^2(\Omega, \mathbb{C}^K)$. *Then the consistency condition* (3) *holds for all* $(x_1, ..., x_N) = X \in \Omega$.

The proof is given in Section 3.1, followed by some remarks about a more geometric way of understanding the consistency condition in Section 3.2.

Step (b): Consistent potentials.

The consistency condition puts strong restrictions on the spin-coupling induced by the potentials. The following example shows the inconsistency for one natural looking choice.

Example: We consider a two-particle system (1) with $V_1 = \alpha_2^\mu A_\mu(x_1, x_2)$ and $V_2 = \alpha_1^\mu B_\mu(x_1, x_2)$ for some smooth, compactly supported functions A_μ, B_μ. This is suggested by the usual way of adding a 4-vector potential to the single-time Dirac equation, which is by adding $\alpha^\mu A_\mu$ to the Hamiltonian. One could think that interaction is achieved by choosing the gamma matrices of the other particle, as done here. But then the consistency condition is

$$\begin{aligned} & \left[\alpha_2^\mu A_\mu, -i\alpha_2^\nu \partial_{2,\nu} + \gamma_2^0 m_2\right] = 0 \\ \iff & -2m_2\gamma_2^\mu A_\mu + i\alpha_2^\nu \alpha_2^\mu \left(\partial_{2,\nu} A_\mu\right) + iA_\mu [\alpha_2^\nu, \alpha_2^\mu]\partial_{2,\nu} = 0. \end{aligned} \tag{12}$$

There is no possibility that the respective terms will cancel each other, so any A_μ different from zero will make the equations inconsistent. In particular, the derivative term with $\partial_{2,\nu}$ has to vanish separately, which will be a crucial ingredient in the proof of theorem 2.4. A similar calculation excludes potentials of the form $V_k \sim F_{\mu\nu}(x_1, x_2)\gamma_1^\mu \gamma_2^\nu$, too.

To have a chance of being consistent, the potentials may only depend on few matrices, which are the identity matrix and γ^5. To see this, we need to reformulate the consistency condition to a more useful version. That the bracket in (3) applied to any solution ψ ought to be zero implies that it must also be zero on every initial value $\varphi = \psi|_{t_1=\ldots=t_N=0}$. The initial values will be defined on a $3N$-dimensional set U, an intersection of Ω with the time-zero hypersurface. The assumption that there are solutions for all initial values in a certain class, e.g. the smooth compactly supported functions, allows us to draw general conclusions.

Theorem 2.4 *We assume:*

(A) *$U \subseteq \mathbb{R}^{3N}$ is open and simply connected. For a multi-time Dirac system* (1) *with continuously differentiable V_k, we have for each $\varphi \in C_c^\infty(U, \mathbb{C}^K)$,*

$$\left([H_j, H_k] - i\frac{\partial V_k}{\partial t_j} + i\frac{\partial V_j}{\partial t_k}\right)\varphi = 0, \qquad \forall k \neq j. \tag{13}$$

Then, for each $k \neq j$, the k-th spin component of the potential V_j is spanned by $\mathbb{1}_k$ and γ_k^5.

The proof is given in Section 4.1. One can directly see that the above example is not in the class of admissible potentials.
Theorem 2.4 allows us to proceed by a basis decomposition. All possible matrix structures that might appear in V_1 and V_2 can be listed and the consistency condition can be explicitly evaluated, as will be done in Section 4.2. In Lemma 4.2, we show that the consistency condition is equivalent to the system of equations (36a) to (36p), and that only eight possibly interacting terms remain.
It turns out that these possibilities for interacting terms in the potentials can not be excluded by general arguments. In fact, interacting potentials that fulfill the consistency condition exist, for example the ones in the following lemma.

Lemma 2.5 *Let C_ν and c_ν be constants for $\nu = 0, 1, 2, 3$ with at least one C_ν and c_ν different from zero, and define $x := x_2 - x_1$. Consider the multi-time Dirac system* (1) *for two particles with potentials*

$$\begin{aligned} V_1 &= \gamma_1^\mu C_\mu \exp\left(2i\gamma_1^5 c_\lambda x^\lambda\right) - m_1\gamma_1^0 \\ V_2 &= \gamma_1^5 \alpha_2^\nu c_\nu. \end{aligned} \tag{14}$$

1. *This system is consistent, i.e.* (3) *holds.*

2. *This system is interacting.*

This is proven in Section 4.3. With this example at hand, it becomes clear that we cannot prove inconsistency of arbitrary interacting potentials. But obviously, the potential V_1 in (14) is not Lorentz invariant. Since the use of multi-time equations aims at a relativistic formulation of quantum mechanics, it is natural to require Poincaré invariance, i.e. Lorentz invariance and translation invariance, of the potentials. We show that the latter excludes the former by finding that every translation invariant potential has to be of a certain shape.

Lemma 2.6 *Suppose the assumptions* (**A**) *of theorem 2.4 hold. If, in addition, the potentials are both interacting and translation invariant, i.e. satisfy*

$$V_k(x_1, x_2) = V_k(x_1 + a, x_2 + a) \quad \forall a \in \mathbb{R}^4, \tag{15}$$

then they are necessarily of the form

$$V_k = M_1 e^{c_{k,\nu} x^\nu} + M_2 e^{-c_{k,\nu} x^\nu} + const. \tag{16}$$

for some $M_1, M_2 \in \mathbb{C}^{K \times K}$ *and* $c_k \in \mathbb{C}^4$*, where* $x = x_1 - x_2$*.*

A slightly stronger version of this lemma will be formulated and proven in Section 4.4. Our main theorem 2.2 can then be proven by a simple collection of facts:

Proof of Theorem 2.2:

- First case: $\Omega = \mathbb{R}^{4N}$. Suppose a system (1) with potentials $V_k \in C^1(\mathbb{R}^{4N}, \mathbb{C}^{K \times K})$ that are interacting has a solution $\psi \in C^2(\mathbb{R}^{4N}, \mathbb{C}^K)$ for all initial values $\varphi \in C_c^\infty(\mathbb{R}^{3N}, \mathbb{C}^K)$. Consequently, by Proposition 2.3, the consistency condition (13) has to be true for all $\varphi \in C_c^\infty(\mathbb{R}^{3N}, \mathbb{C}^K)$. Then, by Lemma 2.6, if the potentials are translation invariant, they are of the form (16), which is not Lorentz invariant. Therefore, the potentials cannot be Poincaré invariant.

- Second case: $\Omega = \mathscr{S}^{(N)}$. The proof for the domain $\mathscr{S}^{(N)}$ goes through as above because the necessary lemmas were all proven for general domains that are open and simply connected, which is true for $\mathscr{S}^{(N)}$.

□

Under the assumptions on higher regularity of solutions, we have thus generalized the results of Petrat and Tumulka [5] in the sense that our theorem 2.2 covers arbitrary multiplication operators with spin-coupling. The class of potentials that are consistent and translation invariant (equation (16)) does not contain any physically interesting potentials, but only potentials that oscillate with the distance of the particles. That these are not Lorentz invariant further motivates to disregard them because multi-time equations are intended for a fully and manifest Lorentz invariant formulation of quantum mechanics. The implications of this result for the formulation of interacting relativistic quantum mechanics were discussed above in the introduction.

3 Proof of the consistency condition

3.1 Proof of Proposition 2.3

Proof of Proposition 2.3: Suppose $\psi \in C^2(\Omega, \mathbb{C}^K)$ solves the equations (1). Let $j \neq k$. By the theorem of Schwarz, the time-derivatives on ψ commute, which for $X \in \Omega$ gives:

$$\left(i\partial_{t_k} i\partial_{t_j} - i\partial_{t_j} i\partial_{t_k}\right)\psi = 0 \Rightarrow i\partial_{t_k}\left(H_j\psi\right) - i\partial_{t_j}\left(H_k\psi\right) = 0 \tag{17}$$

$$\Rightarrow H_j i\partial_{t_k}\psi + \left(i\partial_{t_k}V_j\right)\psi - \left(i\partial_{t_j}V_k\right)\psi - H_k i\partial_{t_j}\psi = 0 \tag{18}$$

$$\Rightarrow \left(H_jH_k + \left(i\partial_{t_k}V_j\right) - \left(i\partial_{t_j}V_k\right) - H_kH_j\right)\psi = 0. \tag{19}$$

In (17) and (19), we used that ψ solves the multi-time equations (1), and (18) follows by the product rule. As $X \in \Omega$ was arbitrary, equation (3) holds on Ω, as claimed. □

Remark:

1. The assumption that the solution ψ is at least twice differentiable in the time direction seems unproblematic because the spatial smoothness of initial data is usually inherited in the time direction due to the nature of physically relevant evolution equations. E.g. for the one-particle Dirac equation with smooth external electromagnetic potential A_μ, it was proven in [24] that solutions that are smooth on one (space-like) Cauchy surface are indeed smooth on all of $\mathbb{R}^4$.

2. This theorem even covers relativistic Coulomb potentials because for the domain $\Omega = \mathscr{S}^{(N)}$, a potential of the form

$$V \sim \frac{1}{(t_k - t_j)^2 - |\mathbf{x}_k - \mathbf{x}_j|^2} \tag{20}$$

   is singular only outside of $\mathscr{S}^{(N)}$, which ensures that $V \in C^\infty(\mathscr{S}^{(N)}, \mathbb{C}^{K\times K})$.

3.2 Geometric view of the consistency condition

In this section, we discuss on a non-rigorous level how the results on the consistency condition can be reformulated with the help of differential geometry (compare Section 2.3 in [5]). For each multi-time argument $(t_1, ..., t_N)$, the multi-time wave function will be an element of the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^{3N}, \mathbb{C}^K)$. We can define a vector bundle E over the base manifold $\mathbb{R}^N$ with identical fibres $\mathscr{H}$ at every point. (This is therefore a trivial vector bundle $E = \mathbb{R}^N \times \mathscr{H}$). A multi-time wave function is then a section of E.

A natural notion of parallel transport on E can be given by the single-time evolution operators $U_k(t_k)$ (which would be $e^{-iH_kt_k}$ for time-independent H_k). This means that we define a connection ∇ on E with components $\nabla_k = \partial_{t_k} + iH_k$, whereby the parallel transport in direction t_k is given by U_k. Solutions of (1) are then sections that are covariantly constant, i.e. satisfy $\nabla\psi = 0$.

The well-definedness of solutions requires that the parallel transport along a closed curve does not change the vector. So we need that for any loop γ, $U_\gamma = \mathbb{1}$. This is equivalent to saying that the vector bundle has a trivial holonomy group, $\mathrm{Hol}(\nabla) = \{\mathbb{1}\}$. By the theorem of Ambrose and Singer [25], the holonomy group is in direct correspondence to the curvature form $F(\nabla)$; in particular: $\mathrm{Hol}(\nabla) = \{\mathbb{1}\} \Leftrightarrow F(\nabla) = 0$. Therefore, the existence of a well-defined solution implies that ∇ is a flat curvature for E. By the formula for calculating the curvature from the connection, this means

$$0 = F_{ij} = \frac{\partial H_i}{\partial t_j} - \frac{\partial H_j}{\partial t_i} - i[H_i, H_j], \tag{21}$$

which is the consistency condition.

4 Spin-coupling potentials

4.1 Proof of Theorem 2.4

Proof of Theorem 2.4: We start with a system (8) and evaluate the consistency condition (13). Let $k \neq j$, then:

$$\begin{aligned} &\left[i\alpha_k^\mu \partial_{k,\mu} - \gamma_k^0 m_k - V_k, i\alpha_j^\nu \partial_{j,\nu} - \gamma_j^0 m_j - V_j\right] && (22)\\ =& \left[i\alpha_k^\mu \partial_{k,\mu} - \gamma_k^0 m_k, -V_j\right] + \left[-V_k, i\alpha_j^\nu \partial_{j,\nu} - \gamma_j^0 m_j\right] + [V_k, V_j] && (23)\\ =& [V_k, V_j] + m_k\left[\gamma_k^0, V_j\right] - m_j\left[\gamma_j^0, V_k\right] - i\left[\alpha_k^\mu \partial_{k,\mu}, V_j\right] + i\left[\alpha_j^\nu \partial_{j,\nu}, V_k\right] && (24)\end{aligned}$$

In (23), we used that the derivatives w.r.t. different coordinates commute by Schwarz. We consider the last term in more detail:

$$\begin{aligned} i\left[\alpha_j^\nu \partial_{j,\nu}, V_k\right] &= i\alpha_j^\nu \partial_{j,\nu} V_k - iV_k \alpha_j^\nu \partial_{j,\nu}\\ &= i\alpha_j^\nu \left(\partial_{j,\nu} V_k\right) + i\alpha_j^\nu V_k \partial_{j,\nu} - iV_k \alpha_j^\nu \partial_{j,\nu}\\ &= i\alpha_j^\nu \left(\partial_{j,\nu} V_k\right) + i\left[\alpha_j^\nu, V_k\right]\partial_{j,\nu}\\ &= i\alpha_j^\nu \left(\partial_{j,\nu} V_k\right) + i\sum_{a=1}^{3}\left[\alpha_j^a, V_k\right]\partial_{j,a}, \end{aligned} \tag{25}$$

where in the last line, the summand with $\nu = 0$ was dropped because $\alpha^0 = \mathbb{1}$ commutes with everything. Doing the same for the second last term yields that the consistency condition is equivalent to

$$\begin{aligned} 0 =& [V_k, V_j] + m_k\left[\gamma_k^0, V_j\right] - m_j\left[\gamma_j^0, V_k\right]\\ &- i\alpha_k^\mu\left(\partial_{k,\mu} V_j\right) + i\alpha_j^\nu\left(\partial_{j,\nu} V_k\right)\\ &- i\sum_{a=1}^{3}\left[\alpha_k^a, V_j\right]\partial_{k,a} + i\sum_{a=1}^{3}\left[\alpha_j^a, V_k\right]\partial_{j,a}. \end{aligned} \tag{26}$$

The derivatives in (26) are in some sense linearly independent, which is made clear in the following auxiliary claim.

Lemma 4.1 *Let $U \subseteq \mathbb{R}^{3N}$ be open. Let $f : U \to \mathbb{C}^K$ be a function and suppose there are complex $K \times K$-matrices $\Lambda_{k,j}(\mathbf{x}_1, ..., \mathbf{x}_N)$ such that*

$$\left(f(\mathbf{x}_1, ..., \mathbf{x}_N) + \sum_{k=1}^{N}\sum_{j=1}^{3}\Lambda_{k,j}\frac{\partial}{\partial x_k^j}\right)\varphi(\mathbf{x}_1, .., .\mathbf{x}_N) = 0, \quad \forall(\mathbf{x}_1, ..., \mathbf{x}_N) \in U, \tag{27}$$

holds for all $\varphi \in C_c^\infty(U, \mathbb{C}^K)$. Then, for all j and k, $\Lambda_{k,j}(\mathbf{x}_1, ..., \mathbf{x}_N) = 0$, and f must be the zero function.

Proof of the Lemma: We choose some fixed k and j and show that $\Lambda_{k,j} = 0$ first. Pick some point $(\mathbf{x}_1, ..., \mathbf{x}_N) = \mathbf{X} \in U$. There exists $\varphi \in C_c^\infty(U, \mathbb{C}^K)$ with the property that $\varphi(\mathbf{X}) = 0$ and $\partial_{l,m}\varphi(\mathbf{X}) = \delta_{lk}\delta_{mj}$. Thus, evaluating (27) at the point $\mathbf{X}$, we have

$$0 = f(\mathbf{X})\varphi(\mathbf{X}) + \sum_{l=1}^{N}\sum_{m=1}^{3} \Lambda_{l,m}(\mathbf{X})\delta_{lk}\delta_{mj} = \Lambda_{k,j}(\mathbf{X}) \tag{28}$$

Because all factors $\Lambda_{k,j}$ are equal to zero, eq. (27) directly implies that f is the zero function. □

Applying this lemma to the consistency condition (26), we obtain that the prefactors of the derivative terms have to vanish separately, which means

$$\left[\alpha_j^a, V_k\right] = 0, \quad \forall k \neq j, \ \forall a \in \{1, 2, 3\}. \tag{29}$$

This will give us the desired constraint on the matrix structures that may appear in each V_k. We note that the following matrices form a basis of the complex 4×4 matrices (for a proof see e.g. [26, p. 53ff.]) :

$$\alpha^\mu, \quad \gamma^5\alpha^\mu, \quad \gamma^\mu, \quad \gamma^5\gamma^\mu, \qquad \mu = 0, 1, 2, 3. \tag{30}$$

Although the matrix V_k is a tensor product of N 4×4-matrices, we can disregard all factors of the tensor product apart from the j-th to check when the condition (29) can be satisfied. We can express V_k in the above basis and just compute all commutators of α^a with basis elements. The following list, where we omit the index j, results:

$$\begin{aligned}
\left[\alpha^a, \alpha^0\right] &= 0\\
\left[\alpha^a, \alpha^b\right] &= 2\gamma^a\gamma^b = -2i\varepsilon_{abc}\gamma^5\alpha^c\\
\left[\alpha^a, \gamma^5\alpha^0\right] &= 0\\
\left[\alpha^a, \gamma^5\alpha^b\right] &= (2 - 2\delta^{ab})\gamma^5\gamma^b\gamma^a = 2i\varepsilon_{abc}\alpha^c\\
\left[\alpha^a, \gamma^0\right] &= -2\gamma^a\\
\left[\alpha^a, \gamma^b\right] &= -2\delta^{ab}\gamma^0\\
\left[\alpha^a, \gamma^5\gamma^0\right] &= -2\gamma^5\gamma^a\\
\left[\alpha^a, \gamma^5\gamma^b\right] &= -2\delta^{ab}\gamma^5\gamma^0.
\end{aligned} \tag{31}$$

If V_k contains combinations of $\alpha_j^0 = \mathbb{1}_j$ and γ_j^5, the commutators in (26) vanish. But the commutators with all other elements of the basis give non-zero and linearly independent matrices, which implies that other matrices cannot be present in V_k in order for condition (29) to be fulfilled. □

4.2 Basis decomposition

By theorem 2.4, the consistency condition implies that V_k only depends on the spin of the j-th particle via the identity matrix or γ_j^5. Therefore, we can expand the potentials as

$$\begin{aligned}
V_1 &= \mathbb{1}_2 V_{11} + \gamma_2^5 V_{15},\\
V_2 &= \mathbb{1}_1 V_{21} + \gamma_1^5 V_{25}.
\end{aligned} \tag{32}$$

In the terms V_{i1} and V_{i5}, all matrices depending on the i-th spin index may appear in principle, so we have

$$\begin{aligned} V_{11} &= \alpha_1^\mu W_{1,\mu} + \gamma_1^5 \alpha_1^\mu Y_{1,\mu} + \gamma_1^\mu A_\mu + \gamma_1^5 \gamma_1^\mu B_\mu \\ V_{15} &= \alpha_1^\mu X_{1,\mu} + \gamma_1^5 \alpha_1^\mu Z_{1,\mu} + \gamma_1^\mu C_\mu + \gamma_1^5 \gamma_1^\mu D_\mu \\ V_{21} &= \alpha_2^\nu W_{2,\nu} + \gamma_2^5 \alpha_2^\nu X_{2,\nu} + \gamma_2^\nu E_\nu + \gamma_2^5 \gamma_2^\nu F_\nu \\ V_{25} &= \alpha_2^\nu Y_{2,\nu} + \gamma_2^5 \alpha_2^\nu Z_{2,\nu} + \gamma_2^\nu G_\nu + \gamma_2^5 \gamma_2^\nu H_\nu, \end{aligned} \tag{33}$$

where $A_0, B_k, C_0, D_k, E_0, F_k, G_0, H_k, W_{i,\mu}, X_{i,\mu}, Y_{i,\mu}, Z_{i,\mu}$ are arbitrary real scalar functions and $A_k, B_0, C_k, D_0, E_k, F_0, G_k, H_0$ are arbitrary functions with purely imaginary values, such that the potentials are self-adjoint. It will soon become understandable why this nomenclature makes sense, especially what W_1, X_1, Y_1, Z_1 have to do with W_2, X_2, Y_2, Z_2.

Lemma 4.2 *Consider a multi-time system* (1) *for two particles for which the assumption **(A)** of Theorem 2.4 holds. Then the potentials can be expanded as*

$$V_1 = \gamma_1^\mu A_\mu + \gamma_1^5 \gamma_1^\mu B_\mu + \gamma_2^5 \left(\gamma_1^\mu C_\mu + \gamma_1^5 \gamma_1^\mu D_\mu \right) + V_{1,ext} \tag{34}$$

$$V_2 = \gamma_2^\nu E_\nu + \gamma_2^5 \gamma_2^\nu F_\nu + \gamma_1^5 \left(\gamma_2^\nu G_\nu + \gamma_2^5 \gamma_2^\nu H_\nu \right) + V_{2,ext} \tag{35}$$

where $V_{i,ext}$ is not interacting and the functions A_μ to H_μ, $\mu = 0, 1, 2, 3$, are scalars. Furthermore, the consistency condition is equivalent to the following system of equations:

$$\partial_{1,\mu} W_{2,\nu} = \partial_{2,\nu} W_{1,\mu} \tag{36a}$$
$$\partial_{1,\mu} X_{2,\nu} = \partial_{2,\nu} X_{1,\mu} \tag{36b}$$
$$\partial_{1,\mu} Y_{2,\nu} = \partial_{2,\nu} Y_{1,\mu} \tag{36c}$$
$$\partial_{1,\mu} Z_{2,\nu} = \partial_{2,\nu} Z_{1,\mu} \tag{36d}$$
$$B_\mu Y_{2,\nu} + D_\mu Z_{2,\nu} = \tfrac{i}{2} \partial_{2,\nu} A_\mu \tag{36e}$$
$$(m_1 \delta_{0\mu} + A_\mu) Y_{2,\nu} + C_\mu Z_{2,\nu} = \tfrac{i}{2} \partial_{2,\nu} B_\mu \tag{36f}$$
$$-B_\mu Z_{2,\nu} - D_\mu Y_{2,\nu} = \tfrac{i}{2} \partial_{2,\nu} C_\mu \tag{36g}$$
$$-(m_1 \delta_{0\mu} + A_\mu) Z_{2,\nu} - C_\mu Y_{2,\nu} = \tfrac{i}{2} \partial_{2,\nu} D_\mu \tag{36h}$$
$$F_\nu X_{1,\mu} + H_\nu Z_{1,\mu} = \tfrac{i}{2} \partial_{1,\mu} E_\nu \tag{36i}$$
$$(m_2 \delta_{0\nu} + E_\nu) X_{1,\mu} + G_\nu Z_{1,\mu} = \tfrac{i}{2} \partial_{1,\mu} F_\nu \tag{36j}$$
$$-F_\nu Z_{1,\mu} - H_\nu X_{1,\mu} = \tfrac{i}{2} \partial_{1,\mu} G_\nu \tag{36k}$$
$$-(m_2 \delta_{0\nu} + E_\nu) Z_{1,\mu} - G_\nu X_{1,\mu} = \tfrac{i}{2} \partial_{1,\mu} H_\nu \tag{36l}$$
$$B_\mu G_\nu = C_\mu F_\nu \tag{36m}$$
$$B_\mu H_\nu = C_\mu (m_2 \delta_{0\nu} + E_\nu) \tag{36n}$$
$$(m_1 \delta_{0\mu} + A_\mu) G_\nu = D_\mu F_\nu \tag{36o}$$
$$(m_1 \delta_{0\mu} + A_\mu) H_\nu = D_\mu (m_2 \delta_{0\nu} + E_\nu) \tag{36p}$$

Proof of Lemma 4.2: Having used Theorem 2.4 already and expanded the potentials as in (33), we now evaluate the missing part of the consistency condition:

$$0 \stackrel{!}{=} [V_k, V_j] + m_k \left[\gamma_k^0, V_j \right] - m_j \left[\gamma_j^0, V_k \right] - i \alpha_k^\mu \partial_{k,\mu} V_j + i \alpha_j^\mu \partial_{j,\mu} V_k \tag{37}$$

We have

$$\begin{aligned} m_1 \left[\gamma_1^0, V_2 \right] &= 2 m_1 \gamma_1^0 \gamma_1^5 V_{25}, \\ m_2 \left[\gamma_2^0, V_1 \right] &= 2 m_2 \gamma_2^0 \gamma_2^5 V_{15}, \end{aligned} \tag{38}$$

and

$$\begin{aligned}[V_1, V_2] &= \left[V_{11}, \gamma_1^5\right] V_{25} + \left[\gamma_2^5, V_{21}\right] V_{15} + \left[V_{15}\gamma_2^5, \gamma_1^5 V_{25}\right] \\ &= \left(-2\gamma_1^5\gamma_1^\mu A_\mu - 2\gamma_1^\mu B_\mu\right) V_{25} \\ &\quad + \left(2\gamma_2^5\gamma_2^\nu E_\nu + 2\gamma_2^\nu F_\nu\right) V_{15} \\ &\quad + 2\alpha_1^\mu\gamma_1^5 X_{1,\mu}\left(\gamma_2^5\gamma_2^\nu G_\nu + \gamma_2^\nu H_\nu\right) + 2\alpha_1^\mu Z_{1,\mu}\left(\gamma_2^5\gamma_2^\nu G_\nu + \gamma_2^\nu H_\nu\right) \\ &\quad + 2\gamma_1^\mu\gamma_1^5 C_\mu\left(\gamma_2^5\alpha_2^\nu Y_{\nu,2} + \alpha_2^\nu Z_{2,\nu}\right) - 2\gamma_1^\mu D_\mu\left(\gamma_2^5\alpha_2^\nu Y_{\nu,2} + \alpha_2^\nu Z_{2,\nu}\right). \end{aligned} \tag{39}$$

The derivative terms are

$$- i\alpha_1^\mu \partial_{1,\mu} V_{21} - i\alpha_1^\mu\gamma_1^5\partial_{1,\mu} V_{25} + i\alpha_2^\nu\partial_{2,\nu} V_{11} + i\alpha_2^\nu\gamma_2^5\partial_{2,\nu} V_{15}. \tag{40}$$

As the 16 matrices in (30) are linearly independent, their tensor products give us $16^2 = 256$ linearly independent matrices that appear in the consistency condition. Their respective prefactors have to vanish separately. This gives the following table, in which every of the 16 cells stands for 16 terms (for $\mu, \nu = 0, 1, 2, 3$) that have to vanish.

$\otimes$	α_2^ν	$\gamma_2^5\alpha_2^\nu$	γ_2^ν	$\gamma_2^5\gamma_2^\nu$
α_1^μ	$-i\partial_{1,\mu}W_{2,\nu} + i\partial_{2,\nu}W_{1,\mu}$	$-i\partial_{1,\mu}X_{2,\nu} + i\partial_{2,\nu}X_{1,\mu}$	$2F_\nu X_{1,\mu} + 2H_\nu Z_{1,\mu} - i\partial_{1,\mu}E_\nu$	$(2m_2\delta_{0\nu} + 2E_\nu)X_{1,\mu} + 2G_\nu Z_{1,\mu} - i\partial_{1,\mu}F_\nu$
$\gamma_1^5\alpha_1^\mu$	$-i\partial_{1,\mu}Y_{2,\nu} + i\partial_{2,\nu}Y_{1,\mu}$	$-i\partial_{1,\mu}Z_{2,\nu} + i\partial_{2,\nu}Z_{1,\mu}$	$2F_\nu Z_{1,\mu} + 2H_\nu X_{1,\mu} + i\partial_{1,\mu}G_\nu$	$(2m_2\delta_{0\nu} + 2E_\nu)Z_{1,\mu} + 2G_\nu X_{1,\mu} + i\partial_{1,\mu}H_\nu$
γ_1^μ	$-2B_\mu Y_{2,\nu} - 2D_\mu Z_{2,\nu} + i\partial_{2,\nu}A_\mu$	$-2B_\mu Z_{2,\nu} - 2D_\mu Y_{2,\nu} - i\partial_{2,\nu}C_\mu$	$-2B_\mu G_\nu + 2C_\mu F_\nu$	$-2B_\mu H_\nu + 2E_\nu C_\mu + 2m_2 C_\mu\delta_{0\nu}$
$\gamma_1^5\gamma_1^\mu$	$-(2m_1\delta_{0\mu} + 2A_\mu)Y_{2,\nu} - 2C_\mu Z_{2,\nu} + i\partial_{2,\nu}B_\mu$	$-(2m_1\delta_{0\mu} + 2A_\mu)Z_{2,\nu} - 2C_\mu Y_{2,\nu} - i\partial_{2,\nu}D_\mu$	$-(2m_1\delta_{\mu 0} + 2A_\mu)G_\nu + 2D_\mu F_\nu$	$-(2A_\mu + 2m_1\delta_{0\mu})H_\nu + (2m_2\delta_{0\nu} + 2E_\nu)D_\mu$

Setting every entry of this table equal to zero gives the required system of equations (36a)–(36p).
It remains to show that the potentials can be expanded as in (34), (35). Let us add up equations (36a) to (36d) with the respective matrices, factorizing $\alpha_1^\mu\alpha_2^\nu$, which leads to

$$\begin{aligned} &- \partial_{1,\mu}W_{2,\nu} + \partial_{2,\nu}W_{1,\mu} + \gamma_2^5\left(-\partial_{1,\mu}X_{2,\nu} + \partial_{2,\nu}X_{1,\mu}\right) \\ &+ \gamma_1^5\left(-\partial_{1,\mu}Y_{2,\nu} + \partial_{2,\nu}Y_{1,\mu}\right) + \gamma_1^5\gamma_2^5\left(-\partial_{1,\mu}Z_{2,\nu} + \partial_{2,\nu}Z_{1,\mu}\right) = 0. \end{aligned} \tag{41}$$

The names we gave to the terms in the potential are suited to make the symmetry of this equation visible. Defining

$$f_{j,\mu} := W_{j,\mu} + \gamma_2^5 X_{j,\mu} + \gamma_1^5 Y_{j,\mu} + \gamma_1^5\gamma_2^5 Z_{j,\mu}, \tag{42}$$

equation (41) becomes

$$\partial_{1,\mu} f_{2,\nu} = \partial_{2,\nu} f_{1,\mu}. \tag{43}$$

Then, we adapt the argument of Petrat and Tumulka [5, p. 34]: Define

$$g_{j,\mu\nu} = \partial_{j,\mu} f_{j,\nu} - \partial_{j,\nu} f_{j,\mu}. \tag{44}$$

For $i \neq j$, we have

$$\partial_{i,\lambda} g_{j,\mu\nu} = \partial_{j,\mu}\partial_{i,\lambda} f_{j,\nu} - \partial_{j,\nu}\partial_{i,\lambda} f_{j,\mu} = \partial_{j,\mu}\partial_{j,\nu} f_{i,\lambda} - \partial_{j,\nu}\partial_{j,\mu} f_{i,\lambda} = 0. \qquad (45)$$

This implies that $g_{j,\mu\nu}$ is a function of x_j only. Define for arbitrary fixed $\tilde{x}_1, \tilde{x}_2$ the function $\tilde{f}_{j,\mu}(x_j) := f_{j,\mu}(x_j, \tilde{x}_i)$ and $h_{j,\mu}(x_1, x_2) := f_{j,\mu}(x_1, x_2) - \tilde{f}_{j,\mu}(x_j)$. Since (45) implies

$$g_{j,\mu\nu} = \partial_{j,\mu} f_{j,\nu} - \partial_{j,\nu} f_{j,\mu} = \partial_{j,\mu}\tilde{f}_{j,\nu} - \partial_{j,\nu}\tilde{f}_{j,\mu}, \qquad (46)$$

we have

$$\partial_{j,\mu} h_{j,\nu} - \partial_{j,\nu} h_{j,\mu} = 0, \quad j = 1, 2. \qquad (47)$$

Moreover, eq. (43) gives us

$$\partial_{1,\mu} h_{2,\nu} - \partial_{2,\nu} h_{1,\mu} = 0. \qquad (48)$$

These two equations together form the integrability condition, from which it follows that a self-adjoint matrix-valued function $M(x_1, x_2)$ exists such that $h_{j,\mu} = \partial_{j,\mu} M(x_1, x_2)$, i.e.

$$f_{j,\mu}(x_1, x_2) = \partial_{j,\mu} M(x_1, x_2) + \tilde{f}_{j,\mu}(x_j). \qquad (49)$$

Therefore, the unitary map $e^{iM(x_1,x_2)}$ maps the potential f_j to the purely external potential $\tilde{f}_j$, which shows that f_j is not interacting according to our definition.
The generalization to the case where the consistency condition only holds on $\mathscr{S}^{(N)}$ works exactly like in [5, p. 35]. □

4.3 A consistent example

As a side remark before we prove Lemma 2.5, note that the connection of the consistent potential with the above basis decomposition is more easily visible if the potential is rewritten as $V_1 = -i\gamma_1^\mu C_\mu \sin(2c_\nu x^\nu) + \gamma_1^5\gamma_1^\mu C_\mu \cos(2c_\nu x^\nu) - m_1\gamma_1^0$.

Proof of Lemma 2.5:

1. We have to evaluate the consistency condition

$$\begin{aligned}
&\left[i\alpha_1^\mu\partial_{1,\mu} - m_1\gamma_1^0 - \gamma_1^\mu C_\mu \exp\left(2i\gamma_1^5 c_\lambda x^\lambda\right) + m_1\gamma_1^0, i\alpha_2^\nu\partial_{2,\nu} - m_2\gamma_2^0 - \gamma_1^5\alpha_2^\nu c_\nu\right] = 0\\
&\iff -\left[\gamma_1^\mu C_\mu \exp\left(2i\gamma_1^5 c_\lambda x^\lambda\right), i\alpha_2^\nu\partial_{2,\nu}\right] + \left[\gamma_1^\mu C_\mu \exp\left(2i\gamma_1^5 c_\lambda x^\lambda\right), \gamma_1^5\alpha_2^\nu c_\nu\right] = 0\\
&\iff \gamma_1^\mu C_\mu \alpha_2^\nu \left(i\partial_{2,\nu} \exp\left(2i\gamma_1^5 c_\lambda x^\lambda\right) + 2\gamma_1^5 c_\nu \exp\left(2i\gamma_1^5 c_\lambda x^\lambda\right)\right) = 0,
\end{aligned}$$

which is indeed true. Note that in the case at hand the consistency condition is satisfied identically, not only applied to certain functions.

2. Now we assume (for a contradiction) that there is a gauge transformation $U(x_1, x_2)$: $\mathbb{C}^K \to \mathbb{C}^K$ that yields non-interacting potentials. Such a map can be written as $U(x_1, x_2) = e^{iM(x_1,x_2)}$ with a self-adjoint $K \times K$-matrix M. We define the transformed quantities

$$\tilde{\psi} := U\psi, \quad \tilde{\gamma^\mu} := U\gamma^\mu U^\dagger. \qquad (50)$$

If ψ is a solution of the system (1), it follows that $\tilde{\psi}$ satisfies

$$(i\tilde{\alpha}_k^\mu\partial_{k,\mu} - \tilde{\gamma_k^0} m_k)\tilde{\psi} = \tilde{V}_k\tilde{\psi} - \tilde{\alpha}_k^\mu(\partial_{k,\mu}\tilde{M})\tilde{\psi}, \qquad (51)$$

where $\tilde{V}$ and $\tilde{M}$ stand for the same expressions as V and M, but with all appearing matrices replaced by the ones with a tilde[1]. Therefore, the condition that the transformed potential only depends on x_k amounts to the requirement that

$$V_k(x_1, x_2) - \alpha_k^\mu \partial_{k,\mu} M(x_1, x_2) \tag{52}$$

is in fact only a matrix-valued function of x_k, so its derivative with respect to another coordinate has to vanish. Using that V_2 is constant, this implies the following two equations:

$$\partial_{1,\lambda} \alpha_2^\mu \partial_{2,\mu} M(x_1, x_2) = 0 \tag{53}$$

$$\partial_{2,\delta} \alpha_1^\nu \partial_{1,\nu} M(x_1, x_2) = c_\delta 2i\gamma_1^5 \gamma_1^\mu C_\mu \exp\left(2i\gamma_1^5 c_\nu x^\nu\right) \tag{54}$$

Now consider the contraction

$$\begin{aligned} &\alpha_1^\lambda \alpha_2^\delta \partial_{1,\lambda} \partial_{2,\delta} M(x_1, x_2) \\ &= \alpha_1^\lambda \left(\alpha_2^\delta \partial_{1,\lambda} \partial_{2,\delta} M(x_1, x_2)\right) = 0 \\ &= \alpha_2^\delta \left(\alpha_1^\lambda \partial_{1,\lambda} \partial_{2,\delta} M(x_1, x_2)\right) = \alpha_2^\delta c_\delta 2i\gamma_1^5 \gamma_1^\mu C_\mu \exp\left(2i\gamma_1^5 c_\nu x^\nu\right) \end{aligned} \tag{55}$$

where we have used, after different regrouping of the summands, equation (53) in the second line and (54) in the third line. This is a contradiction because the C_μ, c_μ are not all zero. Hence, a matrix M with the required properties does not exist. We have therefore proven that the potential is not gauge-equivalent to a non-interacting one, so it is interacting. □

4.4 Classification of consistent potentials

Instead of proving lemma 2.6 directly, we give a slightly stronger reformulation that implies it, but uses the basis decomposition discussed in Section 4.2.

Lemma 4.3 *Suppose the consistency condition is fulfilled (in the sense of **(A)** in theorem 2.4) for a two-particle Dirac system* (1) *for which the gauge transformation which makes W_i, X_i, Y_i, Z_i purely external has already taken place. If the potentials are translation invariant, i.e. satisfy*

$$V_i(x_1, x_2) = V_i(x_1 + a, x_2 + a) \quad \forall a \in \mathbb{R}^4, \tag{56}$$

then all terms $A_\mu, ..., H_\mu$ in the potentials are necessarily of the form

$$C_1 \cdot e^{c_{i,\nu} x^\nu} + C_2 \cdot e^{-c_{i,\nu} x^\nu} \tag{57}$$

for some $C_1, C_2 \in \mathbb{C}$ and $c_i \in \mathbb{C}^4$, where $x = x_1 - x_2$. In the case of A_0 and E_0, a constant term $-m_1$ resp. $-m_2$ is added.

Proof of Lemma 4.3 After the gauge transformation, W_i, X_i, Y_i and Z_i are functions of x_i only. If we assume that the potentials are translation invariant, it follows that these functions have to be constants. Therefore, we can derive second order differential equations for the functions A to H. We show the steps for B_μ and D_μ, the other cases are analogous. Since $V_k \in C^1(\Omega, \mathbb{C}^{K \times K})$, every scalar function $A_\mu, B_\mu, ..., H_\mu, W_{i,\mu}, ..., Z_{i,\mu}$ in the potentials has to be continuously differentiable. Equations (36e) to (36l) imply

[1]Since the gamma matrices are always only defined up to a similarity transformation, the tildes do not really matter and can basically be omitted. Note that a gauge transformation just refers to a (local) change of coordinates in the spinor space.

that the terms A to H are in fact two times continuously differentiable, because the first derivatives are expressible as a sum of continuously differentiable functions.
Therefore, we may differentiate equation (36f) once more. Inserting (36e) and (36g), we obtain

$$\frac{1}{4}\partial_{2,\nu}\partial_{2,\lambda}B_\mu = (Z_{2,\lambda}Z_{2,\nu} - Y_{2,\lambda}Y_{2,\nu})B_\mu + (Y_{2,\nu}Z_{2,\lambda} - Y_{2,\lambda}Z_{2,\nu})D_\mu. \tag{58}$$

Similarly for D_μ:

$$\frac{1}{4}\partial_{2,\nu}\partial_{2,\lambda}D_\mu = (Z_{2,\lambda}Z_{2,\nu} - Y_{2,\lambda}Y_{2,\nu})D_\mu + (Y_{2,\nu}Z_{2,\lambda} - Y_{2,\lambda}Z_{2,\nu})B_\mu \tag{59}$$

Although the derivatives $\partial_{2,\nu}$ and $\partial_{2,\lambda}$ need to commute, the right hand side of these equations is apparently not invariant under exchange of ν and λ. This implies that

$$B_\mu = D_\mu = 0 \ \vee \ Y_{2,\nu}Z_{2,\lambda} - Y_{2,\lambda}Z_{2,\nu} = 0. \tag{60}$$

In the first case, we are already done (the potentials are of the desired form, with the constants being equal to zero). So we go on with the second case, where the differential equation becomes

$$\partial_{2,\nu}\partial_{2,\lambda}B_\mu = 4(Z_{2,\lambda}Z_{2,\nu} - Y_{2,\lambda}Y_{2,\nu})B_\mu, \tag{61}$$

and the same for D_μ. Using $Y_{2,\nu}Z_{2,\lambda} = Y_{2,\lambda}Z_{2,\nu}$, it can be rewritten as

$$\partial_{2,\nu}\partial_{2,\lambda}B_\mu = 2\sqrt{Z_{2,\nu}^2 - Y_{2,\nu}^2} \cdot 2\sqrt{Z_{2,\lambda}^2 - Y_{2,\lambda}^2} \cdot B_\mu. \tag{62}$$

The square root is also defined for negative radicand as $\sqrt{x} := i\sqrt{|x|}$. This has the general solution

$$B_\mu = C_\mu^+ \exp\left(2\sqrt{Z_{2,\alpha}^2 - Y_{2,\alpha}^2}x_2^\alpha\right) + C_\mu^- \exp\left(-2\sqrt{Z_{2,\alpha}^2 - Y_{2,\alpha}^2}x_2^\alpha\right), \tag{63}$$

with free constants $C_\mu^\pm$ that may depend on x_1. Since the potential must be translation independent, the constants must be such that B_μ has the form (57).
We thus have the required form for B and D, and the other terms work analogously. In the case of A and E, one should derive the differential equations for the functions $(m_1\delta_{0\mu} + A_\mu)$ and $(m_2\delta_{0\nu} + E_\nu)$ instead. Then, the consistency condition poses several additional constraints, eqs. (36m)–(36p) amongst others, that were not considered so far. But we will not elucidate on that because we only want to show that the form (57) is *necessary*. □

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Multi-time dynamics of the Dirac-Fock-Podolsky model of QED

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Abstract

Dirac, Fock, and Podolsky [1] devised a relativistic model in 1932 in which a fixed number of N Dirac electrons interact through a second-quantized electromagnetic field. It is formulated with the help of a multi-time wave function $\psi(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N)$ that generalizes the Schrödinger multi-particle wave function to allow for a manifestly relativistic formulation of wave mechanics. The dynamics is given in terms of N evolution equations that have to be solved simultaneously. Integrability imposes a rather strict constraint on the possible forms of interaction between the N particles and makes the rigorous construction of interacting dynamics a long-standing problem, also present in the modern formulation of quantum field theory. For a simplified version of the multi-time model, in our case describing N Dirac electrons that interact through a relativistic scalar field, we prove well-posedness of the corresponding multi-time initial value problem and discuss the mechanism and type of interaction between the charges. For the sake of mathematical rigor we are forced to employ an ultraviolet cut-off in the scalar field. Although this again breaks the desired relativistic invariance, this violation occurs only on the arbitrary small but finite length-scale of this cut-off. In view of recent progress in this field, the main mathematical challenges faced in this work are, on the one hand, the unboundedness from below of the free Dirac Hamiltonians and the unbounded, time-dependent interaction terms, and on the other hand, the necessity of pointwise control of the multi-time wave function.

Keywords: multi-time wave functions, relativistic quantum mechanics, scalar field, quantum electrodynamics, consistency condition, partial differential equations, invariant domains

1 Introduction

1.1 The need for multi-time models

The multi-time formalism for relativistic wave mechanics was first developed in works of Dirac [2, 1] and Bloch [3] and after Tomonaga's famous paper [4] ultimately lead towards the modern relativistic formulation of QFT. At its base, the main observation is that the Schrödiger wave function for a many-body system contains only one time variable t and N position variables $\mathbf{x}_i$, $i = 1, \dots, N$, in other words a configuration of N space-time coordinates $(t, \mathbf{x}_i)$, $i = 1, \dots, N$, on an equal-time hypersurface $t \times \mathbb{R}^3$ in Minkowski space. A Lorentz-boost will in general lead to a configuration of space-time points $(t'_i, \mathbf{x}'_i)$, $i = 1, \dots, N$, with pair-wise distinct t'_i, t'_j, hence, a Schrödinger wave function defined on equal time hypersurfaces will fail to have the desired transformation properties under Lorentz boosts. A natural way to extend the wave function on

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equal-time hypersurfaces is the multi-time wave function $\psi(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N)$, an object which lives on a subset of $\mathbb{R}^{4N}$.

In recent years, there has been a renewed interest in constructing mathematically rigoros multi-time models, see [5] for an overview. Some of the current efforts to understand Dirac's multi-time models focus on the well-posedness of the corresponding initial value problems [6, 7, 8, 9, 10], other works also ask the question how the multi-time formalism could be exploited to avoid the infamous ultraviolet divergence of relativistic QFT and how a varying number of particles by means of creation and annihilation processes can be addressed [11, 12, 13]. Beside being candidate models for fundamental formulations of relativistic wave mechanics, a better mathematical understanding of such multi-time evolutions may also be beneficial regarding more technical discussions, such as the control of scattering estimates on vacuum expectation values of products of interacting field operators; see e.g. [14].

Many contemporary treatments of multi-time models are yet not entirely satisfactory as they either have technical deficiencies, e.g., do not allow to treat unbounded Hamiltonians, or define interactions whose nature are conceptually not entirely clear or experimentally adequate. Also our treatment presented in this work is not fully satisfactory by those standards, as for the sake of mathematical rigor we need to introduce an ultraviolet cut-off that in turn breaks the Lorentz-invariance of the model. Nevertheless, building on previous works, we still achieve a substantial improvement since we can allow for unbounded Hamiltonians in the evolution equations. Furthermore, the violation of Lorentz-invariance only occurs on the finite but arbitrary small length-scale of the cut-off. Since the mathematically rigorous treatment of multi-time evolutions is independent of the ultraviolet divergences of relativistic interaction, we believe that it is advantageous for the progress in both topics to separate the discussion between formulations of multi-time dynamics and the divergences of quantum field theory at first. Later, it may well be that the understanding of multi-time evolution leads to new possibilities to encode relativistic interaction without causing ultraviolet divergences.

This work is divided into three parts. First, we give an informal introduction to the model at hand in subsection 1.2. The mathematical definition of this model is then given in section 2 where we state our main results on existence, uniqueness, and interaction of solutions, i.e., Theorem 1, Theorem 2, and Theorem 3, respectively. The corresponding proofs are provided in section 3.

1.2 The multi-time model

In our choice of model we follow closely the Dirac, Fock, Podolsky (DFP) model given in the paper [1], which we informally introduce in this subsection and formally define in the next one. This model is supposed to describe the relativistic interaction between N persistent Dirac electrons. The only simplification we assume for the model treated in this paper in comparison to the original DFP model is that the electromagnetic interaction is replaced by the one of a scalar field. This allows to avoid the additional complication of electromagnetic gauge freedom. A ready choice for the evolution equations of the multi-time wave function $\psi(x_1, ..., x_N)$ is a system of N Hamiltonian equations,

$$i\partial_{t_j}\psi(x_1, ..., x_N) = \mathcal{H}_j\psi(x_1, ..., x_N), \quad j = 1, ..., N, \tag{1}$$

with a suitable *partial Hamiltonian* $\mathcal{H}_j$ for each particle. In [3], Bloch argued that it is necessary for the existence of solutions to (1) that an integrability condition for the different times t_j, the so-called *consistency condition*

$$[\mathcal{H}_j, \mathcal{H}_k] + i\frac{\partial \mathcal{H}_j}{\partial t_k} - i\frac{\partial \mathcal{H}_k}{\partial t_j} = 0, \quad \forall j \neq k, \tag{2}$$

is satisfied in the domain of ψ, which is usually taken as the set of space-like configurations in $\mathbb{R}^{4N}$.

Let $\mathcal{H}_j^0 = -i\gamma_j^0\boldsymbol{\gamma}_j \cdot \boldsymbol{\nabla}_j + \gamma_j^0 m$ be the free Dirac operator acting on particle j, with the usual gamma matrices γ_j^μ. For the free multi-time evolution with Hamiltonians $\mathcal{H}_j = \mathcal{H}_j^0$, condition (2) is fulfilled. For the introduction of a non-trivial interaction, however, the consistency condition poses a serious obstacle. If one takes as partial Hamiltonians

$$\mathcal{H}_j = \mathcal{H}_j^0 + V_j(x_1, ..., x_N), \tag{3}$$

with interaction potentials, i.e. multiplication operators, V_j, it is hardly possible to fulfill (2). Using this insight, it was shown in [6, 15] that systems of multi-time Dirac equations with relativistic interaction potentials fail to admit solutions.

Already in 1932 in [2], Dirac pointed out an ingenious way to circumvent this problem, namely, by second quantization. He observed that in case the "potential" is not a multiplication operator, but a Fock space valued field operator $\varphi(x)$, the consistency condition (2) can be retained although it will turn out that an interaction is present. The Hamiltonians in question are of the form

$$\mathcal{H}_j = \mathcal{H}_j^0 + \varphi(t_j, \mathbf{x}_j), \tag{4}$$

all containing one and the same second quantized scalar field φ on space-time $\mathbb{R}^4$, fulfilling the wave equation

$$\Box_x \varphi(x) = \left(\partial_t^2 - \triangle_{\mathbf{x}}\right)\varphi(t, \mathbf{x}) = 0, \tag{5}$$

as well as the canonical commutation relation

$$[\varphi(x_j), \varphi(x_k)] = i\Delta(x_j, x_k), \tag{6}$$

with Δ being the Pauli-Jordan function [4, 16] given in (74). It is well-known that (6) implies

$$[\varphi(x_j), \dot{\varphi}(x_k)]_{t_j = t_k} = i\delta^{(3)}(\mathbf{x}_j - \mathbf{x}_k). \tag{7}$$

This ensures the consistency of the system of equations in the sense of (2) since

$$\Delta(x_j, x_k) = 0 \quad \text{if } x_j, x_k \text{ are space-like related.} \tag{8}$$

A natural choice for a representation of the field operator fulfilling (6) is the one on standard Fock space. The multi-time wave-function $\psi(x_1, ..., x_N)$ can then be thought of as taking values in a bosonic Fock space. This second quantization of $\varphi(x)$ is the key feature to understand how the seemingly "free" evolutions in (5) in fact allow to mediate interaction between the Dirac electrons. In fact, an informal computation (see [1]) shows that (5) and (8) imply for the field operator $\varphi_H(x) := \varphi_H(t, \mathbf{x}) = U(t)^\dagger \varphi(0, \mathbf{x}) U(t)$, where $U(t)$ denotes the time evolution of the N-body system on equal-time hypersurfaces, that

$$\left(\partial_t^2 - \triangle_{\mathbf{x}}\right)\varphi_H(t, \mathbf{x}) = -\sum_{j=1}^N \delta^{(3)}\left(\hat{\mathbf{x}}_j(t) - \mathbf{x}\right), \tag{9}$$

where $\hat{\mathbf{x}}_j(t) = U(t)^\dagger \hat{\mathbf{x}}_j U(t)$ denotes the position operator of the k-th electron in the Heisenberg picture. The right-hand side of (9) now demonstrates the effective source terms influencing the scalar field which in turn couples the motion of the N electrons. A rigoros version of this informal computation is given as Theorem 3.

Mathematical challenges. There are three main difficulties we have to overcome for a mathematical solution theory of the model.

1. As it is well-known [17], the scalar field model is badly ultraviolet divergent. A standard way to defer the discussion of this problem and nevertheless continue the mathematical discussion is the introduction of a ultraviolet cut-off in the scalar field. This cut-off, which can be thought of as smearing out the scalar field with a smooth and compactly supported function ρ with diameter $\delta > 0$, ensures well-definedness of the model, however, breaks Lorentz on the length scale δ as it smears out the right-hand side of (8) as can be seen from (28) below. This will furthermore force us to take as domain $\mathscr{S}_\delta$, defined in (19) below, for the multi-time wave function instead of all space-like configurations on $\mathbb{R}^{4N}$. Since $\mathscr{S}_\delta$ is not an open set in $\mathbb{R}^{4N}$ a simple notion of differentiability is not sufficient anymore which is reflected in our choice of solution sense in Definition 1.

2. We need sufficient regularity in the solution candidates to allow for point-wise evaluation. It is decisive for our proofs that we find a dense set $\mathscr{D}$ of smooth functions which is left invariant by the single-time evolutions. Furthermore, the majority of methods employed in the literature on Schrödinger Hamiltonians (see e.g. [18]) rely on boundedness from below, and hence, do not apply to our setting as the free Dirac Hamiltonian is not bounded from below.

3. Since we add unbounded and time-dependent interaction terms to the free Dirac Hamiltonians, already the study of the corresponding single-time equations generated by the Hamiltonians $\mathcal{H}_j(t)$ in (4) is subtle. Abstract theorems such as the one of Kato [19] or Yosida [20, ch. XIV] about the existence of a propagator $U(t,s)$ require time-independence of the domain $\mathrm{dom}(\mathcal{H}_j(t))$, which in our case is unknown.

Beside the introduction of an ultraviolet cut-off, which will be defined in the next section, there is a further difference compared to the original formulation of Dirac, Fock, Podolsky, namely that the multi-time wave function ψ of N particles has N time arguments and not an additional "field time" argument. This is because we formulate the field degrees of freedom in momentum space and in the Dyson picture, leading to a time-dependent $\varphi(t,\mathbf{x})$ but no free field Hamiltonian in $\mathcal{H}_j$. The choice of a field time as in [1] corresponds to choosing a space-like hypersurface Σ (in that paper, only equal-time hypersurfaces Σ_t are considered) on which the field degrees of freedom are evaluated. Our formulation is mathematically convenient since the Hilbert space is fixed and not hypersurface-dependent. It is always possible to choose a hypersurface and perform the Fourier transformation to obtain field modes in position space.

2 Definition of the model and main results

We now put the model described by the informal equations (1), (4), (6) into a mathematical rigoros context and define a solution sense, see Def. 1 below, which will allow us to formulate our main results about existence and uniqueness of solutions. As the model describes the interaction of N electrons with a scalar field, an operator on Fock space, there are two main ingredients we need to define: the field operator and the multi-time evolution equations.

Field operator with Cut-off. We follow the standard quantization procedure. The Fock space is constructed by means of a direct sum of symmetric tensor products of the one-particle Hilbert space $L^2(\mathbb{R}^3,\mathbb{C})$ of complex valued square integrable functions on $\mathbb{R}^3$:

$$\mathscr{F} = \bigoplus_{n=0}^{\infty} L^2(\mathbb{R}^3,\mathbb{C})^{\odot n}, \tag{10}$$

where $\odot$ denotes the symmetric tensor product. In our setting, we think of $\mathbb{R}^3$ as momentum space. The total Hilbert space, in which the wave function $\psi(t_1, \cdot, ..., t_N, \cdot)$ is contained for fixed time $t_1, \ldots, t_N \in \mathbb{R}$, is given by

$$\mathscr{H} = L^2(\mathbb{R}^{3N}, \mathscr{F}^K) \cong L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathscr{F} \cong L^2(\mathbb{R}^{3N}, \mathbb{C}) \otimes \mathscr{F}^K, \tag{11}$$

with $K = 4^N$ denoting the dimension of spinor space of the N Dirac electrons. In view of (10) and (11), we use the notation

$$\begin{aligned} \text{for a.e. } (x_1, ..., x_N) : \psi(x_1, ..., x_N) = \left(\psi^{(n)}(x_1, ..., x_N)\right)_{n \in \mathbb{N}_0}, \\ \text{so that } \left((\mathbf{k}_1, ..., \mathbf{k}_n) \mapsto \psi^{(n)}(x_1, ..., x_N; \mathbf{k}_1, ..., \mathbf{k}_n)\right) \in \mathbb{C}^K \otimes L^2(\mathbb{R}^3, \mathbb{C})^{\odot n} \end{aligned} \tag{12}$$

to denote the n-particles sectors of Fock space $\mathscr{F}$ and distinguish between functions with values in $\mathscr{F}$ and $\mathbb{C}^K$. A dense set in $\mathscr{F}$ are the finite particle vectors $\mathscr{F}_{\text{fin}}$. On this set, we can define for square integrable f, as in Nelson's paper [21], the annihilation

$$\left(\int d^3\mathbf{k}\ f(\mathbf{k}) a(\mathbf{k}) \psi\right)^{(n)} (\mathbf{k}_1, ..., \mathbf{k}_n) = \sqrt{n+1} \int d^3\mathbf{k}\ f(\mathbf{k}) \psi^{(n+1)}(\mathbf{k}, \mathbf{k}_1, ..., \mathbf{k}_n) \tag{13}$$

and creation operators

$$\left(\int d^3\mathbf{k}\ f(\mathbf{k}) a^\dagger(\mathbf{k}) \psi\right)^{(n)} (\mathbf{k}_1, ..., \mathbf{k}_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(\mathbf{k}_j) \psi^{(n-1)}(\mathbf{k}_1, ..., \widehat{\mathbf{k}_j}, ..., \mathbf{k}_n), \tag{14}$$

in which a variable with hat is omitted. The field mass is $\mu \geq 0$ and the energy $\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + \mu^2}$, which allows to define the free field Hamiltonian

$$\left(\mathcal{H}_f \psi\right)^{(n)} (\mathbf{k}_1, ...\mathbf{k}_n) = \sum_{j=1}^{n} \omega(\mathbf{k_j}) \psi(\mathbf{k}_1, ..., \mathbf{k}_n), \tag{15}$$

as self-adjoint operator on its domain $\text{dom}(\mathcal{H}_f) \subset \mathscr{F}$; see [22]. We will later use the notation $\text{dom}(\mathcal{H}_f^\infty) := \bigcap_{j=0}^\infty \text{dom}(\mathcal{H}_f^j)$.

Before we can define the scalar field, we need to introduce the cut-off as final ingredient. Let $B_r(\mathbf{x})$ denote the open ball in $\mathbb{R}^3$ of radius r around $\mathbf{x} \in \mathbb{R}^3$. For this we introduce a smooth and compactly supported real-valued function

$$\rho \in C_c^\infty(\mathbb{R}^3, \mathbb{R}) \text{ such that supp}\,(\rho) \subset B_{\delta/2}(\mathbf{0}), \tag{16}$$

which can later be thought of as smearing out the point-like interaction to be mediated by the scalar field by a charge form factor ρ. The Fourier transform $\hat{\rho}(\mathbf{k})$ is an element of the Schwartz space of function of rapid decay with not necessarily compact support. For each particle index $j = 1, ..., N$, we can now define the time-dependent scalar field

$$\varphi_j(t)\psi := \int d^3\mathbf{k}\ \left[\left(\frac{\hat{\rho}(\mathbf{k})}{\sqrt{\omega(\mathbf{k})}} e^{-i\omega(\mathbf{k})t} e^{i\mathbf{k}\cdot\hat{\mathbf{x}}_j} a(\mathbf{k}) + \frac{\hat{\rho}^\dagger(\mathbf{k})}{\sqrt{\omega(\mathbf{k})}} e^{i\omega(\mathbf{k})t} e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}_j} a^\dagger(\mathbf{k})\right)\psi\right] \tag{17}$$

for sufficiently regular $\psi \in \mathscr{H}$. Here, $\hat{\mathbf{x}}_j$ is the position operator of the j-th particle which acts on a multi-time wave function by $\hat{\mathbf{x}}_j \psi(t_1, \mathbf{x}_1, ..., t_j, \mathbf{x}_j, ...) = \mathbf{x}_j \psi(t_1, \mathbf{x}_1, ..., t_j, \mathbf{x}_j, ...)$. The necessity of the cut-off function $\rho \in C_c^\infty(\mathbb{R}^3)$ can be seen from the fact that if we had chosen $\rho(\mathbf{x}) = \delta^3(\mathbf{x})$ which for reasons of Lorentz invariance would be physically desirable but would imply $\hat{\rho} = (2\pi)^{-3/2}$, the domain of the second summand in $\varphi_j(t)$ would be $\{0\}$, which is a manifestation of the mentioned ultraviolet problem. With a square integrable $\hat{\rho}$, the field operator is self-adjoint on a dense domain; see [22]. An equivalent definition is possible by direct fiber integrals, see [23, 24]. Despite the notation, one should not think of the φ_j as being N different fields, the index just denotes in a brief way that the single scalar field is evaluated at the coordinates of particles j, i.e. at $\mathbf{x}_j$.

This allows to define the one-particle Hamiltonians as follows:

$$\mathcal{H}_j(t) = \mathcal{H}_j^0 + \varphi_j(t), \quad j = 1, ..., N. \tag{18}$$

Multi-Time Evolution Equations and Solution Sense. As domain for our multi-time wave function on configuration space-time, we take those configurations of space-time points which are at equal times or have a space-like distance of at least δ, i.e.

$$\mathscr{S}_\delta := \left\{ (x_1, ..., x_N) \in \mathbb{R}^{4N} \middle| \forall j \neq k : t_j = t_k \text{ or } \|\mathbf{x}_j - \mathbf{x}_k\| > |t_j - t_k| + \delta \right\}. \tag{19}$$

The multi-time wave function will hence be represented as a map $\psi : \mathscr{S}_\delta \to \mathscr{F}^K$.

The natural notion of a solution to our multi-time system (1) would be a smooth function mapping from $\mathscr{S}_\delta$ to the Fock space $\mathscr{F}^K$. However, the above introduced Hilbert space $\mathscr{H}$ on $\mathbb{R}^{3N}$ allows to apply on a lot of functional analytic methods, and thus, simplifies the mathematical analysis considerably. This is why it is helpful to at first define a solution as a map $\psi : \mathbb{R}^N \to \mathscr{H}, (t_1, ..., t_N) \mapsto \psi(t_1, ..., t_N)$ and require it to solve the system (1) on the space-time configurations in $\mathscr{S}_\delta$. The latter involves the difficulty that the domain $\mathscr{S}_\delta$ is not an open set in $\mathbb{R}^{4N}$ so that partial derivatives with respect to time coordinates cannot be straightforwardly defined in this set.

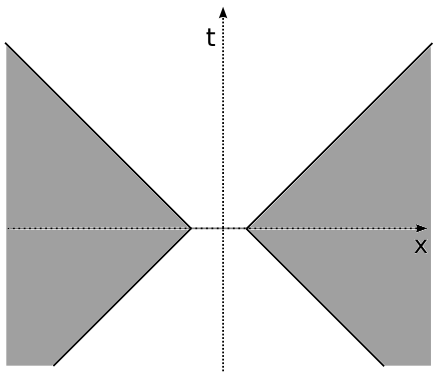

Figure 1: The set $\mathscr{S}_\delta$ is depicted in grey, for two particles in relative coordinates. Because of the line at $t = t_1 - t_2 = 0$, this is obviously not an open set in configuration space-time. At the origin, for example, the partial derivative ∂_{t_1} cannot be computed inside the set.

In order to cope with this difficulty, we adapt a method to define partial derivatives in $\mathscr{S}_\delta$ that was also employed by Petrat and Tumulka [6, sec. 4]. If all times are pair-wise different, the usual partial derivatives exist. However, this is not the case at points where for some $j \neq k$, $t_j = t_k$ while $\|\mathbf{x}_j - \mathbf{x}_k\| \leq \delta$. For those configurations we will only take the derivative with respect to the common time coordinate. This is implemented as follows: Each point $x = (x_1, ..., x_N) \in \mathscr{S}_\delta$ defines a partition of $\{1, ..., N\}$ into non-empty disjoint subsets $P_1, ..., P_L$ by the equivalence relation that is the transitive closure of the relation that holds between j and k exactly if[1] $\|\mathbf{x}_j - \mathbf{x}_k\| \leq |t_j - t_k| + \delta$. We call this the *corresponding partition* to x. By

[1]This gives exactly the partition called FP_{q^4} by Petrat and Tumulka.

(19), all particles in one set P_i of the partition necessarily have the same time coordinate, i.e. $\forall i \in \{1, ..., L\}$ $\forall j, k \in P_i$, we have $t_j = t_k$. We write this common time coordinate as t_{P_i} for each $i = 1, ..., L$.

The partial derivative with respect to t_{P_i} can now be defined for a differentiable function $\psi : \mathbb{R}^N \to \mathscr{H}$ as

$$\left(\frac{\partial}{\partial t_{P_i}}\psi(t_1, ..., t_N)\right)(\mathbf{x}_1, ..., \mathbf{x}_N) := \sum_{j \in P_i} \left(\frac{\partial}{\partial t_j}\psi(t_1, ..., t_N)\right)(\mathbf{x}_1, ..., \mathbf{x}_N), \tag{20}$$

provided that the expression on the right-hand side is well-defined. By this definition, $\frac{\partial}{\partial t_{P_i}}\psi$ can be obtained solely by limits of sequences of configurations inside $\mathscr{S}_\delta$, so changing the function ψ outside of the relevant domain $\mathscr{S}_\delta$ will not matter for the derivative, and thus not affect its status of being a solution. With this notation at hand, we define:

Definition 1 (Solution Sense) *For each set $A \subset \{1, ..., N\}$, define the respective Hamiltonian*

$$\mathcal{H}_A(t) := \sum_{j \in A} \left(\mathcal{H}_j^0 + \varphi_j(t)\right). \tag{21}$$

A solution of the multi-time system *is a function $\psi : \mathbb{R}^N \to \mathscr{H}, (t_1, ..., t_N) \mapsto \psi(t_1, ..., t_N)$ such that the following hold:*

i) Time derivatives: ψ is differentiable.

ii) Pointwise evaluation: For every $(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathscr{S}_\delta$, and for all $j = 1, ..., N$, the following pointwise evaluations are well-defined:

$$\begin{aligned} &\Big(\psi(t_1, ..., t_N)\Big)(\mathbf{x}_1, ..., \mathbf{x}_N), \\ &\Big(\partial_{t_j}\psi(t_1, ..., t_N)\Big)(\mathbf{x}_1, ..., \mathbf{x}_N), \\ &\Big(\mathcal{H}_j(t_j)\psi(t_1, ..., t_N)\Big)(\mathbf{x}_1, ..., \mathbf{x}_N). \end{aligned} \tag{22}$$

iii) Evolution equations: For every $x = (t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathscr{S}_\delta$ with corresponding partition $P_1, ..., P_L$, the equations

$$\left(\frac{\partial}{\partial t_{P_j}}\psi(t_1, ..., t_N)\right)(\mathbf{x}_1, ..., \mathbf{x}_N) = \Big(\mathcal{H}_{P_j}(t_{P_j})\psi\,(t_1, ..., t_N)\Big)(\mathbf{x}_1, ..., \mathbf{x}_N), \quad j = 1, ..., L, \tag{23}$$

where the left hand side is defined by (20)*, are satisfied.*

Due to the unfamiliar structure of the domain $\mathscr{S}_\delta$ and our compact notation, this definition may look complicated at first sight. However, the complication is only due to the introduction of the cut-off ρ which led to the definition of $\mathscr{S}_\delta$. The purpose of the whole effort is simply to restrict the system (1) to those time directions in which taking the derivative is admissible in $\mathscr{S}_\delta$. It may be helpful to take a quick look at Eq. (30) which shows the explicit form of the multi-time system for the special case of $N = 2$. We emphasize that with our notation in (21), the index of the Hamiltonian is actually a set, for example $\mathcal{H}_{\{1,2\}} = \mathcal{H}_1 + \mathcal{H}_2$ denoting the mutual Hamiltonian of particles 1 and 2.

As a final ingredient, we define a dense domain in $\mathscr{H}$:

$$\mathscr{D} := C_c^\infty(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathscr{F} \cap L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathrm{dom}(\mathcal{H}_f^\infty). \tag{24}$$

Our first main result is on the existence of solutions given initial values in $\mathscr{D}$.

Theorem 1 (Existence) *Let $\psi^0 \in \mathscr{D}$. Then there is a solution of the multi-time system ψ in the sense of definition 1 which satisfies $\psi(0,...,0) = \psi^0$ pointwise. In particular, there is such a solution ψ fulfilling*

$$\psi(t_1, \cdot, ..., t_N, \cdot) \in \mathscr{D} \quad \forall (t_1, ..., t_N) \in \mathbb{R}^N. \tag{25}$$

The second main result is on the uniqueness of solutions in $\mathscr{D}$.

Theorem 2 (Uniqueness) *Let $\psi^0 \in \mathscr{D}$. Let ψ_1 and ψ_2 be two solutions of the multi-time system in the sense of definition 1 which both satisfy $\psi_k(0,...,0) = \psi^0$ pointwise for $k = 1, 2$. Then we have for all $(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathscr{S}_\delta$:*

$$\Big(\psi_1(t_1, ..., t_N)\Big)(\mathbf{x}_1, ..., \mathbf{x}_N) = \Big(\psi_2(t_1, ..., t_N)\Big)(\mathbf{x}_1, ..., \mathbf{x}_N). \tag{26}$$

To illustrate that our model is indeed interacting, we provide a rigoros version of Eq. (9) for the case of our model, in other words, the Ehrenfest equation for the scalar field operator.

Theorem 3 *For every $t \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^3$, let us abbreviate the solution to given initial values $\psi^0 \in \mathscr{D}$ at equal times as $\psi^t := U_{\{1,...,N\}}(t,0)\psi^0$ and $\mathcal{H}^t := \mathcal{H}_{\{1,...,N\}}(t)$ and write $\varphi(t,\mathbf{x})$ for the field operator acting as*

$$\varphi(t,\mathbf{x})\psi := \int d^3\mathbf{k} \ \left[\left(\frac{\hat{\rho}(\mathbf{k})}{\sqrt{\omega(\mathbf{k})}} e^{-i\omega(\mathbf{k})t} e^{i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{k}) + \frac{\hat{\rho}^\dagger(\mathbf{k})}{\sqrt{\omega(\mathbf{k})}} e^{i\omega(\mathbf{k})t} e^{-i\mathbf{k}\cdot\mathbf{x}} a^\dagger(\mathbf{k})\right)\psi\right]. \tag{27}$$

Then, the following equation holds:

$$\Box \left\langle \psi^t, \varphi(t,\mathbf{x})\psi^t \right\rangle = -\sum_{k=1}^{N} \left\langle \psi^t, \rho ** \delta(\hat{\mathbf{x}}_k - \mathbf{x})\psi^t \right\rangle, \tag{28}$$

where $\Box := \partial_t^2 - \triangle_{\mathbf{x}}$, and the double convolution defined as in (75) *is here understood as a shorthand notation for*

$$\begin{aligned} \rho ** \delta(\hat{\mathbf{x}}_k - \mathbf{x}) &= \int d^3\mathbf{y}_1 \int d^3\mathbf{y}_2 \ \rho(\mathbf{y}_1)\rho(\mathbf{y}_2)\delta(\hat{\mathbf{x}}_k - \mathbf{y}_1 - (\mathbf{x} - \mathbf{y}_2)). \\ &= \int d^3\mathbf{y}_1 \ \rho(\mathbf{y}_1)\rho(\mathbf{x} - \hat{\mathbf{x}}_k + \mathbf{y}_1). \end{aligned} \tag{29}$$

We observe that the Ehrenfest equation (28) for the scalar fiel features a "source term" on the right hand side. It consists of the N electrons as sources whose point-like nature is smeared out by the form factors ρ comprising the ultraviolet cut-off. The two occurrences of ρ in the double convolution $\rho ** \delta$ arise like this: In the computation, the source term is introduced by means of the commutation relation (8). The latter features two occurrences of φ whereas each φ bares one ρ in its definition in (27).

The remaining section of the paper provides the proofs of the above theorems. It is divided in section 3.1, which explains the strategy of proof regarding existence of solutions, section 3.2, which collects necessary results about the single-time evolution operators, section 3.3, which constructs the multi-time evolution and provides the proof of Theorem 1, section 3.4, which asserts the uniqueness of solutions, i.e., Theorem 2, and finally, section 3.5, which carries out the computation for the proof of Theorem 3.

3 Proofs

3.1 Strategy of proof for existence of solutions

Before treating the general case in the following sections, it is helpful to explain our strategy of proof in the simplest case of $N = 2$ as there we can easily make the index partitions fully explicit and do not obstruct ideas in the compact partitioning notation introduced above. For the treatment of the general case, however, the compact notation will prove very helpful to tackle the additional difficulties.

In the case of $N = 2$, we are looking for a pointwise evaluable solution $\psi : \mathbb{R}^2 \to \mathscr{H}$ to the system

$$\left.\begin{array}{l}\Big(i\partial_{t_1}\psi(t_1,t_2)\Big)(\mathbf{x}_1,\mathbf{x}_2) = \Big(\mathcal{H}_1(t_1)\psi(t_1,t_2)\Big)(\mathbf{x}_1,\mathbf{x}_2)\\ \Big(i\partial_{t_2}\psi(t_1,t_2)\Big)(\mathbf{x}_1,\mathbf{x}_2) = \Big(\mathcal{H}_2(t_2)\psi(t_1,t_2)\Big)(\mathbf{x}_1,\mathbf{x}_2)\end{array}\right\} \text{ if } \|\mathbf{x}_1-\mathbf{x}_2\| > \delta + |t_1 - t_2|,$$
$$\Big(i\partial_t\psi(t,t)\Big)(\mathbf{x}_1,\mathbf{x}_2) = \Big(\mathcal{H}_{\{1,2\}}(t)\psi(t,t)\Big)(\mathbf{x}_1,\mathbf{x}_2) \quad \text{if } t_1 = t_2 = t, \tag{30}$$

where $\mathcal{H}_{\{1,2\}} = \mathcal{H}_1 + \mathcal{H}_2$. Note that there is a little bit of redundancy in this system, since the second case is implied by the first if $t_1 = t_2$ and $\|\mathbf{x}_1 - \mathbf{x}_2\| > \delta + |t_1 - t_2|$. The relevance of the second case comes from the points where the times are equal, but the particles have smaller distance than δ, i.e. the line in figure 1.

The first step is to show that evolution operators $U_{\{1\}}, U_{\{2\}}, U_{\{1,2\}}$, one for each of the single equations in (30), exist. These evolutions satisfy the usual properties of two-parameter propagators and, for all ψ in a suitable domain, generate a time evolution fulfilling

$$i\frac{\partial}{\partial t}U_A(t,s)\psi = \mathcal{H}_A(t)U_A(t,s)\psi, \quad A \in \{\{1\},\{2\},\{1,2\}\}. \tag{31}$$

An essential property of U_A that we will need is that it makes the support of a wave function grow only within its future (or backwards) lightcone, as it is common for Dirac propagators. A further necessary ingredient that has to be proven is the invariance of smooth functions under the time evolutions. This will be established by commutator theorems following Huang [25].

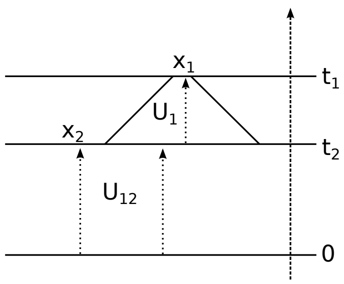

Figure 2: Depiction of the multi-time evolution. First, the initial values are evolved from time 0 to t_2 with the common propagator $U_{\{1,2\}}$, then only the degrees of freedom of particle 1 are brought to time t_1 by applying U_1. This works consistently because x_2 is outside of the backward lightcone of x_1 with an additional distance of δ, as sketched here.

In the second step, a candidate for the solution can directly be constructed with the help of the evolution operators U_A. Given smooth initial values ψ^0 at $t_1 = t_2 = 0$, we define

$$\psi(t_1,t_2) = U_{\{1\}}(t_1,t_2)U_{\{1,2\}}(t_2,0)\psi^0. \tag{32}$$

The idea is: First evolve both particles simultaneously up to time t_2 and then only evolve the first particle to t_1. If more times are added, we need to order them increasingly such that we do not "move back and forth" in the time coordinates. It is necessary, as mentioned above, to prove that the U_A operators keep functions sufficiently regular to be able to define ψ in a pointwise sense and obtain a differentiable function.

By definition, $i\partial_{t_1}\psi(t_1,t_2) = \mathcal{H}_1(t_1)\psi(t_1,t_2)$ holds. If both times are equal, the equation $i\partial_t\psi(t,t) = \mathcal{H}_{\{1,2\}}(t)\psi(t,t)$ is also fulfilled. For the derivative with respect to t_2, one has

$$\Big(i\partial_{t_2}\psi(t_1,t_2)\Big)(\mathbf{x}_1,\mathbf{x}_2) = \Big(U_{\{1\}}(t_1,t_2)\mathcal{H}_2(t_2)U_{\{1,2\}}(t_2,0)\psi^0\Big)(\mathbf{x}_1,\mathbf{x}_2). \tag{33}$$

To show that ψ solves the multi-time equations, U_1 and $\mathcal{H}_2$ have to commute on the configurations with minimal space-like distance δ. By taking another derivative, and after treating some difficulties that originate in the unboundedness of $\mathcal{H}_2(t_2)$, we will be able to reduce this to the consistency condition

$$\left([\mathcal{H}_1(t_1),\mathcal{H}_2(t_2)]\,\psi(t_1,t_2)\right)(\mathbf{x}_1,\mathbf{x}_2) = 0. \tag{34}$$

The crucial ingredients in this step are that the commutators vanish at configurations inside our domain of definition $\mathscr{S}_\delta$, and that the supports grow at most with the speed of light.

3.2 Dynamics of the single-time equations

In this section, we consider a fixed set $A \subset \{1,...,N\}$ with the respective Hamiltonian $\mathcal{H}_A(t)$ defined in (21) and construct a corresponding time evolution operator $U_A(t,s)$. This is contained in the following theorem, which uses the subsequent Lemmas 5 and 6. The subsection continues with important properties of the operator $U_A(t,s)$, namely the spreading of data with at most the speed of light (Lemma 7) and the invariance of certain smooth functions (Lemma 9, Corollary 10), namely those in the important set $\mathscr{D}$ defined in (24). We denote the identity map by $\mathbb{1}$.

Theorem 4 *There exists a unique two-parameter family of unitary operators $U_A(t,s) : \mathscr{H} \to \mathscr{H}$ with the properties that for all $t,s,r \in \mathbb{R}$,*

1. *$U_A(t,t) = \mathbb{1}$,*
2. *$U_A(t,r) = U_A(t,s)U_A(s,r)$,*
3. *If $\psi \in \mathscr{D}$, then $\frac{\partial}{\partial t}U_A(t,s)\psi\Big|_{t=s} = -i\mathcal{H}_A(s)\psi$.*

Remark: The third property in the theorem is slightly weaker than in the common case of time-independent Hamiltonians, where one can prove that the derivative exists for all functions in the domain of the Hamiltonian. But in our case, since we do not know whether $\mathrm{dom}(\mathcal{H}(t))$ is independent of t, we have to reside to a common domain like $\mathscr{D}$.

Proof: We first prove the *existence* of U_A. Consider for a fixed $s \in \mathbb{R}$ the time-independent Hamiltonian

$$\widetilde{\mathcal{H}}_{A,s} := \mathcal{H}_f + \sum_{j\in A}\left(\mathcal{H}_j^0 + \varphi_j(s)\right). \tag{35}$$

It is proven below in Lemma 5 that this Hamiltonian is essentially self-adjoint on the dense domain $\mathscr{D}$. Therefore, there is a strongly continuous unitary one-parameter group $\widetilde{U}_{A,s}$ with the property that if $\psi \in \mathrm{dom}(\widetilde{\mathcal{H}}_{A,s})$, then $\frac{\partial}{\partial t}\widetilde{U}_{A,s}(t)\psi = -i\widetilde{\mathcal{H}}_{A,s}\psi$. We can transform back to the Hamiltonian without tilde by setting

$$U_A(t,s) := e^{i\mathcal{H}_f(t-s)}\widetilde{U}_{A,s}(t-s) \quad \forall t,s \in \mathbb{R}. \tag{36}$$

We have to check that the such defined two-parameter family of unitary operators satisfies the properties listed in the theorem.

1. For all $t \in \mathbb{R}$, $U_A(t,t) = \mathbb{1}$ follows immediately by $\widetilde{U}_{A,s}(0) = \mathbb{1}$.
2. We compute for any $t, s, r \in \mathbb{R}$,

$$\begin{aligned} U_A(t,s)U_A(s,r) &= e^{i\mathcal{H}_f(t-s)}\widetilde{U}_{A,s}(t-s)e^{i\mathcal{H}_f(s-r)}\widetilde{U}_{A,r}(s-r) \\ &= e^{i\mathcal{H}_f(t-r)} \underbrace{e^{i\mathcal{H}_f(r-s)}\widetilde{U}_{A,s}(t-s)e^{i\mathcal{H}_f(s-r)}}_{=\widetilde{U}_{A,r}(t-s) \text{ by Lemma 6, part 2}} \widetilde{U}_{A,r}(s-r) \\ &= e^{i\mathcal{H}_f(t-r)}\widetilde{U}_{A,r}(t-s)\widetilde{U}_{A,r}(s-r) \\ &= U_A(t,r). \end{aligned} \tag{37}$$

3. Let $\psi \in \mathscr{D}$ and $t, s \in \mathbb{R}$, then also $\psi \in \mathrm{dom}(\mathcal{H}_f) \cap \mathrm{dom}(\widetilde{\mathcal{H}}_{A,s})$, and

$$\begin{aligned} &i\partial_t U_A(t,s)\psi(s)\big|_{t=s} \\ &= \left[-\mathcal{H}_f e^{i\mathcal{H}_f(t-s)}\widetilde{U}_{A,s}(t-s)\psi(s) + e^{i\mathcal{H}_f(t-s)}\widetilde{\mathcal{H}}_{A,s}\widetilde{U}_{A,s}(t-s)\psi(s)\right]_{t=s} \\ &= \left[-\mathcal{H}_f\psi(t) + e^{i\mathcal{H}_f(t-s)}\widetilde{\mathcal{H}}_{A,s}e^{-i\mathcal{H}_f(t-s)}\psi(t)\right]_{t=s} \\ &= \left[-\mathcal{H}_f\psi(t) + \widetilde{\mathcal{H}}_{A,t}\psi(t)\right]_{t=s} = \mathcal{H}_A(s)\psi(s), \end{aligned} \tag{38}$$

where we used in the last line the statement of Lemma 6, part 1. This establishes the third property and hence existence.

We now prove *uniqueness* of U_A. Assume there are two families $U_A(t,s)$ and $U'_A(t,s)$ with all required properties. Pick some $\psi^0 \in \mathscr{D}$, then $\psi(t) := U_A(t,0)\psi^0$ and $\psi'(t) := U'_A(t,0)\psi^0$ are differentiable w.r.t to t by the invariance of $\mathscr{D}$ (Corollary 10). By linearity, also $w(t) := \psi(t) - \psi'(t)$ satisfies the differential equation $i\partial_t w(t) = \mathcal{H}_A(t)w(t)$. Note that $w(0) = 0$. Because $\mathcal{H}_A(t)$ is self-adjoint for all times, the norm is preserved during time evolution:

$$i\partial_t \langle w(t), w(t)\rangle = -\langle \mathcal{H}_A(t)w(t), w(t)\rangle + \langle w(t), \mathcal{H}_A(t)w(t)\rangle = 0 \tag{39}$$

Therefore, also $w(t)$ must have norm zero, so $\psi(t) = \psi'(t)\ \forall t \in \mathbb{R}$, which proves that the families $U_A(t,s)$ and $U'_A(t,s)$ are in fact identical. □

We have used the statements of the following two lemmas:

Lemma 5 *Let $t, s \in \mathbb{R}$. The Hamiltonian $\mathcal{H}_A(t)$ and the operator $\widetilde{\mathcal{H}}_{A,s}$ defined in* (35) *are essentially self-adjoint on the domain $\mathscr{D}$ defined in* (24).

The following proof is a generalization of an argument by Arai [24] and a similar argument given in [26, app. C].

Proof: Let $t, s \in \mathbb{R}$. We want to prove essential self-adjointness of $\widetilde{\mathcal{H}}_{A,s}$ using the commutator theorem [27, theorem X.37], nicely proven in [28]. It is easy to see that the same argumentation can then also be applied to $\mathcal{H}_A(t)$, which just has one term less. Consider

$$K_A := \sum_{j \in A} -\triangle_j + \mathcal{H}_f + 1. \tag{40}$$

This operator is essentially self-adjoint on $\mathscr{D}$ due to well-known results (see e.g. [27]) and certainly satisfies $K_A \geq 1$. Therefore, to apply the commutator theorem, we need to prove:

1. $\exists c \in \mathbb{R}$ such that $\forall \phi \in \mathscr{D}$, $\|(\widetilde{\mathcal{H}}_{A,s})\phi\| \leq c\|K_A\phi\|$.
2. $\exists d \in \mathbb{R}$ such that $\forall \phi \in \mathscr{D}$, $|\left\langle \widetilde{\mathcal{H}}_{A,s}\phi, K_\alpha\phi\right\rangle - \left\langle K_A\phi, \widetilde{\mathcal{H}}_{A,s}\phi\right\rangle| \leq d\|K_A^{1/2}\phi\|$.

Proof of 1. We make use of the standard estimates (see e.g. [21]) valid for all $\psi \in \mathrm{dom}(\mathcal{H}_f^{1/2})$ and $f \in L^2(\mathbb{R}^3, \mathbb{C})$,

$$\left\| \int d^3\mathbf{k}\ f(\mathbf{k}) a(\mathbf{k}) \psi \right\| \le \|f\|_2 \left\| \mathcal{H}_f^{1/2} \psi \right\|, \quad \left\| \int d^3\mathbf{k}\ f(\mathbf{k}) a^\dagger(\mathbf{k}) \psi \right\| \le \|f\|_2 \left\| \mathcal{H}_f^{1/2} \psi \right\| + \|f\|_2 \|\psi\|. \quad (41)$$

Now let $\phi \in \mathscr{D}$. We have by the triangle inequality

$$\left\| \widetilde{\mathcal{H}}_{A,s} \phi \right\| \le \sum_{j \in A} \left(\left\| \mathcal{H}_j^0 \phi \right\| + \|\varphi_j \phi\| \right) + \|\mathcal{H}_f \phi\| \,, \quad (42)$$

so we need to bound each of the summands on the right hand side. $\|\mathcal{H}_f \phi\| \le \|K_A \phi\|$ is clear since 1 and $-\triangle$ are positive operators. Next we consider the free Dirac operator,

$$\left\| \mathcal{H}_j^0 \phi \right\| \le m \|\phi\| + \|-i(\boldsymbol{\alpha}_j \cdot \nabla_j)\phi\| \,. \quad (43)$$

The derivative term needs closer inspection,

$$\|-i(\boldsymbol{\alpha}_j \cdot \nabla_j)\phi\|^2 = \left\langle \phi, -(\boldsymbol{\alpha}_j \cdot \nabla_j)^2 \phi \right\rangle = \langle \phi, -\triangle \phi \rangle \,, \quad (44)$$

where only the Laplacian survives because the α-matrices anticommute and the derivatives commute. Continuing with the Cauchy-Schwarz inequality and the elementary inequality $\sqrt{ab} \le \frac{1}{2}(a+b)\ \forall a, b \ge 0$, we obtain

$$\|-i(\boldsymbol{\alpha}_j \cdot \nabla_j)\phi\| \le \sqrt{\langle \phi, -\triangle \phi \rangle} \le \sqrt{\|\phi\| \, \|-\triangle \phi\|} \le \frac{1}{2} \left(\|\phi\| + \|-\triangle \phi\| \right). \quad (45)$$

Again, since all the summands in K_A are positive operators, this directly leads to

$$\left\| \mathcal{H}_j^0 \phi \right\| \le C \, \|K_A \phi\| \,. \quad (46)$$

In the whole article, C denotes an arbitrary positive constant that may be different each time. For the interaction term, we see that the factor $\frac{\hat{\rho}(\mathbf{k})}{\sqrt{\omega(\mathbf{k})}}$ is in L^2 since $\hat{\rho}$ being a Schwartz function ensures rapid decay at infinity and since the singularity at $k = 0$ (present only for $\mu = 0$) is integrable. This allows the use of (41), giving

$$\|\varphi_j \phi\| \le C \left(\left\| \mathcal{H}_f^{1/2} \phi \right\| + \|\phi\| \right), \quad (47)$$

and with one more application of Cauchy-Schwarz,

$$\left\| \mathcal{H}_f^{1/2} \phi \right\| \le \|\phi\|^{1/2} \, \|\mathcal{H}_f \phi\|^{1/2} \le \frac{1}{2} \left(\|\phi\| + \|\mathcal{H}_f \phi\| \right), \quad (48)$$

we are done with the proof that there is a constant c (not depending on ϕ) with $\|(\widetilde{\mathcal{H}}_{A,s})\phi\| \le c\|K_A \phi\|$.
Proof of 2. As in the previous step, we can bound the summands in $\widetilde{\mathcal{H}}_{A,s}$ one by one. We first observe that $\mathcal{H}_f$ and $\mathcal{H}_j^0$ commute with K_A. For the interaction term, we have

$$[\varphi_j, K_A] = [\varphi_j, -\triangle_j] + [\varphi_j, \mathcal{H}_f] \,, \quad (49)$$

so let us compute

$$\begin{aligned} \langle \varphi_j \phi, \triangle_j \phi \rangle - \langle \triangle_j \phi, \varphi_j \phi \rangle &= \sum_{a=1}^{3} \left\langle \frac{\partial}{\partial x_j^a} \phi, \frac{\partial}{\partial x_j^a} \varphi_j \phi \right\rangle - \left\langle \frac{\partial}{\partial x_j^a} \varphi_j \phi, \frac{\partial}{\partial x_j^a} \phi \right\rangle \\ &= 2i \sum_{a=1}^{3} \Im \left\langle \frac{\partial}{\partial x_j^a} \phi, \frac{\partial}{\partial x_j^a} \varphi_j \phi \right\rangle \\ &= 2i \sum_{a=1}^{3} \Im \left\langle \frac{\partial}{\partial x_j^a} \phi, \int d^3\mathbf{k} \left[\left(\frac{-i k_j^a \hat{\rho}(\mathbf{k})}{\sqrt{\omega(\mathbf{k})}} e^{-i\omega(\mathbf{k})t} e^{i\mathbf{k}\cdot\hat{\mathbf{x}}_j} a(\mathbf{k}) + c.c. \right) \phi \right] \right\rangle, \end{aligned} \quad (50)$$

where the last equality holds since $\left\langle \frac{\partial}{\partial x_j^a}\phi, \varphi_j \frac{\partial}{\partial x_j^a}\phi \right\rangle$ is real; and "c.c" denotes the hermitian conjugate of the preceding term. Since $\hat{\rho}$ is a Schwartz function, also $-ik_j^a\hat{\rho}(\mathbf{k})$ is, so we get from the estimate (41)

$$|\langle\varphi_j\phi, \triangle_j\phi\rangle - \langle\triangle_j\phi, \varphi_j\phi\rangle| \leq C\left(\left\|\mathcal{H}_f^{1/2}\phi\right\| + \|\phi\|\right) \leq 2C\left\|K_A^{1/2}\phi\right\|. \tag{51}$$

For the second term in (49), we look at the commutator of φ_j and $\mathcal{H}_f$. This amounts to a time derivative of $\varphi_j(t)$, which gives an expression like in the last line of (50), but where the function $-ik_j^a\hat{\rho}(\mathbf{k})$ is replaced by $-i\omega(\mathbf{k})\hat{\rho}(\mathbf{k})$. This is again a Schwartz function. Using estimate (41) again for that function, we obtain

$$|\langle\varphi_j\phi, \mathcal{H}_f\phi\rangle - \langle\mathcal{H}_f\phi, \varphi_j\phi\rangle| \leq C\left\|K_A^{1/2}\phi\right\|. \tag{52}$$

This means we have shown that there is a constant d (independent of ϕ), such that

$$\left|\left\langle\widetilde{\mathcal{H}}_{A,s}\phi, K_A\phi\right\rangle - \left\langle K_A\phi, \widetilde{\mathcal{H}}_{A,s}\phi\right\rangle\right| \leq d\|K_A^{1/2}\phi\|. \tag{53}$$

This is the second necessary ingredient for the application of the commutator theorem, which gives the statement of the lemma. □

Lemma 6 *The self-adjoint Hamiltonian $\widetilde{\mathcal{H}}_{A,s}$ and the unitary group $\widetilde{U}_{A,s}$ it generates satisfy the following properties for all $r, s, t \in \mathbb{R}$:*

1. $e^{i\mathcal{H}_f(t-s)}\widetilde{\mathcal{H}}_{A,s}^n e^{-i\mathcal{H}_f(t-s)} = \widetilde{\mathcal{H}}_{A,t}^n \quad \forall n \in \mathbb{N}$*, whenever both sides are well-defined.*
2. $e^{i\mathcal{H}_f(r-s)}\widetilde{U}_{A,s}(t-s)e^{i\mathcal{H}_f(s-r)} = \widetilde{U}_{A,r}(t-s)$.

Proof: Let $r, s, t \in \mathbb{R}$.

1. We have for $n = 1$

$$\begin{aligned} e^{i\mathcal{H}_f(t-s)}\widetilde{\mathcal{H}}_{A,s}e^{-i\mathcal{H}_f(t-s)} &= e^{i\mathcal{H}_f(t-s)}\left(\mathcal{H}_f + \sum_{j\in A}\mathcal{H}_j^0 + \varphi_j(s)\right)e^{-i\mathcal{H}_f(t-s)} \\ &= \mathcal{H}_f + \sum_{j\in A}\mathcal{H}_j^0 + e^{i\mathcal{H}_f(t-s)}\varphi_j(s)e^{-i\mathcal{H}_f(t-s)} \\ &= \widetilde{\mathcal{H}}_{A,t}. \end{aligned} \tag{54}$$

   The statement for arbitrary $n \in \mathbb{N}$ follows directly from the $n = 1$ case, which can be seen by inserting the identity $\mathbb{1} = e^{-i\mathcal{H}_f(t-s)}e^{i\mathcal{H}_f(t-s)}$ between the factors of $\widetilde{\mathcal{H}}_{A,s}$,

$$e^{i\mathcal{H}_f(t-s)}\widetilde{\mathcal{H}}_{A,s}^n e^{-i\mathcal{H}_f(t-s)} = \prod_{k=1}^n e^{i\mathcal{H}_f(t-s)}\widetilde{\mathcal{H}}_{A,s}e^{-i\mathcal{H}_f(t-s)} = \widetilde{\mathcal{H}}_{A,t}^n. \tag{55}$$

2. By the analytic vector theorem, the set $\mathscr{A}$ of analytic vectors for $\widetilde{\mathcal{H}}_{A,s}$ is dense. Hence its image under the unitary map $e^{i\mathcal{H}_f(r-s)}$ is also dense. Let $\psi \in e^{i\mathcal{H}_f(r-s)}(\mathscr{A})$. We can write

$$\begin{aligned} e^{i\mathcal{H}_f(r-s)}\widetilde{U}_{A,s}(t-s)e^{i\mathcal{H}_f(s-r)}\psi &= e^{i\mathcal{H}_f(r-s)}\sum_{n=0}^\infty \frac{i^n(t-s)^n}{n!}\widetilde{\mathcal{H}}_{A,s}^n e^{i\mathcal{H}_f(s-r)}\psi \\ &= \sum_{n=0}^\infty \frac{i^n(t-s)^n}{n!}e^{i\mathcal{H}_f(r-s)}\widetilde{\mathcal{H}}_{A,s}^n e^{i\mathcal{H}_f(s-r)}\psi \\ &= \sum_{n=0}^\infty \frac{i^n(t-s)^n}{n!}\widetilde{\mathcal{H}}_{A,r}^n\psi, \end{aligned} \tag{56}$$

where we used part 1 of the lemma in the last step. The series converges, so ψ is analytic for $\widetilde{\mathcal{H}}_{A,r}$, which proves

$$e^{i\mathcal{H}_f(r-s)}\widetilde{U}_{A,s}(t-s)e^{i\mathcal{H}_f(s-r)}\psi = \widetilde{U}_{A,r}(t-s)\psi, \quad \forall\psi \in e^{i\mathcal{H}_f(r-s)}(\mathscr{A}). \tag{57}$$

Equation (57) tells us that the bounded operators $e^{i\mathcal{H}_f(r-s)}\widetilde{U}_{A,s}(t-s)e^{i\mathcal{H}_f(s-r)}$ and $\widetilde{U}_{A,r}(t-s)$ agree on a dense set, which implies that they are equal. □

The next lemma is about the causal structure of our equations. It uses the usual definition of addition of sets,

$$M + R := \{m + r | m \in M, r \in R\}. \tag{58}$$

In order to simplify notation, it is implied that vectors in $\mathbb{R}^{3N}$ and $\mathbb{R}^3$ can be added by just changing the respective j-th coordinate, e.g. $(\mathbf{x}_1, \mathbf{x}_2) + \mathbf{y}_2 \equiv (\mathbf{x}_1, \mathbf{x}_2 + \mathbf{y}_2)$.

Lemma 7

1. *The evolution operators U_A do not propagate data faster than light, i.e. if for $R \subset \mathbb{R}^{3N}$ we have $\operatorname{supp}\psi \subset R$, then for all $t, s \in \mathbb{R}$,*

$$\operatorname{supp}\,(U_A(t,s)\psi) \subset R + \sum_{j\in A} B_{|t-s|}(\mathbf{x}_j). \tag{59}$$

2. *Let ψ be the solution of $i\partial_t\psi = \mathcal{H}_A(t)\psi$ with smooth initial values given as $\psi(0,...,0) = \psi^0$. Then for all $t \in \mathbb{R}$, $\psi(t, \mathbf{x}_1, ..., t, \mathbf{x}_N)$ is uniquely determined by specifying initial conditions on $\sum_{j\in A} \overline{B}_{|t|}(\mathbf{x}_j)$.*

Proof:

1. This lightcone property of the free Dirac equation is well-known (compare [29, theorem 2.20]). The claim for our model is a direct generalization to the many-particle case of the functional analytic arguments in [23, theorem 3.4]. (Note that it is also feasible to adapt the arguments using current conservation in [6, lemma 14] since the continuity equation holds for our model, as well.)

2. This follows directly from 1. since if ψ and ψ' are two solutions whose initial values ψ^0 and ψ'^0 agree on $\sum_{j\in A} \overline{B}_{|t|}(\mathbf{x}_j)$, then

$$\operatorname{supp}\,(\psi^0 - \psi'^0) \subset \mathbb{R}^{3N} \setminus \sum_{j\in A} \overline{B}_{|t|}(\mathbf{x}_j) \tag{60}$$

implies by (59)

$$\operatorname{supp}\,(U_A(t,0)(\psi^0 - \psi'^0)) \subset \mathbb{R}^{3N} \setminus \sum_{j\in A} \overline{B}_{|t|}(\mathbf{x}_j) + \sum_{j\in A} B_{|t|}(\mathbf{x}_j) = \mathbb{R}^{3N} \setminus \{(\mathbf{x}_1, ..., \mathbf{x}_N)\}, \tag{61}$$

which is the claim. □

Another necessary information is which domains stay invariant under the time evolutions we have just constructed. The idea is to exploit a theorem by Huang [25, thm. 2.3], which we cite here adopted to our notation.

Theorem 8 ***(Huang).*** *Let K be a positive self-adjoint operator and define $Z_j(t) = K^{j-1}[\mathcal{H}_A(t), K]\,K^{-j}$. Suppose that $Z_k(t)$ is bounded with $\|Z_k(\cdot)\| \in L^1_{loc}(\mathbb{R})$ for all $k \leq j$. Then $U_A(t,s)[\operatorname{dom}(K^j)] = \operatorname{dom}(K^j)$.*

We will use a family of comparison operators for $j \in \mathbb{N}$, abbreviating $\sum_{k=1}^{N} -\triangle_k =: -\triangle$,

$$K_n := (-\triangle)^n + (\mathcal{H}_f)^n + 1. \tag{62}$$

The operator K_n resembles the $n-th$ power of the operator K_A we defined in (40) for the commutator theorem. Its domain of self-adjointness is denoted by $\mathrm{dom}(K_n)$.

Lemma 9 *The family of operators $U_A(t,s)$ with $t, s \in \mathbb{R}$ leaves the set $\mathrm{dom}(K_n)$ invariant for all $n \in \mathbb{N}$.*

Proof: Let $n \in \mathbb{N}$. It is known that K_n is self-adjoint and strictly positive. We prove the invariance of $\mathrm{dom}(K^n)$ using Thm. 8, hence we only need the case $j = 1$ and need to bound $Z_1(t) = [\mathcal{H}_A(t), K_n]K_n^{-1}$.
Note that, since K_n is positive, 0 is in its resolvent set. This means that $K_n : \mathrm{dom}(K_n) \to \mathscr{H}$ is bijective, so its inverse $K_n^{-1} : \mathscr{H} \to \mathrm{dom}(K_n)$ is bounded by the closed graph theorem. Because the Laplacian commutes with the free Dirac operator (in the sense of self-adjoint operators, which can e.g. be seen by their resolvents), this carries over to $(-\triangle)^n$ and the commutator gives

$$[\mathcal{H}_A(t), K_n] = \sum_{j\in A} [\varphi_j(t), (-\triangle)^n] + \sum_{j\in A} \left[\varphi_j(t), \mathcal{H}_f^n\right]. \tag{63}$$

The commutator terms give rise to derivatives of the field terms φ, similarly as in the calculation (50). It becomes apparent that arbitrary derivatives with respect to time or space variables lead to the multiplication of $\hat{\rho}(\mathbf{k})$ in (17) by a product of k^a and $\omega(\mathbf{k})$ factors, which still keep the rapid decay at infinity. Therefore, also the derivative is a quantum field with an L^2-function as cut-off function. This means that the bound (47) can analogously be applied to the commutator and we have some $C > 0$ with

$$\|[\mathcal{H}_A(t), K_n]\,\eta\| \le C\left(\|\mathcal{H}_f\eta\| + \|\eta\|\right) \quad \forall \eta \in \mathrm{dom}(K). \tag{64}$$

By the inequality of arithmetic and geometric mean,

$$\|\mathcal{H}_f\eta\| = \|\sqrt[n]{\mathcal{H}_f^n}\eta\| \le C(\|\mathcal{H}_f^n\eta\| + \|\eta\|) \le C(\|K_n\eta\| + \|\eta\|) \tag{65}$$

Since $K_n^{-1}\psi \in \mathrm{dom}(K_n)$, we can apply this to $Z_1(t)$,

$$\|Z_1(t)\psi\| = \left\|\left([\mathcal{H}_A(t), K_n]\right) K_n^{-1}\psi\right\| \le C\left(\|K_nK_n^{-1}\psi\| + \|K_n^{-1}\psi\|\right) = C\left(1 + \|K_n^{-1}\|_{op}\right)\|\psi\|, \tag{66}$$

which implies that $Z_1(t)$ is bounded with $\|Z_1(\cdot)\| \in L^1_{loc}(\mathbb{R})$. Hence, application of Theorem 8 yields the claim. □

Corollary 10 *The family of operators $U_A(t,s)$ with $t, s \in \mathbb{R}$ leaves the set $\mathscr{D}$, defined in* (24), *invariant.*

Proof: By Lemma 9, $U_A(t,s)$ with $t, s \in \mathbb{R}$ leaves $\mathrm{dom}(K_n)$ invariant for each $n \in \mathbb{N}$. We claim that

$$\mathrm{dom}(K_n) = \mathrm{dom}((-\triangle)^n) \otimes \mathscr{F} \cap L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathrm{dom}(\mathcal{H}_f^n). \tag{67}$$

The operator K_n is of the form $(-\triangle)^n \otimes \mathbb{1} + \mathbb{1} \otimes \mathcal{H}_f^n + 1$, where the bounded operator 1 is irrelevant for the domain. By [30, chap. VIII.10], an operator of this structure on a tensor product space is essentially self-adjoint on the domain $\mathrm{dom}((-\triangle)^n) \otimes \mathscr{F} \cap L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathrm{dom}(\mathcal{H}_f^n)$. The domain of self-adjointness arises when we take the closure of that operator. It is, however, known from [31, p. 160] that a sum of positive operators is already closed on the domain (67). Thus, (67) is actually the domain of self-adjointness of K_n.

Let $\psi \in \mathscr{D}$, then also $\psi \in \mathrm{dom}(K_n)$ for all $n \in \mathbb{N}$. Thus, $U_A(t,s)\psi \in \mathrm{dom}(K_n)$ for all $n \in \mathbb{N}$. For the Fock space part, this directly gives

$$U_A(t,s)\psi \in \bigcap_{n=1}^{\infty} L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathrm{dom}(\mathcal{H}_f^n) = L^2(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathrm{dom}(\mathcal{H}_f^\infty). \tag{68}$$

In the L^2-part, we first note that Lemma 7 gives an upper bound on the growth of supports, so compactness of the support is preserved under the time evolution $U_A(t,s)$. Secondly, we have

$$U_A(t,s)\psi \in \bigcap_{n=1}^{\infty} \mathrm{dom}((-\triangle)^n) \otimes \mathscr{F} \subset C^\infty(\mathbb{R}^{3N}, \mathbb{C}^K) \otimes \mathscr{F}, \tag{69}$$

which follows from Sobolev's lemma as contained in the proposition in [27, chap. IX.7]. These two facts imply that the time evolution leaves C_c^∞ invariant. Thus we infer $U_A(t,s)\psi \in \mathscr{D}$. □

Another result that will be helpful later is that not only the time evolutions leave the set $\mathscr{D}$ invariant, but also the terms in the Hamilton operators themselves.

Lemma 11 *The set $\mathscr{D}$ is left invariant by $\mathcal{H}_f$, $\mathcal{H}_j^0$ and $\varphi_j(t)$ for each $1 \leq j \leq N$ and $t \in \mathbb{R}$.*

Proof:

1. $\mathcal{H}_j^0$ only acts on the first tensor component and on that one, it leaves C_c^∞-functions invariant because it is a linear combination of partial derivatives and the identity.
2. $\mathcal{H}_f$ only acts on the second tensor component and on that one, it leaves $\mathrm{dom}(\mathcal{H}_f^\infty)$ invariant by definition.
3. First we note that φ_j does not increase supports. Now let $k \in \mathbb{N}, t \in \mathbb{R}$ and $\psi \in \mathrm{dom}(\mathcal{H}_f^{k+1})$. Then, using the same estimates as in the proof of Lemma 5,

$$\left\|\mathcal{H}_f^k\ \varphi_j(t)\psi\right\| \leq \left\|\varphi_j(t)\mathcal{H}_f^k\psi\right\| + \left\|\frac{\partial^k}{\partial t^k}\varphi_j(t)\psi\right\| \leq C\left(\left\|\mathcal{H}_f^{k+1}\psi\right\| + \|\mathcal{H}_f\psi\| + \|\psi\|\right) < \infty, \tag{70}$$

which shows that $\varphi_j(t)\psi \in \mathrm{dom}(\mathcal{H}_f^k)$ for every $t \in \mathbb{R}$. An analogous argument can be done for the operators $\mathcal{H}_j^0$, which together implies that $\varphi_j(t)$ leaves $\mathscr{D}$ invariant. □

3.3 Construction of the multi-time evolution

The construction of the solution of our multi-time system (23) relies on the consistency condition which we prove now.

Lemma 12 *Let $\psi \in \mathscr{D}$ and A, B be disjoint subsets of $\{1, ..., N\}$, then the consistency condition*

$$[\mathcal{H}_A(t_A), \mathcal{H}_B(t_B)]\, \psi(\mathbf{x}_1, ..., \mathbf{x}_N) = 0 \tag{71}$$

is satisfied whenever $\forall j \in A, k \in B : \|\mathbf{x}_j - \mathbf{x}_k\| > \delta + |t_A - t_B|$.

Proof: Let $t_A, t_B \in \mathbb{R}$. The commutator reads

$$[\mathcal{H}_A(t_A), \mathcal{H}_B(t_B)] = \left[\sum_{j\in A} \mathcal{H}_j^0 + \varphi_j(t_A), \sum_{k\in B} \mathcal{H}_k^0 + \varphi_k(t_B)\right] = \sum_{j\in A, k\in B} [\varphi_j(t_A), \varphi_k(t_B)]\,, \tag{72}$$

since, by definition, the free Dirac Hamiltonians commute with the other terms. We will now show that each of the summands in the double sum applied to $\psi \in \mathscr{D}$ vanishes when evaluated at $(\mathbf{x}_1, ..., \mathbf{x}_N) \in \mathbb{R}^{3N}$ with $\forall j \in A, k \in B : \|\mathbf{x}_j - \mathbf{x}_k\| > \delta + |t_A - t_B|$.

It is well-known (e.g. [27, thm X.41]) that field operators as defined in (17) satisfy the CCR, which means

$$\begin{aligned}
&[\varphi_j(t_A),\varphi_k(t_B)]\,\psi(\mathbf{x}_1,...,\mathbf{x}_N)\\
&= i\Im\int \frac{d^3\mathbf{k}}{\omega(\mathbf{k})}\,\hat\rho(\mathbf{k})^\dagger\hat\rho(\mathbf{k})e^{i\omega(\mathbf{k})t_A - i\mathbf{k}\cdot\mathbf{x}_j}e^{-i\omega(\mathbf{k})t_B+i\mathbf{k}\cdot\mathbf{x}_k}\psi(\mathbf{x}_1,...,\mathbf{x}_N)\\
&= \frac{1}{2}\int\frac{d^3\mathbf{k}}{\omega(\mathbf{k})}\left(\hat\rho(\mathbf{k})^\dagger\hat\rho(\mathbf{k})e^{i\omega(\mathbf{k})(t_A-t_B)}e^{-i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_k)} - \text{ c.c}\right)\psi(\mathbf{x}_1,...,\mathbf{x}_N)\\
&= \frac{1}{2}\int\frac{d^3\mathbf{k}}{\omega(\mathbf{k})}\Big(\int d^3\mathbf{y}_1d^3\mathbf{y}_2\rho(\mathbf{y}_1)e^{-i\mathbf{k}\cdot\mathbf{y}_1}\rho(\mathbf{y}_2)e^{i\mathbf{k}\cdot\mathbf{y}_2}e^{i\omega(\mathbf{k})(t_A-t_B)}e^{-i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_k)}\\
&\qquad - \text{c.c}\Big)\psi(\mathbf{x}_1,...,\mathbf{x}_N),
\end{aligned} \tag{73}$$

upon insertion of the Fourier transforms. We compare this to the so-called Pauli-Jordan function [32, p. 88], i.e. the distribution

$$\Delta(x_j,x_k) := c\int\frac{d^3\mathbf{k}}{\omega(\mathbf{k})}\left(e^{i\omega(\mathbf{k})(t_j-t_k)-i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_k)} - \text{ c.c.}\right), \tag{74}$$

where $c = \frac{i}{16\pi^3}$. It is known that $\Delta(x_1,x_2)=0$ whenever x_1 is space-like to x_2 [32, p. 89]. We define a double convolution by

$$\begin{aligned}
&(\rho**\Delta)(t_j,\mathbf{x}_j,t_k,\mathbf{x}_k) := \int d^3\mathbf{y}_1d^3\mathbf{y}_2\;\rho(\mathbf{y}_1)\rho(\mathbf{y}_2)\Delta(t_j,\mathbf{x}_j-\mathbf{y}_1,t_k,\mathbf{x}_k-\mathbf{y}_2)\\
&= c\int\frac{d^3\mathbf{k}}{\omega(\mathbf{k})}\int d^3\mathbf{y}_1d^3\mathbf{y}_2\rho(\mathbf{y}_1)\rho(\mathbf{y}_2)\left(e^{i\omega(\mathbf{k})(t_j-t_k)-i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{y}_1-\mathbf{x}_k+\mathbf{y}_2)} - \text{ c.c.}\right),
\end{aligned} \tag{75}$$

which is a well-defined integral since $\rho\in C_c^\infty(\mathbb{R}^3)$. Comparison to (73) yields

$$\frac{2}{c}\,[\varphi_j(t_A),\varphi_k(t_B)]\,\psi(\mathbf{x}_1,...,\mathbf{x}_N) = (\rho**\Delta)(t_A,\mathbf{x}_j,t_B,\mathbf{x}_k)\psi(\mathbf{x}_1,...,\mathbf{x}_N). \tag{76}$$

We know that $\|\mathbf{x}_j-\mathbf{x}_k\| > |t_A-t_B|+\delta$ and by (16), $\rho(\mathbf{y})\neq 0$ only if $\|\mathbf{y}\| < \frac{\delta}{2}$. Thus the argument of the function Δ in the double convolution (75) satisfies

$$\begin{aligned}
\|\mathbf{x}_j-\mathbf{y}_1-(\mathbf{x}_k-\mathbf{y}_2)\| &\geq \|\mathbf{x}_k-\mathbf{x}_j\| - \|\mathbf{y}_1\| - \|\mathbf{y}_2\|\\
&\geq \|\mathbf{x}_j-\mathbf{x}_k\| - \delta\\
&> |t_A-t_B|,
\end{aligned} \tag{77}$$

i.e. it is space-like, which implies that $(\rho**\Delta)(t_A,\mathbf{x}_j,t_B,\mathbf{x}_k)=0$ and hence also the commutator is zero. □

With all the previous results at hand, the existence of solutions can be treated constructively. We first prove a lemma which contains the crucial ingredient for the subsequent theorem.

Lemma 13 *Let $\zeta\in\mathscr{D}$. Let A,B be arbitrary subsets of $\{1,...,N\}$ with $A\cap B=\emptyset$, let $t_B\geq s\geq t_A$, then*

$$\left([\mathcal{H}_A(t_A),U_B(t_B,s)]\,\zeta\right)(\mathbf{x}_1,...,\mathbf{x}_N)=0. \tag{78}$$

holds at every point $(\mathbf{x}_1,...,\mathbf{x}_N)\in\mathbb{R}^{3N}$ for which $\forall j\in A,k\in B$, $\|\mathbf{x}_j-\mathbf{x}_k\|>\delta+t_B-t_A$.

The idea of the proof is to take the derivative of the commutator in (78) with respect to t_B to get an expression where the consistency condition proven in Lemma 12 becomes useful. However, it is not immediately clear if a term of the form $\mathcal{H}_A(t_A)U_B(t_B,s)$ is differentiable or even continuous in t_B because $\mathcal{H}_A$ is not a continuous operator. Therefore, we have to take a detour and approximate $\mathcal{H}_A$ by bounded operators. A similar approximation by bounded operators is used in the proof of the Hille-Yosida theorem in [33, ch. 7.4].

Proof: Let $A, B \subset \{1, ..., N\}$ with $A \cap B = \emptyset$, $s, t_A, t_B \in \mathbb{R}$ with $t_B \geq s \geq t_A$, $\zeta \in \mathscr{D}$ and $(\mathbf{x}_1, ..., \mathbf{x}_N) \in \mathbb{R}^{3N}$ such that $\forall j \in A, k \in B$: $\|\mathbf{x}_j - \mathbf{x}_k\| > \delta + t_B - t_A$.

We abbreviate $\sum_{k\in A} \varphi_k(t) =: \varphi_A(t)$ for $t \in \mathbb{R}$. First note that the free Dirac terms in $\mathcal{H}_A$ trivially commute, so

$$([U_B(t_B, s), \mathcal{H}_A(t_A)]\,\zeta)\,(\mathbf{x}_1, ..., \mathbf{x}_N) = ([U_B(t_B, s), \varphi_A(t_A)]\,\zeta)\,(\mathbf{x}_1, ..., \mathbf{x}_N). \tag{79}$$

Now define for $\varepsilon > 0, t \in \mathbb{R}$ a family of auxiliary operators

$$\varphi_A^\varepsilon(t) := \frac{\varphi_A(t)}{1 + i\varepsilon\varphi_A(t)}, \tag{80}$$

which are well-defined since $\varphi_A(t)$ is self-adjoint for all t [22]. For $\lambda \in \mathbb{R}, \varepsilon > 0$,

$$\left|\frac{\lambda}{1 + i\varepsilon\lambda}\right| \leq \frac{1}{\varepsilon} \quad \Longrightarrow \|\varphi_A^\varepsilon(t)\| \leq \frac{1}{\varepsilon} \tag{81}$$

where the implication follows by the spectral theorem. The difference of field operator φ_A and its approximation φ_A^ε can be recast into

$$(\varphi_A(t_A) - \varphi_A^\varepsilon(t_A)) = \frac{\varphi_A(t_A) + i\varepsilon\varphi_A(t_A)^2}{1 + i\varepsilon\varphi_A(t_A)} - \frac{\varphi_A(t_A)}{1 + i\varepsilon\varphi_A(t_A)} = \frac{i\varepsilon}{1 + i\varepsilon\varphi_A(t_A)}\varphi_A(t_A)^2 \tag{82}$$

and we note the bound for all $\varepsilon > 0$:

$$\left\|\frac{1}{1 + i\varepsilon\varphi_A(t_A)}\right\| \leq 1. \tag{83}$$

Because $U_B(t_B, s)\zeta \in \mathscr{D}$ by corollary 10, we find the bound

$$\begin{aligned} \|[U_B(t_B, s), \varphi_A(t_A) - \varphi_A^\varepsilon(t_A)]\,\zeta\| \leq\ & \|(\varphi_A(t_A) - \varphi_A^\varepsilon(t_A))\zeta\| \\ & + \|(\varphi_A(t_A) - \varphi_A^\varepsilon(t_A))U_B(t_B, s)\zeta\| \\ & \leq \varepsilon\left(\|\varphi_A(t_A)^2\zeta\| + \|\varphi_A(t_A)^2 U_B(t_B, s)\zeta\|\right). \end{aligned} \tag{84}$$

Since we can take $\varepsilon \to 0$, the norm of the left hand side has to vanish. Because we furthermore know that $[U_B(t_B, s), \varphi_A(t_A) - \varphi_A^\varepsilon(t_A)]$ is a continuous function, the following implication holds:

$$([U_B(t_B, s), \varphi_A^\varepsilon(t_A)]\,\zeta)\,(\mathbf{x}_1, ..., \mathbf{x}_N) = 0\ \forall\varepsilon > 0 \Rightarrow ([U_B(t_B, s), \varphi_A(t_A)]\,\zeta)\,(\mathbf{x}_1, ..., \mathbf{x}_N) = 0. \tag{85}$$

Thus it remains to prove that the commutator defined for $t \in \mathbb{R}$,

$$\Omega_t := [U_B(t, s), \varphi_A^\varepsilon(t_A)]\,\zeta, \tag{86}$$

vanishes at $(\mathbf{x}_1, ..., \mathbf{x}_N)$. Note that Ω_t depends on ε, which we do not write for brevity. As a merit of our approximation, $t \mapsto \Omega_t$ is a continuous map $\mathbb{R} \to \mathscr{H}$. We proceed in four steps:

1. Construct an auxiliary function ϕ_t that solves for $\eta \in \mathscr{D}$

$$i\partial_t \langle \eta, \phi_t \rangle = \langle \eta, [\varphi_B(t), \varphi_A^\varepsilon(t_A)]\, U_B(t, s)\eta \rangle + \langle \mathcal{H}_B(t)\eta, \phi_t \rangle. \tag{87}$$

2. Show that $\forall \eta \in \mathscr{D} : i\partial_t \langle \eta, \phi_t - \Omega_t \rangle = \langle \mathcal{H}_B(t)\eta, \phi_t - \Omega_t \rangle$.

3. Show that the weak equation proven in step 2 has a unique solution, thus $\phi_t = \Omega_t$.

4. Investigate the support properties of ϕ_t and conclude that Ω_t vanishes at $(\mathbf{x}_1, ..., \mathbf{x}_N)$.

Step 1: We introduce the abbreviation for $t \in \mathbb{R}$

$$f_t := [\varphi_B(t), \varphi_A^\varepsilon(t_A)]\, U_B(t,s)\zeta \tag{88}$$

and recognize that the function $f : \mathbb{R} \to \mathscr{H}, t \mapsto f_t$ is bounded and measurable. Define

$$\phi_t := \int_s^t d\tau\; e^{i\mathcal{H}_f(t-s)} e^{-i(\mathcal{H}_f+\mathcal{H}_B(s))(t-\tau)} e^{-i\mathcal{H}_f(\tau-s)} f_\tau. \tag{89}$$

For $\eta \in \mathscr{D}, t \in \mathbb{R}$, we compute using Fubini's theorem,

$$\begin{aligned} i\partial_t \langle \eta, \phi_t \rangle =& i\partial_t \int_s^t d\tau \left\langle e^{i\mathcal{H}_f(\tau-s)} e^{i(\mathcal{H}_f+\mathcal{H}_B(s))(t-\tau)} e^{-i\mathcal{H}_f(t-s)}\eta, f_\tau \right\rangle \\ =& \left\langle e^{i\mathcal{H}_f(t-s)} e^{i(\mathcal{H}_f+\mathcal{H}_B(s))(t-t)} e^{-i\mathcal{H}_f(t-s)}\eta, f_t \right\rangle \\ &+ \int_s^t d\tau \left\langle e^{i\mathcal{H}_f(\tau-s)} \mathcal{H}_B(s) e^{i(\mathcal{H}_f+\mathcal{H}_B(s))(t-\tau)} e^{-i\mathcal{H}_f(t-s)}\eta, f_\tau \right\rangle \\ =& \langle \eta, f_t \rangle + \langle \mathcal{H}_B(t)\eta, \phi_t \rangle . \end{aligned} \tag{90}$$

Step 2: A calculation similar to the one above is now possible for $\Omega_t, t \in \mathbb{R}$:

$$\begin{aligned} i\partial_t \langle \eta, \Omega_t \rangle =& i\partial_t \left(\langle U_B(s,t)\eta, \varphi_A^\varepsilon(t_A)\zeta \rangle - \left\langle \varphi_A^\varepsilon(t_A)^\dagger \eta, U_B(t,s)\zeta \right\rangle \right) \\ =& \langle U_B(s,t)\mathcal{H}_B(t)\eta, \varphi_A^\varepsilon(t_A)\zeta \rangle - \left\langle \varphi_A^\varepsilon(t_A)^\dagger \eta, \mathcal{H}_B(t) U_B(t,s)\zeta \right\rangle \\ &- \langle \mathcal{H}_B(t)\eta, \varphi_A^\varepsilon(t_A) U_B(t,s)\zeta \rangle + \langle \mathcal{H}_B(t)\eta, \varphi_A^\varepsilon(t_A) U_B(t,s)\zeta \rangle \\ =& \langle \mathcal{H}_B(t)\eta, \Omega_t \rangle + \langle \eta, [\mathcal{H}_B(t), \varphi_A^\varepsilon(t_A)]\, U_B(t,s)\zeta \rangle \\ =& \langle \mathcal{H}_B(t)\eta, \Omega_t \rangle + \langle \eta, [\varphi_B(t), \varphi_A^\varepsilon(t_A)]\, U_B(t,s)\zeta \rangle + \sum_{k\in B} \left\langle \eta, \underbrace{\left[\mathcal{H}_k^0, \varphi_A^\varepsilon(t_A)\right]}_{=0} \zeta \right\rangle \\ =& \langle \eta, f_t \rangle + \langle \mathcal{H}_B(t)\eta, \Omega_t \rangle . \end{aligned} \tag{91}$$

This together with (90) yields that the difference $\phi_t - \Omega_t$ is a weak solution of the Dirac equation in the sense that $\forall \eta \in \mathscr{D}$:

$$i\partial_t \langle \eta, \phi_t - \Omega_t \rangle = \langle \mathcal{H}_B(t)\eta, \phi_t - \Omega_t \rangle \quad . \tag{92}$$

Step 3: For all $s \in \mathbb{R}$, $U_B(s,s) = \mathbb{1}$ implies $\Omega_s = 0$ and by definition, $\phi_s = 0$. To show that Ω_t and ϕ_t are actually equal for all times $t \in \mathbb{R}$, it thus suffices to prove uniqueness of solutions to Eq. (92).
To this end, let $\rho : \mathbb{R} \to \mathcal{H}, t \mapsto \rho_t$ be continuous and for every $\eta \in \mathscr{D}$ a solution to

$$i\partial_t \langle \eta, \rho_t \rangle = \langle \mathcal{H}_B(t)\eta, \rho_t \rangle . \tag{93}$$

We claim that then, for all $t \in \mathbb{R}$, $\rho_t = U_B(t,s)\rho_s$. To see this we consider $t \mapsto \langle U_B(t,s)\eta, \rho_t \rangle$, we prove that this is differentiable with zero derivative. For $h > 0$, we find

$$\begin{aligned} &\frac{1}{h} \left\| \langle U_B(t+h,s)\eta, \rho_{t+h} \rangle - \langle U_B(t,s)\eta, \rho_t \rangle \right\| \\ \le& \left\| \frac{1}{h} \langle U_B(t+h,s)\eta - U_B(t,s)\eta, \rho_{t+h} \rangle - \langle i\mathcal{H}_B(t) U_B(t,s)\eta, \rho_{t+h} \rangle \right\| \\ &+ \left\| \frac{1}{h} \langle U_B(t,s)\eta, \rho_{t+h} - \rho_t \rangle - i \langle \mathcal{H}_B(t) U_B(t,s)\eta, \rho_{t+h} \rangle \right\| \\ \le& \left\| \frac{1}{h} (U_B(t+h,s)\eta - U_B(t,s)\eta) - i\mathcal{H}_B(t) U_B(t,s)\eta \right\| \|\rho_{t+h}\| \\ &+ \left\| \frac{1}{h} \langle U_B(t,s)\eta, \rho_{t+h} - \rho_t \rangle - i \langle \mathcal{H}_B(t) U_B(t,s)\eta, \rho_t \rangle \right\| + \left\| \langle \mathcal{H}_B(t) U_B(t,s)\eta, \rho_{t+h} - \rho_t \rangle \right\|. \end{aligned} \tag{94}$$

The first term goes to zero as $h \to 0$ because $\eta \in \mathscr{D}$ and since ρ_t is continuous, the norm ρ_{t+h} is bounded in a neighbourhood of t. The second term vanishes using (93), noting that also $U_B(t,s)\eta \in \mathscr{D}$ by Corollary 10. The last term also goes to zero by continuity of ρ_t. We have thus proven that

$$\partial_t \langle U_B(t,s)\eta, \rho_t\rangle = 0 \ \Rightarrow \langle \eta, U_B(s,t)\rho_t\rangle = const. \tag{95}$$

This implies the desired uniqueness statement $\langle \eta, U_B(t,s)\rho_s - \rho_t\rangle = 0$ for all $\eta \in \mathscr{D}$. Since $\mathscr{D} \subset \mathscr{H}$ is dense, $\rho_t = U_B(t,s)\rho_s$ follows.
In the special case of (92), the initial value is $\rho_s = \phi_s - \Omega_s = 0$. Furthermore, $t \mapsto \Omega_t - \phi_t$ is continuous, hence

$$\forall t \in \mathbb{R} : \phi_t - \Omega_t = 0. \tag{96}$$

Step 4: Thanks to Eq. (89), we now have an explicit formula for Ω_t by means of $\Omega_t = \phi_t$. Next, we investigate its support.
To treat the commutator term in (88), we insert two identities:

$$\begin{aligned}
[\varphi_B(t), \varphi_A^\varepsilon(t_A)] = &\frac{1}{1+i\varepsilon\varphi_A(t_A)}(1+i\varepsilon\varphi_A(t_A))\varphi_B(t)\varphi_A(t_A)\frac{1}{1+i\varepsilon\varphi_A(t_A)} \\
&- \frac{1}{1+i\varepsilon\varphi_A(t_A)}\varphi_A(t_A)\varphi_B(t)(1+i\varepsilon\varphi_A(t_A))\frac{1}{1+i\varepsilon\varphi_A(t_A)} \\
= &\frac{1}{1+i\varepsilon\varphi_A(t_A)}\left[\varphi_B(t), \varphi_A(t_A)\right]\frac{1}{1+i\varepsilon\varphi_A(t_A)}.
\end{aligned} \tag{97}$$

The operator $\frac{1}{1+i\varepsilon\varphi_A(t_A)}$ does not increase the domain of functions since it is the resolvent of $\varphi_A(t_A)$ that can be written as a direct fiber integral, compare [23, thm. 3.4] and [34, thm. XIII.85]. Hence, Lemma 12 guarantees that $f_t(\mathbf{x}_1, ..., \mathbf{x}_N) = 0$ whenever $\|\mathbf{x}_j - \mathbf{x}_k\| > \delta + |t - t_A|$ for all $j \in A, k \in B$.

The spatial support is not altered by the $\mathcal{H}_f$ operators and their exponentials, so we have

$$\mathrm{supp}\left(e^{-i\mathcal{H}_f(\tau-s)}f_\tau\right) \subset \left\{(\mathbf{x}_1, ..., \mathbf{x}_N) \in \mathbb{R}^{3N} \middle| \exists j \in A, k \in B : \|\mathbf{x}_j - \mathbf{x}_k\| \le \delta + \tau - t_A\right\}. \tag{98}$$

Applying Lemma 7, this support can grow by at most $\sum_{k\in B} B_{t-\tau}(\mathbf{x}_j)$ when acted on by $e^{-i(\mathcal{H}_f + \mathcal{H}_B(s))(t-\tau)}$. So this implies

$$\mathrm{supp}\left(e^{-i(\mathcal{H}_f+\mathcal{H}_B(s))(t-\tau)}e^{-i\mathcal{H}_f(\tau-s)}f_\tau\right) \subset \left\{(\mathbf{x}_1, ..., \mathbf{x}_N) \in \mathbb{R}^{3N} \middle| \begin{array}{c} \exists j \in A, k \in B : \\ \|\mathbf{x}_j - \mathbf{x}_k\| \le \delta + t - t_A \end{array}\right\}. \tag{99}$$

Consider $\Omega_{t_B} = \phi_{t_B}$. By (99), the integrand in Eq. (89) vanishes whenever $\|\mathbf{x}_j - \mathbf{x}_k\| > \delta + t_B - t_A$. This is satisfied for $(\mathbf{x}_1, ..., \mathbf{x}_N)$ by assumption, which yields

$$\Omega_t(\mathbf{x}_1, ..., \mathbf{x}_N) = \left(\left[U_B(t,s), \varphi_A^\varepsilon(t_A)\right]\zeta\right)(\mathbf{x}_1, ..., \mathbf{x}_N) = 0 \tag{100}$$

for every positive ε, and thus with (85) the claim of the lemma. □

We are now ready to prove the existence Theorem 1. In addition to the claim in Thm. 1 we also prove the following extended claim that states the form of the solution.

Theorem 14 *For each $\psi^0 \in \mathscr{D}$, there exists a solution ψ of the multi-time system in the sense of Def. 1 on $\mathscr{S}_\delta$ with initial data $\psi(0, ..., 0) = \psi^0$ and with $\psi(t_1, ..., t_N) \in \mathscr{D}$.*
Let σ be a permutation on $\{1, ..., N\}$ such that $t_{\sigma(1)} \ge t_{\sigma(2)} \ge \cdots \ge t_{\sigma(N)}$, then one such solution is given by

$$\begin{aligned}
&\psi(t_1, ..., t_N) \\
&= U_{\{\sigma(1)\}}(t_{\sigma(1)}, t_{\sigma(2)}) \dots U_{\{\sigma(1),...,\sigma(N-1)\}}(t_{\sigma(N-1)}, t_{\sigma(N)}) U_{\{1,2,...,N\}}(t_{\sigma(N)}, 0)\psi^0.
\end{aligned} \tag{101}$$

For the proof, it will be helpful to abbreviate formulas like (101) using the $\bigcirc$-symbol for the ordered product of operators, $\bigcirc_{k=1}^{l} A_k := A_1 A_2 ... A_l$. In this notation, expression (101) reads

$$\left(\left(\bigcirc_{k=1}^{N-1} U_{\{\sigma(j)|j\leq k\}}(t_{\sigma(k)}, t_{\sigma(k+1)})\right) U_{\{1,...,N\}}(t_{\sigma(N)}, 0)\psi^0\right)(\mathbf{x}_1, ..., \mathbf{x}_N). \tag{102}$$

Compare also fig. 2 for a depiction of the successive application of the U_A operators in a simple case.

Proof: Let $\psi^0 \in \mathscr{D}$, and define $\psi : \mathbb{R}^N \to \mathscr{H}$ by Eq. (101). Property $U_A(t,t) = \mathbb{1}$ stated in Theorem 4 ensures $\psi(0, ..., 0) = \psi^0$, so the correct initial value is attained. $\psi^0 \in \mathscr{D}$ implies that for all $t_1, ..., t_N \in \mathbb{R}$, $\psi(t_1, ..., t_N) \in \mathscr{D}$ since $\mathscr{D}$ is preserved by the operators U_A by virtue of Corollary 10.

We now show the three points from Definition 1.

i) Since $\psi : \mathbb{R}^N \to \mathscr{D} \subset \mathscr{H}$, we may infer by Theorem 4 part 3 that ψ is differentiable.

ii) Let $j \in \{1, ..., N\}$. By Lemma 11 also $\mathcal{H}_j(t_j)\psi(t_1, ..., t_N) \in \mathscr{D}$, so both expressions are pointwise evaluable. The same is true for $\partial_{t_j}\psi(t_1, ..., t_N)$ since it amounts to a successive application of U_A operators and of $\mathcal{H}_j$, which all leave $\mathscr{D}$ invariant.

iii) We now have to check that ψ satisfies the respective equations (23) in S_δ. Given a set $A \subset \{1, ..., N\}$ and a time $t_A \in \mathbb{R}$, consider a configuration $(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathscr{S}_\delta$ where $t_j = t_A \ \forall j \in A$. We assume w.l.o.g. that the times are already ordered $t_1 \geq t_2 \geq \cdots \geq t_N$, so that the permutation in (101) is the identity. Let $a := \min(A)$ and $b := \max(A)$, then

$$\begin{aligned}\psi(t_1, ..., t_N) = &\left(\bigcirc_{k=1}^{a-2} U_{\{j|j\leq k\}}(t_k, t_{k+1})\right) U_{\{j|j\leq a-1\}}(t_{a-1}, t_A) U_{\{j|j\leq b\}}(t_A, t_{b+1}) \\ &\left(\bigcirc_{k=b+1}^{N-1} U_{\{j|j\leq k\}}(t_k, t_{k+1})\right) U_{\{1,...,N\}}(t_N, 0)\psi^0\end{aligned} \tag{103}$$

We take the derivative of (103) with respect to t_A and use that for $\zeta \in \mathscr{D}$,

$$i\frac{d}{dt}U_B(s,t)\zeta = -U_B(s,t)\mathcal{H}_B(t)\zeta, \quad \forall\ s, t \in \mathbb{R}, B \subset \{1, ..., N\}, \tag{104}$$

which follows directly from the properties of the time evolution operators. Abbreviating

$$\psi' := U_{\{j|j\leq b\}}(t_A, t_{b+1}) \left(\bigcirc_{k=b+1}^{N-1} U_{\{j|j\leq k\}}(t_k, t_{k+1})\right) U_{\{1,...,N\}}(t_{\sigma(N)}, 0)\psi^0, \tag{105}$$

we obtain

$$\begin{aligned}&i\frac{\partial}{\partial t_A}\psi(t_1, ..., t_N) \\ &= \left(\left(\bigcirc_{k=1}^{a-2} U_{\{j|j\leq k\}}(t_k, t_{k+1})\right) U_{\{j|j\leq a-1\}}(t_{a-1}, t_A) \ \left(-\mathcal{H}_{\{j|j\leq a-1\}}(t_A) + \mathcal{H}_{\{j|j\leq b\}}(t_A)\right)\psi'\right) \\ &= \mathcal{H}_A(t_A)\psi(t_1, ..., t_N) + \left(\left[\bigcirc_{k=1}^{a-1} U_{\{j|j\leq k\}}(t_k, t_{k+1}), \mathcal{H}_A(t_A)\right]\psi'\right).\end{aligned} \tag{106}$$

We rewrite the second term as

$$\begin{aligned}&\left[\bigcirc_{k=1}^{a-1} U_{\{j|j\leq k\}}(t_k, t_{k+1}), \mathcal{H}_A(t_A)\right]\psi' \\ &= \sum_{l=1}^{a-1}\left(\bigcirc_{k=1}^{l-1} U_{\{j|j\leq k\}}(t_k, t_{k+1})\right)\left[U_{\{j|j\leq l\}}(t_l, t_{l+1}), \mathcal{H}_A(t_A)\right]\left(\bigcirc_{k=l+1}^{a-1} U_{\{j|j\leq k\}}(t_k, t_{k+1})\right)\psi',\end{aligned} \tag{107}$$

where empty products such as $\bigcirc_{k=1}^{0}$ denote $\mathbb{1}$. Lemma 13 implies that for any $\zeta \in \mathscr{D}$ and $l < a$,

$$\operatorname{supp}\left(\left[U_{\{j|j\leq l\}}(t_l, t_{l+1}), \mathcal{H}_A(t_A)\right]\zeta\right) \subset \{(\mathbf{x}_1, ..., \mathbf{x}_N) | \exists k \in A, j \leq l : \|\mathbf{x}_j - \mathbf{x}_k\| \leq \delta + t_l - t_A\}. \tag{108}$$

The support properties of the evolution operators (Lemma 7) imply that if $\operatorname{supp}(\xi) \subset R$, then $\operatorname{supp}\left(\bigcirc_{k=1}^{l-1} U_{\{j|j\leq k\}}(t_k, t_{k+1})\xi\right)$ is a subset of

$$\left\{(\mathbf{y}_1, ..., \mathbf{y}_N) \in \mathbb{R}^{3N} \middle| \exists (\mathbf{x}_1, ...\mathbf{x}_N) \in R : \begin{array}{c} \mathbf{x}_j = \mathbf{y}_j \text{ if } j > l. \\ \|\mathbf{x}_j - \mathbf{y}_j\| \leq t_j - t_l \text{ if } j \leq l. \end{array} \right\} \tag{109}$$

Now we see that the support growth described by (109) is exactly such that the term $\left[\bigcirc_{k=1}^{a-1} U_{\{j|j\leq k\}}(t_k, t_{k+1}), \mathcal{H}_A(t_A)\right] \psi'(\mathbf{x}_1, ..., \mathbf{x}_N) = 0$, whenever $\|\mathbf{x}_j - \mathbf{x}_k\| > \delta + |t_j - t_k|$ holds for all $j \in A, k \notin A$. Thus (106) evaluated inside of $\mathscr{S}_\delta$ becomes

$$\left(i \frac{\partial}{\partial t_A} \psi(t_1, ..., t_N)\right) (\mathbf{x}_1, ..., \mathbf{x}_N) = \left(\mathcal{H}_A(t_A) \psi(t_1, ..., t_N)\right) (\mathbf{x}_1, ..., \mathbf{x}_N), \tag{110}$$

which proves that ψ indeed is a solution of the multi-time system (23). □

3.4 Uniqueness of solutions

Uniqueness of solutions can be proven by induction over the particle number, using the key features of our multi-time system that the Hamiltonians $\mathcal{H}_k$ are self-adjoint and that the propagation speed is bounded by the speed of light (see Lemma 7).

Proof of Theorem 2: Let ψ_1, ψ_2 be solutions to (23) in the sense of Def. 1 with $\psi_1(0, ..., 0) = \psi_2(0, ..., 0) = \psi^0$. Due to linearity, $\omega := \psi_1 - \psi_2$ is a solution to (23) in the sense of Def. 1 with initial value $\omega(0, ..., 0) = \psi^0 - \psi^0 = 0$. In particular, the point-wise evaluations of ω as in (22) are also well-defined. By induction over $L \in \{1, ..., N\}$, we prove the statement:
$\mathbf{A(L)}$: *At all points* $(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathscr{S}_\delta$ *with at most* L *different time coordinates, we have* $(\omega(t_1, ..., t_N))(\mathbf{x}_1, ..., \mathbf{x}_N) = 0$.
For the **base case** $\mathbf{A(1)}$, we consider configurations with all times equal, where ω satisfies

$$i\partial_t \omega(t, ..., t) = \mathcal{H}_{\{1,...,N\}}(t)\omega(t, ..., t). \tag{111}$$

By the uniqueness statement in Theorem 4, this implies

$$\omega(t, ..., t) = U_{\{1,...,N\}}(t, 0)\omega^0 = 0. \tag{112}$$

$\mathbf{A(L)} \implies \mathbf{A(L+1)}$: We assume that $A(L)$ holds, and let $(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) \in \mathscr{S}_\delta$ with exactly $L+1$ different time coordinates. This means there is a unique partition of $\{1, ..., N\}$ into disjoint sets $\Pi_1, ..., \Pi_{L+1}$ which groups together particles with the same time coordinate in an ascending way:

$$\begin{aligned} \Pi_1 &:= \left\{ j \in \{1, ..., N\} \middle| t_j = \min_{k\in\{1,...,N\}} t_k \right\} \\ \Pi_2 &:= \left\{ j \in \{1, ..., N\} \middle| t_j = \min_{k\in\{1,...,N\}\setminus\Pi_1} t_k \right\} \\ &\dots \\ \Pi_m &:= \left\{ j \in \{1, ..., N\} \middle| t_j = \min_{k\in\{1,...,N\}\setminus\cup_{i=1}^{m-1}\Pi_i} t_k \right\}. \end{aligned} \tag{113}$$

Denote the largest time by t_{L+1} and the second largest one by t_L. We define the backwards lightcone with respect to the particles in Π_{L+1} as follows,

$$B := \left\{ (y_1, ..., y_N) \in \mathbb{R}^{4N} \middle| \begin{array}{c} y_j = x_j \text{ if } j \notin \Pi_{L+1} \\ \forall j \in \Pi_{L+1} : y_j^0 = \tau \text{ with } t_L \leq \tau \leq t_{L+1}, \\ |\mathbf{y}_j - \mathbf{x}_j| \leq t_{L+1} - \tau \end{array} \right\}. \tag{114}$$

We show that $B \subset \mathscr{S}_\delta$. If $(y_1, ..., y_N) \in B$, consider $j \in \Pi_{L+1}$ and $k \notin \Pi_{L+1}$, then

$$\begin{aligned} |y_k^0 - y_j^0| + \delta &= \tau - t_k + \delta = (\tau - t_{L+1}) + (t_{L+1} - t_k + \delta) \\ &< -|\mathbf{y}_j - \mathbf{x}_j| + |\mathbf{x}_k - \mathbf{x}_j| \leq |\mathbf{x}_k - \mathbf{y}_j| = |\mathbf{y}_k - \mathbf{y}_j|. \end{aligned} \tag{115}$$

Thus, all points in B are still in our domain $\mathscr{S}_\delta$. In particular, we have

$$\left(i\partial_\tau \omega(y_1^0, ..., y_N^0)\right)(\mathbf{y}_1, ..., \mathbf{y}_N) = \left(\mathcal{H}_{\Pi_{L+1}}(\tau)\omega(y_1^0, ..., y_N^0)\right)(\mathbf{y}_1, ..., \mathbf{y}_N) \quad \forall (y_1, ..., y_N) \in B. \tag{116}$$

Since B contains the domain of dependence, i.e. the set that uniquely determines the value of ω at $(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N)$ according to Lemma 7, Theorem 4 tells us that

$$\omega(x_1, ..., x_N) = \left(U_{\Pi_{L+1}}(t_{L+1}, t_L)\omega^{t_L}\right)(\mathbf{x}_1, ..., \mathbf{x}_N), \tag{117}$$

where ω^{t_L} denotes the function ω evaluated at the time coordinates as in $(t_1, ..., t_N)$ but where t_{L+1} is replaced by t_L. This only has L different times and is thus given according to the induction hypothesis $A(L)$ as $\omega^{t_L} = 0$ in the whole domain of dependence. Consequently,

$$(\omega(t_1, ..., t_N))(\mathbf{x}_1, ..., \mathbf{x}_N) = 0, \tag{118}$$

which concludes the uniqueness proof. □

3.5 Interaction

We now demonstrate that our model is indeed interacting, providing a rigoros version of Eq. (9).

Proof of Theorem 3 Let $t \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^3$. The first step just uses that ψ^t solves the Dirac equation,

$$i\partial_t \left\langle \psi^t, \varphi(t,\mathbf{x})\psi^t \right\rangle = \left\langle -\mathcal{H}^t\psi^t, \varphi(t,\mathbf{x})\psi^t \right\rangle + \left\langle \psi^t, \varphi(t,\mathbf{x})\mathcal{H}^t\psi^t \right\rangle + \left\langle \psi^t, i\dot{\varphi}(t,\mathbf{x})\psi^t \right\rangle. \tag{119}$$

We already encountered $\dot{\varphi}$, the time-derivative of the operator φ, in the proof of Lemma 5. Since $\mathcal{H}^t$ and $\varphi(t,\mathbf{x})$ commute at equal times, only the third summand survives and the second derivative is

$$\begin{aligned} \partial_t^2 \left\langle \psi^t, \varphi(t,\mathbf{x})\psi^t \right\rangle &= -i\partial_t \left\langle \psi^t, i\dot{\varphi}(t,\mathbf{x})\psi^t \right\rangle \\ &= i\left\langle \mathcal{H}^t\psi^t, \dot{\varphi}(t,\mathbf{x})\psi^t \right\rangle - i\left\langle \psi^t, \dot{\varphi}(t,\mathbf{x})\mathcal{H}^t\psi^t \right\rangle + \left\langle \psi^t, \ddot{\varphi}(t,\mathbf{x})\psi^t \right\rangle \\ &= i\left\langle \psi^t, \left[\mathcal{H}^t, \dot{\varphi}(t,\mathbf{x})\right]\psi^t \right\rangle + \left\langle \psi^t, \triangle_{\mathbf{x}}\varphi(t,\mathbf{x})\psi^t \right\rangle. \end{aligned} \tag{120}$$

Hence,

$$\square \left\langle \psi^t, \varphi(t,\mathbf{x})\psi^t \right\rangle = i\left\langle \psi^t, \left[\mathcal{H}^t, \dot{\varphi}(t,\mathbf{x})\right]\psi^t \right\rangle = i\sum_{k=1}^{N} \left\langle \psi^t, \left[\varphi_k(t), \dot{\varphi}(t,\mathbf{x})\right]\psi^t \right\rangle. \tag{121}$$

So we need to compute, with the integration variable $x = (\mathbf{x}_1, ..., \mathbf{x}_N)$,

$$\begin{aligned} & i\left\langle \psi^t, \left[\varphi_k(t), \dot{\varphi}(t,\mathbf{v})\right]\psi^t \right\rangle \\ &= i\int d^{3N}x\ \psi^{t\dagger}(x) \int \frac{d^3\mathbf{k}}{2\omega(\mathbf{k})} \left(\hat{\rho}^\dagger(\mathbf{k})\hat{\rho}(\mathbf{k}) i\omega(\mathbf{k}) e^{-i\mathbf{k}(\mathbf{x}_k - \mathbf{v})} - c.c.\right)\psi^t(x) \\ &= -\frac{1}{2}\int d^{3N}x\ \psi^{t\dagger}(x) \int d^3\mathbf{k}\ \hat{\rho}^\dagger(\mathbf{k})\hat{\rho}(\mathbf{k}) \left(e^{-i\mathbf{k}(\mathbf{x}_k - \mathbf{v})} + e^{i\mathbf{k}(\mathbf{x}_k - \mathbf{v})}\right)\psi^t(x). \end{aligned} \tag{122}$$

Denoting the function $\mathbf{y} \mapsto \rho(\mathbf{y} + \mathbf{v} - \mathbf{x}_k)$ by ω, we have $\hat{\omega}(\mathbf{k}) = \hat{\rho}(\mathbf{k}) e^{i\mathbf{k}(\mathbf{x}_k - \mathbf{v})}$. Thus, the above formula can be rewritten with the help of the Plancherel theorem,

$$\begin{aligned}
&= -\frac{1}{2} \int d^{3N}x \ \psi^{t\dagger}(x) \left(\langle \hat{\rho}, \hat{\omega} \rangle_{L^2(\mathbb{R}^3)} + \langle \hat{\omega}, \hat{\rho} \rangle_{L^2(\mathbb{R}^3)} \right) \psi^t(x) \\
&= -\frac{1}{2} \int d^{3N}x \ \psi^{t\dagger}(x) \left(\langle \rho, \omega \rangle_{L^2(\mathbb{R}^3)} + \langle \omega, \rho \rangle_{L^2(\mathbb{R}^3)} \right) \psi^t(x) \\
&= - \int d^{3N}x \ \psi^{t\dagger}(x) \, \langle \rho, \omega \rangle_{L^2(\mathbb{R}^3)} \, \psi^t(x). \\
&= - \int d^{3N}x \ \psi^{t\dagger}(x) \int d^3\mathbf{y}_1 \rho(\mathbf{y}_1) \rho(\mathbf{v} - \mathbf{x_k} + \mathbf{y}_1) \psi^t(x)
\end{aligned} \tag{123}$$

We have used that ρ and ω are real-valued. The result contains the term we wrote as $\rho{*}{*}\delta(\mathbf{x}_k - \mathbf{v})$ in (29). Inserting this into (121) gives

$$\begin{aligned}
\Box \left\langle \psi^t, \varphi(t, \mathbf{x}) \psi^t \right\rangle &= - \sum_{k=1}^{N} \int d^{3N}x \ \psi^{t\dagger}(x) \int d^3\mathbf{y}_1 \rho(\mathbf{y}_1) \rho(\mathbf{x} - \mathbf{x_k} + \mathbf{y}_1) \psi^t(x) \\
&\equiv - \sum_{k=1}^{N} \left\langle \psi^t, \rho * * \delta(\hat{\mathbf{x}}_k - \mathbf{x}) \psi^t \right\rangle ,
\end{aligned} \tag{124}$$

which concludes the proof. □

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The Mass Shell of the Nelson Model without Cut-Offs

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Abstract

The massless Nelson model describes non-relativistic, spinless quantum particles interacting with a relativistic, massless, scalar quantum field. The interaction is linear in the field. We analyze its one particle sector. First, we construct the renormalized mass shell of the non-relativistic particle for an arbitrarily small infrared cut-off that turns off the interaction with the low energy modes of the field. No ultraviolet cut-off is imposed. Second, we implement a suitable Bogolyubov transformation of the Hamiltonian in the infrared regime. This transformation depends on the total momentum of the system and is non-unitary as the infrared cut-off is removed. For the transformed Hamiltonian we construct the mass shell in the limit where both the ultraviolet and the infrared cut-off are removed. Our approach is constructive and leads to explicit expansion formulae which are amenable to rigorously control the S-matrix elements.

Keywords: Multiscale Perturbation Theory, Nelson Model, Renormalization, Ultraviolet Divergence, Infrared Catastrophe.

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Contents

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1 Introduction and Definition of the Model

We study the mass shell of a non-relativistic spinless quantum particle interacting with the quantized field of relativistic, massless, scalar bosons, where the interaction is linear in the field. This model originated as an effective description of the interaction between non-relativistic nucleons and mesons. It is usually referred to as 'Nelson model' since E. Nelson (see [Nel64]) showed how to remove the ultraviolet cut-off that turns off the interaction with the high frequency modes of the field. The limiting Hamiltonian is defined starting from the quadratic form associated with the so-called Gross transformed Hamiltonian. The latter is obtained from the Nelson Hamiltonian through a unitary dressing transformation [Gro62] after subtracting a constant which is divergent in the ultraviolet (UV) limit. This means that only a ground state energy renormalization is necessary in order to define the local interaction. This model for only one nucleon is known as the one particle sector of the translation invariant Nelson model.

In recent years this model has been extensively studied with regard to quantum electrodynamics (QED). In fact, when the bosons are massless particles (i.e. 'scalar photons') the model can be seen as a scalar version of the effective theory (non-relativistic QED) that describes a non-relativistic electron interacting with the quantized radiation field. In the study of the translation invariant, massless Nelson model an ultraviolet cut-off of the order of the rest mass energy of the electron is usually imposed. Otherwise relativistic corrections to the electron dynamics and electron-positron pair creation should be taken into account. In spite of these simplifications, the massless Nelson model gives non-perturbative insights on the infrared properties of QED.

It is an interesting mathematical problem to clarify whether the results concerning the infrared region, which have been obtained in presence of an ultraviolet cut-off, can be extended to the 'renormalized' Nelson model (i.e. without an ultraviolet cut-off). As presented in [HHS05] these questions do not in general have a straightforward answer.

For the one particle sector of the renormalized Nelson model the study of the mass shell was carried out by Cannon few years after the appearance of Nelson's paper. In [Can71] it is proven that a perturbed mass shell exists for sufficiently small values of the coupling constant g and in the spectral region (E, P) for $|P| < 1$. Here, E and P are the spectral variables of the Hamiltonian and of the total momentum operator, respectively. In fact, starting from translation invariance, one considers the natural decomposition of the Hilbert space on the spectrum of the total momentum operator and studies the existence of the ground state of the fiber Hamiltonians H_P for $|P| < 1$. In his paper, Cannon relies on the spectral gap of the fiber Hamiltonians induced by a meson mass. The mass shell of the nucleon is then defined by analytic perturbation theory of the ground state eigenvector fiber by fiber for $|P| < 1$ and sufficiently small g. The interaction is in fact a small perturbation of type B – i.e. in the form sense – with respect to the free Hamiltonian. For this type of perturbation it is in principle possible to control the perturbed spectral projection and to give a meaning to the formal expansion of the ground state vector of the perturbed Hamiltonian. The price for this is a very cumbersome formula (see [Kat95]) making his result almost intractable for applications to scattering theory. As a matter of fact, no explicit expression for the perturbed mass shell is provided in [Can71].

Finally, for the massless Nelson model, the result concerning the existence of the mass shell was extended by Fröhlich to arbitrarily small infrared cut-off with no restriction on the coupling constant. The method used in [Frö73] is based on a lattice approximation of the boson momentum space which is eventually removed, a technique inspired by earlier works of Glimm and Jaffe. However, Fröhlich's expression for the fiber eigenvectors is only implicit. In recent years the P-dependence of the ground state energy in the massless Nelson model and in non-relativistic QED has been studied in presence of an ultraviolet regularization. [BCFS07] and [Che08] use the isospectral renormalization group whereas [AH10] relies on statistical mechanics methods.

We accomplish three main goals: (1) By using a multiscale technique for small values of the coupling constant and for a fixed infrared cut-off $\kappa > 1$ (in units where the electron mass m, the Planck's constant $\hbar$, and the speed of light c all equal one) we first derive the results by Cannon for the massless Nelson model. Rather than using regular perturbation theory for quadratic forms we employ a multiscale technique for operators inspired by [Piz03]. Our construction yields more explicit expressions for the 'renormalized' mass shell. In particular, they are amenable to rigorously control the S-matrix elements under the removal of the UV cut-off and to compare them with physicists' perturbation formulae.

(2) We then show how to construct the mass shell for the renormalized model when the interaction is extended to frequency ranges down to an arbitrarily small infrared cut-off. This result at a small but fixed value of the coupling constant g is beyond the reach of the method employed by Cannon [Can71] because the spectral gap shrinks to zero as the infrared cut-off is removed.

(3) The final part of our analysis concerns the properties of the mass shell in the infrared limit where it is well-known that no *proper* mass shell is present, a fact usually referred to as the *infrared catastrophe*. Following the strategy developed in [Piz03], we implement a suitable Bogolyubov transformation for the field variables corresponding to frequencies below the threshold $\kappa > 1$. In contrast to Gross' dressing this transformation depends on the P-fiber and is not unitary in the infrared limit. Fiber by fiber, we obtain a transformed Hamiltonian where the interaction is not linear in the field anymore both because of the Gross transformation in the UV region (frequencies larger than κ) and because of the infrared dressing transformation (frequencies smaller than κ). Each transformed Hamiltonian has a ground state in the infrared limit, the construction of which requires a delicate control of the interplay between high and low frequency modes. The control of the mass shell associated with these *unphysical* fiber Hamiltonians is crucial to analyze the infraparticle behavior of the renormalized electron in the massless Nelson model and to provide an asymptotic expansion for the scattering amplitudes in 'Compton scattering', free from both ultraviolet and infrared divergences.

Definition of the model. The Hilbert space of the model is

$$\mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}; dx) \otimes \mathcal{F}(h),$$

where $\mathcal{F}(h)$ is the Fock space of scalar bosons

$$\mathcal{F}(h) := \bigoplus_{j=0}^{\infty} \mathcal{F}^{(j)}, \qquad \mathcal{F}^{(0)} := \mathbb{C}, \qquad \mathcal{F}^{j\geq 1} := \bigodot_{l=1}^{j} h, \qquad h := L^2(\mathbb{R}^3, \mathbb{C}; dk),$$

where $\odot$ denotes the symmetric tensor product. Let $a(k), a^*(k)$ be the usual Fock space annihilation and creation operators satisfying the canonical commutation relations (CCR)

$$[a(k), a^*(l)] = \delta(k-l), \qquad [a(k), a(l)] = [a^*(k), a^*(l)] = 0.$$

The kinematics of the system is described by: (a) The position x and the momentum p of the non-relativistic particle that satisfy the Heisenberg commutation relations. (b) The scalar field Φ and its conjugate momentum where

$$\Phi(y) := \int dk\, \rho(k) \left(a(k)e^{iky} + a^*(k)e^{-iky}\right), \qquad \rho(k) := \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}}, \qquad \omega(k) := |k|.$$

The dynamics is generated by the Hamiltonian of the Nelson model,

$$H|_\tau^\Lambda := \frac{p^2}{2} + H^f + g\Phi|_\tau^\Lambda(x)$$

where

$$H^f := \int dk\, \omega(k) a^*(k) a(k)$$

is the free field Hamiltonian, and

$$g\Phi|_\tau^\Lambda(x) := g \int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\tau} dk\, \rho(k) \left(a(k)e^{ikx} + a^*(k)e^{-ikx}\right), \qquad \rho(k) := \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}}, \tag{1}$$

is the interaction term for $0 \leq \tau < \Lambda < \infty$; here $g \in \mathbb{R}$ is the coupling constant and for the domain of integration we use the notation $\mathcal{B}_\sigma := \{k \in \mathbb{R}^3 \,|\, |k| < \sigma\}$ for any $\sigma > 0$. Note that for $\Lambda = \infty$ the formal expression of the interaction $\Phi|_\kappa^\Lambda$ is not a well-defined operator on $\mathcal{H}$ because the form factor $\rho(k)$ is not square integrable.

We briefly recall some well-known facts about this model. For $0 \leq \tau < \Lambda < \infty$ the operator $H|_\tau^\Lambda$ is self-adjoint and its domain coincides with the one of $H_0 := \frac{p^2}{2} + H^f$ (see also Proposition 1.1 below). The total momentum operator of the system is

$$P := p + P^f := p + \int dk\, k\, a^*(k) a(k)$$

where P^f is the field momentum. Due to translational invariance of the system the Hamiltonian and the total momentum operator commute. Hence, the Hilbert space $\mathcal{H}$ can be decomposed on the joint spectrum of the three components of the total momentum operator, i.e.

$$\mathcal{H} = \int^{\oplus} dP\, \mathcal{H}_P$$

where $\mathcal{H}_P$ is a copy of the Fock space $\mathcal{F}$ carrying the (Fock) representation corresponding to annihilation and creation operators

$$b(k) := a(k)e^{ikx}, \qquad b^*(k) := a^*(k)e^{-ikx}.$$

We will use the same symbol $\mathcal{F}$ for all Fock spaces. The fiber Hamiltonian can be expressed as

$$H_P|_\tau^\Lambda := \frac{1}{2}\left(P - P^f\right)^2 + H^f + g\int_{\mathcal{B}_\Lambda\setminus\mathcal{B}_\tau} dk\,\rho(k)\,(b(k) + b^*(k))\,.$$

By construction, the fiber Hamiltonian maps its domain in $\mathcal{H}_P$ into $\mathcal{H}_P$. Finally, for later use we define

$$H_{P,0} := \frac{(P - P^f)^2}{2} + H^f, \qquad \Delta H_P|_\tau^\Lambda := H_P|_\tau^\Lambda - H_{P,0}. \tag{2}$$

The Gross transformation. We use a frequency

$$1 < \kappa < 2$$

to separate the ultraviolet and the infrared regimes. The renormalization of the Hamiltonian must cure the divergence which appears in the second order correction to the ground state energy as $\Lambda \to \infty$. This logarithmically divergent term

$$V_{\text{self}}|_\kappa^\Lambda := -\frac{g^2}{[2(2\pi)^3]}\int_{\mathcal{B}_\Lambda\setminus\mathcal{B}_\kappa} dk\,\frac{1}{|k|\left[\frac{|k|^2}{2} + |k|\right]} \tag{3}$$

can be separated from the rest of the Hamiltonian by a Bogolyubov transformation $e^{-T|_\kappa^\Lambda}$, acting on all frequencies above κ, whose skew-adjoint generator is given by

$$T|_\kappa^\Lambda := \int_{\mathcal{B}_\Lambda\setminus\mathcal{B}_\kappa} dk\,\beta(k)\,(b(k) - b^*(k))\,, \qquad \beta(k) := -g\frac{\rho(k)}{\frac{|k|^2}{2} + \omega(k)}. \tag{4}$$

Note that for any $1 < \kappa < \Lambda \leq \infty$, the operators $T|_\kappa^\Lambda$, $T^*|_\kappa^\Lambda$ are well-defined on $D(H_{P,0})$. For $1 < \kappa < \Lambda < \infty$ the Hamiltonian $H_P|_\kappa^\Lambda$ transforms as follows:

$$H'_P|_\kappa^\Lambda := e^{T|_\kappa^\Lambda} H_P|_\kappa^\Lambda e^{-T|_\kappa^\Lambda} - V_{\text{self}}|_\kappa^\Lambda \tag{5}$$

$$\begin{aligned} &= \frac{1}{2}\left(P - P^f\right)^2 + H^f + \frac{1}{2}[(B|_\kappa^\Lambda)^2 + (B^*|_\kappa^\Lambda)^2] + B^*|_\kappa^\Lambda \cdot B|_\kappa^\Lambda \\ &\quad - (P - P^f)\cdot B|_\kappa^\Lambda - B^*|_\kappa^\Lambda \cdot (P - P^f) \end{aligned} \tag{6}$$

where

$$B|_\kappa^\Lambda := \int_{\mathcal{B}_\Lambda\setminus\mathcal{B}_\kappa} dk\;k\beta(k)b(k). \tag{7}$$

It is important to note that the operator equality (6) holds on $D(H_{P,0})$ as proven in [Nel64, Lemma 3]. In the following sections we will study the renormalized Hamiltonian

$$H'_P|_\kappa^\Lambda + g\Phi|_\tau^\kappa \tag{8}$$

The proofs of [Nel64, Lemma 2 and 3] imply:

Proposition 1.1. *For $0 \leq \tau < \Lambda < \infty$, the operators $H_P|_\tau^\Lambda$ and $H'_P|_\kappa^\Lambda + g\Phi|_\tau^\kappa$ are self-adjoint and their domain coincide with the one of $H_{P,0}$.*

By [Nel64, Main Theorem] there exists an ultraviolet renormalized Hamiltonian:

Theorem 1.2. *For all $\tau \geq 0$, there is a unique self-adjoint operator $H_P|_\tau^\infty$ on $\mathcal{F}$ that generates the unitary group defined by*

$$e^{-itH_P|_\tau^\infty} := \text{s-lim}_{\Lambda\to\infty} e^{-it(H_P|_\tau^\Lambda - V_{\text{self}}|_\kappa^\Lambda)}, \quad t \in \mathbb{R}.$$

The domain of $H_P|_\tau^\infty$ is a dense subset of the domain of $H_{P,0}^{1/2}$, and $H_P|_\tau^\infty$ is bounded from below.

However, we will not make use of Theorem 1.2. In the case of $|P| < P_{max}$ defined in (9) and for sufficiently small $|g|$ this result will follow from our multiscale analysis.

2 Main Results

Since the particle is non-relativistic we restrict the total momentum to the ball

$$|P| \leq P_{\max} := \frac{1}{4}. \tag{9}$$

The ultraviolet and infrared scaling. We shall introduce a scaling that divides the interaction term into slices of boson momenta for which, step by step, we apply analytic perturbation theory. In the ultraviolet regime, this scaling is defined by the sequence

$$\sigma_n := \kappa\beta^n, \qquad 1 < \beta, \qquad n \in \mathbb{N},$$

while in the infrared regime we use

$$\tau_m := \kappa\gamma^m, \qquad 0 < \gamma < \frac{1}{2}, \qquad m \in \mathbb{N}.$$

With respect to these scalings we shall use the following notation for Hamiltonians and Fock spaces:

IR	UV	Hamiltonian	Fock space
κ	σ_n	$H'_P\|_0^n := H'_P\|_\kappa^{\sigma_n}$	$\mathcal{F}\|_0^n := \mathcal{F}(L^2(\mathcal{B}_{\sigma_n} \setminus \mathcal{B}_\kappa))$
τ_m	σ_n	$H'_P\|_m^n := H'_P\|_0^n + g\Phi\|_{\tau_m}^\kappa$	$\mathcal{F}\|_m^n := \mathcal{F}(L^2(\mathcal{B}_{\sigma_n} \setminus \mathcal{B}_{\tau_m}))$

The normalized vacuum vector in each of these Fock spaces is denoted by the same symbol Ω. We shall exclusively use the index n to denote the ultraviolet cut-off σ_n and the index m to denote the infrared cut-off τ_m, e.g.

$$\mathcal{F}|_{n-1}^n := \mathcal{F}(L^2(\mathcal{B}_{\sigma_n} \setminus \mathcal{B}_{\sigma_{n-1}})), \qquad \mathcal{F}|_m^{m-1} := \mathcal{F}(L^2(\mathcal{B}_{\tau_{m-1}} \setminus \mathcal{B}_{\tau_m})).$$

For a vector ψ in $\mathcal{F}|_0^{n-1}$ and an operator O on $\mathcal{F}|_0^{n-1}$ we shall use the same symbol to denote the vector $\psi \otimes \Omega$ in $\mathcal{F}|_0^n$ and the operator $O \otimes \mathbb{1}_{\mathcal{F}|_{n-1}^n}$ on $\mathcal{F}|_0^n$, respectively.

Moreover, the Fock space slices and the related interaction terms are given by

	Slice	Interaction	Fock space
UV	$[\sigma_{n-1}, \sigma_n)$	$\Delta H'_P\|^n_{n-1} := H'_P\|^n_0 - H'_P\|^{n-1}_0$	$\mathcal{F}\|^n_{n-1}$
IR	$(\tau_m, \tau_{m-1}]$	$g\Phi\|^{m-1}_m := g\Phi\|^{\tau_{m-1}}_{\tau_m}$	$\mathcal{F}\|^{m-1}_m$

Similarly we shall use $|^n_m$, $|^n_{n-1}$, $|^{m-1}_m$ instead of $|^{\sigma_n}_{\tau_m}$, $|^{\sigma_n}_{\sigma_{n-1}}$, $|^{\tau_{m-1}}_{\tau_m}$, respectively, as short-hand notation to denote the range of boson momenta associated with the interaction.

For a self-adjoint operator A which is bounded from below we define the spectral gap as

$$\mathrm{Gap}\,(A) := \inf\{\mathrm{Spec}\,(A) \setminus \{\inf \mathrm{Spec}\,(A)\}\} - \inf \mathrm{Spec}\,(A)\,.$$

Moreover, we denote

$$E_P|^n_m := \inf \mathrm{Spec}\,(H_P|^n_m \upharpoonright \mathcal{F}|^n_m)\,, \qquad E'_P|^n_m := \inf \mathrm{Spec}\,(H'_P|^n_m \upharpoonright \mathcal{F}|^n_m) = E_P|^n_m - V_{\mathrm{self}}|^n_0 \tag{10}$$

where $\mathrm{Spec}\,(A \upharpoonright X)$ denotes the spectrum of the linear operator A restricted to the subspace X. If $E'_P|^n_m$ is a non-degenerate eigenvalue of the Hamiltonian $H'_P|^n_m$ we shall denote a (possibly unnormalized) corresponding eigenvector by $\Psi'_P|^n_m$. In this situation we have

$$\mathrm{Gap}\,(H'_P|^n_m \upharpoonright \mathcal{F}|^n_m) = \inf_{\psi \perp \Psi'_P|^n_m} \langle H'_P|^n_m - E'_P|^n_m \rangle_\psi$$

where the infimum is taken over the vectors ψ in the domain of $H'_P|^n_m \upharpoonright \mathcal{F}|^n_m$, and we have used the notation

$$\langle A \rangle_\psi = \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle}$$

for any operator A and $\psi \in D(A)$.

The Mass Shell of $H'_P|^\infty_0$. The multiscale perturbation theory that we use here relies on the control of the spectral gap as more and more slices of the interaction Hamiltonian are added. In the construction of the mass shell eigenvectors one observes a major difference between removing the ultraviolet and the infrared cut-off. In the infrared limit the main problem is that the gap closes and the infimum of the spectrum is not an eigenvalue anymore (see [Piz03]). In the ultraviolet limit the main problem is that the whole spectrum moves towards $-\infty$. The latter is caused by the well-known logarithmic divergence in (3). In order to gain control on the gap it is necessary to extract this divergent term which, as it is also well-known, can be accomplished via the Gross transformation. At first, we shall therefore apply the multiscale perturbation theory to the Gross transformed Hamiltonians $H'_P|^n_0$, and then use unitarity to inherit all results for the back-transformed Nelson Hamiltonians

$$H_P|^n_0 := e^{-T|^n_0} H'_P|^n_0 e^{T|^n_0} + V_{\mathrm{self}}|^n_0, \quad n \in \mathbb{N}.$$

The iterative analytic perturbation theory, which was successfully applied for the infrared regime [Piz03], can be adapted to the ultraviolet regime using the following induction:

Suppose that, for a given and appropriately chosen real sequence $(\xi_n)_{n\in\mathbb{N}}$ bounded from below by a positive constant, we know that the following holds for the $(n-1)$-th step of the induction:

(i) $\Psi'_P|_0^{n-1}$ is the unique ground state of $H'_P|_0^{n-1}$ with energy $E'_P|_0^{n-1}$.

(ii) $\text{Gap}\left(H'_P|_0^{n-1} \upharpoonright \mathcal{F}|_0^{n-1}\right) \geq \xi_{n-1}$.

In order to show the induction step $(n-1) \Rightarrow n$, we first estimate the new spectral gap while adding the slice $\mathcal{F}|_{n-1}^n$ of boson Fock space without modifying the Hamiltonian. An a priori variational argument yields $\text{Gap}\left(H'_P|_0^{n-1} \upharpoonright \mathcal{F}|_0^n\right) \geq \xi_{n-1}$. With this at hand we apply analytic perturbation theory à la Kato to construct the ground state of $H'_P|_0^n \upharpoonright \mathcal{F}|_0^n$. More precisely, we show that the Neumann series of the resolvent

$$\frac{1}{H'_P|_0^n - z} = \frac{1}{H'_P|_0^{n-1} - z} \sum_{j=0}^{\infty} [-\Delta H'_P|_{n-1}^n \frac{1}{H'_P|_0^{n-1} - z}]^j \tag{11}$$

is well-defined for all z in the domain

$$\frac{1}{2}\xi_n \leq |E'_P|_0^{n-1} - z| \leq \xi_n < \xi_{n-1}.$$

Step by step we show the convergence of the Neumann series for a sufficiently small $|g|$ (and β sufficiently close to one) but uniformly in n. In the control of the resolvent in (11) a convenient definition of $(\xi_n)_{n\in\mathbb{N}}$ turns out to be crucial. Kato's perturbation theory ensures the existence of a projection $Q'_P|_0^n$ onto the unique ground state $\Psi'_P|_0^n$ with eigenvalue $E'_P|_0^n$. Since an a priori variational argument yields $E'_P|_0^n \leq E'_P|_0^{n-1}$, we conclude that $\text{Gap}\left(H'_P|_0^n \upharpoonright \mathcal{F}|_0^n\right) \geq \xi_n$.

This way we construct a convergent sequence of ground states corresponding to $H'_P|_0^n$, $n \in \mathbb{N}$,

$$\Psi'_P|_0^n := Q'_P|_0^n Q'_P|_0^{n-1} \cdots Q'_P|_0^1 \Omega$$

where Ω is the ground state of $H'_{P,0}$. The projections $Q'_P|_0^n$ will be given explicitly in (76). Finally, the unitarity of the Gross transformation implies that

$$\Psi_P|_0^n := e^{-T|_0^n} \Psi'_P|_0^n, \ n \in \mathbb{N},$$

is a sequence of ground states of $H_P|_0^n$ that also converges, say to a $\Psi_P|_0^\infty \in \mathcal{F}$. Furthermore, we prove the convergence of $H'_P|_0^n$ in the norm resolvent sense to a limiting Hamiltonian $H'_P|_0^\infty$, the unique ground state of which is $\Psi'_P|_0^\infty$. Precisely, we prove:

Theorem 2.1. *Let $|P| \leq P_{\max}$. There is a constant $g_{\max} > 0$ such such that for all $|g| < g_{\max}$ the following holds true:*

(i) The sequence of operators $(H_P|_0^n - V_{\text{self}}|_0^n)_{n\in\mathbb{N}}$ converges in the norm resolvent sense to a self-adjoint operator $H_P|_0^\infty$ acting on $\mathcal{F}$.

(ii) The limit $\Psi_P|_0^\infty := \lim_{n\to\infty} \Psi_P|_0^n$ exists in $\mathcal{F}$ and is non-zero.

(iii) $E_P|_0^\infty := \lim_{n\to\infty}(E_P|_0^n - V_{\text{self}}|_0^n)$ exists.

(iv) $E_P|_0^\infty$ is the non-degenerate ground state energy of the Hamiltonian $H_P|_0^\infty$ with corresponding ground state $\Psi_P|_0^\infty$. Moreover, the spectral gap of $H_P|_0^\infty \upharpoonright \mathcal{F}|_0^\infty$ is bounded from below by $\frac{1}{16}\kappa$.

The Mass Shell of $H'_P|_m^\infty$ for $m \in \mathbb{N}$. Starting from the ground states $\Psi'_P|_0^n$ of the Hamiltonian $H'_P|_0^n$, we continue to add interaction slices $g\Phi|_{\tau_m}^{\tau_{m-1}}$, $m \in \mathbb{N}$, now below the frequency κ and construct the family of ground states $\Psi'_P|_m^n$ of the Hamiltonians $H'_P|_m^n$ with eigenvalue $E'_P|_m^n$, i.e.

$$H'_P|_m^n \Psi'_P|_m^n = E'_P|_m^n \Psi'_P|_m^n.$$

For arbitrarily large but fixed $m \in \mathbb{N}$, we prove results analogous to Theorem 2.1: Norm resolvent convergence of $(H'_P|_m^n)_{n\in\mathbb{N}}$ is shown in Lemma 5.2. The existence of $\Psi'_P|_m^\infty$, $m \in \mathbb{N}$, is shown in Theorem 5.8. In particular, the spectral gap of $H'_P|_m^n$ is bounded from below by a constant times τ_m uniformly for all $n \in \mathbb{N} \cup \{\infty\}$. This is proven in Lemma 5.5.

The Mass Shell of $H_P^{W'}|_\infty^\infty$. As it is well-known (see [Frö73, Piz03]), for every $n \in \mathbb{N} \cup \{\infty\}$ the ground state $\frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|}$ weakly converge to zero as $m \to \infty$. This is linked to the infamous infrared catastrophe problem in QED. In fact, in the infrared limit the interaction turns out to be *marginal* according to renormalization group terminology. On the other hand it was proven in [Frö73] that

$$b(k)\Psi'_P|_m^n = g\,\rho(k)\frac{1}{E'_P|_m^n - |k| - H'_{P-k}|_m^n}\Psi'_P|_m^n \tag{12}$$

which implies that

$$b(k)\Psi'_P|_m^n \approx \alpha_m(\nabla E'_P|_m^n, k)\Psi'_P|_m^n, \qquad \alpha_m(Q,k) := -g\,\frac{\rho(k)}{\omega(k)}\frac{\mathbb{1}_{\mathcal{B}_\kappa\setminus\mathcal{B}_{\tau_m}}(k)}{1-\widehat{k}\cdot Q} \tag{13}$$

up to higher order terms as $k \to 0$. This motivates a strategy to analyze the infrared limit by using the Bogolyubov transformation $W_m(\nabla E'_P|_m^n)$ defined as follows: for $Q \in \mathbb{R}^3$, $|Q| < 1$,

$$W_m(Q)\; b^\#(k)\; W_m(Q)^* := b^\#(k) + \alpha_m(Q,k) \quad b^\#(k) = b(k), b^*(k). \tag{14}$$

Instead of studying $H'_P|_m^n$ directly one considers the transformed Hamiltonian

$$H_P^{W'}|_m^n := W_m(\nabla E'_P|_m^n)\; H'_P|_m^n\; W_m(\nabla E'_P|_m^n)^*. \tag{15}$$

Note that the transformation acts non-trivially only on boson momenta below κ. For any finite m, the operator $W_m(Q)$ is unitary but this property does not hold anymore in the limit $m \to \infty$. Furthermore, for $Q \neq Q'$ the function $\alpha_m(Q,k) - \alpha_m(Q',k)$ is not square integrable as $m \to \infty$.

Most importantly, the interaction term

$$H_P^{W'}|_m^n - H_{P,0} \tag{16}$$

of the transformed Hamiltonian is now *superficially marginal* in the infrared limit, in contrast to the interaction $H'_P|_m^n - H_{P,0}$. At a fixed ultraviolet cut-off and at a small coupling constant g, it has been proven in [Piz03] that the sequence of ground states $(\phi_P|_m^n)_{m\in\mathbb{N}}$, i.e.

$$H_P^{W'}|_m^n \phi_P|_m^n = E'_P|_m^n \phi_P|_m^n, \tag{17}$$

converges in the limit $m \to \infty$ while the spectral gap closes. Consequently, infrared asymptotic freedom holds. This result requires a sophisticated proof by induction. In the present paper we prove the same result while simultaneously removing the ultraviolet cut-off. Before sketching the main technical difficulties in dealing with the construction of the states $\phi_P|_\infty^\infty$ let us briefly explain their physical relevance.

With the states $\phi_P|_m^n$ and the Bogolyubov transformation $W_m(\nabla E'_P|_m^n)$ at hand it is possible to control the properties of the physical mass shell given by the states $\Psi'_P|_m^n$ in the infrared limit, i.e. $m \to \infty$, namely the dependence on the total momentum P. This spectral information represents the key ingredient to construct the scattering states for the so-called *infraparticles* (see [Piz03] and [CFP09]). The QED analogue of the transformation of the field variables in (14) is related to the Liénard-Wiechert fields carried by the charged particle and to the infrared radiation emitted in Compton scattering; see [CFP09] for precise mathematical statements.

More technically, while simultaneously removing the infrared and the ultraviolet cut-off in $\phi_P|_m^n$ a major difficulty arises in the induction mentioned above. In fact, the proof of the limit of $\phi_P|_m^n$ as $m \to \infty$ relies on a suitable rearrangement of the terms in the Hamiltonian $H_P^{W'}|_m^n$ given by

$$H_P^{W'}|_m^n = \frac{1}{2}\Gamma_P|_m^{n\,2} + H^f - \nabla E'_P|_m^n \cdot P^f + C_{P,m}^{(n)} + R_P|_m^n\,, \tag{18}$$

see (85) in Section 6, where the vector operator $\Gamma_P|_m^n$ has the crucial property

$$\langle \phi_P|_m^n, \Gamma_P|_m^n \phi_P|_m^n \rangle = 0. \tag{19}$$

However, the operator $\Gamma_P|_m^n$ is ill-defined in the limit $n \to \infty$. This suggests the following strategy for the simultaneous removal of the cut-offs, for sufficiently small g but uniform in n and m:

(i) First show that $(\phi_P|_m^n)_{m\in\mathbb{N}}$ is a Cauchy sequence uniformly in n;

(ii) then provide bounds of the form

$$\|\phi_P|_m^n - \phi_P|_m^{n-1}\| \le f_1(n,m), \tag{20}$$

and

$$|\nabla E'_P|_m^n - \nabla E'_P|_m^{n-1}| \le f_2(n,m), \tag{21}$$

where $f_1(n,m)$ and $f_2(n,m)$ are such that for the scaling $n(m) := \alpha m$ with α sufficiently large both $(\phi_P|_m^{n(m)})_{n\in\mathbb{N}}$ and $(\nabla E'_P|_m^{n(m)})_{n\in\mathbb{N}}$ are Cauchy sequences.

This program will be carried out in Sections 6 and 7. It will yield the second main result:

Theorem 2.2. *Let $|P| \le P_{\max}$. For $|g|$ sufficiently small the following holds true:*

(i) There exists an $\alpha_{\min} > 0$ such that for any integer $\alpha' > \alpha_{\min}$ and $n(m) = \alpha' m$, the limit

$$\phi_P|_\infty^\infty := \lim_{m\to\infty} \phi_P|_m^{n(m)}$$

exists in $\mathcal{F}$ and is non-zero.

(ii) $E'_{P,\infty} := \lim_{m\to\infty} E'_P|_m^\infty$ exists and is the ground state energy corresponding to the eigenvector $\phi_P|_\infty^\infty$ of the self-adjoint operator

$$H_P^{W'}|_\infty^\infty := \lim_{m\to\infty} H_P^{W'}|_m^{n(m)},$$

where the limit is understood in the norm resolvent sense.

At this point, we emphasize that at least within the scope of the presented multiscale technique, the given scaling to remove both UV and IR cut-offs simultaneously is natural. The method indeed relies on the control of the spectral gap, and as the gap closes in the IR limit, the UV limit must be taken at a comparatively fast enough rate.

For the notation throughout this paper, the reader is advised to consult the list below.

Notation.

1. By convention $0 \notin \mathbb{N}$.
2. The symbol C denotes any universal constant. Any appearing C is independent of the indices m and n and of all parameters in the paper, i.e. g, β, γ and ζ, at least in prescribed neighborhoods.
3. The bars $|\cdot|$, $\|\cdot\|$ denote the euclidean and the Fock space norm, respectively. The brackets $\langle\cdot,\cdot\rangle$ denote the scalar product of vectors in $\mathcal{F}$. Given a subspace $\mathcal{K} \subseteq \mathcal{F}$ and an operator A on $\mathcal{F}$ we use the notation
$$\|A\|_{\mathcal{K}} = \|A \upharpoonright \mathcal{K}\|.$$
4. For a vector operator $A = (A^{(1)}, A^{(2)}, A^{(3)})$ with components $A^{(i)} : D(A^{(i)}) \to \mathcal{F}$, $1 \le i \le 3$, we use the notation
$$\|A\psi\|^2 = \sum_{i=1}^{3} \|A^{(i)}\psi\|^2.$$

3 Tools

We recall some standard operator inequalities which are frequently used. For every square integrable function f the estimates

$$\begin{aligned} \left\| \int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\tau} dk\ f(k) b(k)\psi \right\| &\le \left(\int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\tau} dk \left| \frac{f(k)}{\sqrt{|k|}} \right|^2 \right)^{1/2} \|(H^f|_\tau^\Lambda)^{1/2}\psi\|, \\ \left\| \int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\tau} dk\ f(k) b^*(k)\psi \right\| &\le \left(\int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\tau} dk \left| \frac{f(k)}{\sqrt{|k|}} \right|^2 \right)^{1/2} \|(H^f|_\tau^\Lambda)^{1/2}\psi\| \\ &\quad + \left(\int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\tau} dk\, |f(k)|^2 \right)^{1/2} \|\psi\| \end{aligned} \tag{22}$$

hold true for all $0 \le \tau < \Lambda \le \infty$ and ψ in the domain of $H_{P,0}^{1/2}$ whenever the integrals on the right-hand side of (22) are well defined.

The following two results are crucial ingredients in the proofs presented in the next sections. The first one, Theorem 3.1, is a classical result by L. Gross that turns out to be the main non-perturbative ingredient for the gap estimates that we obtain by iterative analytic perturbation theory; see Sections 4 and 5.

Theorem 3.1. *For* $0 \leq \tau < \Lambda < \infty$ *and all* $P \in \mathbb{R}^3$ *the ground state energies* $E_P|_\tau^\Lambda := \inf \mathrm{Spec}\left(H_P|_\tau^\Lambda\right)$ *fulfill* $E_0|_\tau^\Lambda \leq E_P|_\tau^\Lambda$.

Proof. See [Gro72, Theorem 8]. □

The second one, Lemma 3.2, plays a role in Sections 5, 6, 7 where we consider the interaction both in the ultraviolet and in the infrared regime. It is a crucial ingredient to prove statements (i), (ii) in Corollary 5.4 . We stress that the multiscale technique which we apply in Section 4 to remove the ultraviolet cut-off at $m = 0$ does not refer to Corollary 5.4 (i),(ii), and only relies on Theorem 3.1 and on a weaker estimate given in (48) that follows from (22).

Lemma 3.2. *There exist finite constants* $c_a, c_b > 0$ *such that*

$$\langle \psi, H_{P,0}\psi\rangle \leq \frac{1}{1-|g|c_a}\Big[\langle \psi, H'_P|_m^n \psi\rangle + |g|c_b \langle \psi, \psi\rangle\Big] \tag{23}$$

for $|g| \leq 1, \frac{1}{c_a}$ *and* $\psi \in D(H_{P,0}^{1/2})$ *with* $m, n \in \mathbb{N}$.

Proof. See Appendix A. □

4 Ground States of the Gross Transformed Hamiltonians $H'_P|_0^\infty$

This section provides the proof of Theorem 2.1 in Section 2. We start by introducing a sequence of gap bounds.

Definition 4.1. *We define the sequence of gap bounds*

$$\xi_n := \frac{1}{8}\kappa\left(1 - \sum_{j=1}^{n} \Delta\xi_j\right), \qquad \Delta\xi_n := \frac{(\beta-1)^2}{2\beta}\frac{n}{\beta^n} \tag{24}$$

for $n \in \mathbb{N}$ *with the scaling parameter* $\beta > 1$. *Furthermore, we impose the constraint*

$$|g| \leq (\beta - 1), \qquad 1 < \beta < 2. \tag{25}$$

The definition of the sequence of gap bounds $(\xi_n)_{n\in\mathbb{N}}$ in (24) will be motivated in Lemma 4.5. Note that $\sum_{j=1}^\infty \Delta\xi_j = \frac{1}{2}$ implies

$$\frac{1}{16}\kappa \leq \xi_n \leq \frac{1}{8}\kappa. \tag{26}$$

Remark 4.2. *In this section the constraints* $|P| < P_{\max}$ *and* $1 < \kappa < 2$ *are implicitly assumed.*

Lemma 4.3. *For an integer* $n > 1$ *assume:*

(i) $E'_P|_0^{n-1}$ *is the non-degenerate eigenvalue of* $H'_P|_0^{n-1} \restriction \mathcal{F}|_0^{n-1}$ *with eigenvector* $\Psi'_P|_0^{n-1}$.

(ii) $\mathrm{Gap}\left(H'_P|_0^{n-1} \restriction \mathcal{F}|_0^{n-1}\right) \geq \xi_{n-1}$.

(iii) $E'_P|_0^{n-1}$ *is differentiable in* P *and* $|\nabla E'_P|_0^{n-1}| \leq C_{\nabla E} \equiv \frac{3}{4}$.

This implies that $E'_P|_0^{n-1}$ *is also the non-degenerate ground state energy of* $H'_P|_0^{n-1} \restriction \mathcal{F}|_0^n$ *with eigenvector* $\Psi'_P|_0^{n-1} \otimes \Omega$*. Furthermore,*

$$\mathrm{Gap}\left(H'_P|_0^{n-1} \restriction \mathcal{F}|_0^n\right) \geq \inf_{\mathcal{F}|_0^n \ni \psi \perp \Psi'_P|_0^{n-1} \otimes \Omega} \left\langle H'_P|_0^{n-1} - \theta H^f|_{n-1}^n - E'_P|_0^{n-1} \right\rangle_\psi \geq \xi_{n-1} \tag{27}$$

where $0 < \theta < \frac{1}{8}$ *and the infimum is taken over* $\psi \in D(H_{P,0})$.

Proof. Using (i), a direct computation yields

$$H'_P|_0^{n-1}(\Psi'_P|_0^{n-1} \otimes \Omega) = E'_P|_0^{n-1}(\Psi'_P|_0^{n-1} \otimes \Omega)$$

as the interaction is cut off at σ_{n-1}. Hence, $E'_P|_0^{n-1}$ is an eigenvalue of $H'_P|_0^{n-1} \restriction \mathcal{F}|_0^n$ with eigenvector $\Psi'_P|_0^{n-1} \otimes \Omega$. Let us consider

$$\inf_{\mathcal{F}|_0^n \ni \psi \perp \Psi'_P|_0^{n-1} \otimes \Omega} \left\langle H'_P|_0^{n-1} - E'_P|_0^{n-1} \right\rangle_\psi . \tag{28}$$

As the Gross transformation is unitary and does not affect $\mathcal{F}|_{n-1}^n$, and since $H^f|_{n-1}^n$ is positive, we have

$$(28) \geq \inf_{\mathcal{F}|_0^n \ni \psi \perp \Psi_P|_0^{n-1} \otimes \Omega} \left\langle H_P|_0^{n-1} - \theta H^f|_{n-1}^n - E_P|_0^{n-1} \right\rangle_\psi . \tag{29}$$

We subtract the term $\theta H^f|_{n-1}^n$ for a technical reason which will become clear in Lemma 4.5.

Now, the right-hand side of (29) is bounded from below by

$$\min\left\{ \mathrm{Gap}\left(H'_P|_0^{n-1} \restriction \mathcal{F}|_0^{n-1}\right), \inf_{\psi = \varphi \otimes \eta} \left\langle H_P|_0^{n-1} - \theta H^f|_{n-1}^n - E_P|_0^{n-1} \right\rangle_\psi \right\},$$

where $\varphi \in \mathcal{F}|_0^{n-1}$, $\eta \in \mathcal{F}|_{n-1}^n$, $\varphi \otimes \eta$ belongs to $D(H_{P,0})$ and η is a vector with a definite, strictly positive number of bosons. For $m \geq 1$ bosons in the vector η we estimate

$$\begin{aligned}
&\inf_{\psi = \varphi \otimes \eta} \left\langle H_P|_0^{n-1} - \theta H^f|_{n-1}^n - E_P|_0^{n-1} \right\rangle_\psi \\
&\geq \inf_{\varphi, k_j \in [\sigma_{n-1}, \sigma_n)} \left\langle \frac{1}{2}\left(P - P^f - \sum_{j=1}^m k_j\right)^2 + H^f + g\Phi|_0^{n-1} + (1-\theta)\sum_{j=1}^m |k_j| - E_P|_0^{n-1} \right\rangle_\varphi \\
&\geq \inf_{k_j \in [\sigma_{n-1}, \sigma_n)} \left[(1-\theta)\sum_{j=1}^m |k_j| + E_{P - \sum_{j=1}^m k_j}|_0^{n-1} - E_P|_0^{n-1} \right] && (30) \\
&\geq (1 - \theta - C_{\nabla E})\sigma_{n-1} \geq \frac{1}{8}\kappa && (31)
\end{aligned}$$

where the steps (30) and (31) follow from:

1. $\sigma_{n-1} \geq \kappa$, $0 < \theta < \frac{1}{8}$ and $C_{\nabla E} = \frac{3}{4}$.
2. The estimate

$$E_{P - \sum_{j=1}^m k_j}|_0^{n-1} - E_P|_0^{n-1} = E_{P - \sum_{j=1}^m k_j}|_0^{n-1} - E_0|_0^{n-1} + E_0|_0^{n-1} - E_P|_0^{n-1} \geq E_0|_0^{n-1} - E_P|_0^{n-1}$$

which holds by Theorem 3.1.

3. The estimate
$$E'_0|_0^{n-1} - E_P|_0^{n-1} \geq - \sup_{|Q|\leq P_{\max}} |\nabla E'_Q|_0^n| \geq -C_{\nabla E}$$
since $E'_P|_0^{n-1}$ is differentiable in P and $|P| < 1$.

First, this implies that (28) is bounded from below by $\min\left\{\xi_{n-1}, \frac{\kappa}{8}\right\} = \xi_{n-1}$; see (26). Second, it turns out that $\Psi'_P|_0^{n-1}$ is the non-degenerate ground state of $H'_P|_0^{n-1} \restriction \mathcal{F}|_0^n$ with

$$\mathrm{Gap}\left(H'_P|_0^{n-1} \restriction \mathcal{F}|_0^n\right) \geq \xi_{n-1}.$$

□

Remark 4.4. *Under the assumptions of Lemma 4.3 it follows that for* $j, n \in \mathbb{N}$

$$E'_P|_0^n = \inf \mathrm{Spec}\,(H'_P|_0^n \restriction \mathcal{F}|_0^n) = \inf \mathrm{Spec}\left(H'_P|_0^n \restriction \mathcal{F}_{n+j}\right).$$

Lemma 4.5. *Let* $n \geq 1$*. For* $n = 1$*, set* $H'_P|_0^{n-1} := H'_{P,0}$*,* $E'_P|_0^{n-1} := P^2/2$*, and* $\xi_{n-1} := \kappa/2$*. Assume that for some universal constant* $C_{E'}$ *the bound* $|E'_P|_0^{n-1}| < C_{E'}$ *holds true. Then there exist* $\beta_{\max} > 1$ *and* $g_{\max} > 0$ *such that, for all* $1 < \beta \leq \beta_{\max}$ *and* $|g| \leq g_{\max}$*, the assumptions (i), (ii) in Lemma 4.3 imply that*

$$\frac{1}{H'_P|_0^n - z} \restriction \mathcal{F}|_0^n, \qquad \frac{\xi_n}{2} \leq |E'_P|_0^{n-1} - z| \leq \xi_n, \tag{32}$$

is well-defined.

Proof. Let z be in the domain given in (32). In order to control the expansion of the resolvent $(H'_P|_0^n - z)^{-1}$, i.e.

$$\frac{1}{H'_P|_0^{n-1} - z} \sum_{j=0}^{\infty} \left[-\Delta H'_P|_{n-1}^n \frac{1}{H'_P|_0^{n-1} - z} \right]^j \restriction \mathcal{F}|_n^0,$$

it is sufficient to prove that

$$\left\| \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \Delta H'_P|_{n-1}^n \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} < 1. \tag{33}$$

As we shall show now, this can be achieved by a convenient choice of β and g (uniformly in n) using the gap bounds $(\xi_n)_{n\in\mathbb{N}}$ from Definition 4.1. We can express the interaction term by

$$\begin{aligned} \Delta H'_P|_{n-1}^n = & \frac{1}{2}\left((B|_{n-1}^n)^2 + (B^*|_{n-1}^n)^2 \right) + B|_0^{n-1} \cdot B|_{n-1}^n + B^*|_{n-1}^n \cdot B^*|_0^{n-1} \\ & - (P - P^f) \cdot B|_{n-1}^n - B^*|_{n-1}^n \cdot (P - P^f) \\ & + B^*|_{n-1}^n \cdot B|_{n-1}^n + B^*|_0^{n-1} \cdot B|_{n-1}^n + B^*|_{n-1}^n \cdot B|_0^{n-1}. \end{aligned} \tag{34}$$

Hence, the left-hand side of (33) is bounded by

$$\left\| B|_{n-1}^{n} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \times \tag{35}$$

$$\times \left[\left\| B^*|_{n-1}^{n} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} + \left\| B|_{n-1}^{n} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \right. \tag{36}$$

$$+ 2 \left\| B^*|_0^{n-1} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} + 2 \left\| B|_0^{n-1} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} + \tag{37}$$

$$\left. + 2 \left\| (P - P^f) \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \right]. \tag{38}$$

Notice that the standard inequalities in (22) yield

$$\begin{aligned} \|B|_m^n \psi\| &\le |g|\, C \left(\frac{1}{\sigma_m} - \frac{1}{\sigma_n} \right)^{1/2} \|(H^f|_m^n)^{1/2} \psi\|, \\ \|B^*|_m^n \psi\| &\le |g|\, C \left(\left(\frac{1}{\sigma_m} - \frac{1}{\sigma_n} \right)^{1/2} \|(H^f|_m^n)^{1/2} \psi\| + (\ln \sigma_n - \ln \sigma_m)^{1/2} \|\psi\| \right) \end{aligned} \tag{39}$$

for all ψ in the domain of $H_{P,0}^{1/2}$. Then expression (35)-(38) can be controlled as follows:

1. We estimate

$$\left\| B|_{n-1}^{n} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \le |g| C \left(\frac{\beta - 1}{\sigma_n} \right)^{1/2} \left\| (H^f|_{n-1}^{n})^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}. \tag{40}$$

Furthermore, since $H^f|_{n-1}^n$ and $H'_P|_0^{n-1}$ commute, we have that

$$\begin{aligned} &\left\| (H^f|_{n-1}^{n})^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \\ &\le \theta^{-1/2} \left\| \left(\frac{\theta H^f|_{n-1}^n}{H'_P|_0^{n-1} - \theta H^f|_{n-1}^n - E'_P|_0^{n-1} + \theta H^f|_{n-1}^n + E'_P|_0^{n-1} - z)} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \\ &\le \theta^{-1/2} \left\| \left(\frac{\theta H^f|_{n-1}^n}{\xi_{n-1} - \xi_n + \theta H^f|_{n-1}^n)} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \le \theta^{-1/2} \end{aligned} \tag{41}$$

for, e.g. $\theta = \frac{1}{16}$. This is true because of Lemma 4.3, the constraints on z given in (32), and the bound $\Delta\xi_n = \xi_{n-1} - \xi_n > 0$ (see Definition 4.1).

2. Next we consider the bounds

$$\left\| B|_0^{n-1} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \le |g| C \left\| (H^f|_0^{n-1})^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}, \tag{42}$$

and

$$\left\| B^*|_0^{n-1} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \leq |g| C \Bigg(\left\| (H^f|_0^{n-1})^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} + \left(\ln \beta^{n-1} \right)^{1/2} \left\| \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \Bigg). \tag{43}$$

Terms including $H^f|_0^{n-1}$ or $(P - P^f)$ can be estimated as follows:

$$\left\| (H^f|_0^{n-1})^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \leq \left\| H_{P,0}^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}, \tag{44}$$

$$\left\| (P - P^f) \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n} \leq \sqrt{2} \left\| H_{P,0}^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}. \tag{45}$$

In order to estimate the right-hand side in (44) and (45), we observe that the standard inequalities (39) readily imply that there exists a n-indepedent finite constant c_{uv} such that, for $|g| \leq 1$ and $|g| < \frac{1}{c_{uv}}$, $\psi \in D(H_{P,0}^{1/2})$ and $n \in \mathbb{N}$, it holds

$$\langle \psi, H_{P,0} \psi \rangle \leq \frac{1}{1 - |g| c_{uv}} \Big[\langle \psi, H'_P|_0^n \psi \rangle + g^2 c_{uv}^2 \ln \sigma_n \langle \psi, \psi \rangle \Big]. \tag{46}$$

Consequently, for $|g|$ sufficiently small, we can estimate

$$\left\| H_{P,0}^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}^2 \leq C \sup_{\|\psi\|=1} \left\langle \psi, \left[1 + (|z| + |g| \ln \sigma_n) \left| \frac{1}{H'_P|_0^{n-1} - z} \right| \right] \psi \right\rangle \tag{47}$$

where $\psi \in \mathcal{F}|_0^n$. Moreover, the right-hand side of

$$|z| \leq |E'_P|_0^{n-1} - z| + |E'_P|_0^{n-1}|$$

is uniformly bounded because, first, $|E'_P|_0^{n-1} - z| \leq \xi_{n-1} \leq \frac{1}{2}\kappa$, and, second, $|E'_P|_0^{n-1}| \leq C_{E'}$ by assumption. Hence, we get

$$\left\| H_{P,0}^{1/2} \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}^2 \leq C \left(1 + (1 + |g| \ln \sigma_n) \left\| \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}^2 \right). \tag{48}$$

Finally, the remaining norm in (48) can be controlled by

$$\left\| \left(\frac{1}{H'_P|_0^{n-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|_0^n}^2 \leq \max \left\{ \frac{1}{|E'_P|_0^{n-1} - z|}, \frac{1}{\mathrm{Gap}\left(H'_P|_0^{n-1} \upharpoonright \mathcal{F}|_0^n \right) - |E'_P|_0^{n-1} - z|} \right\} \leq \frac{C}{\Delta \xi_n} \tag{49}$$

which is due to Lemma 4.3 and the domain of z given in (32).

We recall that by Definition 4.1 the sequence $(\Delta\xi_n)_{n\in\mathbb{N}}$ tends to zero, which is a necessary ingredient in the induction scheme in the proof of Theorem 2.1. Hence, the terms proportional to $(\Delta\xi_n)^{-1/2}$ must be treated cautiously. It turns out that the sum of the terms in (35)-(38) is bounded by

$$O\left(|g|\left(\frac{(\beta-1)}{\sigma_n\Delta\xi_n}\right)^{1/2}\right)+O\left(|g|\left(\frac{(\beta-1)\ln\beta^{n-1}}{\sigma_n\Delta\xi_n}\right)^{1/2}\right)\le|g|^{1/2}C\left(\frac{(\beta-1)^2n}{\beta^n\Delta\xi_n}\right)^{1/2} \tag{50}$$

for $|g|\le(\beta-1)$; see (25). This dictates the choice $\Delta\xi_n := \frac{(\beta-1)^2}{2\beta}\frac{n}{\beta^n}$ made in Definition 4.1. Hence, for all $n\in\mathbb{N}$ we get

$$\left\|\left(\frac{1}{H'_P|_0^{n-1}-z}\right)^{1/2}\Delta H'_P|_{n-1}^n\left(\frac{1}{H'_P|_0^{n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}|_0^n}\le|g|^{1/2}C\left(\frac{(\beta-1)^2n}{\beta^n\,\Delta\xi_n}\right)^{1/2}\le|g|^{1/2}C. \tag{51}$$

Therefore, (33) holds for $|g|$ sufficiently small which proves the claim. ◻

Definition 4.6. *For $n\in\mathbb{N}$ we define the contour*

$$\Gamma_n := \left\{z\in\mathbb{C}\;\middle|\;|E'_P|_0^{n-1}-z|=\frac{1}{2}\xi_n\right\}.$$

The bound in (50) was delicate because the outer boundary of the domain of z might be close to the spectrum. However, when considering z being further away from the spectrum we get a much better estimate:

Corollary 4.7. *Let g, β fulfill the conditions of Lemma 4.5 and $z\in\Gamma_n$ or $z=E'_P|_0^n+i\lambda$ with $\lambda\in\mathbb{R}, |\lambda|=1$ for $n\in\mathbb{N}$. The following estimates hold true*

$$\left\|\left(\frac{1}{H'_P|_0^{n-1}-z}\right)^{1/2}\Delta H'_P|_{n-1}^n\left(\frac{1}{H'_P|_0^{n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}|_0^n}\le C|g|\left(\frac{(\beta-1)n}{\beta^n}\right)^{1/2}, \tag{52}$$

$$\left\|\frac{1}{H'_P|_0^n-z}-\frac{1}{H'_P|_0^{n-1}-z}\right\|_{\mathcal{F}|_0^n}\le C|g|\left(\frac{(\beta-1)n}{\beta^n}\right)^{1/2}. \tag{53}$$

Proof. It is enough to notice that in the estimate of the left-hand side of (52) one can just replace $\Delta\xi_n$ in (50) by a constant and use that $1<\beta<2$, see (25). For $|g|$ small enough, the inequality in (53) follows from (52). ◻

With these lemmas at hand we prove the induction step for the removal of the ultraviolet cut-off.

Theorem 4.8. *Let g, β fulfill the assumptions of Lemma 4.5. Then for $|g|$ sufficiently small the following holds true for all $n\in\mathbb{N}$:*

(i) $E'_P|_0^n := \inf\operatorname{Spec}\left(H'_P|_0^n\restriction\mathcal{F}|_0^n\right)$ *is a non-degenerate eigenvalue of* $H'_P|_0^n\restriction\mathcal{F}|_0^n$.

(ii) $\operatorname{Gap}\left(H'_P|_0^n\restriction\mathcal{F}|_0^n\right)\ge\xi_n$.

(iii) The vectors

$$\Psi'_P|_0^0 := \Omega,$$
$$\Psi'_P|_0^j := Q'_P|_0^j \Psi'_P|_0^{j-1}, \qquad Q'_P|_0^j := -\frac{1}{2\pi i}\oint_{\Gamma_j} \frac{dz}{H'_{P,j} - z}, \qquad j \geq 1, \tag{54}$$

are well-defined and $\Psi'_P|_0^n$ is the unique ground state of $H'_P|_0^n \upharpoonright \mathcal{F}|_0^n$.

(iv) The following holds:

$$\left\|\Psi'_P|_0^n - \Psi'_P|_0^{n-1}\right\| \leq C|g|\left(\frac{(\beta-1)n}{\beta^n}\right)^{1/2}, \tag{55}$$
$$\|\Psi'_P|_0^n\| \geq C_{\Psi'} \tag{56}$$

where $0 < C_{\Psi'} < 1$.

(v) $E'_P|_0^n$ is analytic in P for all $n \in \mathbb{N}$ and the following bounds hold true

$$|E'_P|_0^n - E'_P|_0^{n-1}| \leq C|g|^2 \frac{(\beta-1)n}{\beta^n}, \qquad |E'_P|_0^n| < C_{E'}\left(> \frac{P^2}{2}\right), \tag{57}$$
$$|\nabla E'_P|_0^n - \nabla E'_P|_0^{n-1}| \leq C|g|^2 \frac{(\beta-1)n}{\beta^n}, \qquad |\nabla E'_P|_0^n| \leq C_{\nabla E}\left(= \frac{3}{4}\right), \tag{58}$$

where $E'_P|_0^0 \equiv \frac{P^2}{2}$ and $\nabla E'_P|_0^0 \equiv P$.

Proof. We prove this by induction: Statements (i)-(v) for $(n-1)$ will be referred to as assumptions A(i)-A(v) while the same statements for n are claims C(i)-C(v). For $n = 1$ the claims can be verified by direct computation and by using Lemma 4.5. Let $n > 1$ and suppose A(i)-A(v) hold.

1. Because of A(i), A(ii), and A(v) Lemma 4.3 states that

$$\operatorname{Gap}\left(H'_P|_0^{n-1} \upharpoonright \mathcal{F}|_0^n\right) \geq \xi_{n-1}.$$

   Lemma 4.5 ensures that the resolvent $(H'_P|_0^n - z)^{-1}$ is well-defined for $\frac{1}{2}\xi_n \leq |E'_P|_0^{n-1} - z| \leq \xi_n$.

2. Hence, Kato's theorem yields claims C(i) and C(iii). As a consequence, the spectrum of $H'_P|_0^n \upharpoonright \mathcal{F}|_0^n$ is contained in $\{E'_P|_0^n\} \cup (E'_P|_0^{n-1} + \xi_n, \infty)$ because $E'_P|_0^n \leq E'_P|_0^{n-1}$ by (iii) of Corollary 5.4 for $m = 0$, which proves claim C(ii).

3. Next, we prove C(iv). By A(iii) we have

$$\|\Psi'_P|_0^n - \Psi'_P|_0^{n-1}\| \leq \|(Q'_n - Q'_{n-1})\Psi'_P|_0^{n-1}\| = O\left(|g|\left(\frac{(\beta-1)n}{\beta^n}\right)^{1/2}\right) \tag{59}$$

   where we have used Lemma 4.7 and that $\|\Psi'_P|_0^{n-1}\| \leq 1$ holds by construction. Furthermore, starting from the identity

$$\|\Psi'_P|_0^n\|^2 = \|\Psi'_P|_0^{n-1}\|^2 + \|\Psi'_P|_0^n - \Psi'_P|_0^{n-1}\|^2 + 2\,\mathrm{Re}\left\langle \Psi'_P|_0^{n-1}, \Psi'_P|_0^n - \Psi'_P|_0^{n-1}\right\rangle \tag{60}$$

we conclude that

$$\|\Psi'_P|_0^n\|^2 - \|\Psi'_P|_0^{n-1}\|^2 = O\left(|g|^2 \frac{(\beta-1)n}{\beta^n}\right). \tag{61}$$

Finally, since $\|\Psi'_P|_0^0\| = 1$ by definition,

$$\|\Psi'_P|_0^n\|^2 \geq 1 - \sum_{j=1}^{n} \left| \|\Psi'_P|_0^j\|^2 - \|\Psi'_P|_0^{j-1}\|^2 \right| \geq 1 - C|g|^2 \sum_{j=0}^{n} \frac{(\beta-1)j}{\beta^j} \geq 1 - O(|g|) \geq C_{\Psi'} > 0$$

for some positive constant $C_{\Psi'}$, and $|g|$ sufficiently small and subject to the constraint $|g| \leq (\beta - 1)$; see (25).

4. In order to prove C(v), first by using (52) and (56) we can estimate the energy shift as follows

$$|E'_P|_0^n - E'_P|_0^{n-1}| = \left| \frac{\left\langle \Psi'_P|_0^n, \Delta H'_P|_{n-1}^n \Psi'_P|_0^{n-1} \right\rangle}{\left\langle \Psi'_P|_0^n, \Psi'_P|_0^{n-1} \right\rangle} \right| = O\left(|g|^2 \frac{(\beta-1)n}{\beta^n}\right)$$

This readily implies

$$|E'_P|_0^n| \leq \frac{P^2}{2} + C|g|^2 \sum_{j=0}^{n} \frac{(\beta-1)j}{\beta^j} \leq C_{E'} \tag{62}$$

for some constant $C_{E'}$.

Since $(H'_P|_0^n)_{|P| \leq P_{\max}}$ is an analytic family of type A and $E'_P|_0^n$ is an isolated eigenvalue, $E'_P|_0^n$ is an analytic function of P and

$$\nabla E'_P|_0^n = P - \left\langle [P^f + B|_0^n + B^*|_0^n] \right\rangle_{\Psi'_P|_0^n}. \tag{63}$$

By using equations (40), (41), (42), (45), (46) for $z \in \Gamma_n$ (see Definition 4.6), and (59), for $|g|$ sufficiently small one can easily prove that

$$\begin{aligned} \nabla E'_P|_0^n - \nabla E'_P|_0^{n-1} &= -\langle [B|_{n-1}^n + B^*|_{n-1}^n] \rangle_{\Psi'_P|_0^n} \\ &\quad + \left\langle [P - P^f + B|_0^{n-1} + B^*|_0^{n-1}] \right\rangle_{\Psi'_P|_0^n} - \left\langle [P - P^f + B|_0^{n-1} + B^*|_0^{n-1}] \right\rangle_{\Psi'_P|_0^{n-1}} \\ &= O\left(|g|^2 \frac{(\beta-1)n}{\beta^n}\right) \end{aligned}$$

and finally the bound $|\nabla E'_P|_0^n| \leq \frac{3}{4} = C_{\nabla E}$. □

We can now prove the first main result.

Proof of Theorem 2.1 in Section 2.

(i) Recall that $\Psi_P|_0^n := e^{-T|_0^n}\Psi'_P|_0^n$. By unitarity of the Gross transformation

$$\begin{aligned}\|\Psi_P|_0^n - \Psi_P|_0^{n-1}\| &= \|\Psi'_P|_0^n - e^{T|_{n-1}^n}\Psi'_P|_0^{n-1}\| \\ &\leq \|(e^{T|_{n-1}^n} - 1)\Psi'_P|_0^{n-1}\| + \|\Psi'_P|_0^n - \Psi'_P|_0^{n-1}\|\end{aligned}$$

holds. The convergence of $(\Psi'_P|_0^n)_{n\in\mathbb{N}}$ to a non-zero vector (see Theorem 4.8) and

$$\begin{aligned}\|(e^{T|_{n-1}^n} - 1)\Psi'_P|_0^{n-1}\| &\leq \int_0^1 d\lambda\, \|e^{\lambda T|_{n-1}^n} T|_{n-1}^n \Psi'_P|_0^{n-1}\| \\ &\leq \|T|_{n-1}^n \Psi'_P|_0^{n-1}\| \xrightarrow[n\to\infty]{} 0\end{aligned}$$

imply the claim.

(ii) Again the unitarity of the Gross transformation and (5) implies

$$E_P|_0^n - V_{\mathrm{self}}|_0^n := \inf \mathrm{Spec}\,(H_P|_0^n \upharpoonright \mathcal{F}|_0^n) - V_{\mathrm{self}}|_0^n = E'_P|_0^n. \tag{64}$$

Since the right-hand side of (57) in Theorem 4.8 is summable, the sequence $(E'_P|_0^n)$ is convergent.

(iii) By Corollary 4.7 the resolvent $(H'_P|_0^n - z)^{-1}$, for $z = E'_P|_0^n + i\lambda$, $\lambda \in \mathbb{R}$ and $|\operatorname{Im}\lambda| = 1$, converges as $n \to \infty$. Furthermore, for every n the range of $(H'_P|_0^n - z)^{-1}$ is given by $D(H_{P,0})$ which is dense in $\mathcal{F}$. Hence, the Trotter-Kato Theorem [RS81, Theorem VIII.22] ensures the existence of a limiting self-adjoint Hamiltonian $H'_P|_0^\infty$ on $\mathcal{F}$. Because of the unitarity of the Gross transformation, the family of Hamiltonians $H_P|_0^n - V_{\mathrm{self}}|_0^n$, $n \in \mathbb{N}$, converges to $H_P|_0^\infty := e^{-T|_\kappa^\infty} H'_P|_0^\infty e^{T|_\kappa^\infty}$ in the norm resolvent sense as $n \to \infty$.

(iv) By (iii), $\Psi_P|_0^\infty$ is a ground state of $H_P|_0^\infty$. Moreover, Theorem 4.8 ensures

$$\mathrm{Spec}\,((H'_P|_0^n - E'_P|_0^n) \upharpoonright \mathcal{F}|_0^n) \subset \{0\} \cup (\xi_n, \infty).$$

Since $\xi_n \geq \frac{1}{16}\kappa$ the set $(-\infty, 0) \cup (0, \frac{1}{16}\kappa)$ is not part of the spectrum of $(H'_P|_0^n - E'_P|_0^n) \upharpoonright \mathcal{F}|_0^n$ for any $n \in \mathbb{N}$. As the spectrum cannot suddenly expand in the limit [RS81, Theorem VIII.24], this proves the claimed gap bound. The gap bound and the resolvent convergence imply that $E'_P|_0^\infty$ is a non-degenerate eigenvalue.

□

5 Ground States of the Gross Transformed Hamiltonians $H'_P|_m^\infty$ for $m \in \mathbb{N}$

So far we have studied the Gross transformed Hamiltonian $H'_P|_0^n$ for an arbitrary large n. In the following we want to add interaction slices below the frequency κ. As a preparation for this we state some important properties of the Hamiltonian

$$H'_P|_m^n := H'_P|_0^n + g\Phi|_m^0$$

for any $m \in \mathbb{N} \cup \{\infty\}$ and $n \in \mathbb{N}$. Note that for all such cut-offs the operator $H'_P|_m^n$ is a Kato small perturbation of $H_{P,0}$ and therefore self-adjoint on $D(H_{P,0})$. We collect these facts including the limiting case $n \to \infty$ in the next lemma.

Remark 5.1. *In this section we implicitly assume the constraints $|P| < P_{\max}$ and $1 < \kappa < 2$. Furthermore, g and β are such that all the results of Section 4 hold true.*

Lemma 5.2. *Let $|g|$ be sufficiently small. For $n \in \mathbb{N}$, $m \in \mathbb{N} \cup \{\infty\}$ there exists $\lambda \in \mathbb{R}$ such the operator*

$$\frac{1}{H'_P|^n_m - E'_P|^n_0 \pm i\lambda}$$

has range $D(H_{P,0})$ and converges in norm as $n \to \infty$. Therefore, the sequence of operators $H'_P|^n_m$, $n \in \mathbb{N}$, converges to a self-adjoint operator acting on $\mathcal{F}$ in the norm resolvent sense.

Proof. Let $m \in \mathbb{N} \cup \{\infty\}$. The only non-straightforward case is $n \to \infty$. First, we show the validity of the Neumann expansion

$$\frac{1}{H'_P|^n_m - E'_P|^n_0 \pm i\lambda} = \frac{1}{H'_P|^n_0 + g\Phi|^0_m - E'_P|^n_0 \pm i\lambda} = R_n \sum_{j=0}^{\infty} (S R_n)^j \tag{65}$$

for

$$R_n := \frac{1}{H'_P|^n_0 - E'_P|^n_0 \pm i\lambda} \qquad \text{and} \qquad S = -g\Phi|^0_m.$$

With the standard inequalities (22) we estimate

$$\|S R_n\| \leq C|g| \left\| (H^f|^0_m)^{1/2} \left(\frac{1}{H'_P|^n_0 - E'_P|^n_0 \pm i\lambda} \right)^{1/2} \right\| \left(\frac{1}{|\lambda|} \right)^{1/2} + C|g| \frac{1}{|\lambda|}. \tag{66}$$

Fix a θ' such that $1 - \theta' - C_{\nabla E} > 0$. From an analogous computation as conducted in the proof of Lemma 4.3 one finds

$$\inf_{\|\psi\|=1} \left\langle \psi, (H'_P|^n_0 - \theta' H^f|^0_m - E'_P|^n_0)\psi \right\rangle \geq 0$$

where the infimum is taken over $\psi \in D(H_{P,0})$. Consequently, we get that

$$\left\| \left(\frac{\theta' H^f|^0_m}{H'_P|^n_0 - \theta' H^f|^0_m - E'_P|^n_0 + \theta' H^f|^0_m \pm i\lambda} \right)^{1/2} \right\|^2 \leq \frac{1}{|\lambda|}$$

holds because $H^f|^0_m$ and $H'_P|^n_0$ commute. For $|\lambda|$ sufficiently large this gives

$$(66) \leq \frac{|g|C\theta'^{-1/2} + |g|C}{|\lambda|} < 1 \tag{67}$$

so that the Neumann expansion in (65) is well-defined for all $n \in \mathbb{N}$. Moreover, the limit of (65) for $n \to \infty$ exists because:

1. The sequence $(R_n)_{n\in\mathbb{N}}$, converges in norm; see Theorem 2.1
2. $\|R_l S\|, \|S R_l\| < 1$ for all $l \in \mathbb{N}$, see (67)

3. For any $j \geq 1$ we have

$$\|R_l(SR_l)^{j+1} - R_n(SR_n)^{j+1}\| \leq \|SR_l\| \, \|R_l(SR_l)^j - R_n(SR_n)^j\| + \|R_nS\|^{j+1} \, \|R_l - R_n\|.$$

For all $n \in \mathbb{N}$ the range of the resolvent $(H'_P|^n_m - E'_P|^n_0 \pm i\lambda)^{-1}$ equals $D(H_{P,0})$ and therefore it is dense. Finally the Trotter-Kato Theorem [RS81, Theorem VIII.22] ensures the existence of a self-adjoint limiting operator $H'_P|^\infty_m$ bounded from below. □

For the Hamiltonian $H'_P|^n_m$, where the infrared cut-off τ_m is arbitrarily small but strictly larger than zero, we construct the corresponding ground state $\Psi'_P|^n_m$. For this construction we introduce a new parameter ζ and provide necessary constraints on the infrared scaling parameter γ depending on the coupling constant g.

Definition 5.3. *We consider an infrared scaling parameter γ that obeys*

$$0 < \gamma < \frac{1}{2}, \qquad |g| \leq \gamma^2, \qquad \sum_{j=1}^{\infty} \gamma^{\frac{j}{4}}(1+j) \leq \frac{1}{2}. \tag{68}$$

Furthermore, we fix the auxiliary constant $0 < \zeta < \frac{1}{16}$ such that

$$1 - \theta - C_{\nabla E} \geq 2\zeta$$

where $0 < \theta < \frac{1}{8}$ and $C_{\nabla E} = \frac{3}{4}$.

As we shall see later, the upper bound on ζ is constrained by the ultraviolet gap estimate; see (iv) in Theorem 2.1.

In the iterative construction of the ground state we use Corollary 5.4 below that relies on Lemma 3.2 and on Theorem 3.1 for statements (i),(ii). The estimate in (iii) is based on a simple variational argument.

Corollary 5.4. *Let $|g|$ be sufficiently small. For all $n, m \in \mathbb{N}$ the following holds true:*

(i) $-|g|c_b \leq E'_P|^n_m \leq \frac{1}{2}P^2$, *where c_b is the constant introduced in Lemma 3.2.*

(ii) *There is a $g_{\max} > 0$ such that for $0 \leq |g| < g_{\max}$ and all $k \in \mathbb{R}^3$*

$$E'_{P-k}|^n_m - E'_P|^n_m \geq -C_{\nabla E}|k|. \tag{69}$$

(iii) *Assume that $E'_P|^{n+1}_m, E'_P|^n_{m+1}$, and $E'_P|^n_m$ are eigenvalues of $H'_P|^{n+1}_m \upharpoonright \mathcal{F}|^{n+1}_m$, $H'_P|^n_{m+1} \upharpoonright \mathcal{F}|^n_{m+1}$, and $H'_P|^n_m \upharpoonright \mathcal{F}|^n_m$, respectively; then $E'_P|^{n+1}_m, E'_P|^n_{m+1} \leq E'_P|^n_m$.*

Proof. See Appendix A. □

Lemma 5.5. *Let $|g|$ be sufficiently small and $n \in \mathbb{N} \cup \{\infty\}$. For an integer $m \geq 1$, assume:*

(i) *$E'_P|^n_{m-1}$ is the non-degenerate eigenvalue of $H'_P|^n_{m-1} \upharpoonright \mathcal{F}|^n_{m-1}$ with eigenvector $\Psi'_P|^n_{m-1}$.*

(ii) $\mathrm{Gap}\left(H'_P|^n_{m-1} \upharpoonright \mathcal{F}|^n_{m-1}\right) \geq \zeta\tau_{m-1}$.

This implies that $E'_P|^n_{m-1}$ is also the non-degenerate ground state energy of $H'_P|^n_{m-1} \upharpoonright \mathcal{F}|^n_m$ with eigenvector $\Psi'_P|^n_{m-1} \otimes \Omega$. Furthermore, it holds:

$$\begin{aligned}\mathrm{Gap}\,(H'_P|^n_{m-1} \upharpoonright \mathcal{F}|^n_m) &\geq \inf_{\mathcal{F}|^n_m \ni \psi \perp \Psi'_P|^n_{m-1} \otimes \Omega} \left\langle H'_P|^n_{m-1} - \theta H^f|^{m-1}_m - E'_P|^n_{m-1} \right\rangle_\psi \\ &\geq 2\zeta\tau_m \end{aligned} \tag{70}$$

where the infimum is taken over $\psi \in D(H_{P,0})$.

Proof. Mimicking the steps in the proof Lemma 4.3 and the inequality in (69) we get the bound

$$\inf_{\mathcal{F}|^n_m \ni \psi \perp \Psi'_P|^n_{m-1} \otimes \Omega} \left\langle H'_P|^n_0 + g\Phi|^0_{m-1} - \theta H^f|^{m-1}_m - E'_P|^n_{m-1} \right\rangle_\psi \geq (1 - \theta - C_{\nabla E})\tau_m \geq 2\zeta\tau_m.$$

This gives the estimate

$$\mathrm{Gap}\,(H'_P|^n_{m-1} \upharpoonright \mathcal{F}|^n_m) = \mathrm{Gap}\left(\left(H'_P|^n_0 + g\Phi|^0_{m-1}\right) \upharpoonright \mathcal{F}|^n_m\right) \geq \min\{\zeta\tau_{m-1}, 2\zeta\tau_m\} = 2\zeta\tau_m$$

where in the last step we have used that $\gamma < \frac{1}{2}$; see (68). This proves the claim for any finite n, m. But the resolvent convergence proved in Lemma 5.2 ensures that the statements remain true in the limit $n \to \infty$ as the spectrum cannot suddenly expand in the limit [RS81, Theorem VIII.24]. □

Lemma 5.6. *For $n \in \mathbb{N} \cup \{\infty\}$ and $m \geq 1$ there is a $g_{\max} > 0$ such that, for $|g| < g_{\max}$ and γ fulfilling the constraints in (68), the assumptions of Lemma 5.5 imply that the resolvent*

$$\frac{1}{H'_P|^n_m - z},$$

restricted to $\mathcal{F}|^n_m$, is well-defined in the domain

$$\frac{1}{4}\zeta\tau_m \leq |E'_P|^n_{m-1} - z| \leq \zeta\tau_m. \tag{71}$$

Proof. It is sufficient to show that

$$\left\| \left(\frac{1}{H'_P|^n_{m-1} - z}\right)^{1/2} g\Phi|^{m-1}_m \left(\frac{1}{H'_P|^n_{m-1} - z}\right)^{1/2} \right\|_{\mathcal{F}|^n_m} \tag{72}$$

is less than one for all z in the given domain. For g sufficiently small this is true because:

1. By standard inequalities in (22) the estimate

$$\left\| g\Phi|^{m-1}_m \left(\frac{1}{H'_P|^n_{m-1} - z}\right)^{1/2} \right\|_{\mathcal{F}|^n_m} \leq |g| C\,((1-\gamma)\tau_{m-1})^{1/2} \left\| (H^f|^{m-1}_m)^{1/2} \left(\frac{1}{H'_P|^n_{m-1} - z}\right)^{1/2} \right\|_{\mathcal{F}|^n_m} \tag{73}$$

holds true. Since $H^f|^{m-1}_m$ commutes with $H'_P|^n_{m-1}$ and using (70), the spectral theorem yields

$$\left\| (H^f|^{m-1}_m)^{1/2} \left(\frac{1}{H'_P|^n_{m-1} - z}\right)^{1/2} \right\|_{\mathcal{F}|^n_m} \leq C. \tag{74}$$

2. Using Lemma 5.5 we get

$$\left\| \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \right\|^2_{\mathcal{F}|^n_m} \leq \max \left\{ \frac{1}{\frac{1}{4}\zeta\tau_m}, \frac{1}{\zeta\tau_m} \right\} \leq \frac{4}{\zeta\tau_m}. \tag{75}$$

Combining (73), (74), and (75) we find

$$(72) \leq C|g| \left(\frac{\tau_{m-1}}{\tau_m} \right)^{1/2} = C|g|\gamma^{-1/2} \leq C|g|^{3/4}.$$

where we have used the constraints in (68). This proves the claim. □

Inside the domain where the resolvent is well-defined, let us now introduce the integration contour that is used to iteratively construct the ground state vectors in Theorem 5.8 below.

Definition 5.7. *For $m \in \mathbb{N}$ we define the contour*

$$\Delta_m := \left\{ z \in \mathbb{C} \;\middle|\; |E'_P|^n_{m-1} - z| = \frac{1}{2}\zeta\tau_m \right\}.$$

Theorem 5.8. *Let $n \in \mathbb{N} \cup \{\infty\}$ and g, γ sufficiently small such that the constraints in (68) are fulfilled. Then for all $m \geq 0$ the following holds true:*

(i) $E'_P|^n_m := \inf \operatorname{Spec}\left(H'_P|^n_m \upharpoonright \mathcal{F}|^n_m \right)$ *is the non-degenerate ground state energy of* $H'_P|^n_m \upharpoonright \mathcal{F}|^n_m$.

(ii) $\operatorname{Gap}\left(H'_P|^n_m \upharpoonright \mathcal{F}|^n_m \right) \geq \zeta\tau_m$.

(iii) The vectors

$$\Psi'_P|^n_0 := \Psi'_P|^n_0,$$
$$\Psi'_P|^n_m := Q'_P|^n_m \Psi'_P|^n_{m-1}, \qquad Q'_P|^n_m := -\frac{1}{2\pi i} \oint_{\Delta_m} \frac{dz}{H'_P|^n_m - z}, \qquad m \geq 1, \tag{76}$$

are well-defined and non-zero. The vector $\Psi'_P|^n_m$ is the unique ground state of $H'_P|^n_m \upharpoonright \mathcal{F}|^n_m$.

Proof. The proof is by induction and it relies on Corollary 5.4, Lemma 5.5, and Lemma 5.6. Since the rationale can be inferred from similar steps in the proof of Theorem 4.8, we do not provide the details.
The main difference with respect to Theorem 4.8 is the fact the sequence of vectors does not converge. Moreover, here we only prove that the norm of the vector $\Psi'_P|^n_m$ is nonzero for all finite m that follows from the bound $\|\Psi'_P|^n_m\| \geq C\|\Psi'_P|^n_{m-1}\|$. The same type of argument is shown for the vectors $\phi_P|^n_m$ (with n finite) in the next section. We refer the reader to equations (100)–(106). □

An auxiliary result needed for the next section is:

Lemma 5.9. *Let $|g|$ be sufficiently small. Then for all $n, m \in \mathbb{N}$*

(i)

$$\left| E'_P|^n_{m+1} - E'_P|^n_m \right| \leq Cg^2\gamma^m \tag{77}$$

(ii)

$$\left|\nabla E'_P|^n_m\right| \le C_{\nabla E} \tag{78}$$

hold true, where $\nabla E'_P|^n_m$ *is given by*

$$\nabla E'_P|^n_m = P - \left\langle [P^f + B|^n_0 + B^*|^n_0] \right\rangle_{\Psi'_P|^n_m} . \tag{79}$$

Proof. (i) The claim can be seen from:

(a) The gap estimate (70) and (i) in Corollary 5.4.

(b) The bound

$$\theta H^f|^m_{m+1} + g\Phi|^m_{m+1} + g^2 \int_{\mathcal{B}_{\tau_m} \setminus \mathcal{B}_{\tau_{m+1}}} dk \frac{\rho(k)^2}{\theta\omega(k)} \ge 0$$

which can be inferred from completion of the square.

(c) The inequality

$$\int_{\mathcal{B}_{\tau_m} \setminus \mathcal{B}_{\tau_{m+1}}} dk \frac{\rho(k)^2}{\theta\omega(k)} \le \frac{C}{\theta}\gamma^m.$$

(ii) Since $(H'_P|^n_m)_{|P| \le P_{\max}}$, is an analytic family of type A and $E'_P|^n_m$ is an isolated eigenvalue, equation (79) holds by analytic perturbation theory. Moreover, (78) follows immediately from Corollary 5.4 (ii).

□

6 Ground States of the Transformed Hamiltonians $H^{W'}_P|^n_\infty$ for $n \in \mathbb{N}$

This section provides the key result for Section 7 where we remove both limits simultaneously. Here (Section 6) we generalize the strategy employed in [Piz03] to perform the limit of a vanishing infrared cut-off τ_m uniformly in the ultraviolet cut-off σ_n.

Remark 6.1. *In this section we implicitly assume the constraints* $|P| < P_{\max}$ *and* $1 < \kappa < 2$. *Furthermore,* g, β*, and* γ *are such that all the results of Sections 4 and 5 hold true.*

Preliminaries. We collect the definitions of the transformed operators and vectors, and we explain some of their properties:

Hamiltonian	Fock space
$H^{W'}_P\|^n_m := W_m(\nabla E'_P\|^n_m)\ H'_P\|^n_m\ W_m(\nabla E'_P\|^n_m)^*$	$\mathcal{F}\|^n_m := \mathcal{F}(L^2(\mathcal{B}_{\sigma_n} \setminus \mathcal{B}_{\tau_m}))$
$\widetilde{H}^{W'}_P\|^n_m := W_m(\nabla E'_P\|^n_{m-1})\ H'_P\|^n_m\ W_m(\nabla E'_P\|^n_{m-1})^*$	$\mathcal{F}\|^n_m$

Notice that

$$\widetilde{H}_P^{W'}|_m^n = W_m(\nabla E'_P|_{m-1}^n) W_m(\nabla E'_P|_m^n)^* H_P^{W'}|_m^n W_m(\nabla E'_P|_m^n) W_m(\nabla E'_P|_{m-1}^n)^*. \tag{80}$$

The transformation $W_m(Q)$, $Q \in \mathbb{R}^3$ and $|Q| \leq 1$, was defined in (14) and it is unitary for all finite m. For $n, m \in \mathbb{N}$ we iteratively define the vectors

$$\begin{aligned} \phi_P|_0^n &:= \frac{\Psi'_P|_0^n}{\|\Psi'_P|_0^n\|}, \\ \widetilde{\phi}_P|_m^n &:= \widetilde{Q}'_P|_m^n \phi_P|_{m-1}^n, \qquad \widetilde{Q}'_P|_m^n := -\frac{1}{2\pi i} \oint_{\Delta_m} \frac{dz}{\widetilde{H}_P^{W'}|_m^n - z} \\ \phi_P|_m^n &:= W_m(\nabla E'_P|_m^n) W_m(\nabla E'_P|_{m-1}^n)^* \widetilde{\phi}_P|_m^n \end{aligned} \tag{81}$$

where the contour Δ_m was introduced in Definition 5.7. This family of vectors is well-defined because of the unitarity of the transformations W_m and of the results of Section 5. If the vectors $\phi_P|_m^n$ and $\widetilde{\phi}_P|_m^n$ are non-zero they are by construction the (unnormalized) ground states of $H_P^{W'}|_m^n$ and $\widetilde{H}_P^{W'}|_m^n$, respectively. Assuming that these vectors are non-zero we introduce the following auxiliary definitions:

$$\begin{aligned} A_{P,m}^{(n)} &:= \int dk\, k \alpha_m(\nabla E'_P|_m^n, k)[b(k) + b^*(k)], \qquad C_{P,m}^{(k,n)} := \int dk\, k \alpha_m(\nabla E'_P|_m^n, k)^2, \\ C_{P,m}^{(\omega,n)} &:= \int dk\, \omega(k) \alpha_m(\nabla E'_P|_m^n, k)^2, \qquad C_{P,m}^{(\rho,n)} := 2g \int dk\, \rho(k) \alpha_m(\nabla E'_P|_m^n, k). \end{aligned} \tag{82}$$

where the function

$$\alpha_m(\nabla E'_P|_m^n, k) := -g\, \frac{\rho(k)}{\omega(k)} \frac{\mathbb{1}_{\mathcal{B}_\kappa \setminus \mathcal{B}_{\tau_m}}(k)}{1 - \widehat{k} \cdot \nabla E'_P|_m^n}$$

was introduced in (13). Furthermore, we define

$$\begin{aligned} R_P|_m^n &:= -\nabla E'_P|_m^n \cdot (B|_0^n + B^*|_0^n) - \frac{1}{2}\left([B|_0^n, P - P^f] + [P - P^f, B^*|_0^n] + [B|_0^n, B^*|_0^n]\right), \\ \Pi_P|_m^n &:= P^f + A_{P,m}^{(n)} + B|_0^n + B^*|_0^n \\ &= W_m(\nabla E'_P|_m^n)\left(P^f + B|_0^n + B^*|_0^n\right) W_m(\nabla E'_P|_m^n)^* - C_{P,m}^{(k,n)}, \end{aligned} \tag{83}$$

$$\begin{aligned} \Gamma_P|_m^n &:= \Pi_P|_m^n - \langle \Pi_P|_m^n \rangle_{\phi_P|_m^n}, \\ C_{P,m}^{(n)} &:= \frac{P^2}{2} - \frac{1}{2}(P - \nabla E'_P|_m^n)^2 - \nabla E'_P|_m^n \cdot C_{P,m}^{(k,n)} + C_{P,m}^{(\omega,n)} + C_{P,m}^{(\rho,n)}. \end{aligned} \tag{84}$$

Using these abbreviations and a formal computation carried out in Appendix B, one can prove that the identity

$$H_P^{W'}|_m^n = \frac{1}{2} \Gamma_P|_m^{n\,2} + H^f - \nabla E'_P|_m^n \cdot P^f + C_{P,m}^{(n)} + R_P|_m^n \tag{85}$$

holds on $D(H_{P,0})$ for all $n, m \in \mathbb{N}$. As in [Piz03] the ‘normal ordered’ operator $\Gamma_P|_m^n$ will play a crucial role in the next steps.

Analogously, one can verify that on $D(H_{P,0})$ and for $n, m \in \mathbb{N}$ the following identity holds true:

$$\widetilde{H}_P^{W'}|_m^n = \frac{1}{2}\left(\Gamma_P|_{m-1}^n + \widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)} + \widetilde{C}_{P,m}^{(k,n)} - C_{P,m-1}^{(k,n)}\right)^2 + H^f - \nabla E_P'|_{m-1}^n \cdot P^f + \widetilde{C}_{P,m}^{(n)} + R_P|_{m-1}^n; \quad (86)$$

here we have similarly introduced, for any fixed $n \in \mathbb{N}$,

$$\begin{aligned} \widetilde{A}_{P,m}^{(n)} &:= \int dk\, k\alpha_m(\nabla E_P|_{m-1}^n, k)[b(k) + b^*(k)], \qquad \widetilde{C}_{P,m}^{(k,n)} := \int dk\, k\alpha_m(\nabla E_P'|_{m-1}^n, k)^2, \\ \widetilde{C}_{P,m}^{(\omega,n)} &:= \int dk\, \omega(k)\alpha_m(\nabla E_P|_{m-1}^n, k)^2, \qquad \widetilde{C}_{P,m}^{(\rho,n)} := 2g\int dk\, \rho(k)\alpha_m(\nabla E_P|_{m-1}^n, k), \end{aligned} \quad (87)$$

which differ from those in (82) only in the argument of α_m. We also define

$$\begin{aligned} \widetilde{\Pi}_P|_m^n &:= P^f + \widetilde{A}_{P,m}^{(n)} + B|_0^n + B^*|_0^n \\ &= W_m(\nabla E_P'|_{m-1}^n)\left(P^f + B|_0^n + B^*|_0^n\right) W_m(\nabla E_P'|_{m-1}^n)^* - \widetilde{C}_{P,m}^{(k,n)}, \\ \widetilde{\Gamma}_P|_m^n &:= \widetilde{\Pi}_P|_m^n - \left\langle \widetilde{\Pi}_P|_m^n \right\rangle_{\widetilde{\phi}_P|_m^n}, \\ \widetilde{C}_{P,m}^{(n)} &:= \frac{P^2}{2} - \frac{1}{2}(P - \nabla E_P'|_{m-1}^n)^2 - \nabla E_P'|_{m-1}^n \cdot C_{P,m}^{(k,n)} + \widetilde{C}_{P,m}^{(\omega,n)} + \widetilde{C}_{P,m}^{(\rho,n)}. \end{aligned} \quad (88)$$

Notice that using (79) we have the following identities

$$\langle \Pi_P|_m^n \rangle_{\phi_P|_m^n} = P - \nabla E_P'|_m^n - C_{P,m}^{(k,n)}, \quad (89)$$

$$\Gamma_P|_m^n = W_m(\nabla E_P'|_m^n)\left(P^f + B|_0^n + B^*|_0^n\right) W_m(\nabla E_P'|_m^n)^* - P + \nabla E_P'|_m^n, \quad (90)$$

$$\widetilde{\Gamma}_P|_m^n = W_m(\nabla E_P'|_{m-1}^n) W_m(\nabla E_P'|_m^n)^* \Gamma_P|_m^n W_m(\nabla E_P'|_m^n) W_m(\nabla E_P'|_{m-1}^n)^*, \quad (91)$$

$$\widetilde{\Gamma}_P|_m^n - \Gamma_P|_{m-1}^n = (\nabla E_P'|_m^n - \nabla E_P'|_{m-1}^n) + (\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)}) + (\widetilde{C}_{P,m}^{(k,n)} - C_{P,m-1}^{(k,n)}). \quad (92)$$

To start with, we show that for any finite m, the vectors $\phi_P|_m^n$ and $\widetilde{\phi}_P|_m^n$ are non-zero. Namely, by starting from $\phi_P|_0^n$, we estimate the norm difference

$$\|\widetilde{\phi}_P|_m^n - \phi_P|_{m-1}^n\| = \left\| -\frac{1}{2\pi i} \oint_{\Delta_m} \frac{dz}{\widetilde{H}_P^{W'}|_m^n - z} \phi_P|_{m-1}^n - \phi_P|_{m-1}^n \right\|. \quad (93)$$

In (93) we expand the resolvent with respect to

$$\Delta\widehat{H}_P^{W'}|_m^{m-1} := \widetilde{H}_P^{W'}|_m^n - H_P^{W'}|_{m-1}^n - \widetilde{C}_{P,m}^{(n)} + C_{P,m-1}^{(n)} \quad (94)$$

$$= \frac{1}{2}\left(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)} + \widetilde{C}_{P,m}^{(k,n)} - C_{P,m-1}^{(k,n)}\right)^2 + \quad (95)$$

$$+ \frac{1}{2}\left[\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)}, \Gamma_P|_{m-1}^n\right] + \quad (96)$$

$$+ \left(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)}\right) \cdot \Gamma_P|_{m-1}^n + \left(\widetilde{C}_{P,m}^{(k,n)} - C_{P,m-1}^{(k,n)}\right) \cdot \Gamma_P|_{m-1}^n. \quad (97)$$

Given the form of $\Delta\widehat{H}_P^{W'}|_m^{m-1}$ it is convenient to replace the integration contour Δ_m with $\widehat{\Delta}_m$ defined below:

Definition 6.2. *For $m \in \mathbb{N}$ define*

$$\widehat{\Delta}_m := \left\{ z - (C^{(n)}_{P,m-1} - \widetilde{C}^{(n)}_{P,m}) \;\middle|\; z \in \Delta_m \right\}.$$

In the same fashion as Theorem 5.8 we ensure the bounds

$$\frac{1}{4}\zeta\tau_m \leq |E'_P|^n_{m-1} - z + \widetilde{C}^{(n)}_{P,m} - C^{(n)}_{P,m-1}| \leq \zeta\tau_m. \tag{98}$$

for z in the original integration contour Δ_m. For this we observe that

$$|\widetilde{C}^{(n)}_{P,m} - C^{(n)}_{P,m-1}| \leq g^2 C\tau_{m-1}, \tag{99}$$

and hence, for $|g|$ sufficiently small,

$$\zeta\tau_m \geq \frac{1}{2}\zeta\tau_m + g^2 C\tau_{m-1} \geq |E'_P|^n_{m-1} - z + \widetilde{C}^{(n)}_{P,m} - C^{(n)}_{P,m-1}| \geq \frac{1}{2}\zeta\tau_m - g^2 C\tau_{m-1} \geq \frac{1}{4}\zeta\tau_m$$

where in the last step we have used the constraints in (68). The upper bound (98) follows from (99) by a similar argument. Hence, we can use the shifted contours $\widehat{\Delta}_m$ instead of Δ_m and estimate

$$\|\widetilde{\phi}_P|^n_m - \phi_P|^n_{m-1}\| \leq \left\| \frac{1}{2\pi i} \oint_{\widehat{\Delta}_m} dz \sum_{j=1}^{\infty} \left(\frac{1}{E'_P|^n_{m-1} - z} \right)^{1/2} \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \times \right. \tag{100}$$

$$\left. \times \left[\left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} (-\Delta\widehat{H}^{W'}_n|^{m-1}_m) \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \right]^j \phi_P|^n_{m-1} \right\|$$

$$\leq C\gamma^m \sup_{z \in \widehat{\Delta}_m} \left| \frac{1}{E'_P|^n_{m-1} - z} \right|^{1/2} \left\| \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} \times \tag{101}$$

$$\times \sum_{j=1}^{\infty} \left\| \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \Delta\widehat{H}^{W'}_n|^{m-1}_m \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \right\|^{j-1}_{\mathcal{F}|^n_m} \times \tag{102}$$

$$\times \left\| \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \Delta\widehat{H}^{W'}_n|^{m-1}_m \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \phi_P|^n_{m-1} \right\|. \tag{103}$$

Firstly, the gap estimate in (75) immediately yields

$$\sup_{z \in \widehat{\Delta}_m} \left| \frac{1}{E'_P|^n_{m-1} - z} \right|^{1/2} \left\| \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} \leq \frac{C}{\gamma^m}$$

so that (101) is bounded by a constant. Secondly, we show that the series in (102) is convergent. We remark that $(\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1})$ commutes with $W_{m-1}(\nabla E'_P|^n_{m-1})$ so that

$$\left\| \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \left(\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} \right) \cdot \Gamma_P|^n_{m-1} \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m}$$

$$= \left\| \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \left(\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} \right) \cdot \left(P^f + B|^n_0 + B^*|^n_0 + \nabla E'_P|^n_{m-1} - P \right) \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m},$$

where we used again the unitarity of W_{m-1}. Since $(\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1})$ commutes with $B|^n_0$, $B^*|^n_0$ it is enough to bound

$$\left\| \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \left(\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} \right) \cdot [P^f - P + B|^n_0] \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m}$$

$$\leq C \left\| \left(\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} \right) \cdot \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} \times \tag{104}$$

$$\times \left[\left\| H^{1/2}_{P,0} \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} + \left\| B|^n_0 \left(\frac{1}{H'_P|^n_{m-1} - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} \right] \tag{105}$$

The factor (104) can be bounded by $C|g|\gamma^{(m-1)/2}$, similarly to (73). Both terms in (105) can be estimated as $C|g|\gamma^{-m/2}$ using inequalities (22)-(23) and the uniform bound on $|E'_P|^n_m|$ given by Corollary 5.4; see an analogous argument in (48) that exploits the bound in (46). All the remaining terms can be controlled in a similar fashion. Hence, for $|g|$ sufficiently small and γ satisfying the constraint (68), we conclude that

$$\|\widetilde{\phi}_P|^n_m\| \geq C \|\phi_P|^n_{m-1}\| \tag{106}$$

for a strictly positive constant C.

Key result. Theorem 6.3 below is the key tool needed for proving the second main result of this paper, namely that the ground states $(\phi_P|^n_m)_{m\in\mathbb{N}}$ converge to a non-zero vector. This theorem relies on several lemmas (Lemma 6.4, Lemma 6.5, and Lemma 6.6) that will be proven later on.

Recall that the symbol C denotes any universal constant. Throughout the computation it will be important to distinguish the constants C_i, $1 \leq i \leq 7$.

Theorem 6.3. *For $|g|$, γ, and ζ sufficiently small and fulfilling the constraints in Definition 5.3 the following holds true for all $n \in \mathbb{N}$, $m \geq 1$:*

(i) $\|\phi_P|^n_m - \widetilde{\phi}_P|^n_m\| \leq m\gamma^{\frac{m}{4}}$ *and* $\|\widetilde{\phi}_P|^n_m - \phi_P|^n_{m-1}\| \leq \gamma^{\frac{m}{4}}$,

(ii) $\|\phi_P|^n_m\| \geq 1 - \sum_{j=1}^m \gamma^{\frac{j}{4}}(1+j) \qquad (\geq \frac{1}{2})$,

(iii) Let $z \in \widehat{\Delta}_{m+1}$ *and* $\delta := \frac{1}{2}$ *then*

$$|g|^\delta \left| \left\langle \Gamma^{(i)}_P|^n_m \phi_P|^n_m, \frac{1}{H^{W'}_P|^n_m - z} \Gamma^{(i)}_P|^n_m \phi_P|^n_m \right\rangle \right| \leq \gamma^{-\frac{m}{2}}, \qquad i = 1, 2, 3.$$

Proof. We prove this by induction: Statements (i)-(iii) for $(m-1)$ shall be referred to as assumptions A(i)-A(iii) while the same statements for m are referred to as claims C(i)-C(iii).

A straightforward computation yields the case $m = 1$.

Let $m \geq 2$ and suppose A(i)-A(iii) hold. We start proving claims C(i) and C(ii).

1. Due to the inequality in (101)-(103), the estimate

$$\|\widetilde{\phi}_P|_m^n - \phi_P|_{m-1}^n\| \le C_1 \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \Delta\widehat{H}_n^{W'}|_m^{m-1} \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \phi_P|_{m-1}^n \right\|$$

holds true for $|g|$ sufficiently small, uniformly in n and m. Furthermore, Lemma 6.5 states that

$$\begin{aligned} &\left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \Delta\widehat{H}_n^{W'}|_m^{m-1} \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \phi_P|_{m-1}^n \right\| \\ &\qquad \le |g| C_2 \gamma^{\frac{m-2}{2}} \left(1 + \sum_{i=1}^{3} \left| \left\langle \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n, \frac{1}{H_P^{W'}|_{m-1}^n - z} \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\rangle \right|^{\frac{1}{2}} \right) \end{aligned}$$

which together with the induction assumption A(iii) yields

$$\|\widetilde{\phi}_P|_m^n - \phi_P|_{m-1}^n\| \le |g| C_1 C_2 \gamma^{\frac{m-2}{2}} \left(1 + 3|g|^{-\frac{\delta}{2}} \gamma^{-\frac{m-1}{4}}\right).$$

For $|g|$ sufficiently small and γ satisfying the constraints in (68) we have

$$\|\widetilde{\phi}_P|_m^n - \phi_P|_{m-1}^n\| \le \gamma^{\frac{m}{4}}. \tag{107}$$

Finally, from (107), A(ii) and (68) we conclude

$$\|\widetilde{\phi}_P|_m^n\| \ge \|\phi_P|_{m-1}^n\| - \|\widetilde{\phi}_P|_m^n - \phi_P|_{m-1}^n\| \ge 1 - \sum_{j=1}^{m-1} \gamma^{\frac{j}{4}}(1+j) - \gamma^{\frac{m}{4}} \ge \frac{1}{2}. \tag{108}$$

2. We observe that

$$\begin{aligned} \|\phi_P|_m^n - \widetilde{\phi}_P|_m^n\| &\le \|[W_m(\nabla E'_P|_m^n) W_m(\nabla E'_P|_{m-1}^n)^* - \mathbb{1}_{\mathcal{F}|_m^n}]\, \widetilde{\phi}_P|_m^n\| \\ &\le \left\| [W_m(\nabla E'_P|_m^n) - W_m(\nabla E'_P|_{m-1}^n)]\, \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \right\| \end{aligned} \tag{109}$$

holds because the vectors $\Psi'_P|_m^n$ and $W_m(\nabla E'_P|_{m-1}^n)^* \widetilde{\phi}_P|_m^n$ are parallel and $\|\widetilde{\phi}_P|_m^n\| \le 1$. Lemma 6.6 yields

$$(109) \le |g|\, C_3 m\, |\ln\gamma| \left|\nabla E'_P|_m^n - \nabla E'_P|_{m-1}^n\right|. \tag{110}$$

The difference of the gradients of the ground state energies in (110) is estimated in Lemma 6.7 which states that

$$\begin{aligned} |\nabla E'_P|_m^n - \nabla E'_P|_{m-1}^n| \le g^2 C_4 \gamma^{\frac{m-1}{2}} &+ \sup_{z\in\widehat{\Delta}_m} \left\| \left(\frac{1}{H_P^{W'}|_m^n - z}\right)^{1/2} \Delta\widehat{H}_n^{W'}|_m^{m-1} \left(\frac{1}{H_P^{W'}|_m^n - z}\right)^{1/2} \phi_P|_{m-1}^n \right\| \\ &+ C \frac{\|\phi_P|_{m-1}^n - \widetilde{\phi}_P|_m^n\|}{\|\phi_P|_{m-1}^n\|^2 \|\widetilde{\phi}_P|_m^n\|^2}. \end{aligned}$$

Hence, using Lemma 6.5, (107), (108) as well as assumptions A(ii) and A(iii), one finds that

$$\|\phi_P|_m^n - \widetilde{\phi}_P|_m^n\| \leq |g|C_3 m|\ln\gamma| \left(g^2 C_4 \gamma^{m-1} + |g|C_2\gamma^{\frac{m-2}{2}}(1+3|g|^{-\frac{\delta}{2}}\gamma^{-\frac{m-1}{4}}) + C_5\gamma^{\frac{m}{4}}\right)$$

which implies

$$\|\phi_P|_m^n - \widetilde{\phi}_P|_m^n\| \leq m\gamma^{\frac{m}{4}} \tag{111}$$

for $|g|$ sufficiently small and γ fulfilling the constraints in (68).

Estimates (107) and (111) prove C(i). C(ii) follows along the same lines as (108) using the bound in (111).

Finally, we prove claim C(iii). Let $z \in \widehat{\Delta}_{m+1}$ and $i = 1, 2, 3$. Using the unitarity of the transformations W_m we get

$$\left|\left\langle \Gamma_P^{(i)}|_m^n \phi_P|_m^n, \frac{1}{H_P^{W'}|_m^n - z}\Gamma_P^{(i)}|_m^n \phi_P|_m^n\right\rangle\right| = \left|\left\langle \widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n, \frac{1}{\widetilde{H}_P^{W'}|_m^n - z}\widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n\right\rangle\right|,$$

see identities (80)-(91). For $|g|$ sufficiently small, i.e., $|g|$ of order γ^2, we can expand the resolvent $(\widetilde{H}_P^{W'}|_m^n - z)^{-1}$ by the same reasoning as for (100)-(103) even for $z \in \widehat{\Delta}_{m+1}$ because of the bound on the energy shifts

$$\left|E'_P|_{m+1}^n - E'_P|_m^n\right| \leq C g^2 \gamma^m, \tag{112}$$

given by Lemma 5.9, and because of (71). Hence, using (94) we find

$$\begin{aligned}
&\left|\left\langle \widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n, \frac{1}{\widetilde{H}_P^{W'}|_m^n - z}\widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n\right\rangle\right| \\
&\leq \sum_{j=1}^{\infty} \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} [\Delta\widehat{H}_n^{W'}|_m^{m-1} + \widetilde{C}_{P,m}^{(n)} - C_{P,m-1}^{(n)}] \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \right\|_{\mathcal{F}|_m^n}^{j-1} \times \\
&\quad \times \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n \right\|^2 \\
&\leq C \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n \right\|^2
\end{aligned} \tag{113}$$

Furthermore,

$$\left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n \right\|^2 \leq 2 \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\|^2 + \tag{114}$$

$$+ 2 \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} (\widetilde{\Gamma}_P^{(i)}|_m^n \widetilde{\phi}_P|_m^n - \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n) \right\|^2. \tag{115}$$

Term (114): Exploiting the property

$$\langle \phi_P|_{m-1}^n, \Gamma_P|_{m-1}^n \phi_P|_{m-1}^n \rangle = 0$$

and the spectral theorem, one can show that the term on the right-hand side of (114) fulfills

$$\left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z} \right)^{1/2} \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\|^2 = \left\langle \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n, \left| \frac{1}{H_P^{W'}|_{m-1}^n - z} \right| \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\rangle$$

$$\leq C \left| \left\langle \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n, \frac{1}{H_P^{W'}|_{m-1}^n - z} \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\rangle \right| \tag{116}$$

$$\leq C \left| \left\langle \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n, \frac{1}{H_P^{W'}|_{m-1}^n - y} \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\rangle \right| \tag{117}$$

$$+ C \frac{\sup_{y \in \widehat{\Delta}_m, z \in \widehat{\Delta}_{m+1}} |z-y|}{\operatorname{dist}\left(z, \operatorname{Spec}\left(H'_P|_{m-1}^n \upharpoonright \mathcal{F}|_{m-1}^n\right) \setminus \{E'_P|_{m-1}^n\}\right)} \left| \left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \frac{1}{H'_P|_{m-1}^n - y} \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle \right| \tag{118}$$

$$\leq C_7 \left| \left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \frac{1}{H'_P|_{m-1}^n - y} \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle \right|. \tag{119}$$

for $y \in \widehat{\Delta}_m$ (recall that $z \in \widehat{\Delta}_{m+1}$). In passing from (116) to (117) we have used the property $\left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \phi_P|_{m-1}^n \right\rangle = 0$ which implies that the vector $\Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n$ has spectral support (with respect to $H_P^{W'}|_{m-1}^n$) contained in the interval $(E'_P|_{m-1}^n + \zeta\tau_{m-1}, \infty)$, and hence:

a)

$$\left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \left| \frac{1}{H'_P|_{m-1}^n - y} \right| \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle \leq C \left| \left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \frac{1}{H'_P|_{m-1}^n - y} \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle \right|$$

b)

$$\left| \left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \frac{1}{H'_P|_{m-1}^n - z} \frac{1}{H'_P|_{m-1}^n - y} \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle \right|$$
$$\leq \frac{1}{\operatorname{dist}\left(z, \operatorname{Spec}\left(H'_P|_{m-1}^n \upharpoonright \mathcal{F}|_{m-1}^n\right) \setminus \{E'_P|_{m-1}^n\}\right)} \left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \left| \frac{1}{H'_P|_{m-1}^n - y} \right| \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle.$$

In the step from (116)-(118) we used inequality (112). Therefore, we can conclude that

$$(114) \leq C_7 \left| \left\langle \Gamma_P|_{m-1}^n \phi|_{m-1}^n, \frac{1}{H'_P|_{m-1}^n - y} \Gamma_P|_{m-1}^n \phi|_{m-1}^n \right\rangle \right|. \tag{120}$$

Term (115): We first observe that

$$(115) \leq 4 \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z} \right)^{1/2} (\widetilde{\Gamma}_P^{(i)}|_m^n - \Gamma_P^{(i)}|_{m-1}^n) \widetilde{\phi}_P|_m^n \right\|^2 + \tag{121}$$

$$+ 4 \left\| \left(\frac{1}{H_P^{W'}|_{m-1}^n - z} \right)^{1/2} \Gamma_P^{(i)}|_{m-1}^n (\widetilde{\phi}_P|_m^n - \phi_P|_{m-1}^n) \right\|^2. \tag{122}$$

In order to estimate (121) we use the identity in (92) and the following ingredients:

c) The bound on $|\nabla E'_P|^n_m - \nabla E'_P|^n_{m-1}|$ from Lemma 6.7

d) The estimate in (99), i.e. $|\widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}| \leq g^2 C\gamma^{m-1}$

e) The bound

$$\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - z}\right)^{1/2} \int dk\, k[\alpha_m(\nabla E'_P|^n_{m-1}, k) - \alpha_{m-1}(\nabla E'_P|^n_{m-1}, k)](b(k) + b^*(k))\right\|^2_{\mathcal{F}|^n_m} \leq g^2 C\gamma^{m-3}.$$

Hence, we obtain

$$(121) \leq \frac{C}{\tau_{m+1}}\Bigg[g^2\tau^{1/2}_{m-1} + \sup_{y\in\widehat{\Delta}_m}\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \Delta\widehat{H}^{W'}_n|^{m-1}_m \left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \phi_P|^n_{m-1}\right\| + \tag{123}$$

$$+ \frac{\|\phi_P|^n_{m-1} - \widetilde{\phi}_P|^n_m\|}{\|\phi_P|^n_{m-1}\|^2\|\widetilde{\phi}_P|^n_m\|^2}\Bigg]^2 + \tag{124}$$

$$+ \frac{C}{\tau_{m+1}}\left[g^2C\gamma^{m-1}\right]^2 \tag{125}$$

$$+ g^2C\gamma^{m-3} \tag{126}$$

where (123)-(124), (125) and (126) are related to ingredients c), d) and e) respectively.

For the remaining term (122) we use analytic perturbation theory to find

$$\sqrt{(122)} \leq C\tau_m \sup_{y\in\widehat{\Delta}_m}\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - z}\right)^{1/2} \Gamma^{(i)}_P|^n_{m-1}\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2}\right\|_{\mathcal{F}|^n_m} \times$$
$$\times \sum_{j=1}^{\infty}\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \Delta\widehat{H}^{W'}_n|^{m-1}_m\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2}\right\|^{j-1}_{\mathcal{F}|^n_m} \times$$
$$\times \left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \Delta\widehat{H}^{W'}_n|^{m-1}_m\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \phi_P|^n_{m-1}\right\| \left|\frac{1}{E'_P|^n_{m-1} - y}\right|^{1/2}$$
$$\leq \frac{C}{\gamma^{\frac{1}{2}}}\frac{1}{\gamma^{\frac{m}{2}}} \sup_{y\in\widehat{\Delta}_m}\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \Delta\widehat{H}^{W'}_n|^{m-1}_m\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2} \phi_P|^n_{m-1}\right\|,$$

where we have used the estimates in (101)-(103) for $y \in \widehat{\Delta}_m$, and, using the identity in (90)

$$\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1} - z}\right)^{1/2} \Gamma^{(i)}_P|^n_{m-1}\left(\frac{1}{H^{W'}_P|^n_{m-1} - y}\right)^{1/2}\right\|_{\mathcal{F}|^n_m} \tag{127}$$
$$= \left\|\left(\frac{1}{H'_P|^n_{m-1} - z}\right)^{1/2} [P^f - P + \nabla E'_P|^n_{m-1} + B|^n_0 + B^*|^n_0]\left(\frac{1}{H'_P|^n_{m-1} - y}\right)^{1/2}\right\|_{\mathcal{F}|^n_m}$$
$$\leq C\tau^{-1}_m\gamma^{-1/2}. \tag{128}$$

The inequality in (128) can be derived by combining the first inequality in (39) with Lemma 3.2.

Using Lemma 6.5, Assumption A(iii), the estimates (107), (108) and the constraints (68) we get

$$(121) \leq C\left[g^4\gamma^{-2} + g^2\gamma^{-3}\left(1 + \gamma^{-\frac{m-1}{2}} g^{-\delta}\right) + \gamma^{-\frac{m+2}{2}} + g^4\gamma^{m-3} + g^2\gamma^{m-3}\right] \leq \frac{C}{\gamma^{\frac{m+2}{2}}},$$
$$(122) \leq Cg^2\gamma^{-3}(1 + \gamma^{-\frac{m-1}{2}}|g|^{-\delta}) \leq \frac{C}{\gamma^{\frac{m+2}{2}}},$$

and hence,

$$(115) \leq \frac{C_6}{\gamma^{\frac{m+2}{2}}}. \tag{129}$$

Finally, we collect inequalities (120), (129) and make use of assumption A(iii) to derive

$$|g|^\delta \left|\left\langle \Gamma_P^{(i)}|_m^n \phi_P|_m^n, \frac{1}{H_P^{W'}|_m^n - z} \Gamma_P^{(i)}|_m^n \phi_P|_m^n \right\rangle\right| \leq C_7\gamma^{-\frac{m-1}{2}} + |g|^\delta \frac{C_6}{\gamma^{\frac{m+2}{2}}} \leq \gamma^{-\frac{m}{2}}$$

for γ and $|g|$ sufficiently small and fulfilling the constraints in (68). This proves claim C(iii). □

We shall now provide the lemmas we have used.

Lemma 6.4. *Let $|g|$ be sufficiently small. For $n, m \in \mathbb{N}$ the following expectation values are uniformly bounded:*

$$\left|\langle \phi_P|_m^n, \Pi_P|_m^n \phi_P|_m^n \rangle\right|, \left|\left\langle \widetilde{\phi}_P|_m^n, \widetilde{\Pi}_P|_m^n \widetilde{\phi}_P|_m^n \right\rangle\right| \leq C,$$

Proof. We only prove the bound for the first term. The second can be bounded analogously. Let $n, m \in \mathbb{N}$. By definition of the transformations W_m and using the fact that the vectors

$$\Psi'_P|_m^n, \quad W_m(\nabla E'_P|_m^n)^* \phi_P|_m^n, \quad W_m(\nabla E'_P|_{m-1}^n)^* \widetilde{\phi}_P|_m^n$$

are parallel and their norm is less than one, we have

$$\left|\langle \phi_P|_m^n, \Pi_P|_m^n \phi_P|_m^n \rangle\right|$$
$$\leq C\left|\left\langle \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|}, \left[P^f + B|_0^n + B^*|_0^n - C_{P,m}^{(k,n)}\right] \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \right\rangle\right| \leq C[|P| + |\nabla E'_P|_m^n| + |C_{P,m}^{(k,n)}|].$$

where the last inequality holds by Lemma 5.9. □

Lemma 6.5. *Let $|g|, \zeta, \gamma$ be sufficiently small. Furthermore, let $n \in \mathbb{N}$, $m \geq 2$ and $z \in \widehat{\Delta}_m$. Then*

$$\left\|\left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \Delta\widehat{H}_n^{W'}|_m^{m-1} \left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2} \phi_P|_{m-1}^n\right\|$$
$$\leq |g|C\gamma^{\frac{m-2}{2}} \left(1 + \sum_{i=1}^3 \left|\left\langle \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n, \frac{1}{H_P^{W'}|_{m-1}^n - z} \Gamma_P^{(i)}|_{m-1}^n \phi_P|_{m-1}^n \right\rangle\right|^{\frac{1}{2}}\right) \tag{130}$$

holds true, where $\Delta\widehat{H}_n^{W'}|_m^{m-1}$ is defined in (94).

Proof. Recall the expression for $\Delta\widehat{H}_n^{W'}|_m^{m-1}$ given in (95)-(97) . With the usual estimates one can show that

$$\left\|\left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2}((95)+(96))\left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2}\phi_P|_{m-1}^n\right\| \leq |g|C\gamma^{\frac{m-1}{2}}. \tag{131}$$

Next, we control the first term in (97). First, observe that

$$\begin{aligned}&\left\|\left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2}(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)})\cdot\Gamma_P|_{m-1}^n\left(\frac{1}{H_P^{W'}|_{m-1}^n - z}\right)^{1/2}\phi_P|_{m-1}^n\right\|^2\\&= \frac{1}{|E'_P|_{m-1}^n - z|}\left\langle(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)})\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n, \left|\frac{1}{H_P^{W'}|_{m-1}^n - z}\right|(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)})\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n\right\rangle.\end{aligned} \tag{132}$$

Second, we recall that $\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)}$ contains boson creation operators restricted to the range $(\tau_m, \tau_{m-1}]$ in momentum space. Therefore,

$$\left\langle\phi_P|_{m-1}^n, \widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)}\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n\right\rangle = 0,$$

which implies

$$(132) \leq \frac{C}{\gamma^m}\left|\left\langle(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)})\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n, \frac{1}{H_P^{W'}|_{m-1}^n - z}(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)})\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n\right\rangle\right| \tag{133}$$

by using the spectral theorem and the gap estimate for $H_P^{W'}|_{m-1}^n \upharpoonright \mathcal{F}|_m^n$. Note further that

$$(\widetilde{A}_{P,m}^{(n)} - A_{P,m-1}^{(n)})\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n = \int dk\,(\alpha_m(\nabla E'_P|_{m-1}^n) - \alpha_{m-1}(\nabla E'_P|_{m-1}^n))b^*(k)k\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n.$$

Using the pull-through formula we get

$$\frac{1}{H_P^{W'}|_{m-1}^n - z}b^*(k) = b^*(k)\frac{1}{H_P^{W'}|_{m-1}^n + \frac{1}{2}k^2 + k\cdot\Gamma_P|_{m-1}^n + |k| - \nabla E'_P|_{m-1}^n\cdot k - z}$$

so that we can rewrite the right-hand side of (133) as follows:

$$\begin{aligned}(133) = \frac{C}{\gamma^m}\int dk\,&\left[\alpha_m(\nabla E'_P|_{m-1}^n) - \alpha_{m-1}(\nabla E'_P|_{m-1}^n)\right]^2\times\\&\times\left\langle k\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n, \frac{1}{H_P^{W'}|_{m-1}^n + \frac{1}{2}k^2 + k\cdot\Gamma_P|_{m-1}^n + |k| - \nabla E'_P|_{m-1}^n\cdot k - z}k\cdot\Gamma_P|_{m-1}^n\phi_P|_{m-1}^n\right\rangle.\end{aligned} \tag{134}$$

In order to expand the resolvent in (134) in terms of $k\cdot\Gamma_P|_{m-1}^n$ we have to provide the bound

$$\left\|\left(\frac{1}{H_P^{W'}|_{m-1}^n + f_{P,m-1}(k) - z}\right)^{1/2}k\cdot\Gamma_P|_{m-1}^n\left(\frac{1}{H_P^{W'}|_{m-1}^n + f_{P,m-1}(k) - z}\right)^{1/2}\right\|_{\mathcal{F}|_m^n} < 1 \tag{135}$$

for $\tau_m < |k| \le \tau_{m-1}$ and $z \in \widehat{\Delta}_m$, where we have defined

$$f_{P,m-1}(k) := \frac{1}{2}k^2 + |k|(1 - \nabla E'_P|^n_{m-1} \cdot \widehat{k}).$$

Recall that

$$\Gamma_P|^n_{m-1} = P^f + A^{(n)}_{P,m-1} + B|^n_0 + B^*|^n_0 - \langle \Pi_P|^n_{m-1} \rangle_{\phi_P|^n_{m-1}}.$$

The necessary estimates are:

1. For $|g|$ sufficiently small, the lower bound

$$f_{P,m-1}(k) - |E'_P|^n_{m-1} - z| > |k| \left(1 - \nabla E'_P|^n_{m-1} \cdot \widehat{k} - \frac{1}{2}\zeta - g^2\gamma^{-1}C\right) > 0 \tag{136}$$

   holds because z belongs to the shifted contour $\widehat{\Delta}_m$ so that

$$|E'_P|^n_{m-1} - z| \le \frac{1}{2}\zeta\tau_m + g^2 C\tau_{m-1}.$$

   The inequality in (136) implies

$$\left\| \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|^2_{\mathcal{F}|^n_{m-1}} \le \frac{1}{|k| \left(1 - \nabla E'_P|^n_{m-1} \cdot \widehat{k} - \frac{1}{2}\zeta - g^2\gamma^{-1}C\right)}.$$

2. By the unitarity of $W_{m-1}(\nabla E'_P|^n_{m-1})$ and using $[B|^n_0, W_{m-1}(\nabla E'_P|^n_{m-1})] = 0$ as well as the standard inequalities (22), we have

$$\left\| k \cdot B|^n_0 \left(\frac{1}{H^{W'}_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \le |g|\ |k|\ C \left\| H^{1/2}_{P,0} \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}}.$$

3. By definition of the transformation $W_{m-1}(\nabla E'_P|^n_{m-1})$ and the transformation formulae (198),

$$W_{m-1}(\nabla E'_P|^n_{m-1})(P - P^f)W_{m-1}(\nabla E'_P|^n_{m-1})^* = P - P^f - A^{(n)}_{P,m-1} - C^{(k,n)}_{P,m-1}$$

   holds on $D(H_{P,0})$. Hence, we have the bound

$$\begin{aligned}
&\left\| k \cdot (P^f + A^{(n)}_{P,m-1}) \left(\frac{1}{H^{W'}_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \\
&\quad \le |k| \left\| (P - P^f) \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \\
&\qquad + |k|(|P| + g^2 C) \left\| \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \\
&\quad \le |k| \sqrt{2} \left\| H^{1/2}_{P,0} \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} \\
&\qquad + |k|(|P| + g^2 C) \left\| \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}}.
\end{aligned}$$

4. Using the a priori estimate (23) in Lemma 3.2 one derives

$$\left\| H_{P,0}^{1/2} \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}}$$
$$\leq \frac{1}{\sqrt{1-|g|c_a}} \left(\left\| (H'_P|^n_{m-1})^{1/2} \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|^2_{\mathcal{F}|^n_{m-1}} + |g|c_b \left\| \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|^2_{\mathcal{F}|^n_{m-1}} \right)^{1/2}.$$

Collecting these estimates, we find:

$$\left\| \left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} k \cdot \Gamma_P|^n_{m-1} \left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \tag{137}$$

$$\leq |k| \left\| \left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \times \tag{138}$$

$$\times \left[\frac{\sqrt{2} + |g|C}{\sqrt{1-|g|c_a}} \left(\left\| (H'_P|^n_{m-1})^{1/2} \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|^2_{\mathcal{F}|^n_{m-1}} + \right.\right.$$
$$\left.\left. + |g|c_b \left\| \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|^2_{\mathcal{F}|^n_{m-1}} \right)^{1/2} + (|P| + g^2 C) \left\| \left(\frac{1}{H_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \right].$$

Note that

$$\left\| (H'_P|^n_{m-1})^{1/2} \left(\frac{1}{H'_P|^n_{m-1} + f_{P,m-1}(k) - z} \right)^{1/2} \right\|_{\mathcal{F}|^n_{m-1}} \leq \left(1 + \frac{|E'_P|^n_{m-1}|}{f_{P,m-1}(k) - |E'_P|^n_{m-1} - z|} \right)^{1/2}.$$

Finally we obtain

$$(137) \leq \frac{1}{\left(1 - \nabla E'_P|^n_{m-1} \cdot \widehat{k} - \frac{1}{2}\zeta - g^2\gamma^{-1}C\right)} \times$$
$$\times \left[\frac{\sqrt{2} + |g|C}{\sqrt{1-|g|c_a}} \left(|E'_P|^n_{m-1}| + \tau_{m-1}\left(1 - \nabla E'_P|^n_{m-1} \cdot \widehat{k} - \frac{1}{2}\zeta - Cg^2\gamma^{-1}\right) + gc_b \right)^{1/2} + (|P| + g^2 C) \right]$$

so that

$$\lim \sup_{|g|,\gamma,\zeta \to 0} (137) \leq \frac{2P_{\max}}{1 - P_{\max}} < \frac{2}{3}$$

for $P_{\max} < \frac{1}{4}$. By continuity, inequality (135) holds for g, ζ, γ in a neighborhood of zero.

Going back to equation (134) we can proceed with the expansion (in $k \cdot \Gamma_P|^n_{m-1}$) of the resolvent:

$$(133) \leq Cg^2\gamma^{m-2} \sup_{\tau_m \leq |k| \leq \tau_{m-1}} \sum_{i,l=1}^{3} \left\langle \left[\left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z}\right)^{1/2}\right]^* \Gamma_P^{(i)}|^n_{m-1}\phi_P|^n_{m-1}, \right. \tag{139}$$

$$\sum_{j=0}^{\infty}\left[\left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z}\right)^{1/2} k \cdot \Gamma_P|^n_{m-1}\left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z}\right)^{1/2}\right]^j \times$$

$$\left. \times \left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z}\right)^{1/2} \Gamma_P^{(l)}|^n_{m-1}\phi_P|^n_{m-1} \right\rangle$$

$$\leq Cg^2\gamma^{m-2}\sum_{i=1}^{3} \sup_{\tau_m \leq |k| \leq \tau_{m-1}} \left\| \left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z}\right)^{1/2} \Gamma_P^{(i)}|^n_{m-1}\phi_P|^n_{m-1} \right\|^2 . \tag{140}$$

Since $f_{P,m-1}(k) \geq 0$ and because of the property $\left\langle \phi_P|^n_{m-1}, \Gamma_P|^n_{m-1}\phi_P|^n_{m-1}\right\rangle = 0$ it follows that

$$\left\| \left(\frac{1}{H_P^{W'}|^n_{m-1} + f_{P,m-1}(k) - z}\right)^{1/2} \Gamma_P^{(i)}|^n_{m-1}\phi_P|^n_{m-1} \right\|^2 \leq C \left| \left\langle \Gamma_P^{(i)}|^n_{m-1}\phi_P|^n_{m-1}, \frac{1}{H_P^{W'}|^n_{m-1} - z}\Gamma_P^{(i)}|^n_{m-1}\phi_P|^n_{m-1} \right\rangle \right| .$$

Combining the estimates in (140) and (131) yields the claim of the lemma. □

Lemma 6.6. *For all $n, m \in \mathbb{N}$ and $Q, Q' \in \mathbb{R}^3$ with $|Q|, |Q'| \leq 1$ the estimate*

$$\|[W_m(Q) - W_m(Q')]\, \Psi'_P|^n_m\| \leq |g|C|Q - Q'|| \ln \tau_m|$$

holds.

Proof. The Bogolyubov transformations W_m defined in (14) can be explicitly written as

$$W_m(Q) = \exp\left(\int dk\, \alpha_m(Q,k)(b(k) - b^*(k))\right),$$

so that

$$\|[W_m(Q) - W_m(Q')]\, \Psi'_P|^n_m\| \leq \left\| \int dk\, [\alpha_m(Q,k) - \alpha_m(Q',k)](b(k) - b^*(k))\, \Psi'_P|^n_m \right\| \tag{141}$$

In order to estimate this term we employ:

1. The identity (12) in [Frö73, Equation (1.26)] that relies on the bound $E'_{P-k}|^n_m - E'_P|^n_m \geq -C_{\nabla E}|k|$, $|P| \leq P_{\max}$, from Corollary 5.4(iii).
2. By definition of α_m it holds
$$\int dk \left|\alpha_m(Q,k) - \alpha_m(Q',k)\right| \frac{1}{|k|^{3/2}} \leq |g|C|Q - Q'|\, |\ln\kappa - \ln\tau_m|.$$
3. $\|\Psi'_P|^n_m\| \leq 1$

With these estimates, the claim is proven. □

Lemma 6.7. *Let $|g|$ be sufficiently small. For $n, m \in \mathbb{N}$ the following estimate holds:*

$$|\nabla E'_P|^n_m - \nabla E'_P|^n_{m-1}| \\ \leq g^2 C \tau^{1/2}_{m-1} + C \sup_{z \in \widehat{\Delta}_m} \left\| \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \Delta \widehat{H}^{W'}_n|^{m-1}_m \left(\frac{1}{H^{W'}_P|^n_{m-1} - z} \right)^{1/2} \phi_P|^n_{m-1} \right\| + C \frac{\|\phi_P|^n_{m-1} - \widetilde{\phi}_P|^n_m\|}{\|\phi_P|^n_{m-1}\|^2 \|\widetilde{\phi}_P|^n_m\|^2}.$$

Proof. Let $n, m \in \mathbb{N}$. Using Lemma 5.9 we have

$$\nabla E'_P|^n_m - \nabla E'_P|^n_{m-1} = \left\langle P^f + B|^n_0 + B^*|^n_0 \right\rangle_{\Psi'_P|^n_{m-1}} - \left\langle P^f + B|^n_0 + B^*|^n_0 \right\rangle_{\Psi'_P|^n_m}$$

which by unitarity of the transformation $W_{m-1}(\nabla E'_P|^n_{m-1})$ and $W_m(\nabla E'_P|^n_{m-1})$ can be rewritten as

$$\nabla E'_P|^n_m - \nabla E'_P|^n_{m-1} = \langle \Pi_P|^n_{m-1} \rangle_{\phi_P|^n_{m-1}} - \left\langle \widetilde{\Pi}_P|^n_m \right\rangle_{\widetilde{\phi}_P|^n_m} + \widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}.$$

We have already noted that $|\widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}| \leq g^2 C \tau_{m-1}$. Moreover, we observe

$$\left| \langle \Pi_P|^n_{m-1} \rangle_{\phi_P|^n_{m-1}} - \left\langle \widetilde{\Pi}_{P,m} \right\rangle_{\widetilde{\phi}_P|^n_m} \right| = \left| \frac{\left\langle \phi_P|^n_{m-1}, \Pi_P|^n_{m-1} \phi_P|^n_{m-1} \right\rangle}{\|\phi_P|^n_{m-1}\|^2} - \frac{\left\langle \widetilde{\phi}_P|^n_m, \widetilde{\Pi}_P|^n_m \widetilde{\phi}_P|^n_m \right\rangle}{\|\widetilde{\phi}_P|^n_m\|^2} \right|$$

$$\leq \|\phi_P|^n_{m-1}\|^{-2} \left| \langle \phi_P|^n_{m-1}, \Pi_P|^n_{m-1} \phi_P|^n_{m-1} \rangle - \left\langle \widetilde{\phi}_P|^n_m, \widetilde{\Pi}_P|^n_m \widetilde{\phi}_P|^n_m \right\rangle \right| + \tag{142}$$

$$+ \left| \left\langle \widetilde{\phi}_P|^n_m, \widetilde{\Pi}_P|^n_m \widetilde{\phi}_P|^n_m \right\rangle \right| \left| \|\phi_P|^n_{m-1}\|^{-2} - \|\widetilde{\phi}_P|^n_m\|^{-2} \right|. \tag{143}$$

We know that the norms $\|\phi_P|^n_{m-1}\|$ and $\|\widetilde{\phi}_P|^n_m\|$ are by construction smaller than one and non-zero. Using Lemma 6.4 we find

$$(143) \leq C \frac{\|\phi_P|^n_{m-1} - \widetilde{\phi}_P|^n_m\|}{\|\phi_P|^n_{m-1}\|^2 \|\widetilde{\phi}_P|^n_m\|^2}.$$

In order to bound the term (142) we use

$$\|\phi_P|^n_{m-1}\|^2 (142) = \left| \left\langle \left(\phi_P|^n_{m-1} - \widetilde{\phi}_P|^n_m \right), \Pi_P|^n_{m-1} \phi_P|^n_{m-1} \right\rangle + \right. \tag{144}$$

$$+ \left\langle \widetilde{\phi}_P|^n_m, \left[\Pi_P|^n_{m-1} - \widetilde{\Pi}_P|^n_m \right] \phi_P|^n_{m-1} \right\rangle + \tag{145}$$

$$\left. + \left\langle \widetilde{\phi}_P|^n_m, \widetilde{\Pi}_P|^n_m \left(\phi_P|^n_{m-1} - \widetilde{\phi}_P|^n_m \right) \right\rangle \right|. \tag{146}$$

The term (145) is bounded by

$$|(145)| \leq \left| \left\langle \widetilde{\phi}_P|^n_m, \left[\widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} \right] \phi_P|^n_{m-1} \right\rangle \right| \leq |g| C \tau^{1/2}_{m-1}$$

because by the standard inequalities (22)

$$\left\|\int dk\; k[\alpha_m(\nabla E'_P|^n_{m-1},k)-\alpha_{m-1}(\nabla E'_P|^n_{m-1},k)]b(k)\phi_P|^n_{m-1}\right\|$$
$$\leq C\left(\int dk\;\left|\frac{k[\alpha_m(\nabla E'_P|^n_{m-1},k)-\alpha_{m-1}(\nabla E'_P|^n_{m-1},k)]}{|k|^{1/2}}\right|^2\right)^{1/2}\left\|(H^f|^{m-1}_m)\left(\frac{1}{H^{W'}_P|^n_{m-1}-i}\right)^{1/2}\phi_P|^n_{m-1}\right\|\leq |g|C\tau^{1/2}_{m-1}.$$

Terms (144) and (146) can be treated in the same way, and we only demonstrate the bound on the former. Using analytic perturbation theory we get

$$\begin{aligned}&\left|\left\langle\left(\phi_P|^n_{m-1}-\widetilde{\phi}_P|^n_m\right),\Pi_P|^n_{m-1}\phi_P|^n_{m-1}\right\rangle\right| &(147)\\
&\leq C\tau_m\sup_{z\in\widehat{\Delta}_m}\sum_{j=1}^{\infty}\left|\left\langle\left[\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\Delta\widehat{H}^{W'}_n|^{m-1}_m\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\right]^j\phi_P|^n_{m-1},\right.\right.\\
&\qquad\left.\left.,\left[\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\right]^*\Pi_P|^n_{m-1}\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\phi_P|^n_{m-1}\right\rangle\right|\\
&\leq C\tau_m\sup_{z\in\widehat{\Delta}_m}\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\Delta\widehat{H}^{W'}_n|^{m-1}_m\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\phi_P|^n_{m-1}\right\|\times\\
&\qquad\times\left\|\left[\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\right]^*\Pi_P|^n_{m-1}\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\right\|_{\mathcal{F}|^n_m}. &(148)\end{aligned}$$

The term in (148) can be controlled similarly to (127) in the ultraviolet regime so that we finally have

$$\left\|\left[\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\right]^*\Pi_P|^n_{m-1}\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\right\|_{\mathcal{F}|^n_m}\leq C\tau^{-1}_m. \tag{149}$$

Combining these results, we obtain the estimate

$$\left|\left\langle\left(\phi_P|^n_{m-1}-\widetilde{\phi}_P|^n_m\right),\Pi_P|^n_{m-1}\phi_P|^n_{m-1}\right\rangle\right|\leq C\sup_{z\in\widehat{\Delta}_m}\left\|\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\Delta\widehat{H}^{W'}_n|^{m-1}_m\left(\frac{1}{H^{W'}_P|^n_{m-1}-z}\right)^{1/2}\phi_P|^n_{m-1}\right\|,$$

which concludes the proof. □

7 Ground States of the Transformed Hamiltonians $H^{W'}_P|^\infty_\infty$

In this section, we finally remove both the UV and the IR cut-off (σ_n and τ_m, respectively). In our study of the removal of the IR cut-off in Section 6 we have proven that

$$\|\phi_P|^n_m-\phi_P|^n_{m-1}\|\leq(m+1)\gamma^{\frac{m}{4}}$$

holds for any $n\in\mathbb{N}$. We shall now provide the analogous bound

$$\|\phi_P|^n_m-\phi_P|^{n-1}_m\|\leq CmK^{3m+1}|\ln\gamma|^{m+1}\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2} \tag{150}$$

as the UV cut-off is shifted from σ_{n-1} to σ_n. The constant $K \geq 1$ will be introduced in Theorem 7.5. The latter bound, derived in Corollary 7.6, holds for any IR cut-off τ_m and uses a particular scaling $\mathbb{N} \ni n := n(m) > \alpha m$ for

$$\alpha := \frac{-\ln|\gamma|}{\ln\beta} \geq 1. \tag{151}$$

These two estimates will enable us to prove the second main result Theorem 2.2 at the end of this section.

Remark 7.1. *In this section we implicitly assume the constraints $|P| < P_{\max}$ and $1 < \kappa < 2$. Furthermore, g, β, and γ are such that all the results of Sections 4, 5 , and 6 hold true.*

In order to control the norm difference $\|\phi_P|_m^n - \phi_P|_m^{n-1}\|$ we notice that for $m \geq 1$ the vectors $\phi_P|_m^n$ can be rewritten in the following way

$$\phi_P|_m^n = W_m(\nabla E'_P|_m^n)\, Q'_P|_m^n W|_m^{m-1}(\nabla E'_P|_{m-1}^n)^* \cdots Q'_P|_2^n W|_2^1(\nabla E'_P|_1^n)^* Q'_P|_1^n\; W|_1^0(\nabla E'_P|_0^n)^* \frac{\Psi'_P|_0^n}{\|\Psi'_P|_0^n\|},$$

where $Q'_P|_m^n$ is defined in (76) and

$$W|_m^{m'}(Q)^* := W_m(Q)^* W_{m'}(Q), \qquad W|_1^0(Q)^* = W_1(Q).$$

The following definition will be convenient.

Definition 7.2. *For $n \in \mathbb{N}$ and $m \geq 1$, we define*

$$\eta_P|_m^n := W_m(\nabla E'_P|_m^n)^* \phi_P|_m^n, \tag{152}$$

and $\eta_P|_0^n := \phi_P|_0^n = \Psi_P|_0^n / \|\Psi_P|_0^n\|$ in the case $m = 0$.

Note that by construction we have the identity

$$\eta_P|_{m+1}^n = Q'_P|_{m+1}^n W|_{m+1}^m (\nabla E'_P|_m^n)^* \eta_P|_m^n, \tag{153}$$

and moreover, since the transformation W_m is unitary and due to Theorem 6.3, the bounds

$$1 \geq \|\phi_P|_m^n\| = \|\eta_P|_m^n\| \geq \frac{1}{2} \tag{154}$$

hold true for all $m, n \in \mathbb{N}$. First, we prove two a priori lemmas that can be combined to yield Theorem 7.5.

Lemma 7.3. *For any $m \in \mathbb{N}$, let $\mathbb{N} \ni n > \alpha m \geq 1$. There exists a constant K_1 such that for $|g|$ sufficiently small the following estimates hold true:*

$$\|\eta_P|_{m+1}^n - \eta_P|_{m+1}^{n-1}\| \leq \|\eta_P|_m^n - \eta_P|_m^{n-1}\| + K_1 \left[\left(\frac{n}{\beta^n \gamma^{m+1}} \right)^{1/2} + \left| \nabla E'_P|_m^n - \nabla E'_P|_m^{n-1} \right| \right]. \tag{155}$$

Proof. By using (152) and (153) we get the bound

$$\left\|\eta_P|^n_{m+1} - \eta_P|^{n-1}_{m+1}\right\| \le \left\|\left(Q'_P|^n_{m+1} - Q'_P|^{n-1}_{m+1}\right) W|^m_{m+1}(\nabla E'_P|^n_m)^* \eta_P|^n_m\right\| \tag{156}$$

$$+ \left\|Q'_P|^{n-1}_{m+1}\left(W|^m_{m+1}(\nabla E'_P|^n_m)^* - W|^m_{m+1}(\nabla E'_P|^{n-1}_m)^*\right)\eta_P|^n_m\right\| \tag{157}$$

$$+ \left\|Q'_P|^{n-1}_{m+1} W|^m_{m+1}(\nabla E'_P|^{n-1}_m)^* \left(\eta_P|^n_m - \eta_P|^{n-1}_m\right)\right\|. \tag{158}$$

Furthermore, the expansion

$$\begin{aligned} Q'_P|^n_{m+1} - Q'_P|^{n-1}_{m+1} = -\frac{1}{2\pi i}\oint_{\Delta_{m+1}} dz \Bigg\{ &\left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2} \times \\ &\times \sum_{j=1}^{\infty}\left[\left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2} \Delta H'|^n_{n-1}\left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2}\right]^j \times \\ &\times \left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2}\Bigg\}, \end{aligned} \tag{159}$$

can be controlled by noting that

$$\left\|\left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2}\right\|^2_{\mathcal{F}|^n_{m+1}} \le \frac{2}{\zeta\tau_{m+1}} \tag{160}$$

(see Lemma 5.5), which yields

$$\sup_{z\in\Delta_{m+1}}\left\|\left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2} \Delta H'|^n_{n-1}\left(\frac{1}{H'_P|^{n-1}_{m+1} - z}\right)^{1/2}\right\|_{\mathcal{F}|^n_{m+1}} \le C|g|\left(\frac{n}{\beta^n\zeta\tau_{m+1}}\right)^{1/2} \tag{161}$$

by a similar computation as for (50). Now, by the choice $n > \alpha m$ and $|g|$ sufficiently small, the right-hand side in (161) is strictly smaller than 1. Hence, we get

$$\|Q'_P|^n_{m+1} - Q'_P|^{n-1}_{m+1}\| \le C|g|\left(\frac{n}{\beta^n\zeta\tau_{m+1}}\right)^{1/2}.$$

Moreover, under the constraint in (68) we get the bound

$$(157) \le C|g||\ln\gamma|\left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right| \le C\left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right|$$

by a similar procedure as used in the proof of Lemma 6.6. The remaining term (158) can be estimated using the unitarity of W_m. This concludes the proof. □

Lemma 7.4. *For any $m \in \mathbb{N}$, let $\mathbb{N} \ni n > \alpha m \ge 1$. There exists a constant K_2 such that for $|g|$ sufficiently small the following estimate holds true:*

$$\left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right| \le K_2\left[\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2} + \|\eta_P|^n_m - \eta_P|^{n-1}_m\| + \left|\nabla E'_P|^n_{m-1} - \nabla E'_P|^{n-1}_{m-1}\right|\right]. \tag{162}$$

Proof. Let us start with the equality

$$\left|\nabla E'_P|_m^n - \nabla E'_P|_m^{n-1}\right| = \left|\left\langle P^f + B|_0^n + B^*|_0^n\right\rangle_{\Psi'_P|_m^n} - \left\langle P^f + B|_0^{n-1} + B^*|_0^{n-1}\right\rangle_{\Psi'_P|_m^{n-1}}\right|. \tag{163}$$

As $\Psi'_P|_m^n$ and $\eta_P|_m^n$ belong to the same ray in $\mathcal{H}_P$, we obtain

$$(163) = \left|\left\langle P^f + B|_0^n + B^*|_0^n\right\rangle_{\eta_P|_m^n} - \left\langle P^f + B|_0^{n-1} + B^*|_0^{n-1}\right\rangle_{\eta_P|_m^{n-1}}\right|.$$

In order to shorten the formulae we define

$$V_n := P^f + B|_0^n + B^*|_0^n$$

so that

$$(163) \le \frac{1}{\|\eta_P|_m^{n-1}\|^2}\left|\langle \eta_P|_m^n, V_n\eta_P|_m^n\rangle - \left\langle \eta_P|_m^{n-1}, V_{n-1}\eta_P|_m^{n-1}\right\rangle\right| \tag{164}$$

$$+ \left|\frac{1}{\|\eta_P|_m^n\|^2} - \frac{1}{\|\eta_P|_m^{n-1}\|^2}\right| \left|\langle \eta_P|_m^n, V_n\eta_P|_m^n\rangle\right|. \tag{165}$$

Furthermore, by the definitions in (82), (83) and (152) we have

$$\left|\langle \eta_P|_m^n, V_n\eta_P|_m^n\rangle\right| = \left|\langle \phi_P|_m^n, \Pi_P|_m^n\phi_P|_m^n\rangle + C_{P,m}^{(k,n)}\|\phi_P|_m^n\|^2\right| \le C\,, \tag{166}$$

where we used Lemma 6.4. Hence, by (154) we get the estimate

$$(165) \le C\frac{\|\eta_P|_m^n - \eta_P|_m^{n-1}\|}{\|\eta_P|_m^n\|^2\|\eta_P|_m^{n-1}\|^2} \le C\|\eta_P|_m^n - \eta_P|_m^{n-1}\|. \tag{167}$$

Next, we proceed with

$$(164) \le C\Big[\left|\left\langle(\eta_P|_m^n - \eta_P|_m^{n-1}), V_n\eta_P|_m^n\right\rangle\right| \tag{168}$$

$$+ \left|\left\langle \eta_P|_m^{n-1}, (V_n - V_{n-1})\eta_P|_m^n\right\rangle\right| \tag{169}$$

$$+ \left|\left\langle \eta_P|_m^{n-1}, V_{n-1}(\eta_P|_m^n - \eta_P|_m^{n-1})\right\rangle\right|\Big]. \tag{170}$$

First, we observe that

$$(169) \le C\left|\left\langle \eta_P|_m^{n-1}, (B|_{n-1}^n + B^*|_{n-1}^n)\eta_P|_m^n\right\rangle\right| \le C\left|E'_P|_m^n - i\right|^{1/2}\left|\left\langle \eta_P|_m^{n-1}, B|_{n-1}^n\left(\frac{1}{H'_P|_m^n - i}\right)^{1/2}\eta_P|_m^n\right\rangle\right|$$

holds. Invoking the standard inequalities in (39) and the boundedness of

$$\left\|H_{P,0}^{1/2}\left(\frac{1}{H'_P|_m^n - i}\right)^{1/2}\right\| \le C\,, \tag{171}$$

which holds by Lemma 3.2, one has

$$\left\| B|^n_{n-1} \left(\frac{1}{H'_P|^n_m - i} \right)^{1/2} \right\|_{\mathcal{F}|^n_m} \leq C|g| \left(\frac{1}{\beta^n} \right)^{1/2}.$$

Hence, since the ground state energies are bounded from above and below by Corollary 5.4,

$$(169) \leq C \left(\frac{1}{\beta^n} \right)^{1/2} \tag{172}$$

holds true. Terms (168) and (170) can be treated similarly. By recalling the identity in (153) we can write

$$\begin{aligned}
(168) &= \left| \left\langle (Q'_P|^n_m W|^{m-1}_m (\nabla E'_P|^n_{m-1})^* \eta_P|^n_{m-1} - Q'_P|^{n-1}_m W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \eta_P|^{n-1}_{m-1}), V_n \eta_P|^n_m \right\rangle \right| \\
&\leq \left| \left\langle (Q'_P|^n_m - Q'_P|^{n-1}_m) W|^{m-1}_m (\nabla E'_P|^n_{m-1})^* \eta_P|^n_{m-1}, V_n \eta_P|^n_m \right\rangle \right| && (173) \\
&\quad + \left| \left\langle Q'_P|^{n-1}_m \left(W|^{m-1}_m (\nabla E'_P|^n_{m-1})^* - W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \right) \eta_P|^n_{m-1}, V_n \eta_P|^n_m \right\rangle \right| && (174) \\
&\quad + \left| \left\langle Q'_P|^{n-1}_m W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \left(\eta_P|^n_{m-1} - \eta_P|^{n-1}_{m-1} \right), V_n \eta_P|^n_m \right\rangle \right|. && (175)
\end{aligned}$$

Observe that

$$\begin{aligned}
&\left\langle Q'_P|^{n-1}_m W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \left(\eta_P|^n_{m-1} - \eta_P|^{n-1}_{m-1} \right), V_n \eta_P|^n_m \right\rangle \\
&\qquad = \left\langle W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \left(\eta_P|^n_{m-1} - \eta_P|^{n-1}_{m-1} \right), Q'_P|^{n-1}_m V_n \eta_P|^n_m \right\rangle \\
&\qquad = \frac{1}{\|\eta_P|^{n-1}_m\|^2} \left\langle W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \left(\eta_P|^n_{m-1} - \eta_P|^{n-1}_{m-1} \right), \eta_P|^{n-1}_m \right\rangle \left\langle \eta_P|^{n-1}_m, V_n \eta_P|^n_m \right\rangle.
\end{aligned}$$

With

$$\begin{aligned}
\left| \left\langle \eta_P|^{n-1}_m, V_n \eta_P|^n_m \right\rangle \right| &\leq C \left| E'_P|^n_m - i \right|^{1/2} \left| \left\langle \eta_P|^{n-1}_m, H^{1/2}_{P,0} \left(\frac{1}{H'_P|^n_m - i} \right)^{1/2} \eta_P|^n_m \right\rangle \right| \\
&\quad + C \left| E'_P|^{n-1}_m - i \right|^{1/2} \left| \left\langle \eta_P|^{n-1}_m, \left(\frac{1}{H'_P|^{n-1}_m - i} \right)^{1/2} H^{1/2}_{P,0} \eta_P|^n_m \right\rangle \right|
\end{aligned}$$

and (171), we obtain the first estimate

$$(175) \leq C \|\eta_P|^n_{m-1} - \eta_P|^{n-1}_{m-1}\| \left| \left\langle \eta_P|^{n-1}_m, V_n \eta_P|^n_m \right\rangle \right| \leq C \|\eta_P|^n_{m-1} - \eta_P|^{n-1}_{m-1}\|.$$

Furthermore, (174) can be bounded by

$$\begin{aligned}
(174) &\leq C \left\| \left(W|^{m-1}_m (\nabla E'_P|^n_{m-1})^* - W|^{m-1}_m (\nabla E'_P|^{n-1}_{m-1})^* \right) \eta_P|^n_{m-1} \right\| \left| \left\langle \eta_P|^{n-1}_m, V_n \eta_P|^n_m \right\rangle \right| \\
&\leq C|g| |\ln \gamma| \left| \nabla E'_P|^n_{m-1} - \nabla E'_P|^{n-1}_{m-1} \right| \leq C \left| \nabla E'_P|^n_{m-1} - \nabla E'_P|^{n-1}_{m-1} \right|
\end{aligned}$$

where the constraints (68) has been used again. Finally, using the resolvent expansion in (159) we get

$$(173) \leq C \tau_m^{\frac{1}{2}} \left(\frac{n}{\beta^n \gamma^m} \right)^{1/2} \left| E'_P|^n_m - i \right|^{1/2} \sup_{z \in \Delta_m} \left\| \left[\left(\frac{1}{H'_P|^{n-1}_m - z} \right)^{1/2} \right]^* V_n \left(\frac{1}{H'_P|^n_m - i} \right)^{1/2} \eta_P|^n_m \right\|$$

and the standard inequalities in (22) and Lemma 3.2 yield

$$(173) \leq C\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2}.$$

Carrying out the same argument for term (170) one obtains

$$(168) + (170) \leq C\left[\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2} + \|\eta_P|^n_m - \eta_P|^{n-1}_m\| + \left|\nabla E'_P|^n_{m-1} - \nabla E'_P|^{n-1}_{m-1}\right|\right]$$

which, together with estimate (172), proves the claim. □

Theorem 7.5. *There exist constants* $K \geq \max(K_1, K_2, 5)$, $g_* > 0$ *and* $\frac{1}{2} > \gamma_* > 0$ *such that for* $|g| \leq g_*$ *and* $\gamma \leq \gamma_*$ *the following estimates hold true for all finite* $n \in \mathbb{N}$ *and* $\mathbb{N} \ni m < n/\alpha$*:*

(i) $\left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right| \leq K^{3m+1}\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2}$.

(ii) $\|\eta_P|^n_m - \eta_P|^{n-1}_m\| \leq K^{3m+1}\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2}$.

Proof. Let $n \in \mathbb{N}$ and fix $K \geq \max(K_1, K_2, 5)$. We prove the claim by induction in m for $m < n/\alpha$. Statements (i)-(ii) for m will be referred to as assumptions A(i)-A(ii) while the same statements for $m+1$ are claims C(i)-C(ii). We recall that $\eta_P|^n_0 \equiv \phi_P|^n_0 \equiv \Psi'_P|^n_0/\|\Psi'_P|^n_0\|$ so that C(i) and C(ii) for $m = 0$ are consequence of (58) and (55) for $|g|$ sufficiently small. The induction step $m \Rightarrow (m+1)$ for $(m+1) < \frac{n}{\alpha}$ is a straightforward consequence of inequalities (162) and (155): For C(i) we estimate

$$\begin{aligned}
\left|\nabla E'_P|^n_{m+1} - \nabla E'_P|^{n-1}_{m+1}\right| &\leq K_2\left[\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2} + \|\eta_P|^n_{m+1} - \eta_P|^{n-1}_{m+1}\| + \left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right|\right] \\
&\leq K_2\Bigg[\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2} + \left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right| \\
&\qquad + \|\eta_P|^n_m - \eta_P|^{n-1}_m\| + K_1\left[\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2} + \left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right|\right]\Bigg] \\
&\leq K(K+1)\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2} + K(K+1)\left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right| \\
&\quad + K\|\eta_P|^n_m - \eta_P|^{n-1}_m\|.
\end{aligned}$$

Hence, A(i) and A(ii) and $\gamma < \frac{1}{2}$ imply

$$\left|\nabla E'_P|^n_{m+1} - \nabla E'_P|^{n-1}_{m+1}\right| \leq K^{3(m+1)+1}\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2}\left[\left(\frac{1}{K^2} + \frac{1}{K^3}\right) + \left(\frac{1}{K} + \frac{1}{K^2}\right) + \frac{1}{K^2}\right],$$

which by the assumption on K proves C(i). For C(ii), using (155) again, we get

$$\begin{aligned}
\|\eta_P|^n_{m+1} - \eta_P|^{n-1}_{m+1}\| &\leq \|\eta_P|^n_m - \eta_P|^{n-1}_m\| + K_1\left[\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2} + \left|\nabla E'_P|^n_m - \nabla E'_P|^{n-1}_m\right|\right] \\
&\leq K^{3(m+1)+1}\left(\frac{n}{\beta^n\gamma^{m+1}}\right)^{1/2}\left[\frac{1}{K^3} + \frac{1}{K^3} + \frac{1}{K^2}\right],
\end{aligned}$$

which by the assumption on K and $\gamma < \frac{1}{2}$ proves C(ii) and concludes the proof. □

Corollary 7.6. *Let $n > \alpha m \geq 1$. For $|g|$ and γ as in Theorem 7.5 the estimate*

$$\|\phi_P|_m^n - \phi_P|_m^{n-1}\| \leq CmK^{3m+1}\left(\frac{n}{\beta^n\gamma^m}\right)^{1/2}$$

holds true.

Proof. By Definition 7.2 and the unitarity of the transformations W_m we have that

$$\|\phi_P|_m^n - \phi_P|_m^{n-1}\| \leq \|[W_m(\nabla E'_P|_m^n) - W_m(\nabla E'_P|_m^{n-1})]\eta_P|_m^n\| + \|\eta_P|_m^n - \eta_P|_m^{n-1}\|. \tag{176}$$

The lower bound on the norm of $\eta_P|_m^n$ in (154) together with Lemma 6.6 and the constraints (68) yield the estimate

$$\|[W_m(\nabla E'_P|_m^n) - W_m(\nabla E'_P|_m^{n-1})]\eta_P|_m^n\| \leq Cm\left|\nabla E'_P|_m^n - \nabla E'_P|_m^{n-1}\right|.$$

The claim then follows from a direct application of Theorem 7.5. □

Before we can prove the second main result, we must show the convergence of the fiber Hamiltonians under the simultaneous removal of the UV and IR cut-off, $H_P^{W'}|_m^{n(m)} \to H_P^{W'}|_\infty^\infty$. For this, we need a slightly faster scaling $n(m)$.

Lemma 7.7. *Under the same assumptions of Theorem 7.5, there exist $\bar{\alpha} \geq \alpha$ such that for any $\mathbb{N} \ni \alpha' > \bar{\alpha}$ and $n(m) = \alpha' m$, the Hamiltonians $(H_P^{W'}|_m^{n(m)})_{m\in\mathbb{N}}$ converge in the norm resolvent sense as $m \to \infty$.*

Proof. The convergence of the resolvent of $H_P^{W'}|_m^{n(m)}$ consists of direct applications of results of Section 4, Section 6 and the present section. Let $z = i\lambda$ with $|\lambda| > 1$. First, we observe that for all $m \in \mathbb{N}$ the range of $(H_P^{W'}|_m^{n(m)} - z)^{-1}$ equals $D(H_{P,0})$ which is dense in $\mathcal{F}$. By the Trotter-Kato Theorem [RS81, Theorem VIII.22] it suffices to prove that the family of resolvents $([H_P^{W'}|_m^{n(m)} - z]^{-1})_{m\in\mathbb{N}}$ is convergent. We begin with

$$\begin{aligned}\left\|\frac{1}{H_P^{W'}|_m^l - z} - \frac{1}{H_P^{W'}|_m^{l-1} - z}\right\| &\leq \left\|\frac{1}{H'_P|_m^l - z} - \frac{1}{H'_P|_m^{l-1} - z}\right\| \\ &+ \left\|\frac{1}{W_m(\nabla E'_P|_m^l)^* H'_P|_m^{l-1} W_m(\nabla E'_P|_m^l) - z} - \frac{1}{W_m(\nabla E'_P|_m^{l-1})^* H'_P|_m^{l-1} W_m(\nabla E'_P|_m^{l-1}) - z}\right\|\end{aligned}$$

where we used unitarity of W_m in the first line. Mimicking Corollary 4.7, the first term is bounded above by

$$C|g|\left(\frac{l}{\beta^l}\right)^{1/2}.$$

With the standard inequalities, the second term is bounded by

$$C|g|\left\|\frac{1}{(H_P|_m^{l-1} - z)^{1/2}}\right\| \cdot \left\|(H^f)^{1/2}\frac{1}{(H_P|_m^{l-1} - z)^{1/2}}\right\| \cdot \frac{1}{\tau_m^{1/2}}\left|\nabla E'_P|_m^l - \nabla E'_P|_m^{l-1}\right|,$$

which can be further bounded by

$$C|g|\frac{1}{|\operatorname{Im} z|}\gamma^{-m/2}K^{3m+1}\left(\frac{l}{\beta^l\gamma^m}\right)^{1/2}$$

with the help of Lemma 3.2 and Theorem 7.5. Hence, it holds

$$\left\| \frac{1}{H_P^{W'}|_m^{n(m)} - z} - \frac{1}{H_P^{W'}|_m^{n(m-1)} - z} \right\| \leq \alpha' C|g|K\,(\alpha' m)^{1/2} \left(\frac{K^3}{\gamma \beta^{\alpha'/2}} \right)^m \tag{177}$$

where

$$\frac{K^3}{\gamma \beta^{\alpha'/2}} < 1$$

for $\alpha' \geq \bar{\alpha}$ and $\bar{\alpha}$ sufficiently large.

Moreover, using the explicit expressions (85), (86), Lemma 3.2, the bound

$$\left| \nabla E'_P|_m^n - \nabla E'_P|_{m-1}^n \right| \leq C\gamma^{m/4} \tag{178}$$

at fixed n from Lemma 6.7, and a resolvent expansion one can show that

$$\begin{aligned} &\left\| \frac{1}{H_P^{W'}|_m^{n(m-1)} - z} - \frac{1}{\widetilde{H}_P^{W'}|_m^{n(m-1)} - z} \right\| \\ &\qquad \leq \frac{C}{|\operatorname{Im} z|} \left\| \left(\frac{1}{H_P^{W'}|_m^{n(m-1)} - z} \right)^{1/2} \left[\widetilde{H}_P^{W'}|_m^{n(m-1)} - H_P^{W'}|_m^{n(m-1)} \right] \left(\frac{1}{H_P^{W'}|_m^{n(m-1)} - z} \right)^{1/2} \right\| \end{aligned} \tag{179}$$

where the right-hand side in (179) can be controlled in terms of (178).

Furthermore, we observe that

$$\left\| \frac{1}{\widetilde{H}_P^{W'}|_m^{n(m-1)} - z} - \frac{1}{H_P^{W'}|_{m-1}^{n(m-1)} - z} \right\| \leq \frac{C|g|\gamma^{(m-1)/2}}{|\operatorname{Im} z|}. \tag{180}$$

by operator estimates similar to those used to control (102).

Finally, for $\alpha' \geq \bar{\alpha}$ and $\bar{\alpha}$ sufficiently large, the estimates in (177),(179) and (180) imply that the family of resolvents $([H_P^{W'}|_m^{n(m)} - z]^{-1})_{m \in \mathbb{N}}$ is a Cauchy sequence in the norm topology, which concludes the proof. □

We can now prove the second main result, namely the convergence of the ground state vectors $\phi_P|_m^n$ as $n, m \to \infty$ with $n \equiv n(m)$.

Proof of Theorem 2.2 in Section 2.

(i) Define

$$\alpha_{\min} := \max \left\{ \left| \frac{6 \ln K - \ln |\gamma|}{\ln \beta} \right|, \bar{\alpha} \right\}. \tag{181}$$

For any $\mathbb{N} \ni \alpha' > \alpha_{\min}$, let $n(m) = \alpha' m$. By Theorem 6.3 and Corollary 7.6 we can estimate

$$\begin{aligned} \|\phi_P|_m^{n(m)} - \phi_P|_{m-1}^{n(m-1)}\| &\leq \|\phi_P|_{m-1}^{n(m-1)} - \phi_P|_m^{n(m-1)}\| + \sum_{l=\alpha'(m-1)}^{\alpha' m} \|\phi_P|_m^l - \phi_P|_m^{l-1}\| \\ &\leq m\gamma^{\frac{m-1}{4}} + \alpha' \left[CmK^{3m+1} \left(\frac{\alpha' m}{\beta^{\alpha'(m-1)}\gamma^m} \right)^{1/2} \right] \\ &\leq m\gamma^{\frac{m-1}{4}} + m^{3/2}\alpha'^{3/2} CK\beta^{\alpha'/2} \left(\frac{K^3}{(\beta^{\alpha'}\gamma)^{1/2}} \right)^m \end{aligned}$$

Due to (181) the term $\frac{K^3}{(\beta^{\alpha'}\gamma)^{1/2}} < 1$ so that $(\phi_P|_m^{n(m)})_{m\in\mathbb{N}}$ is a Cauchy sequence. We denote its limit by $\phi_P|_\infty^\infty$. Finally Theorem 6.3 ensures that the vector $\phi_P|_\infty^\infty$ has norm larger than $\frac{1}{2}$.

(ii) Let $E'_P|_\infty^\infty := \lim_{m\to\infty} E'|_m^\infty$ which exists by Corollary 5.4. By Lemma 7.7 and (i), $E'_P|_\infty^\infty$ is the eigenvalue corresponding to the eigenvector $\phi_P|_\infty^\infty$ of $H_P^{W'}|_\infty^\infty$. Furthermore,

$$\operatorname{Spec}\left(H_P^{W'}|_m^n\right) = \operatorname{Spec}\left(H'_P|_m^n\right) \subseteq [E'_P|_m^n, \infty).$$

By the nonexpansion property of the norm resolvent convergence for self-adjoint operators [RS81, Theorem VIII.24], this implies that $\phi_P|_\infty^\infty$ is ground state of $H_P^{W'}|_\infty^\infty$ and $E'_P|_\infty^\infty$ is the ground state energy.

□

A Proofs of Lemma 3.2 and Corollary 5.4

Proof of Lemma 3.2. Let $\psi \in D(H_{P,0}^{1/2})$. We start with the identity

$$\langle \psi, H_{P,0}\psi \rangle = \langle \psi, H'_P|_m^n \psi \rangle - \langle \psi, \Delta H'_P|_0^n \psi \rangle - \left\langle \psi, g\Phi|_m^0 \psi \right\rangle \tag{182}$$

where

$$\begin{aligned} \langle \psi, \Delta H'_P|_0^n \psi \rangle &= \left\langle \psi, \left[\frac{1}{2}\left((B|_0^n)^2 + (B^*|_0^n)^2 \right) + B^*|_0^n \cdot B|_0^n - (P - P^f) \cdot B|_0^n - B^*|_0^n \cdot (P - P^f) \right] \psi \right\rangle \\ &= \operatorname{Re}\left[\left\langle \psi, (B|_0^n)^2 \psi \right\rangle + \langle B|_0^n \psi, B|_0^n \psi \rangle - 2\left\langle (P - P^f)\psi, B|_0^n \psi \right\rangle \right]. \end{aligned}$$

We denote the number operator of bosons in the momentum range $[\kappa, \sigma_n)$ by

$$N|_0^n := \int_{\mathcal{B}_{\sigma_n}\setminus\mathcal{B}_\kappa} dk\; b(k)^* b(k)$$

and express the vector $\psi \in \mathcal{F}$ as a sequence $(\psi^j)_{j\geq 0}$ of j-particle wave functions $\psi^j \in L^2(\mathbb{R}^{3j}, \mathbb{C})$, $j \geq 1$, and $\psi^0 \in \mathbb{C}$. Following [Nel64, Proof of Lemma 5] it is convenient to consider an estimate of the following type

$$\begin{aligned} \operatorname{Re}\left\langle \psi, (B|_0^n)^2 \psi \right\rangle &= \operatorname{Re}\left\langle (N|_0^n + 3)^{1/2}\psi, (N|_0^n + 3)^{-1/2}(B|_0^n)^2 \psi \right\rangle \\ &\leq \left\| (N|_0^n + 3)^{1/2}\psi \right\| \left\| (N|_0^n + 3)^{-1/2}(B|_0^n)^2 \psi \right\|. \end{aligned} \tag{183}$$

We consider the two norms in (183) separately. For $I \subset \mathbb{R}_0^+$ let $\mathbb{1}_I(k) \equiv \mathbb{1}_I(|k|)$ denote the characteristic function of I. Schwarz's inequality gives

$$
\begin{aligned}
&\left\| (N|_0^n + 3)^{-1/2} \left(B|_0^n\right)^2 \psi \right\|^2 \\
&\quad \leq c_1 g^4 \sum_{j=0}^{\infty} \int dk_1 \ldots \int dk_{j+2} \frac{(j+1)(j+2)\omega(k_{j+1})^{1/2} \mathbb{1}_{[\kappa,\infty)}(k_{j+1}) \omega(k_{j+2})^{1/2} \mathbb{1}_{[\kappa,\infty)}(k_{j+2})}{\sum_{i=1}^{j} \mathbb{1}_{[\kappa,\infty)}(k_i) + 3} \times \\
&\qquad\qquad \times \left| \psi^{(j+2)}(k_1 \ldots k_{j+2}) \right|^2 \\
&\quad = c_1 g^4 \sum_{j=0}^{\infty} \int dk_1 \ldots \int dk_{j+2} \frac{(j+1)(j+2)\omega(k_{j+1})^{1/2} \omega(k_{j+2})^{1/2} \mathbb{1}_{[\kappa,\infty)}(k_{j+1}) \mathbb{1}_{[\kappa,\infty)}(k_{j+2})}{\sum_{i=1}^{j+2} \mathbb{1}_{[\kappa,\infty)}(k_i) + 1} \times \\
&\qquad\qquad \times \left| \psi^{(j+2)}(k_1 \ldots k_{j+2}) \right|^2 \\
&\quad \leq c_1 g^4 \sum_{j=0}^{\infty} \int dk_1 \ldots \int dk_{j+2} (j+1)(j+2) \frac{1}{2} \left[\omega(k_{j+1}) \mathbb{1}_{[\kappa,\infty)}(k_{j+2}) + \omega(k_{j+2}) \mathbb{1}_{[\kappa,\infty)}(k_{j+1}) \right] \times \\
&\qquad\qquad \times \frac{\left| \psi^{(j+2)}(k_1 \ldots k_{j+2}) \right|^2}{\sum_{i=1}^{j+2} \mathbb{1}_{[\kappa,\infty)}(k_i) + 1}. \qquad (184)
\end{aligned}
$$

for an n-independent and finite constant

$$
c_1 := \left(\int dk \left| k \frac{\rho(k)}{\frac{|k|^2}{2} + \omega(k)} \frac{\mathbb{1}_{[\kappa,\infty)}(k)}{\omega(k)^{1/4}} \right|^2 \right)^{1/2}.
$$

Using the symmetry we get

$$
\begin{aligned}
(184) &= g^4 c_1 \sum_{j=0}^{\infty} \int dk_1 \ldots \int dk_{j+2} \sum_{l=1}^{j+2} \sum_{m \neq l} \omega(k_l) \mathbb{1}_{[\kappa,\infty)}(k_m) \frac{\left| \psi^{(j+2)}(k_1 \ldots k_{j+2}) \right|^2}{\sum_{i=1}^{j+2} \mathbb{1}_{[\kappa,\infty)}(k_i) + 1} \\
&\leq g^4 c_1 \sum_{j=0}^{\infty} \int dk_1 \ldots \int dk_{j+2} \left[\sum_{l=1}^{j+2} \omega(k_l) \right] \frac{\sum_{m=1}^{j+2} \mathbb{1}_{[\kappa,\infty)}(k_m)}{\sum_{i=1}^{j+2} \mathbb{1}_{[\kappa,\infty)}(k_i) + 1} \left| \psi^{(j+2)}(k_1 \ldots k_{j+2}) \right|^2 \\
&\leq g^4 c_1 \left\| \left(H^f \right)^{1/2} \psi \right\|^2.
\end{aligned}
$$

For the remaining term in (183) we compute

$$
\langle \psi, (N|_0^n + 3)\psi \rangle \leq \frac{1}{\kappa} \left\langle \psi, H^f \psi \right\rangle + 3 \langle \psi, \psi \rangle. \qquad (185)
$$

Moreover, we estimate

$$
\left| \left\langle \psi, (P - P^f) B|_0^n \psi \right\rangle \right| \leq \|(P - P^f)\psi\| \, \|B|_0^n \psi\| \leq \sqrt{2} \|H_{P,0}^{1/2} \psi\| \, \|B|_0^n \psi\| \qquad (186)
$$

where by the standard inequalitites in (39)

$$
\|B|_0^n \psi\| \leq |g| c_2 \|(H^f)^{1/2} \psi\| \qquad (187)
$$

holds true for an n-independent and finite constant

$$c_2 := \left(\int dk \, \left| k \frac{\rho(k)}{\frac{|k|^2}{2} + \omega(k)} \frac{\mathbb{1}_{[\kappa,\infty)}(k)}{\omega(k)^{1/2}} \right|^2 \right)^{1/2} .$$

Finally, using the standard inequalities in (22) again, we find

$$\left| \left\langle \psi, g\Phi|_m^0 \psi \right\rangle \right| \leq 2|g|c_3 \, \|\psi\| \, \|(H^f)^{1/2}\psi\| \leq |g|c_3 \left(\langle \psi, H_{P,0}\psi \rangle + \langle \psi, \psi \rangle \right) \tag{188}$$

for an m-independent and finite constant

$$c_3 := \left(\int dk \, \left| \frac{\rho(k)\mathbb{1}_{[0,\kappa)}(k)}{\omega(k)^{1/2}} \right| \right)^{1/2}$$

Hence, for $|g| \leq 1$ the identity (182) and the estimates (183)-(188) yield the bound

$$\left| \langle \psi, \Delta H'_P|_0^n \psi \rangle \right| + \left| \left\langle \psi, g\Phi|_m^0 \psi \right\rangle \right| \leq |g| \left[c_a \langle \psi, H_{P,0}\psi \rangle + c_b \langle \psi, \psi \rangle \right] \tag{189}$$

for m and n-independent positive constants c_a and c_b. For $|g| < \frac{1}{c_a}$ inequality (189) proves the claim. □

Proof of Corollary 5.4.

(i) We note that $E'_P|_m^n \leq \left\langle \Omega, H'_P|_m^n \Omega \right\rangle = \frac{P^2}{2}$ and, furthermore, by applying Lemma 3.2 we observe that for any $\phi \in D(H_{P,0}^{1/2})$, $\|\phi\| = 1$,

$$0 \leq (1 - |g|c_a) \langle \phi, H_{P,0}\phi \rangle \leq \langle \phi, H'_P|_m^n \phi \rangle + |g|c_b.$$

(ii) First we study the case $|k| < 1$ where we follow a strategy similar to [CFP09, Section VI]:

$$\begin{aligned} E'_{P-k}|_m^n - E'_P|_m^n &= \inf_{\|\varphi\|=1} \left[\langle \varphi, (H'_{P-k}|_m^n - H'_P|_m^n)\varphi \rangle + \langle \varphi, H'_P|_m^n \varphi \rangle - E'_P|_m^n \right] \\ &\geq \inf_{\|\varphi\|=1} \left[\frac{k^2}{2} - |k| \left| \left\langle \varphi, (P - P^f + B|_0^n + B^*|_0^n)\varphi \right\rangle \right| + \langle \varphi, H'_P|_m^n \varphi \rangle - E'_P|_m^n \right] \end{aligned}$$

where the infimum is meant to be taken over $\varphi \in D(H_{P,0}^{1/2}) \cap \mathcal{F}|_m^n$ only. By the standard estimates (39) we get

$$\left| \left\langle \varphi, (P - P^f + B|_0^n + B^*|_0^n)\varphi \right\rangle \right| \leq (\sqrt{2} + 2|g|C) \|H_{P,0}^{1/2}\varphi\| \tag{190}$$

where C does not depend on n since $B^*|_0^n$ can be seen to act to the left as $B|_0^n$ and the integral in (39) converges for any $n \in \mathbb{N} \cup \{\infty\}$. Using Lemma 3.2 it turns out that $E'_{P-k}|_m^n - E'_P|_m^n$ is bounded from below by

$$\begin{aligned} &\inf_{\|\varphi\|=1} \left[\frac{k^2}{2} - |k| \frac{\sqrt{2} + 2C|g|}{\sqrt{1 - |g|c_a}} \sqrt{\left\langle \varphi, H'_P|_m^n \varphi \right\rangle + |g|c_b} + \langle \varphi, H'_P|_m^n \varphi \rangle - E'_P|_m^n \right] \\ &\qquad \geq \inf_{\lambda \geq 0} \left[\frac{k^2}{2} - |k| \frac{\sqrt{2} + 2C|g|}{\sqrt{1 - |g|c_a}} \sqrt{\lambda + E'_P|_m^n + |g|c_b} + \lambda \right] =: \inf_{\lambda \geq 0} f(\lambda) \end{aligned}$$

where

$$f(\lambda) := \frac{k^2}{2} - |k| \, \frac{\sqrt{2} + 2C|g|}{\sqrt{1 - |g|c_a}} \, \sqrt{\lambda + E'_P|_m^n + |g|c_b} + \lambda \tag{191}$$

The infimum can be attained either at $\lambda^* = 0$ or at λ^* such that $f'(\lambda^*) = 0$, i.e.

$$\lambda^* = \frac{|k|^2}{4} \frac{(\sqrt{2} + 2C|g|)^2}{1 - |g|c_a} - (E'_P|_m^n + |g|c_b) \tag{192}$$

Case $\lambda^* = 0$: Since

$$f(0) \geq -|k| \frac{\sqrt{2} + 2C|g|}{\sqrt{1 - |g|c_a}} \sqrt{E'_P|_m^n + |g|c_b}$$

and, by claim (ii),

$$0 \leq E'_P|_m^n + |g|c_b \leq \frac{P^2}{2} + |g|c_b \leq \frac{P_{\max}^2}{2} + |g|c_b \, ,$$

we obtain the lower bound

$$f(0) \geq -|k| \frac{\sqrt{2} + 2C|g|}{\sqrt{1 - |g|c_a}} \left(\frac{P_{\max}}{\sqrt{2}} + O(|g|) \right) = -|k| P_{\max} \left(1 + O(|g|)\right) . \tag{193}$$

Case $\lambda^* > 0$: To evaluate

$$f(\lambda^*) = \frac{k^2}{2} \left(1 - \frac{1}{2} \frac{(\sqrt{2} + 2C|g|)^2}{1 - |g|c_a} \right) - (E'_P|_m^n + |g|c_b)$$

we consider that λ^* given in (192) is assumed to be larger than zero. This implies that

$$f(\lambda^*) > \frac{k^2}{2} \left(1 - \frac{(\sqrt{2} + 2C|g|)^2}{1 - |g|c_a} \right) = -k^2 \left(\frac{1}{2} + O(g) \right) > -|k| \left(\frac{1}{2} + O(g) \right) \tag{194}$$

where we have used that $|k| < 1$.

Recall that $P_{\max} = \frac{1}{4}$. Therefore, taking the minimum of both lower bounds (193) and (194) for $|g|$ sufficiently small proves that, for all $|k| < 1$,

$$E'_{P-k}|_m^n - E'_P|_m^n \geq -c|k| \, , \tag{195}$$

for any $c > \frac{1}{2}$, and in particular for $c = C_{\nabla E} := \frac{3}{4}$.
For the case $|k| \geq 1$ Theorem 3.1 implies:

$$E'_{P-k}|_m^n - E'_P|_m^n = (E'_{P-k}|_m^n - E'_0|_m^n) + (E'_0|_m^n - E'_P|_m^n) \geq E'_0|_m^n - E'_P|_m^n \tag{196}$$

$$\geq -C_{\nabla E}|P_{\max}| \geq -C_{\nabla E}|k|, \tag{197}$$

where the step from (196) to (197) is justified by invoking the result in the case $|k| < 1$, i.e., by replacing $k = P$ in (195) .

(iii) Let $\Psi'_P|_m^n$ be the eigenvector corresponding to $E'_P|_m^n$, then we get

$$E'_P|_m^{n+1} \leq \left\langle \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \otimes \Omega, [H'_P|_0^n + \Delta H'_P|_n^{n+1} + g\Phi|_m^0] \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \otimes \Omega \right\rangle = \left\langle \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|}, H'_P|_0^n \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \right\rangle = E'_P|_m^n$$

as well as

$$E'_P|_{m+1}^n \leq \left\langle \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \otimes \Omega, [H'_P|_m^n + g\Phi|_{m+1}^m] \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \otimes \Omega \right\rangle = \left\langle \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|}, H'_P|_m^n \frac{\Psi'_P|_m^n}{\|\Psi'_P|_m^n\|} \right\rangle = E'_P|_m^n.$$

□

B Transformed Hamiltonians: derivation of identities (85), (86) and (92)

Derivation of identity (85). Let $n, m \in \mathbb{N}$. Recalling (6) we can start with the expression

$$\begin{aligned} H'_P|_m^n = \frac{1}{2}\left(P - P^f\right)^2 + H^f + \frac{1}{2}[(B|_0^n)^2 + (B^*|_0^n)^2] + B^*|_0^n \cdot B|_0^n \\ - (P - P^f) \cdot B|_0^n - B^*|_0^n \cdot (P - P^f) + g\Phi|_m^0. \end{aligned}$$

This Hamiltonian can be written in the form

$$H'_P|_m^n = \frac{1}{2}\left(P - P^f - B|_0^n - B^*|_0^n\right)^2 + H^f + g\Phi|_m^0 + S_{P,n}$$

where we collected terms acting in the ultraviolet region in

$$S_{P,n} := -\frac{1}{2}\left([B|_0^n, P - P^f] + [P - P^f, B^*|_0^n] + [B|_0^n, B^*|_0^n]\right).$$

The conjugation by $W_m(\nabla E'_P|_m^n)$ on these various terms reads

$$\begin{aligned} W_m(\nabla E'_P|_m^n)\, P^f\, W_m(\nabla E'_P|_m^n)^* &= P^f + A_{P,m}^{(n)} + C_{P,m}^{(k,n)} \\ W_m(\nabla E'_P|_m^n)\, H^f\, W_m(\nabla E'_P|_m^n)^* &= H^f + L_{P,m}^{(n)} + C_{P,m}^{(\omega,n)} \\ W_m(\nabla E'_P|_m^n)\, \Phi|_m^0\, W_m(\nabla E'_P|_m^n)^* &= \Phi|_m^0 + C_{P,m}^{(\rho,n)} \\ W_m(\nabla E'_P|_m^n)\, S_{P,n}\, W_m(\nabla E'_P|_m^n)^* &= S_{P,n} \end{aligned} \tag{198}$$

for

$$L_{P,m}^{(n)} := \int dk\, \omega(k)\, \alpha_m(\nabla E'_P|_m^n, k)[b(k) + b^*(k)].$$

and $A_{P,m}^{(n)}, C_{P,m}^{(k,n)}, C_{P,m}^{(\omega,n)}, C_{P,m}^{(\rho,n)}$ given in equations (82).

Using these formulae we find

$$\begin{aligned} W_m(\nabla E'_P|_m^n)\, H'_P|_m^n\, W_m(\nabla E'_P|_m^n)^* = \frac{1}{2}\Big(P - P^f - A_{P,m}^{(n)} - B|_0^n - B^*|_0^n - C_{P,m}^{(k,n)}\Big)^2 \\ + \left(H^f + L_{P,m}^{(n)} + C_{P,m}^{(\omega,n)}\right) + \left(g\Phi|_m^0 + C_m^{(\rho)}\right) + S_{P,n}. \end{aligned}$$

Applying the identity (79) we further have

$$P = \nabla E'_P|^n_m + \left\langle [P^f + B|^n_0 + B^*|^n_0] \right\rangle_{\Psi'_P|^n_m} = \nabla E'_P|^n_m + \left\langle P^f + A^{(n)}_{P,m} + B|^n_0 + B^*|^n_0 \right\rangle_{W_m \Psi'_P|^n_m} + C^{(k,n)}_{P,m}$$
$$= \nabla E'_P|^n_m + \langle \Pi_P|^n_m \rangle_{\phi_P|^n_m} + C^{(k,n)}_{P,m}\,, \tag{199}$$

so that we obtain

$$\begin{aligned} &W_m(\nabla E'_P|^n_m)\; H'_P|^n_m \; W_m(\nabla E'_P|^n_m)^* \\ &\quad= \frac{1}{2}\left(\nabla E'_P|^n_m + \left\langle P^f + A^{(n)}_{P,m} + B|^n_0 + B^*|^n_0 \right\rangle_{\phi_P|^n_m} - \left(P^f + A^{(n)}_{P,m} + B|^n_0 + B^*|^n_0\right)\right)^2 \\ &\quad\quad + H^f + L^{(n)}_{P,m} + C^{(\omega,n)}_{P,m} + g\Phi|^\kappa_{\tau_m} + C^{(\rho)}_m + S_{P,n} \\ &\quad= \frac{1}{2}\Gamma_P|^{n\,2}_m + \frac{1}{2}\nabla E'_P|^{n\,2}_m \\ &\quad\quad + \nabla E'_P|^n_m \cdot \left(\left\langle P^f + A^{(n)}_{P,m} + B|^n_0 + B^*|^n_0 \right\rangle_{\phi_P|^n_m} - \left(P^f + A^{(n)}_{P,m} + B|^n_0 + B^*|^n_0\right)\right) \\ &\quad\quad + H^f + L^{(n)}_{P,m} + C^{(\omega,n)}_{P,m} + g\Phi|^\kappa_{\tau_m} + C^{(\rho,n)}_{P,m} + S_{P,n}. \end{aligned}$$

The transformation W_m was designed to yield the following cancellation

$$-\nabla E'_P|^n_m \cdot A^{(n)}_{P,m} + L_m + g\Phi|^\kappa_{\tau_m} = 0. \tag{200}$$

Hence, using the abbreviations introduced in the beginning of Section 6, we finally arrive at the form

$$H^{W'}_P|^n_m := W_m(\nabla E'_P|^n_m)\; H'_P|^n_m \; W_m(\nabla E'_P|^n_m)^* = \frac{1}{2}\Gamma_P|^{n\,2}_m + H^f - \nabla E'_P|^n_m \cdot P^f + C^{(n)}_{P,m} + R_P|^n_m. \tag{201}$$

By analogous methods as in [Nel64] for the ultraviolet region it can then we verified that this equality actually holds on $D(H_{P,0})$. □

Derivation of Identity (86). From the definition of $\widetilde{H}^{W'}_P|^n_m$, we can write

$$\widetilde{H}^{W'}_P|^n_m = W_m(\nabla E'_P|^n_{m-1})\; W_{m-1}(\nabla E'_P|^n_{m-1})^* \; [H^{W'}_P|^n_{m-1} + g\Phi|^{m-1}_m]\; W_{m-1}(\nabla E'_P|^n_{m-1})\; W_m(\nabla E'_P|^n_{m-1})^*$$

which by virtue of the formulae (198) as well as identity (201) gives

$$\begin{aligned} \widetilde{H}^{W'}_P|^n_m = {} & \frac{1}{2}\left(\Gamma_P|^n_{m-1} + \widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} + \widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}\right)^2 \\ & + H^f + \widetilde{L}^{(n)}_{P,m} - L_{P,m-1} + \widetilde{C}^{(\omega,n)}_{P,m} - C^{(\omega,n)}_{P,m-1} \\ & - \nabla E'_P|^n_{m-1} \cdot \left(P^f + \widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} + \widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}\right) \\ & + g\Phi|^0_m + \widetilde{C}^{(\rho,n)}_{P,m} - C^{(\rho,n)}_{P,m-1} + C^{(n)}_{P,m-1} + R_P|^n_{m-1} \end{aligned}$$

for

$$\widetilde{L}^{(n)}_{P,m} := \int dk\; \omega(k)\; \alpha_m(\nabla E'_P|^n_{m-1}, k)[b(k) + b^*(k)].$$

Due to the cancellation (200) and

$$\widetilde{C}^{(k,n)}_{P,m} = C^{(k,n)}_{P,m-1} - \nabla E'_P|^n_{m-1} \cdot \left(\widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}\right) + \widetilde{C}^{(\omega,n)}_{P,m} - C^{(\omega,n)}_{P,m-1} + \widetilde{C}^{(\rho,n)}_{P,m} - C^{(\rho,n)}_{P,m-1}$$

we finally obtain

$$\widetilde{H}^{W'}_P|^n_m = \frac{1}{2}(\Gamma_P|^n_{m-1} + \widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} + \widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1})^2 + H^f - \nabla E'_P|^n_{m-1} \cdot P^f + \widetilde{C}^{(n)}_{P,m} + R_P|^n_{m-1}.$$

One can verify that this identity holds on $D(H_{P,0})$. □

Derivation of Identity (92). By definitions (84) and (88),

$$\widetilde{\Gamma}_P|^n_m - \Gamma_P|^n_{m-1} = \langle \Pi_P|^n_m \rangle_{\phi_P|^n_{m-1}} - \left\langle \widetilde{\Pi}_P|^n_m \right\rangle_{\widetilde{\phi}_P|^n_m} + \widetilde{\Pi}_P|^n_m - \Pi_P|^n_m.$$

so that (199) yields

$$\widetilde{\Gamma}_P|^n_m - \Gamma_P|^n_{m-1} = \nabla E'_P|^n_m - \nabla E'_P|^n_{m-1} + \widetilde{A}^{(n)}_{P,m} - A^{(n)}_{P,m-1} + \widetilde{C}^{(k,n)}_{P,m} - C^{(k,n)}_{P,m-1}.$$

One can verify that this identity holds on $D(H_{P,0})$. □

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Ultraviolet Properties of the Spinless, One-Particle Yukawa Model

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Abstract

We consider the one-particle sector of the spinless Yukawa model, which describes the interaction of a nucleon with a real field of scalar massive bosons (neutral mesons). The nucleon as well as the mesons have relativistic dispersion relations. In this model we study the dependence of the nucleon mass shell on the ultraviolet cut-off Λ. For any finite ultraviolet cut-off the nucleon one-particle states are constructed in a bounded region of the energy-momentum space. We identify the dependence of the ground state energy on Λ and the coupling constant. More importantly, we show that the model considered here becomes essentially trivial in the limit $\Lambda \to \infty$ regardless of any (nucleon) mass and self-energy renormalization. Our results hold in the small coupling regime.

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Contents

1 Introduction and Definition of the Model

The Yukawa theory provides an effective description of the strong nuclear forces between massive nucleons which are mediated by mesons. The nucleons as well as the mesons have relativistic dispersion relations. It is well-known that the Yukawa theory is plagued by ultraviolet divergences, and so far the fully relativistic model has only been constructed in 1 + 1 dimensions; see [11] and references therein for the details.

In this paper we consider a toy model of the Yukawa theory, referred to as *spinless, one-particle Yukawa model,* obtained by neglecting pair-creation and spin, and we restrict the analysis to the one-nucleon sector. In order to yield a well-defined Hamiltonian for this model one usually introduces a cut-off which removes the problematic meson momenta from the interaction term above a finite threshold energy Λ. While for non-relativistic situations one may argue that a cut-off Λ of the order of the nucleon rest mass should render a satisfying predictive power of the model, a finite cut-off is not justified in the relativistic regime. Though the model we deal with is a caricature of the relativistic interaction between nucleons and mesons, we address the mathematical problem how to control the model uniformly in Λ beyond perturbation theory.

More specifically, we analyze the effect of self-energy and mass renormalization in the limit $\Lambda \to \infty$. It is a common hope that at least for non-relativistic QED, i.e., for the Pauli-Fierz Hamiltonian, the ultraviolet cut-off can possibly be removed by introducing a suitable mass and energy renormalization; see [13]. The believe is that, in contrast to classical electrodynamics where the electron bare mass is sent to negative infinity, in non-relativistic QED the bare mass should tend to zero as $\Lambda \to \infty$ to compensate for the growing electrodynamic mass. Our results show that because of the relativistic dispersion relation of the nucleon this is not the case for the spinless, one-particle Yukawa model. Namely, in a neighborhood of the origin of the (total) momentum space and for small values of the coupling constant, we establish two goals:

1. We identify the dependence of the ground state energy on Λ and the coupling constant g.

2. We show that the nucleon mass shell becomes flat in the limit $\Lambda \to \infty$ up to corrections estimated to be $O_{g\to 0}(|g|^{\frac{1}{2}})$, irrespectively of any scaling of the (nucleon) bare mass m, i.e., $m \equiv m(\Lambda) > 0$.

Our analysis is based on a multi-scale technique which was developed in [12] to treat the infrared divergence of the Nelson model, and which was recently refined in [1] to simultaneously control the infrared and ultraviolet divergences of the same model. We extend this multi-scale technique further and apply it to the spinless, one-particle Yukawa model.

It is interesting to note that for this model the self-energy diverges linearly for $\Lambda \to \infty$ as it is the case for its classical analogue.

Definition of the Model. The Hilbert space of the model is

$$\mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}; dx) \otimes \mathcal{F}(h),$$

where $\mathcal{F}(h)$ is the Fock space of scalar bosons

$$\mathcal{F}(h) := \bigoplus_{j=0}^{\infty} \mathcal{F}^{(j)}, \qquad \mathcal{F}^{(0)} := \mathbb{C}, \qquad \mathcal{F}^{j\geq 1} := \bigodot_{l=1}^{j} h, \qquad h := L^2(\mathbb{R}^3, \mathbb{C}; dk)$$

where $\odot$ denotes the symmetric tensor product. Let $a(k), a^*(k)$ be the usual Fock space annihilation and creation operators satisfying the canonical commutation relations (CCR)

$$[a(k), a(q)^*] = \delta(k-q), \qquad [a(k), a(q)] = 0 = [a(k)^*, a^*(q)], \qquad \forall k, q \in \mathbb{R}^3.$$

The kinematics of the system is described by: (a) The position x and the momentum p of the nucleon that satisfy the Heisenberg commutation relations. (b) The real scalar field Φ and its conjugate momentum.

The dynamics is generated by the Hamiltonian

$$H|_{\kappa}^{\Lambda} := \sqrt{p^2 + m^2} + H^f + g\Phi|_{\kappa}^{\Lambda}(x) \tag{1}$$

where:

- m is the nucleon mass;
- $g \in \mathbb{R}$ is the coupling constant;
- $$H^f := \int dk\, \omega(k) a^*(k) a(k), \qquad \omega(k) \equiv \omega(|k|) := \sqrt{|k|^2 + \mu^2},$$
  is the free field Hamiltonian with μ being the meson mass;
- the interaction term is given by
  $$\Phi|_{\kappa}^{\Lambda}(x) := \phi|_{\kappa}^{\Lambda}(x) + \phi^*|_{\kappa}^{\Lambda}(x), \qquad \phi|_{\kappa}^{\Lambda}(x) := \int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\kappa} dk\, \rho(k) a(k) e^{ikx}, \qquad \rho(k) := \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}} \tag{2}$$
  for $0 \le \kappa < \Lambda$, and for the domain of integration we use the notation $\mathcal{B}_\sigma := \{k \in \mathbb{R}^3 \mid |k| < \sigma\}$ for any $\sigma > 0$;
- we use units such that $\hbar = c = 1$.

Note that for $\Lambda = \infty$ the formal expression of the interaction $\Phi|_{\kappa}^{\Lambda}(x)$ is not a well-defined operator on $\mathcal{H}$ because the form factor $\rho(k)$ is not square integrable. It is well-known (see also Proposition 1.1 below) that for $0 \le \kappa < \Lambda < \infty$ the operator $H|_{\kappa}^{\Lambda}$ is self-adjoint and its domain coincides with the one of $H^{(0)} := \sqrt{p^2 + m^2} + H^f$

We briefly recall some well-known facts about this model. The total momentum operator of the system is

$$P := p + P^f := p + \int dk\, a^*(k) a(k) \tag{3}$$

where P^f is the field momentum. Due to translational invariance of the system the Hamiltonian and the total momentum operator commute. Hence, the Hilbert space $\mathcal{H}$ can be decomposed on the joint spectrum of the three components of the total momentum operator, i.e.,

$$\mathcal{H} = \int^{\oplus} dP\, \mathcal{H}_P$$

here $\mathcal{H}_P$ is a copy of the Fock space $\mathcal{F}$ carrying the (Fock) representation corresponding to annihilation and creation operators

$$b(k) := a(k) e^{ikx}, \quad b^*(k) := a^*(k) e^{-ikx}.$$

We will use the same symbol $\mathcal{F}$ for all Fock spaces. The fiber Hamiltonian can be expressed as

$$H_P|_\kappa^\Lambda := \sqrt{(P - P^f)^2 + m^2} + H^f + g\Phi|_\kappa^\Lambda$$

where

$$\Phi|_\kappa^\Lambda := \phi|_\kappa^\Lambda + \phi^*|_\kappa^\Lambda, \qquad \phi|_\kappa^\Lambda := \int_{\mathcal{B}_\Lambda \setminus \mathcal{B}_\kappa} dk\, \rho(k) b(k),$$

and

$$H^f = \int dk\, \omega(k) b^*(k) b(k), \qquad P^f = \int dk\, k b^*(k) b(k).$$

By construction, the fiber Hamiltonian maps its domain in $\mathcal{H}_P$ into $\mathcal{H}_P$. Finally, for later use we define

$$H_P^{(0)} := H_P^{nuc} + H^f, \qquad H_P^{nuc} := \sqrt{(P - P^f)^2 + m^2}.$$

We restrict our study to the **model parameters**:

$$m > 0, \qquad \mu > 1, \qquad 0 < |g| \leq 1, \qquad 0 < \kappa \leq 1 < \Lambda < \infty, \qquad 0 < P_{max} < \frac{1}{2}, \qquad |P| < P_{max}.$$

The choice $\mu > 1$ and P_{max} less than one is only a technical artifact of the crude estimate (14) in the proof of Lemma 3.1 which provides an easy spectral gap estimate in Lemma 3.3 that we employ in the multi-scale analysis.

Concerning previous results on the spinless, one-particle Yukawa model we refer the reader to [2, 3, 4, 14]. In [2] Eckmann considers the spinless Yukawa model without pair-creation with a regularization of the meson form factor. In contrast to our choice given in (2) the interaction term in his Hamiltonian is given by

$$\int_{|p|,|k|,|p-k| \leq \Lambda} dp \int dk \frac{n^*(p-k)\, a^*(k)\, n(p)}{\sqrt{((p-k)^2 + \mu^2)^{1/2}(k^2 + \mu^2)^{1/2}(p^2 + \mu^2)^{1/2}}} + h.c.$$

where $n^*(p)$ and $n(p)$ denote the nucleon creation and annihilation operators. This implies that the Hamiltonian renormalized by means of a mass operator (for details see [2]) converges in the norm resolvent sense as $\Lambda \to \infty$. Furthermore, in [2] the one-particle scattering states are constructed in the small coupling regime. Also Fröhlich [4] studied the spinless, one-particle Yukawa model but with the meson form factor $\frac{\rho(k)}{|k|^{1/2}}$, for which he showed that the Hamiltonian including a logarithmically divergent self-energy renormalization constant is well defined in the limit $\Lambda \to \infty$ and that the nucleon mass shell is non-trivial.

The behavior of the ground state energy for $\Lambda \to \infty$ has been addressed in [10] and [6] for non-relativistic and pesudo-relativistic QED models. In particular, in [10], for the relativistic dispersion relation the electron self-energy has been proven to obey the same type of dependence on Λ as in our model, but without the restriction to the small coupling regime. Perturbative mass renormalization in non-relativistic QED has been addressed in [7]. Furthermore, mass renormalization based on the binding energy of hydrogen has been discussed in models of quantum electrodynamics in [9].

We also want to mention [8] for a recent application of the iterative analytic perturbation theory to the so-called semi-relativistic Pauli-Fierz model that focusses on the infrared corrections to the electron mass shell.

Notation.

1. The symbol C denotes any positive universal constant and may change its value from line to line.
2. The components of a vector $v \in \mathbb{R}^3$ are denoted by $v = (v_1, v_2, v_3)$.
3. The bars $|\cdot|$, $\|\cdot\|$ denote the euclidean and the Fock space norm, respectively.
4. The brackets $\langle \cdot, \cdot \rangle$ denote the scalar product of vectors in $\mathcal{F}$. Given a subspace $\mathcal{K} \subseteq \mathcal{F}$ and an operator A on $\mathcal{F}$ we use the notation
$$\|A\|_{\mathcal{K}} \equiv \|A \upharpoonright \mathcal{K}\|_{\mathcal{F}} .$$
5. A *hat* over a vector means that the vector is of unit length, i.e., $\widehat{\Psi} := \frac{\Psi}{\|\Psi\|}$.
6. For two vectors ψ, χ we write $\psi \parallel \chi$ if they are parallel and $\psi \perp \chi$ if they are perpendicular.
7. We denote the spectral gap of a self-adjoint operator H restricted to a subspace $\mathcal{K} \subseteq \mathcal{F}$ with unique ground state Ψ and corresponding ground state energy E by
$$\mathrm{Gap}\,(H \upharpoonright \mathcal{K}) := \inf \mathrm{spec}\,(H \upharpoonright \mathcal{K}) \setminus \{E\} - E = \inf_{\psi \perp \Psi} \left\langle \widehat{\psi}, (H - E)\widehat{\psi} \right\rangle$$
where the infimum is taken over the domain of $H \upharpoonright \mathcal{K}$.
8. We use the short-hand notation (γ is defined in (4))
$$H_{P,n} := H_P|^{\Lambda}_{\Lambda\gamma^n}, \qquad \ldots|^m_n = \ldots|^{\Lambda\gamma^m}_{\Lambda\gamma^n}, \qquad \int_a^b dk = \int_{\mathcal{B}_b \setminus \mathcal{B}_a} dk.$$

2 Strategy and Main Results

Our computations are based on von Neumann expansion formulas of the ground state of the Hamiltonians $H_P|^{\Lambda}_{\kappa}$ by *iterative analytic perturbation theory*, that means by a multi-scale procedure that relies on analytic perturbation theory. Indeed, in order to study the Λ-dependence of the mass shell, we need to construct the ground states for a fixed and non-zero value of g that is independent of the cut-off Λ. Note however that unless the coupling constant g is of order $\left(\frac{1}{\Lambda}\right)^{\frac{1}{2}}$ one cannot add the full interaction $g\Phi|^{\Lambda}_{\kappa}$ to the free Hamiltonian $H^{(0)}_P$ in a single shot of perturbation theory. Therefore, instead of adding the interaction in one shot we shall do many intermediate steps in the expansion by slicing up the interaction term of the Hamiltonian into smaller pieces, namely slices corresponding to momentum ranges $[\Lambda\gamma^{n-1}, \Lambda\gamma^n)$ that can be made arbitrarily thin by adjusting a fineness parameter γ
$$\frac{1}{2} < \gamma < 1. \tag{4}$$
It turns out that in this way one can maintain control over the convergence radius of the von Neumann expansions uniformly in Λ. With respect to this slicing we define the Fock spaces:

Definition 2.1. For $n \in \{0\} \cup \mathbb{N}$, we define the Fock spaces

$$\begin{aligned} \mathcal{F} &:= \mathcal{F}\left(L^2\left(\mathbb{R}^3, \mathbb{C}; dk\right)\right), \\ \mathcal{F}_n &:= \mathcal{F}\left(L^2\left(\mathbb{R}^3 \setminus \mathcal{B}_{\Lambda\gamma^n}, \mathbb{C}; dk\right)\right), \\ \mathcal{F}|_n^{n-1} &:= \mathcal{F}\left(L^2\left(\mathcal{B}_{\Lambda\gamma^{n-1}} \setminus \mathcal{B}_{\Lambda\gamma^n}, \mathbb{C}; dk\right)\right). \end{aligned}$$

In all these Fock spaces we shall use the same symbol Ω to denote the vacuum. For a vector ψ in $\mathcal{F}_{n-1}$ and an operator O on $\mathcal{F}_{n-1}$ we shall use the same symbol to denote the vector $\psi \otimes \Omega$ in $\mathcal{F}_n$ and the operator $O \otimes \mathbb{1}_{\mathcal{F}_n^{n-1}}$ on $\mathcal{F}_n$, respectively, where $\mathbb{1}_{\mathcal{F}_n^{n-1}}$ is the identity operator on $\mathcal{F}|_n^{n-1}$ (e.g., $\int_{\Lambda\gamma^{n-1}}^{\Lambda} dk\,\rho(k)b(k) \upharpoonright \mathcal{F}_n \equiv \int_{\Lambda\gamma^{n-1}}^{\Lambda} dk\,\rho(k)b(k) \otimes \mathbb{1}_{\mathcal{F}_n^{n-1}}$).We adapt the notation for the Hamiltonians

$$H_{P,n} := H_P|_{\Lambda\gamma^n}^{\Lambda} = \sqrt{(P - P^f)^2 + m^2} + H^f + g \int_{\Lambda\gamma^n}^{\Lambda} dk\,\rho(k)\,(b(k) + b^*(k)) \;,$$

and note

$$H_{P,n} = H_{P,n-1} + g\Phi|_n^{n-1}, \qquad \Phi|_n^{n-1} := \phi|_n^{n-1} + \phi^*|_n^{n-1}, \qquad \phi|_n^{n-1} := \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\,\rho(k)b(k)\,.$$

Furthermore, for simplicity of our presentation we keep an infrared cut-off

$$\kappa \equiv \Lambda\gamma^N = 1\,,$$

and in the following, for fixed Λ, the fineness parameter γ will be chosen in such a way that

$$N = \frac{\ln\Lambda}{-\ln\gamma} \tag{5}$$

is an integer. Note that by construction $1 \le \Lambda\gamma^n \le \Lambda$ for $0 \le n \le N$.

Remark 2.2. We warn the reader that, though it is not explicit in the notation, the definitions of $\mathcal{F}_n$ and $H_{P,n}$ are $\Lambda-$dependent as well as for other quantities introduced later on (e.g., $E_{P,n}$, $\Psi_{P,n}$).

We introduce:

Definition 2.3. For $P \in \mathbb{R}^3$ and integers $0 \le n \le N$ we define the ground state energies

$$E_{P,n} := \inf\operatorname{spec}(H_{P,n} \upharpoonright \mathcal{F}_n)\,.$$

The desired expansion formulas are a byproduct of the construction of the ground states of the Hamiltonians $H_{P,N} \upharpoonright \mathcal{F}_N$, $|P| < P_{max}$. At the heart of this construction lies an induction argument. Suppose that:

(i) At step $(n-1)$ the vector $\Psi_{P,n-1}$ is the unique ground state of the Hamiltonian $H_{P,n-1} \upharpoonright \mathcal{F}_{n-1}$ with corresponding ground state energy $E_{P,n-1}$.

(ii) For some $\zeta > 0$ the spectral gap can be bounded from below by

$$\operatorname{Gap}(H_{P,n-1} \upharpoonright \mathcal{F}_{n-1}) \ge \zeta\omega(\Lambda\gamma^n)\,.$$

Given the assumptions (i) and (ii) we can derive the implications reported below.

1. In Lemma 3.3 we show through a variational argument that
$$\text{Gap}\left(H_{P,n-1} \upharpoonright \mathcal{F}_n\right) \geq \zeta\omega\left(\Lambda\gamma^n\right).$$
2. Next, we justify the Neumann expansion of the resolvent $\frac{1}{H_{P,n}-z}$ in terms of $\frac{1}{H_{P,n-1}-z}$ and the slice interaction $H_{P,n} - H_{P,n-1}$ for $z \in \mathbb{C}$ in the domain defined by
$$\frac{1}{2}\zeta\omega\left(\Lambda\gamma^{n+1}\right) \leq \left|E_{P,n-1} - z\right| \leq \zeta\omega\left(\Lambda\gamma^{n+1}\right)$$
by a direct computation; see Lemma 3.4. We find
$$\left\|\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2} g\Phi|_n^{n-1}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \leq C|g|$$
uniformly in n and in Λ. The reason for this is that we add interaction slices starting from Λ down to $\Lambda\gamma^N = 1$ in decreasing order so that the contribution of
$$\left\|g\phi|_n^{n-1}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \leq C|g|\left(\Lambda\gamma^{n-1}(1-\gamma)\right)^{1/2}$$
is compensated thanks to the spectral gap estimate and the chosen domain for z which gives
$$\left\|\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \leq C\left(\frac{1}{\Lambda\gamma^n(1-\gamma)}\right)^{1/2}.$$
3. Finally, Theorem 3.6 ensures the existence of a unique ground state
$$\Psi_{P,n} := -\frac{1}{2\pi i}\oint_{\Gamma_{P,n}} \frac{dz}{H_{P,n}-z}\Psi_{P,n-1}$$
$$= -\frac{1}{2\pi i}\sum_{j=0}^{\infty}\oint_{\Gamma_{P,n}} \frac{dz}{H_{P,n-1}-z}\left[-(H_{P,n}-H_{P,n-1})\frac{1}{H_{P,n-1}-z}\right]^j \Psi_{P,n-1} \quad (6)$$
of the Hamiltonian $H_{P,n} \upharpoonright \mathcal{F}_n$ by analytic perturbation theory for sufficiently small $|g|$ uniformly in n and $\Lambda < \infty$, where the contour $\Gamma_{P,n}$ is appropriately chosen around $E_{P,n-1}$; see Definition 3.5.
4. Furthermore, another variational argument guarantees $E_{P,n} \leq E_{P,n-1}$ and, hence, by Kato's theorem
$$\text{Gap}\left(H_{P,n} \upharpoonright \mathcal{F}_n\right) \geq \zeta\omega\left(\Lambda\gamma^{n+1}\right).$$

Along this construction we gain the expansion formula (6) of the ground state $\Psi_{P,n}$ in terms of the previous ground state $\Psi_{P,n-1}$ for each induction step. The above induction is based on the following well-known results:

Proposition 2.4. *For $P \in \mathbb{R}^3$ and any integer $0 \leq n < \infty$ the Hamiltonians $H_P^{nuc}, H^f, H_P^{(0)}, H_{P,n}$ acting on $\mathcal{F}$ are essentially self-adjoint on the domain $D(H_{P=0}^{(0)})$ and bounded from below.*

Theorem 2.5. *For $P \in \mathbb{R}^3$ and integers $0 \leq n < \infty$ the ground state energies fulfill*

$$E_{P,n} \geq E_{0,n}. \tag{7}$$

The inequality in (7) is due to [5].

Remark 2.6. We remark that the construction of the ground state can be implemented for γ arbitrarily close to 1. This feature of our technique will be crucial to derive the results on the limiting regime, as $\Lambda \to \infty$, of the ground state energy and of the effective velocity stated in Theorems (2.7) and (2.8), respectively. Indeed, by (5) it allows us to control any error term that can be bounded by $O(N(1-\gamma)^{1+\varepsilon})$ with $\varepsilon > 0$.

Main Results. As a direct application of the established expansion formulas we can bound the ground state energy from above and from below. The bounds are sharp in the sense that they identify the order of dependence of the ground state energy on the ultraviolet cut-off Λ and the coupling constant g:

Theorem 2.7. *Let $|g|$ be sufficiently small and $|P| < P_{max}$. Define $E_{P,\Lambda} := \inf \operatorname{spec}\left(H_P|_\kappa^\Lambda\right)$. There exist universal constants $a, b > 0$ such that for all $1 < \Lambda < \infty$ it holds*

$$\sqrt{P^2 + m^2} - g^2 b\Lambda \leq E_{P,\Lambda} \leq \sqrt{P^2 + m^2} - g^2 a\Lambda \tag{8}$$

The proof will be given in the end of Section 3.

In our second main result we give an estimate of the effective velocity of the nucleon in a one-particle state:

Theorem 2.8. *Let $|g|$ be sufficiently small and $|P| < P_{max}$. Then, there exist universal constants $c_1, C_1 > 0$ such that the following estimate holds true*

$$\lim sup_{\gamma\to 1} \left|\frac{\partial E_{P,N}}{\partial P_i}\right| \leq \Lambda^{-g^2 c_1} \frac{|P|}{[P^2 + m^2]^{1/2}} + C_1 |g|^{1/2}, \qquad i = 1, 2, 3. \tag{9}$$

The proof will be given in Section (4). A direct consequence of the bound in (9) is

$$\lim sup_{\Lambda\to\infty} \left|\frac{\partial E_{P,\Lambda}}{\partial P_i}\right| \leq C|g|^{1/2}. \tag{10}$$

In order to interpret this result consider that in the free case, i.e., $g = 0$, one finds

$$\left|\frac{\partial E_{P,\Lambda}}{\partial P_i}\right| = \frac{|P_i|}{\sqrt{P^2 + m^2}}.$$

Therefore, Theorem 2.8 states that if the interaction is turned on, even for an arbitrarily small but non-zero $|g|$, the absolute value of the gradient of the ground state energy decreases to an order smaller or equal to $|g|^{1/2}$ in the limit $\Lambda \to \infty$. The physical interpretation of this result is that the mass shell essentially becomes flat and the theory trivial in the limit $\Lambda \to \infty$. Moreover, our proof shows that not even a suitable scaling of the bare mass, i.e., $m \equiv m(\Lambda) > 0$, may prevent the mass shell from becoming essentially flat.

A crucial tool for the above results comes from the non-perturbative estimates that we derive in Theorem (3.7) and Theorem (3.8), respectively:

$$a\Lambda\gamma^{n-1}(1-\gamma) \leq \left\langle \widehat{\Psi}_{P,n-1}, \phi|_n^{n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1} \right\rangle \leq b\Lambda\gamma^{n-1}(1-\gamma)\,, \tag{11}$$

$$c_1(1-\gamma) \leq \alpha_P|_n^{n-1} := \left\langle \widehat{\Psi}_{P,n-1}, \phi|_n^{n-1} \left(\frac{1}{H_{P,n-1} - E_{P,n-1}} \right)^2 \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1} \right\rangle \leq c_2(1-\gamma) \tag{12}$$

which hold for some universal constants $0 < a \leq b < \infty$, $0 < c_1 \leq c_2 < \infty$. In order to get the bounds in (11)-(12) we make use of the spectral information obtained during the construction of the ground states.

The strategy of proof in Theorem 2.8 consists in re-expanding back the vectors in the matrix element yielding the effective velocity. This means that, iteratively, the matrix element

$$\left\langle \widehat{\Psi}_{P,n}, V_i(P) \widehat{\Psi}_{P,n} \right\rangle \equiv \frac{\partial E_{P,n}}{\partial P_i}, \qquad V_i(P) := \frac{P_i - P_i^f}{[(P-P^f)^2 + m^2]^{1/2}}$$

will be expressed in terms of:

1. The analogous quantity on scale $n-1$, i.e.,
$$\left\langle \widehat{\Psi}_{P,n-1}, V_i(P) \widehat{\Psi}_{P,n-1} \right\rangle \tag{13}$$

2. The scalar products
$$A_{P,n-1} := g^2 \left\langle \frac{1}{H_{P,n-1} - E_{P,n-1}} \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1}, V_i(P) \frac{1}{H_{P,n-1} - E_{P,n-1}} \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1} \right\rangle$$
and
$$B_{P,n-1} := 2g^2 \Re \left\langle \widetilde{Q}^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} \phi|_n^{n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1}, V_i(P) \widehat{\Psi}_{P,n-1} \right\rangle$$
where $\widetilde{Q}^{\perp}_{P,n-1}$ is defined in equation (24).

3. A remainder that can be estimated to be $O(|g|^4 (1-\gamma)^{\frac{4}{2}})$.

The hard part of our proof is showing that some a priori estimates on $A_{P,n-1}$ and $B_{P,n-1}$ hold so that they shall not be re-expanded like the leading term (13) but their cumulative contribution can be estimated to be of order $|g|^{\frac{1}{2}}$ as in (9). Two substantially different arguments are devised to control $A_{P,n-1}$ and $B_{P,n-1}$:

- As for $A_{P,n-1}$, due to the velocity operator $V_i(P)$ we can show summability in n after contracting the boson operators $\phi^*|_n^{n-1}$.

- As for $B_{P,n-1}$, by exploiting the presence of the orthogonal projection $\widetilde{Q}^{\perp}_{P,n-1}$ and a suitable *one-step, g−dependent* backwards expansion, we can improve the crude estimate, $O(g^2(1-\gamma))$, that follows from the operator bounds derived in Section 3 by, at least, an extra factor $|g|^{\frac{1}{2}}$.

The product of the coefficients $\{(1-g^2\alpha_P|_n^{n-1})\}_{1\le n\le N}$ that are generated in front of the leading term (13) at each step of the re-expansion gives rise to a damping factor bounded above by $\Lambda^{-g^2c_1}$ as γ tends to 1.

3 Construction of the One-Particle States

We begin our discussion with the construction of the ground states corresponding to the Hamiltonians $H_{P,n} \upharpoonright \mathcal{F}_n$, $0 \le n \le N$. This construction is based on an induction completed in Theorem 3.6. Next, we collect helpful estimates and expansion formulas which also will be used frequently in Section 4. This section ends with Lemma 3.8 where we derive some upper and lower bounds on the ground state energies.

The first lemma provides some a priori estimates on the ground state energies. In particular claim (iii) of Lemma 3.1 will be crucial for the gap estimate in Lemma 3.3.

Lemma 3.1. *For $P \in \mathbb{R}^3$ and any integer $0 \le n < N$ suppose $\Psi_{P,n}$ is the ground state of $H_{P,n} \upharpoonright \mathcal{F}_n$ and $E_{P,n}$ is the corresponding ground state energy. Then:*

(i) $E_{P,n+1} \le E_{P,n}$.

(ii) $-g^2C\Lambda \le E_{P,n} \le \sqrt{P^2+m^2}$.

(iii) $\forall k \in \mathbb{R}^3\,,\ E_{P-k,n} - E_{P,n} \ge -|P|\omega(k)$.

Proof.

(i) By definition of the ground state energy we can estimate

$$E_{P,n+1} - E_{P,n} \le \frac{\langle \Psi_{P,n}, [H_{P,n+1} - H_{P,n}]\,\Psi_{P,n}\rangle}{\langle \Psi_{P,n}, \Psi_{P,n}\rangle} = \frac{\left\langle \Psi_{P,n},\, g\Phi|_{n+1}^{n}\Psi_{P,n}\right\rangle}{\langle \Psi_{P,n}, \Psi_{P,n}\rangle} = 0.$$

(ii) It suffices to observe that

$$E_{P,n} \le \left\langle \widehat{\Psi}_{P,0}, H_{P,n}\widehat{\Psi}_{P,0}\right\rangle = \sqrt{P^2+m^2}$$

and

$$0 \le \sqrt{(P-P^f)^2+m^2} + \int_{\Lambda\gamma^n}^{\Lambda} dk\,\omega(k)\left(b_k^* + g\frac{\rho(k)}{\omega(k)}\right)\left(b_k + g\frac{\rho(k)}{\omega(k)}\right) = H_{P,n} + g^2\int_{\Lambda\gamma^n}^{\Lambda} dk\,\frac{\rho(k)^2}{\omega(k)}$$

where

$$g^2\int_{\Lambda\gamma^n}^{\Lambda} dk\,\frac{\rho(k)^2}{\omega(k)} \le g^2C\Lambda.$$

(iii) Inequality (7) implies

$$E_{P-k,n} - E_{P,n} = E_{P-k,n} - E_{0,n} + E_{0,n} - E_{P,n} \geq E_{0,n} - E_{P,n}$$

and

$$E_{0,n} - E_{P,n} \geq \frac{\langle \Psi_{0,n}, [H_{0,n} - H_{P,n}]\, \Psi_{0,n} \rangle}{\langle \Psi_{0,n}, \Psi_{0,n} \rangle} = \frac{\left\langle \Psi_{0,n}, \left[H_0^{nuc} - H_P^{nuc}\right] \Psi_{0,n} \right\rangle}{\langle \Psi_{0,n}, \Psi_{0,n} \rangle} \geq -|P| \geq -|P|\omega(k) \tag{14}$$

because

$$\left\| \sqrt{P^{f\,2} + m^2} - \sqrt{(P - P^f)^2 + m^2} \right\| \leq |P|$$

and $\omega(k) = \sqrt{k^2 + \mu^2}$ with $\mu > 1$.

□

In our construction we shall single out two parameters needed to control the gap of the Hamiltonians $H_{P,n} \restriction \mathcal{F}_n$, $0 \leq n \leq N$:

Definition 3.2. Define $\frac{1}{8} < \theta < \frac{1}{4}$ and $\zeta > \frac{1}{4}$ such that

$$1 - \theta - P_{\max} \geq \zeta.$$

Later the following lemma will be invoked from the main induction in Theorem 3.6 to provide the gap estimate that is used in the inductive scheme.

Lemma 3.3. *Let $|P| < P_{max}$ and $1 \leq n \leq N$. Assume:*

A(i) $E_{P,n-1}$ is the non-degenerate ground state energy of $H_{P,n-1} \restriction \mathcal{F}_{n-1}$ corresponding to the ground state vector $\Psi_{P,n-1}$.

A(ii) $Gap\,(H_{P,n-1} \restriction \mathcal{F}_{n-1}) \geq \zeta\omega\,(\Lambda\gamma^n)$.

Then:

C(i) $E_{P,n-1}$ is the non-degenerate ground state energy of $H_{P,n-1} \restriction \mathcal{F}_n$ corresponding to the ground state vector $\Psi_{P,n-1} \otimes \Omega$.

C(ii)

$$Gap\,(H_{P,n-1} \restriction \mathcal{F}_n)\,,\ \inf_{\varphi=\psi\otimes\eta} \left\langle \widehat{\varphi}, \left(H_{P,n-1} - \theta H^f|_n^{n-1} - E_{P,n-1}\right)\widehat{\varphi} \right\rangle \geq \zeta\omega\,(\Lambda\gamma^n)$$

where the infimum is taken over $\varphi \in D(H_P^{(0)})$ such that $\psi \in \mathcal{F}_{n-1}$ and $\eta \in \mathcal{F}|_n^{n-1}$ contains a strictly positive number of bosons.

Proof. A direct computation using A(i) shows that $\Psi_{P,n-1} \otimes \Omega$ is eigenvector of $H_{P,n-1} \upharpoonright \mathcal{F}_n$ with corresponding eigenvalue $E_{P,n-1}$. Since $H^f|_n^{n-1}$ is a positive operator one has

$$\inf_{\varphi \perp \Psi_{P,n-1} \otimes \Omega} \langle \widehat{\varphi}, (H_{P,n-1} - E_{P,n-1}) \widehat{\varphi} \rangle \geq \inf_{\varphi \perp \Psi_{P,n-1} \otimes \Omega} \left\langle \widehat{\varphi}, \left(H_{P,n-1} - \theta H^f|_n^{n-1} - E_{P,n-1} \right) \widehat{\varphi} \right\rangle ; \tag{15}$$

we subtract the term $\theta H^f|_n^{n-1}$ for a technical reason which will become clear in Lemma 3.4.

Now, the right-hand side of (15) is bounded from below by

$$\min \left\{ \mathrm{Gap}\left(H_{P,n-1} \upharpoonright \mathcal{F}_{n-1} \right), \inf_{\varphi = \psi \otimes \eta} \left\langle \widehat{\varphi}, \left(H_{P,n-1} - \theta H^f|_n^{n-1} - E_{P,n-1} \right) \widehat{\varphi} \right\rangle \right\}, \tag{16}$$

where $\psi \in \mathcal{F}_{n-1}, \eta \in \mathcal{F}_n^{n-1}, \psi \otimes \eta$ belongs to $D(H_P^{(0)})$, and η is a vector with definite, strictly positive number of bosons. For a vector η with $l \geq 1$ bosons we compute

$$\begin{aligned} &\inf_{\varphi = \psi \otimes \eta} \left\langle \widehat{\varphi}, \left(H_{P,n-1} - \theta H^f|_n^{n-1} - E_{P,n-1} \right) \widehat{\varphi} \right\rangle \\ &\quad \geq \inf_{\psi, \Lambda\gamma^n \leq |k_j| \leq \Lambda\gamma^{n-1}} \left\langle \widehat{\psi}, \left(H_{P - \sum_{j=1}^l k_j, n-1} + (1-\theta) \sum_{j=1}^l \omega(k_j) - E_{P,n-1} \right) \widehat{\psi} \right\rangle \\ &\qquad \geq \inf_{\psi, \Lambda\gamma^n \leq |k_j| \leq \Lambda\gamma^{n-1}} \left(E_{P - \sum_{j=1}^l k_j, n-1} - E_{P,n-1} + (1-\theta) \sum_{j=1}^l \omega(k_j) \right). \end{aligned}$$

Furthermore, Lemma 3.1 implies

$$E_{P - \sum_{j=1}^l k_j, n-1} - E_{P,n-1} \geq -P_{\max} \sum_{j=1}^l \omega(k_j).$$

Hence, by Definition 3.2 the inequality

$$\inf_{\varphi = \psi \otimes \eta} \left\langle \widehat{\varphi}, \left(H_{P,n-1} - \theta H^f|_n^{n-1} - E_{P,n-1} \right) \widehat{\varphi} \right\rangle \geq \zeta \omega \left(\Lambda \gamma^n \right)$$

holds. Now by A(ii) we also get

$$(16) \geq \zeta \omega \left(\Lambda \gamma^n \right). \tag{17}$$

From the estimate in equation (17) we can conclude that $\Psi_{P,n-1} \otimes \Omega$ is the unique ground state of $H_{P,n-1} \upharpoonright \mathcal{F}_n$ with eigenvalue $E_{P,n-1}$ and

$$\mathrm{Gap}\left(H_{P,n-1} \upharpoonright \mathcal{F}_n \right) \geq \zeta \omega \left(\Lambda \gamma^n \right).$$

This proves C(i) and C(ii). □

The second ingredient needed for the main induction in Theorem 3.6 is a control of the resolvent expansion of the Hamiltonians:

Lemma 3.4. *Let $|g|$ be sufficiently small and $|P| < P_{max}$. Suppose further that for $1 \le n \le N$ $E_{P,n-1}$ is the non-degenerate ground state energy of $H_{P,n-1} \upharpoonright \mathcal{F}_{n-1}$ corresponding to the ground state vector $\Psi_{P,n-1}$ and that*

$$Gap\left(H_{P,n-1} \upharpoonright \mathcal{F}_n\right) \ge \zeta\omega\left(\Lambda\gamma^n\right). \tag{18}$$

Then, for $z \in \mathbb{C}$ such that

$$\frac{1}{2}\zeta\omega\left(\Lambda\gamma^{n+1}\right) \le \left|E_{P,n-1} - z\right| \le \zeta\omega\left(\Lambda\gamma^{n+1}\right),$$

the resolvent $\frac{1}{H_{P,n}-z}$ is a well-defined operator on $\mathcal{F}_n$ which equals to

$$\frac{1}{H_{P,n-1}-z}\sum_{j=0}^{\infty}\left[-g\Phi|_n^{n-1}\frac{1}{H_{P,n-1}-z}\right]^j. \tag{19}$$

Proof. We start with the estimate

$$\left\|\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} = \frac{1}{\sqrt{\operatorname{dist}\left(z, \operatorname{spec}\left(H_{P,n-1} \upharpoonright \mathcal{F}_n\right)\right)}}$$
$$\le \left(\max\left\{\frac{2}{\zeta\omega\left(\Lambda\gamma^{n+1}\right)}, \frac{C}{\zeta\omega\left(\Lambda\gamma^n\right) - \zeta\omega\left(\Lambda\gamma^{n+1}\right)}\right\}\right)^{1/2} \le \left(\frac{C}{\zeta\Lambda\gamma^{n+1}(1-\gamma)}\right)^{1/2}$$

where we made use of the assumption in (18). Next, we estimate

$$\left\|g\phi|_n^{n-1}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \le |g|C\left[\Lambda\gamma^{n-1}(1-\gamma)\right]^{1/2}\left\|\left(H^f|_n^{n-1}\right)^{1/2}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n}. \tag{20}$$

The operators $H^f|_n^{n-1}$ and $H_{P,n-1}$ commute, and we may apply the spectral theorem and Lemma 3.3 in order to get

$$\left\|\left(H^f|_n^{n-1}\right)^{1/2}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} = \left\|\left(H^f|_n^{n-1}\right)^{1/2}\left(\frac{1}{H_{P,n-1}-\theta H^f|_n^{n-1} - z + \theta H^f|_n^{n-1}}\right)^{1/2}\right\|_{\mathcal{F}_n} \le \theta^{-1/2}.$$

In consequence, we can estimate

$$\left\|g\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\Phi|_n^{n-1}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \le |g|C(\zeta\gamma^2)^{-1/2}\theta^{-1/2}.$$

Since $\gamma > \frac{1}{2}$, $\zeta > \frac{1}{4}$, and $\theta > \frac{1}{8}$ the coupling constant $|g|$ can be chosen independently of n (and of Λ) such that

$$|g|C(\theta\zeta\gamma^2)^{-1/2} < 1$$

which implies the convergence of the power series on the right-hand side of (19) and, thus, the claim. □

We will now prove that the vectors in the following definition are the unique, non-zero ground states of the Hamiltonians $H_{P,n} \upharpoonright \mathcal{F}_n$, $0 \le n \le N$. (We warn the reader that the spectral projection in (21) will be shown to be well defined in Theorem 3.6.)

Definition 3.5. For $1 \le n \le N$ we define

$$\mathcal{Q}_{P,n} := -\frac{1}{2\pi i}\oint_{\Gamma_{P,n}} \frac{dz}{H_{P,n}-z} \upharpoonright \mathcal{F}_n \qquad \Gamma_{P,n} := \left\{ z \in \mathbb{C} \,\middle|\, \left|E_{P,n-1}-z\right| = \frac{1}{2}\zeta\omega\left(\Lambda\gamma^{n+1}\right)\right\} \tag{21}$$

and recursively

$$\Psi_{P,n} := \mathcal{Q}_{P,n}\Psi_{P,n-1}, \qquad \Psi_{P,0} := \Omega. \tag{22}$$

Note that $\Psi_{P,n}$ are in general unnormalized vectors with $\|\Psi_{P,n}\| \le 1$.

Theorem 3.6. *Let $|g|$ be sufficiently small and $|P| < P_{max}$. For $0 \le n \le N$ it holds:*

(i) $\Psi_{P,n}$ is well-defined, non-zero, and the unique ground state vector of $H_{P,n} \upharpoonright \mathcal{F}_n$ with corresponding eigenvalue

$$E_{P,n} := \inf \operatorname{spec}\left(H_{P,n} \upharpoonright \mathcal{F}_n\right).$$

(ii) $Gap\left(H_{P,n} \upharpoonright \mathcal{F}_n\right) \ge \zeta\omega\left(\Lambda\gamma^{n+1}\right)$.

Proof. A direct computation shows that the claim holds for $n = 0$. Let us assume it holds for $n-1$ with $0 \le n-1 < N-1$:

1. The assumptions allow to apply Lemma 3.3 which states that

$$\operatorname{Gap}\left(H_{P,n-1} \upharpoonright \mathcal{F}_n\right) \ge \zeta\omega\left(\Lambda\gamma^{n}\right).$$

2. Hence, Lemma 3.4 ensures that for $|g|$ small enough but uniform in n (and in Λ) the resolvent

$$\frac{1}{H_{P,n}-z} \upharpoonright \mathcal{F}_n = \frac{1}{H_{P,n-1}-z}\sum_{j=0}^{\infty}\left[-g\Phi|_n^{n-1}\frac{1}{H_{P,n-1}-z}\right]^j \upharpoonright \mathcal{F}_n$$

is well-defined for

$$\frac{1}{2}\zeta\omega\left(\Lambda\gamma^{n+1}\right) \le \left|E_{P,n-1}-z\right| \le \zeta\omega\left(\Lambda\gamma^{n+1}\right). \tag{23}$$

3. For $|g|$ small enough but uniform in n (and in Λ), $\Psi_{P,n}$ defined in (22) is non-zero. Indeed for $0 \le n \le N$ and $z \in \Gamma_{P,n}$ we have

$$\left\|\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2} g\Phi|_n^{n-1}\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \le C|g|(1-\gamma)^{1/2}$$

because for z in the domain $\Gamma_{P,n}$ defined in (21) we get

$$\left\|\left(\frac{1}{H_{P,n-1}-z}\right)^{1/2}\right\|_{\mathcal{F}_n} \le \left(\frac{C}{\Lambda\gamma^{n}}\right)^{1/2}$$

that we can combine with the bound in (20). By Kato's theorem we can conclude that it is the unique ground state of $H_{P,n} \upharpoonright \mathcal{F}_n$ with corresponding ground state energy $E_{P,n}$.

4. Lemma 3.1(i), Kato's theorem, and the domain of z given in (23) provide the estimate

$$\operatorname{Gap}\left(H_{P,n} \upharpoonright \mathcal{F}_n\right) \geq \zeta\omega\left(\Lambda\gamma^{n+1}\right).$$

□

Next we provide expansion formulas which will be used frequently in our computations in Section 4.

Theorem 3.7. *Let $|g|$ be sufficiently small and $|P| < P_{max}$. For $0 \leq n \leq N$ the following statements hold:*

(i) The following equality is satisfied:

$$\begin{aligned}\Psi_{P,n} =& \Psi_{P,n-1} - g\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\Psi_{P,n-1} \\ &+ g^2\widetilde{Q}^{\perp}_{P,n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi|_n^{n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\Psi_{P,n-1} \\ &+ g^2\widetilde{Q}^{\perp}_{P,n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\Psi_{P,n-1} \\ &- g^2\widetilde{Q}_{P,n-1}\phi|_n^{n-1}\left(\frac{1}{H_{P,n-1} - E_{P,n-1}}\right)^2\phi^*|_n^{n-1}\Psi_{P,n-1} + O\left(|g|^3(1-\gamma)^{3/2}\right)\end{aligned}$$

for

$$\widetilde{Q}_{P,n-1} := -\frac{1}{2\pi i}\oint_{\Gamma_{P,n}} dz \frac{1}{H_{P,n-1} - z} \upharpoonright \mathcal{F}_n, \qquad \widetilde{Q}^{\perp}_{P,n-1} := \mathbb{1}_{\mathcal{F}_n} - \widetilde{Q}_{P,n-1} \tag{24}$$

where $\mathbb{1}_{\mathcal{F}_n}$ is the identity operator on $\mathcal{F}_n$.

(ii) The norm of the ground state vectors fulfills the relation

$$\left\|\Psi_{P,n}\right\|^2 = \langle\Psi_{P,n}, \Psi_{P,n}\rangle = \left(1 - g^2\alpha_P|_n^{n-1} + O\left(|g|^4(1-\gamma)^{4/2}\right)\right)\left\|\Psi_{P,n-1}\right\|^2 \tag{25}$$

where

$$\alpha_P|_n^{n-1} := \left\langle\widehat{\Psi}_{P,n-1}, \phi|_n^{n-1}\left(\frac{1}{H_{P,n-1} - E_{P,n-1}}\right)^2\phi^*|_n^{n-1}\widehat{\Psi}_{P,n-1}\right\rangle.$$

(iii) There exist universal constants $0 < c_1 \leq c_2 < \infty$ such that

$$c_1(1-\gamma) \leq \alpha_P|_n^{n-1} \leq c_2(1-\gamma).$$

Proof. Claim (i) can be shown by a direct computation using Definition 3.5. Likewise claim (ii) follows from Definition 3.5 by exploiting the relation

$$\Psi_{P,n} = Q_{P,n}\Psi_{P,n-1} = \frac{\langle\Psi_{P,n}, \Psi_{P,n-1}\rangle}{\langle\Psi_{P,n}, \Psi_{P,n}\rangle}\Psi_{P,n}$$

that holds by construction.

Next, we prove claim (iii). The bound from above is obtained by using the pull-through formula and Lemma 3.1 (iii), i.e.,

$$\alpha_P|_n^{n-1} = \left\langle \widehat{\Psi}_{P,n-1}, \phi|_n^{n-1} \left(\frac{1}{H_{P,n-1} - E_{P,n-1}} \right)^2 \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1} \right\rangle$$
$$= \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\, \rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \left(\frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \right)^2 \widehat{\Psi}_{P,n-1} \right\rangle \leq -C \ln\gamma \leq c_2(1-\gamma) \quad (26)$$

for an appropriately chosen constant c_2; recall that $\frac{1}{2} < \gamma < 1$.

With respect to the bound from below we consider the spectral representation for the self-adjoint operator $H_{P-k,n-1} + \omega(k) - E_{P,n-1}$ and define the spectral projections

$$\chi^+(k) := \chi_{(5\omega(k),+\infty)} \left(H_{P-k,n-1} + \omega(k) - E_{P,n-1} \right), \qquad \chi^-(q) := \mathbb{1}_{\mathcal{F}_{n-1}} - \chi^+(q)$$

where $\chi_{(5\omega(k),+\infty)}$ is the characteristic function being one on the interval $(5\omega(k), +\infty)$ and zero otherwise. We also define the function

$$f(k) := \rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \left(\frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \right)^2 (\chi^+(k) + \chi^-(k))\, \widehat{\Psi}_{P,n-1} \right\rangle$$

that we study for two complementary cases:

(a) In the case $\left\| \chi^+(k) \widehat{\Psi}_{P,n-1} \right\|^2 < \frac{1}{2}$ we get

$$f(k) \geq \rho(k)^2 \left\langle \chi^-(k) \widehat{\Psi}_{P,n-1}, \left(\frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \right)^2 \chi^-(k) \widehat{\Psi}_{P,n-1} \right\rangle \geq \frac{\rho(k)^2}{50\omega(k)^2}. \quad (27)$$

(b) In the other case, i.e., $\left\| \chi^+(k) \widehat{\Psi}_{P,n-1} \right\|^2 \geq \frac{1}{2}$, we start with the trivial inequality

$$f(k) \geq \rho(k)^2 \left\langle \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \widehat{\Psi}_{P,n-1}, \chi^+(k) \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \widehat{\Psi}_{P,n-1} \right\rangle \quad (28)$$

and consider the resolvent formulas

$$\frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} = \frac{1}{H_{P,n-1} + \omega(k) - E_{P,n-1}} - \frac{1}{H_{P,n-1} + \omega(k) - E_{P,n-1}} \Delta_P(k) \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \quad (29)$$

and

$$\frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} = \frac{1}{H_{P,n-1} + \omega(k) - E_{P,n-1}} - \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \Delta_P(k) \frac{1}{H_{P,n-1} + \omega(k) - E_{P,n-1}} \quad (30)$$

where

$$\Delta_P(k) := \sqrt{(P-k-P^f)^2+m^2} - \sqrt{(P-P^f)^2+m^2}\,.$$

Then we apply the expansions in (29) and in (30) to the resolvents on the left and on the right in the scalar product of (28), respectively, and get

$$\begin{aligned} f(k) \geq \rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \frac{1}{H_{P,n-1}+\omega(k)-E_{P,n-1}} \chi^+(k) \frac{1}{H_{P,n-1}+\omega(k)-E_{P,n-1}} \widehat{\Psi}_{P,n-1} \right\rangle \\ -2\Re\rho(k)^2 \Big\langle \widehat{\Psi}_{P,n-1}, \frac{1}{H_{P,n-1}+\omega(k)-E_{P,n-1}} \Delta_P(k) \frac{1}{H_{P-k,n-1}+\omega(k)-E_{P,n-1}} \times \\ \times \chi^+(k) \frac{1}{H_{P,n-1}+\omega(k)-E_{P,n-1}} \widehat{\Psi}_{P,n-1} \Big\rangle \\ +\rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \left| \chi^+(k) \frac{1}{H_{P-k,n-1}+\omega(k)-E_{P,n-1}} \Delta_P(k) \frac{1}{H_{P,n-1}+\omega(k)-E_{P,n-1}} \right|^2 \widehat{\Psi}_{P,n-1} \right\rangle. \end{aligned} \tag{31}$$

Note that

$$\|\Delta_P(k)\| \leq |k|$$

so that neglecting the last positive term in (31) we get the estimate

$$\begin{aligned} f(k) &\geq \frac{\rho(k)^2}{\omega(k)^2} \left\| \chi^+(k)\widehat{\Psi}_{P,n-1} \right\|^2 - \frac{2\rho(k)^2|k|}{5\omega(k)^3} \left\| \chi^+(k)\widehat{\Psi}_{P,n-1} \right\| \\ &\geq \frac{\rho(k)^2}{\omega(k)^2} \left\| \chi^+(k)\widehat{\Psi}_{P,n-1} \right\| \left(\frac{1}{\sqrt{2}} - \frac{2}{5} \right) \geq \frac{(5-2\sqrt{2})\rho(k)^2}{10\omega(k)^2}. \end{aligned} \tag{32}$$

Combining the bounds (27) and (32) we obtain

$$\int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\,\rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \left(\frac{1}{H_{P-k,n-1}+\omega(k)-E_{P,n-1}} \right)^2 \widehat{\Psi}_{P,n-1} \right\rangle \geq -C\ln\gamma \geq c_1(1-\gamma)$$

that gives the bound from below on $\alpha_P|_n^{n-1}$ for an appropriately chosen constant c_1. This together with the bound from above (26) proves the claim. □

With the help of these expansion formulas we get upper and lower bounds on the ground state energy shifts:

Lemma 3.8. *Let $|g|$ be sufficiently small and $|P| < P_{max}$. For $1 \leq n \leq N$ the following holds:*

(i)

$$\begin{aligned} E_{P,n} - E_{P,n-1} &= -\Delta E_P|_n^{n-1} + O\left(|g|^4\Lambda(1-\gamma)^{4/2}\right), \\ \Delta E_P|_n^{n-1} &:= g^2 \left\langle \widehat{\Psi}_{P,n-1}, \phi|_n^{n-1} \frac{1}{H_{P,n-1}-E_{P,n-1}} \phi^*|_n^{n-1} \widehat{\Psi}_{P,n-1} \right\rangle. \end{aligned} \tag{33}$$

(ii) There exist universal constants $a, b > 0$ such that

$$g^2 a\Lambda\gamma^{n-1}(1-\gamma) \leq \Delta E_P|_n^{n-1} \leq g^2 b\Lambda\gamma^{n-1}(1-\gamma).$$

Proof. Claim (i) follows from the expansion formula of Theorem 3.7 applied to

$$E_{P,n} - E_{P,n-1} = \frac{\langle \Psi_{P,n}, [H_{P,n} - H_{P,n-1}]\, \Psi_{P,n-1} \rangle}{\langle \Psi_{P,n}, \Psi_{P,n-1} \rangle} = \frac{\left\langle \Psi_{P,n}, g\Phi|_n^{n-1} \Psi_{P,n-1} \right\rangle}{\langle \Psi_{P,n}, \Psi_{P,n-1} \rangle}.$$

Next, we show claim (ii). The bound from above follows by using the pull-through formula, i.e.,

$$\Delta E_P|_n^{n-1} = g^2 \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\, \rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \widehat{\Psi}_{P,n-1} \right\rangle \tag{34}$$

and the estimate

$$g^2 \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\, \rho(k)^2 \left\langle \widehat{\Psi}_{P,n-1}, \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \widehat{\Psi}_{P,n-1} \right\rangle \le g^2 b \Lambda \gamma^{n-1} (1-\gamma). \tag{35}$$

that uses Lemma 3.1 (iii). The bound from below of (34) can be shown by a similar argument as in (iii) of Theorem 3.7. Therefore we omit the proof. □

The established upper and lower bounds given in Lemma 3.8 enable us to prove the first main result.

Proof of Theorem 2.7. Using (i) of Lemma 3.8 we find

$$E_{P,N} = E_{P,0} - \sum_{n=1}^{N} \Delta E_P|_n^{n-1} + O\left(N|g|^4 \Lambda (1-\gamma)^{4/2}\right),$$

where by construction $E_{P,0} = \sqrt{P^2 + m^2}$.

The inequalities in (ii) of Lemma 3.8 imply

$$E_{P,N} \le \sqrt{P^2 + m^2} - g^2 a \Lambda (1-\gamma) \sum_{n=1}^{N} \gamma^{n-1} + |g|^4 C \Lambda N (1-\gamma) \tag{36}$$

as well as

$$E_{P,N} \ge \sqrt{P^2 + m^2} - g^2 b \Lambda (1-\gamma) \sum_{n=1}^{N} \gamma^{n-1} - |g|^4 C \Lambda \ln \Lambda (1-\gamma). \tag{37}$$

Notice that by the same argument used in Lemma 3.3 one can conclude that $E_{P,N} = \inf \operatorname{spec}\left(H_{P,N} \upharpoonright \mathcal{F}_j\right)$ for all $j \ge N$. Since $N = \frac{\ln \Lambda}{-\ln \gamma}$ and the estimates in (36) and (37) hold for γ arbitrarily close to 1, they imply the inequalities in (8). □

4 The Effective Velocity and the Mass Shell

In this last section we provide the proof of Theorem 2.8, the starting point of which is the expression of the first derivative of the ground state energies $E_{P,n}$ that follows from analytic perturbation theory in P as stated in the proposition below:

Proposition 4.1. *Suppose $E_{P,n}$ is the non-degenerate isolated eigenvalue corresponding to the ground state $\Psi_{P,n}$. Then, the equation*

$$\frac{\partial E_{P,n}}{\partial P_i} = \left\langle \widehat{\Psi}_{P,n}, V_i(P)\widehat{\Psi}_{P,n} \right\rangle , \qquad V_i(P) := \frac{P_i - P_i^f}{[(P-P^f)^2 + m^2]^{1/2}} \tag{38}$$

holds true for components $i = 1, 2, 3$.

Proof. See Lemma 3.7 in [4]. □

In order to control the scalar product in (38) the following definition will be convenient:

Definition 4.2. For each $\Lambda\gamma^{n-1}$ we consider the energy level

$$\min\left\{\Lambda, \frac{\Lambda\gamma^{n-1}}{g^{\epsilon}}\right\}, \qquad 0 < \epsilon \le 1/2 \ , \tag{39}$$

and $l \in \mathbb{N} \cup \{0\}$ such that

$$\Lambda\gamma^{l} \le \min\left\{\Lambda, \frac{\Lambda\gamma^{n-1}}{g^{\epsilon}}\right\} < \Lambda\gamma^{l-1} .$$

We define

$$\Xi_{n-1} := \Lambda\gamma^{l} . \tag{40}$$

The energy scale Ξ_{n-1} will be used in a convenient *backwards expansion* to gain a certain power of $|g|$ in some estimates. From now on, we use the notation

$$H_{P,\Xi_{n-1}} := H_P|^{\Lambda}_{\Xi_{n-1}}, \qquad \Psi_{P,\Xi_{n-1}} := \Psi_{P,l} .$$

The following lemma gives a justification for this type of expansion:

Lemma 4.3. *Let $|g|$ be sufficiently small, $|P| < P_{max}$, and $0 < \epsilon \le 1/2$. For $z \in \Gamma_{P,n-1}$ the bound*

$$\left\| \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} g\Phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \le |g|^{\delta} C, \qquad \delta := 1 - \frac{\epsilon}{2}, \tag{41}$$

holds true. Consequently, the expansion formulas

$$\begin{aligned} \Psi^{(\Xi_{n-1})}_{P,n-1} &:= Q_{P,n-1}\Psi_{P,\Xi_{n-1}}, \\ Q_{P,n-1} &:= -\frac{1}{2\pi i}\oint_{\Gamma_{P,n-1}} \frac{dz}{H_{P,n-1} - z} \upharpoonright \mathcal{F}_{n-1} \\ &= -\frac{1}{2\pi i}\oint_{\Gamma_{P,n-1}} \frac{dz}{H_{P,\Xi_{n-1}} - z} \sum_{j=0}^{\infty} \left[-g\Phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - z} \right]^j \upharpoonright \mathcal{F}_{n-1} \end{aligned} \tag{42}$$

hold true and

$$\|\Psi^{(\Xi_{n-1})}_{P,n-1}\|^2 \ge (1 - O(|g|^{4\delta}))\|\Psi_{P,\Xi_{n-1}}\|^2 . \tag{43}$$

Proof. With the help of Lemma 3.8 we infer the bound

$$\left|E_{P,n-1} - E_{P,\Xi_{n-1}}\right| \leq Cg^2\Xi_{n-1}. \tag{44}$$

Hence, by the definition of Ξ_{n-1} in (39) and $0 < \epsilon \leq 1/2$, $|g|$ can be chosen sufficiently small but uniformly in n such that both ground state energies, $E_{P,n-1}$ and $E_{P,\Xi_{n-1}}$, lie inside the contour $\Gamma_{P,n-1}$. We estimate

$$\sup_{z\in\Gamma_{P,n-1}} \left\| \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} g\Phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}}$$
$$\leq 2|g| \sup_{z\in\Gamma_{P,n-1}} \left\| \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \cdot \sup_{z\in\Gamma_{P,n-1}} \left\| \phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}}.$$

A similar computation as in Lemma 3.3 gives

$$\mathrm{Gap}\,(H_{P,\Xi_{n-1}} \upharpoonright \mathcal{F}_{n-1}) \geq \zeta\omega\,(\Lambda\gamma^n) \tag{45}$$

such that for sufficiently small $|g|$ one has the bound

$$\left\| \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \leq \left(\frac{C}{\Lambda\gamma^n}\right)^{1/2} \tag{46}$$

by using inequality (i) in Lemma 3.1. Furthermore, one can bound

$$\left\| \phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \leq C\Xi^{1/2}_{n-1} \left\| \left(H^f|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}}\right)^{1/2} \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \leq C\Xi^{1/2}_{n-1}\theta^{-1/2}.$$

Hence, we may conclude that

$$\left\| \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} g\Phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \left(\frac{1}{H_{P,\Xi_{n-1}} - z}\right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \leq |g|C \begin{cases} \left(\frac{\Lambda\gamma^{n-1}}{\Lambda\gamma^n g^\epsilon}\right)^{1/2} & \text{for } \frac{\Lambda\gamma^{n-1}}{g^\epsilon} < \Lambda \\ \left(\frac{\Lambda}{\Lambda\gamma^n}\right)^{1/2} & \text{for } \frac{\Lambda\gamma^{n-1}}{g^\epsilon} \geq \Lambda \end{cases} \leq |g|^\delta C.$$

This ensures the validity of the expansion formulas (42) as well as the relation in (43). □

We can now prove our second main result:

Proof of Theorem 2.8. The strategy of proof is an expansion using the formulas provided by Theorem 3.7. As a first observation we note that by the spectral theorem the bounds

$$\|V_i(P)\| \leq 1 \quad \forall P \in \mathbb{R}^3, \qquad \left|\frac{\partial E_{P,n}}{\partial P_i}\right| \leq 1 \quad \text{for} \quad |P| < P_{max} \tag{47}$$

hold. These inequalities will be employed frequently without further notice.

With the help of Theorem 3.7 we find the following expansion for all $N \geq n \geq 1$:

$$\left\langle \widehat{\Psi}_{P,n}, V_i(P)\widehat{\Psi}_{P,n}\right\rangle = \frac{\langle \Psi_{P,n}, V_i(P)\Psi_{P,n}\rangle}{\langle \Psi_{P,n}, \Psi_{P,n}\rangle} \tag{48}$$

$$= \frac{1 + g^2 \alpha_P|_n^{n-1} + \mathcal{O}\left(|g|^4(1-\gamma)^{4/2}\right)}{\langle \Psi_{P,n-1}, \Psi_{P,n-1}\rangle}\Big[\langle \Psi_{P,n-1}, V_i(P)\Psi_{P,n-1}\rangle +$$

$$+ g^2 \left\langle \frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\Psi_{P,n-1}, V_i(P)\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\Psi_{P,n-1}\right\rangle$$

$$+ g^2 \left\langle \widetilde{Q}^{\perp}_{P,n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi|_n^{n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\Psi_{P,n-1}, V_i(P)\Psi_{P,n-1}\right\rangle + h.c.$$

$$- g^2 \left\langle \widetilde{Q}_{P,n-1}\phi|_n^{n-1}\left(\frac{1}{H_{P,n-1} - E_{P,n-1}}\right)^2 \phi^*|_n^{n-1}\Psi_{P,n-1}, V_i(P)\Psi_{P,n-1}\right\rangle + h.c. \tag{49}$$

$$+ \mathcal{O}\left(|g|^4(1-\gamma)^{4/2}\right)\Big].$$

We observe that

$$(49) = -2g^2\alpha_P|_n^{n-1}\langle \Psi_{P,n-1}, V_i(P)\Psi_{P,n-1}\rangle$$

because

$$g^2 \left\langle \widetilde{Q}_{P,n-1}\phi|_n^{n-1}\left(\frac{1}{H_{P,n-1} - E_{P,n-1}}\right)^2 \phi^*|_n^{n-1}\Psi_{P,n-1}, V_i(P)\Psi_{P,n-1}\right\rangle = g^2\alpha_P|_n^{n-1}\langle \Psi_{P,n-1}, V_i(P)\Psi_{P,n-1}\rangle .$$

Hence, we can rewrite (48) as

$$\left\langle \widehat{\Psi}_{P,n}, V_i(P)\widehat{\Psi}_{P,n}\right\rangle = \left(1 - g^2\alpha_P|_n^{n-1} + \mathcal{O}\left(|g|^4(1-\gamma)^{4/2}\right)\right)\left\langle \widehat{\Psi}_{P,n-1}, V_i(P)\widehat{\Psi}_{P,n-1}\right\rangle \tag{50}$$

$$+ g^2 \left\langle \frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P,n-1}, V_i(P)\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P,n-1}\right\rangle \tag{51}$$

$$+ g^2 2\Re \left\langle \widetilde{Q}^{\perp}_{P,n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi|_n^{n-1}\frac{1}{H_{P,n-1} - E_{P,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P,n-1}, V_i(P)\widehat{\Psi}_{P,n-1}\right\rangle \tag{52}$$

$$+ \mathcal{O}\left(|g|^4(1-\gamma)^{4/2}\right).$$

Next, we proceed iteratively by expanding $\left\langle \widehat{\Psi}_{P,n}, V_i(P)\widehat{\Psi}_{P,n}\right\rangle$ at each step from $n = N$ to $n = 0$. Meanwhile, we define

$$A_{P,n-1} := (51), \qquad B_{P,n-1} := (52).$$

As a result of the iteration we find the following expansion

$$\left\langle \widehat{\Psi}_{P,N}, V_i(P)\widehat{\Psi}_{P,N}\right\rangle = \prod_{j=1}^{N}\left(1 - g^2\alpha_P|_{N-j+1}^{N-j}\right)\left\langle \widehat{\Psi}_{P,0}, V_i(P)\widehat{\Psi}_{P,0}\right\rangle$$

$$+ \sum_{j=2}^{N-1}\left(1 - g^2\alpha_P|_N^{N-1}\right)\dots\left(1 - g^2\alpha_P|_{N-j+1}^{N-j}\right)\left[A_{P,N-j-1} + B_{P,N-j-1}\right]$$

$$+ \left(1 - g^2\alpha_P|_N^{N-1}\right)\left[A_{P,N-2} + B_{P,N-2}\right] + \left[A_{P,N-1} + B_{P,N-1}\right] + \mathcal{O}\left(|g|^4 N(1-\gamma)^{4/2}\right). \tag{53}$$

21

Let us assume one could show the bounds

$$\left|A_{P,N-j}\right| \le g^2 C \frac{1-\gamma}{\Lambda\gamma^{N-j+1}}, \tag{54}$$
$$\left|B_{P,N-j}\right| \le |g|^{5/2} C(1-\gamma) \tag{55}$$

where we stress that the universal constant C is independent of the mass m. Then, using the following ingredients

- (iii) of Theorem 3.7,
- $N = \frac{\ln\Lambda}{-\ln\gamma}$,
- the basic estimates

$$\prod_{j=1}^{N}\left(1 - g^2\alpha_P|_{N-j+1}^{N-j}\right) \le \prod_{j=1}^{N}\left(1 - g^2 c_1(1-\gamma)\right) \le \Lambda^{-g^2 c_1 \frac{(1-\gamma)}{-\ln\gamma}},$$

$$\sum_{j=2}^{N-1}\left(1 - g^2\alpha_P|_N^{N-1}\right)\ldots\left(1 - g^2\alpha_P|_{N-j+1}^{N-j}\right) + \left(1 - g^2\alpha_P|_N^{N-1}\right) + 1 \le \sum_{j=0}^{N-1}\left(1 - g^2 c_1(1-\gamma)\right)^j$$
$$\le \frac{1}{g^2 c_1(1-\gamma)},$$

and using $\Lambda\gamma^N = 1$

$$\sum_{j=2}^{N-1}\left(1 - g^2\alpha_P|_N^{N-1}\right)\ldots\left(1 - g^2\alpha_P|_{N-j+1}^{N-j}\right)\frac{1-\gamma}{\Lambda\gamma^{N-j}} + \left(1 - g^2\alpha_P|_N^{N-1}\right)\frac{1-\gamma}{\Lambda\gamma^{N-1}} + \frac{1-\gamma}{\Lambda\gamma^N}$$
$$\le C(1-\gamma)\sum_{j=0}^{N-1}\gamma^j \le C,$$

the bounds in (54)-(55) are seen to imply

$$\left|\left\langle\widehat{\Psi}_{P,N}, V_i(P)\widehat{\Psi}_{P,N}\right\rangle\right| \le \Lambda^{-g^2 c_1 \frac{(1-\gamma)}{-\ln\gamma}} \frac{|P|}{\left[P^2+m^2\right]^{1/2}} + C|g|^{1/2} + C|g|^4 \ln\Lambda(1-\gamma), \tag{56}$$

where we recall that $\left|\left\langle\widehat{\Psi}_{P,0}, V_i(P)\widehat{\Psi}_{P,0}\right\rangle\right| = \frac{|P_i|}{\left[P^2+m^2\right]^{1/2}}$.

As the fineness parameter γ can be chosen arbitrarily close to one the bound in (9) is proven. We show now that the bounds (54)-(55) hold true.

Bound (54): Defining $P_\lambda := \lambda P$ and its components $P_{\lambda i} := \lambda P_i$, $1 \le i \le 3$, we start with the identity

$$A_{P,n-1} = \int_0^1 d\lambda \frac{d}{d\lambda} g^2 \left\langle \frac{1}{H_{P_\lambda,n-1} - E_{P_\lambda,n-1}} \phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}, V_i(P_\lambda)\frac{1}{H_{P_\lambda,n-1} - E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}\right\rangle \tag{57}$$

that holds because of analytic perturbation theory in P (see Lemma 3.7 in [4]) and

$$\left\langle \frac{1}{H_{0,n-1}-E_{0,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{0,n-1}, V_i(0)\frac{1}{H_{0,n-1}-E_{0,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{0,n-1}\right\rangle = 0$$

by symmetry under rotational invariance of $H_{0,n-1}$, $E_{0,n-1}$ and $\widehat{\Psi}_{0,n-1}$. In order to estimate the integrand

$$\begin{aligned}
&g^2\frac{d}{d\lambda}\left\langle \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}, V_i(P_\lambda)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}\right\rangle = \\
&= \lim_{h\to 0}\frac{g^2}{h}\Bigg[\left\langle \frac{1}{H_{P_{\lambda+h},n-1}-E_{P_{\lambda+h},n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_{\lambda+h},n-1}, V_i(P_{\lambda+h})\frac{1}{H_{P_{\lambda+h},n-1}-E_{P_{\lambda+h},n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_{\lambda+h},n-1}\right\rangle \\
&\qquad - \left\langle \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}, V_i(P_\lambda)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}\right\rangle\Bigg] \quad (58)
\end{aligned}$$

we first observe that in expression (58), at least for small $|h|$, the vector $\widehat{\Psi}_{P_{\lambda+h},n-1}$ can be replaced by the vector $\widehat{\Upsilon}_{P_{\lambda+h},n-1}$ where

$$\Upsilon_{P_{\lambda+h},n-1} := -\frac{1}{2\pi i}\oint_{\Gamma_{P,n-1}} \frac{dz}{H_{P_{\lambda+h,n-1}}-z}\Psi_{P_\lambda,n-1}\,.$$

Notice that $\Upsilon_{P_{\lambda+h},n-1} \parallel \Psi_{P_{\lambda+h},n-1}$ and $\Upsilon_{P_{\lambda+h},n-1}\big|_{h=0} = \Psi_{P_\lambda,n-1}$. Hence, we need to estimate three types of terms:

$$\begin{aligned}
&\lim_{h\to 0}\frac{g^2}{h}\Bigg\langle\left[\frac{1}{H_{P_{\lambda+h},n-1}-E_{P_{\lambda+h},n-1}} - \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\right]\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}, \\
&\qquad\qquad V_i(P_\lambda)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}\Bigg\rangle, \quad (59)
\end{aligned}$$

$$\lim_{h\to 0}\frac{g^2}{h}\left\langle \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\left[\widehat{\Upsilon}_{P_{\lambda+h},n-1}-\widehat{\Upsilon}_{P_\lambda,n-1}\right], V_i(P_\lambda)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Upsilon}_{P_\lambda,n-1}\right\rangle, \quad (60)$$

$$\lim_{h\to 0}\frac{g^2}{h}\left\langle \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}, [V_i(P_{\lambda+h})-V_i(P_\lambda)]\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}\right\rangle, \quad (61)$$

In order to estimate term (59) we observe that the expression is well defined because the vector $\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}$ is orthogonal to the ground state vector of both the Hamiltonians $H_{P_{\lambda+h},n-1}$ and $H_{P_\lambda,n-1}$. Hence, we verify that

$$\begin{aligned}
&\lim_{h\to 0}\frac{1}{h}\left[\frac{1}{H_{P_{\lambda+h},n-1}-E_{P_{\lambda+h},n-1}} - \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\right] \\
&= \lim_{h\to 0}\frac{1}{h}\left[\frac{1}{H_{P_{\lambda+h},n-1}-E_{P_{\lambda+h},n-1}}\left(H_{P_\lambda,n-1}-H_{P_{\lambda+h},n-1}-E_{P_\lambda,n-1}+E_{P_{\lambda+h},n-1}\right)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\right] \\
&= \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\left(-\frac{d}{d\lambda}\sqrt{(P_\lambda-P^f)^2+m^2}+\frac{d}{d\lambda}E_{P_\lambda,n-1}\right)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}} \\
&= \frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}}\sum_{i=1}^{3}P_{\lambda\,i}\left(-V_i(P_\lambda)+\frac{\partial E_{P,n-1}}{\partial P_i}\bigg|_{P\equiv P_\lambda}\right)\frac{1}{H_{P_\lambda,n-1}-E_{P_\lambda,n-1}} \quad (62)
\end{aligned}$$

23

holds true when applied to the vector $\phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}$. At first we treat the term proportional to $\sum_{i=1}^3 P_{\lambda\, i} V_i(P_\lambda)$. Using (iii) in Lemma 3.1, the estimate in (47), and the pull-through formula, we get the estimate

$$g^2 \left| \left\langle V_i(P_\lambda) \frac{1}{H_{P_\lambda,n-1} - E_{P_\lambda,n-1}} \phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1}, \right.\right.$$
$$\left.\left. \frac{1}{H_{P_\lambda,n-1} - E_{P_\lambda,n-1}} \sum_{j=1}^3 P_{\lambda\, j} V_j(P_\lambda) \frac{1}{H_{P_\lambda,n-1} - E_{P_\lambda,n-1}} \phi^*|_n^{n-1}\widehat{\Psi}_{P_\lambda,n-1} \right\rangle \right|$$
$$= g^2 \left| \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk \rho(k)^2 \left\langle V_i(P_\lambda - k) \left(\frac{1}{H_{P_\lambda - k,n-1} - E_{P_\lambda,n-1} + \omega(k)} \right) \widehat{\Psi}_{P_\lambda,n-1}, \right.\right.$$
$$\left.\left. \left(\frac{1}{H_{P_\lambda - k,n-1} - E_{P_\lambda,n-1} + \omega(k)} \right) \sum_{j=1}^3 P_{\lambda\, j} V_j(P_\lambda - k) \frac{1}{H_{P_\lambda - k,n-1} - E_{P_\lambda,n-1} + \omega(k)} \widehat{\Psi}_{P_\lambda,n-1} \right\rangle \right|$$
$$\leq g^2 C \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk \frac{1}{|k|^4} \leq g^2 \frac{C(1-\gamma)}{\Lambda\gamma^n}.$$

The remaining term in (59) being proportional to $\sum_{i=1}^3 P_{\lambda\, i} \left(\frac{\partial E_{P,n-1}}{\partial P_i} \big|_{P \equiv P_\lambda} \right)$ can be estimated in the same way. In consequence, we get

$$|(59)| \leq g^2 \frac{C(1-\gamma)}{\Lambda\gamma^n}. \tag{63}$$

Next, we consider term (60). Using the differentiability in λ again we find

$$\lim_{h\to 0} \frac{\Upsilon_{P_{\lambda+h},n-1} - \Upsilon_{P_\lambda,n-1}}{h} = -\frac{1}{2\pi i} \lim_{h\to 0} \frac{1}{h} \oint_{\Gamma_{P,n-1}} dz \left[\frac{1}{H_{P_{\lambda+h},n-1} - z} - \frac{1}{H_{P_\lambda,n-1} - z} \right] \Psi_{P_\lambda,n-1}$$
$$= -\frac{1}{2\pi i} \lim_{h\to 0} \frac{1}{h} \oint_{\Gamma_{P,n-1}} dz \left[\frac{1}{H_{P_\lambda,n-1} - z} \left(H_{P_{\lambda,n-1}} - H_{P_{\lambda+h,n-1}} \right) \frac{1}{H_{P_\lambda,n-1} - z} \right] \Psi_{P_\lambda,n-1}$$
$$= -\frac{1}{2\pi i} \oint_{\Gamma_{P,n-1}} dz \left[\frac{1}{H_{P_\lambda,n-1} - z} \left(-\sum_{i=1}^3 P_{\lambda\, i} V_i(P_\lambda) \right) \frac{1}{H_{P_\lambda,n-1} - z} \right] \Psi_{P_\lambda,n-1}$$
$$= -Q^\perp_{P_\lambda,n-1} \frac{1}{H_{P_\lambda,n-1} - E_{P_\lambda,n-1}} \sum_{i=1}^3 P_{\lambda\, i} V_i(P_\lambda) \Psi_{P_\lambda,n-1} \tag{64}$$

and

$$\lim_{h\to 0} \frac{1}{h} \left[\frac{1}{\left\|\Upsilon_{P_{\lambda+h},n-1}\right\|} - \frac{1}{\left\|\Upsilon_{P_\lambda,n-1}\right\|} \right] = -\frac{1}{\left\|\Upsilon_{P_\lambda,n-1}\right\|^3} \lim_{h\to 0} \Re \left\langle \frac{\Upsilon_{P_{\lambda+h},n-1} - \Upsilon_{P_\lambda,n-1}}{h}, \Upsilon_{P_\lambda,n-1} \right\rangle = 0. \tag{65}$$

Equations (64) and (65), the pull-through formula, and the gap estimate in Theorem 3.6 give

$$|(60)| \leq g^2 \frac{C(1-\gamma)}{\Lambda\gamma^n}. \tag{66}$$

In the estimate of the third term, i.e., term (61), we exploit the additional decay which we gain through the derivative of $V_i(P_\lambda)$, i.e.,

$$\lim_{h\to 0} \frac{1}{h} [V_i(P_{\lambda+h}) - V_i(P_\lambda)] = \frac{P_{\lambda\, i} - V_i(P_\lambda) \sum_{j=1}^3 V_j(P_\lambda) P_{\lambda\, j}}{\sqrt{(P_\lambda - P^f)^2 + m^2}}.$$

Thus, we can rewrite and estimate (61) as follows

$$\Big|g^2\int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\,\rho(k)^2\Big\langle\widehat{\Psi}_{P_\lambda,n-1},\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\times$$
$$\Big[\frac{P_{\lambda\,i}-V_i(P_\lambda-k)\sum_{j=1}^3 V_j(P_\lambda-k)P_{\lambda\,j}}{\sqrt{(P_\lambda-P^f-k)^2+m^2}}\Big]\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\widehat{\Psi}_{P_\lambda,n-1}\Big\rangle\Big|$$
$$\leq Cg^2P_{max}\Big|\int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\,\rho(k)^2\Big\langle\widehat{\Psi}_{P,n-1},\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\times$$
$$\times\frac{1}{\sqrt{(P_\lambda-P^f-k)^2+m^2}}\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\widehat{\Psi}_{P_\lambda,n-1}\Big\rangle\Big| \tag{67}$$

where we have used the pull-through formula. Next we consider the spectral measure $d\mu_k(\xi)\equiv f_k(\xi)d\xi$ (where $f_k(\xi)\geq 0$ a.e.) associated with the vector

$$\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\widehat{\Psi}_{P_\lambda,n-1}$$

in the joint spectral representation of the components of the operator P^f where ξ is the spectral variable. The measure is defined by

$$(0\leq)\ \|\chi_\Omega\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\widehat{\Psi}_{P_\lambda,n-1}\|^2=:\int_{\sigma(P^f)} d\xi\,f_k(\xi)\chi_\Omega(\xi)\ \leq\frac{C}{|k|^2}$$

for every measurable set $\Omega\subseteq\sigma(P^f)$ where $\chi_\Omega(\xi)$ is the characteristic function of the set Ω and χ_Ω is the corresponding spectral projection. Thus we can write (67) as follows

$$(67)\ =\ Cg^2\int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\,\frac{1}{|k|}\Big\|\Big[\frac{1}{\sqrt{(P_\lambda-P^f-k)^2+m^2}}\Big]^{\frac{1}{2}}\frac{1}{H_{P_\lambda-k,n-1}+\omega(k)-E_{P_\lambda,n-1}}\widehat{\Psi}_{P_\lambda,n-1}\Big\|^2$$
$$=\ Cg^2\int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}}\int d\Omega_k d|k|\frac{1}{|k|}\int_{\sigma(P^f)} d\xi\ f_k(\xi)\,\frac{1}{\sqrt{(P_\lambda-\xi-k)^2+m^2}} \tag{68}$$

By knowing that

$$\int_{\sigma(P^f)} d\xi\ f_k(\xi)\,\frac{1}{\sqrt{(P_\lambda-\xi-k)^2+m^2}}<+\infty$$

we can interchange the integration in $d\xi$ with the angular integration in the variable k, i.e.,

$$(68)=Cg^2\int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}}|k|d|k|\int_{\sigma(P^f)} d\xi\int_0^{2\pi} d\varphi\int_0^{\pi} d\theta\sin\theta\,f_k(\xi)\,\frac{1}{\sqrt{(P_\lambda-\xi)^2+k^2-2\cos\theta|P_\lambda-\xi|\,|k|+m^2}}$$

where θ denotes the angle between the vector k and the vector $P_\lambda-\xi$ and φ the azimuthal angle with respect to an arbitrarily chosen vector orthogonal to $P_\lambda-\xi$. We split the integration in the variable θ into two regions: $\theta\in\left[\frac{\pi}{3},\pi\right]$ and $\theta\in\left[0,\frac{\pi}{3}\right]$. For $\theta\in\left[\frac{\pi}{3},\pi\right]$ being $\cos\theta\in\left[-1,\frac{1}{2}\right]$ we observe that

$$(P_\lambda-\xi)^2+k^2-2\cos\theta|P_\lambda-\xi|\,|k|\geq(P_\lambda-\xi)^2+k^2-|P_\lambda-\xi|\,|k|\geq\frac{3}{4}k^2$$

and, consequently,

$$\int_{\sigma(P^f)} d\xi \int_0^{2\pi} d\varphi \int_{\pi/3}^{\pi} d\theta \, \sin\theta \, f_k(\xi) \, \frac{1}{\sqrt{(P_\lambda - \xi)^2 + k^2 - 2\cos\theta |P_\lambda - \xi| \, |k| + m^2}} \tag{69}$$

$$\leq C \int_{\sigma(P^f)} d\xi \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \, \sin\theta \, f_k(\xi) \, \frac{1}{|k|} \tag{70}$$

$$\leq \frac{C}{|k|} \int d\Omega_k \int_{\sigma(P^f)} d\mu_k(\xi) \tag{71}$$

$$\leq \frac{C}{|k|^3} \tag{72}$$

Notice that the constant C in (72) can be chosen to be independent of the mass m. Next, we treat the integration over $\theta \in \left[0, \frac{\pi}{3}\right]$ where $\cos\theta \in \left[\frac{1}{2}, 1\right]$ and

$$(P_\lambda - \xi)^2 + k^2 - 2\cos\theta |P_\lambda - \xi| \, |k| \geq \left[(P_\lambda - \xi)^2 + k^2\right](1 - \cos\theta)$$

we find

$$\begin{aligned} \int_{\sigma(P^f)} d\xi \int_0^{2\pi} d\varphi \int_0^{\pi/3} d\theta \, \sin\theta \, f_k(\xi) \, \frac{1}{\sqrt{[(P_\lambda - \xi)^2 + k^2](1 - \cos\theta) + m^2}} \\ \leq \int_{\sigma(P^f)} d\xi \int_0^{2\pi} d\varphi \int_0^{\pi/3} d\theta \, \sin\theta \frac{1}{|k|} \, f_k(\xi) \, \frac{1}{\sqrt{(1 - \cos\theta)}} \\ \leq C \int_{\sigma(P^f)} d\xi \int_0^{2\pi} d\varphi \int_0^{\pi/3} d\theta \frac{1}{|k|} \, f_k(\xi) \\ \leq \frac{C}{|k|^3} \end{aligned} \tag{73}$$

Notice that also the constant C in (73) can be chosen to be independent of the mass m. Combining the results for the two integration domains, i.e., (69) and (73), we arrive at

$$(68) \leq g^2 C \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} d|k| \frac{1}{|k|^2} \leq g^2 C \frac{1 - \gamma}{\Lambda\gamma^n}. \tag{74}$$

Hence, we have proven the bound in (61).

With the three bounds in (63), (66) and (74) we can control the integrand (59)-(61), and hence, the integral given in (57) which proves the bound in (54).

Bound (55): As a next step we proceed with the bound of (55) where by using the pull-through formula we get

$$
\begin{aligned}
&\left|B_{P,n-1}\right| \\
&= g^2 \left| 2\Re \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\, \rho(k)^2 \left\langle Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} \frac{1}{H_{P-k,n-1} + \omega(k) - E_{P,n-1}} \widehat{\Psi}_{P,n-1}, V_i(P) \widehat{\Psi}_{P,n-1} \right\rangle \right| \\
&\qquad \le g^2 C \int_{\Lambda\gamma^n}^{\Lambda\gamma^{n-1}} dk\, \frac{1}{k^2} \left\| \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,n-1} \right\| \\
&\qquad\qquad \le g^2 C \Lambda \gamma^{n-1} (1-\gamma) \left\| \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,n-1} \right\| . \qquad (75)
\end{aligned}
$$

We shall now show that

$$
\left\| \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,n-1} \right\| \le C \frac{|g|^{1/2}}{\Lambda \gamma^n} \qquad (76)
$$

holds true, so that, by inserting this bound in (75), we get the desired m-independent estimate in (55).

In order to gain a certain power of $|g|$ we re-expand the left-hand side of (76) backwards from energy level $\Lambda\gamma^{n-1}$ to Ξ_{n-1}, as defined in (40), with the help of Lemma 4.3 for an ϵ, $0 < \epsilon \le \frac{1}{2}$, and $\delta = 1 - \frac{\epsilon}{2}$ which will be fixed later. We know that

- $\left\| \left(\frac{1}{H_{P,\Xi_{n-1}} - z} \right)^{1/2} g \Phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \left(\frac{1}{H_{P,\Xi_{n-1}} - z} \right)^{1/2} \right\|_{\mathcal{F}_{n-1}} \le |g|^{\delta} C \quad$ for $z \in \Gamma_{P,n-1}$ (see (41)),
- $\Psi^{(\Xi_{n-1})}_{P,n-1}$ and $\Psi_{P,n-1}$ are two vectors belonging to the same ray with $\|\Psi^{(\Xi_{n-1})}_{P,n-1}\|^2 \ge (1 - O(|g|^{4\delta})) \|\Psi_{P,\Xi_{n-1}}\|^2$ (see (42)).

Thus, denoting the length of the contour $\Gamma_{P,n-1}$ by $|\Gamma_{P,n-1}|$, we find for $|g|$ sufficiently small

$$
\begin{aligned}
\left\| \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,n-1} \right\| &= \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}^{(\Xi_{n-1})}_{P,n-1} \right\| \\
&\le C \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \\
+ C \left\| \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} \right\|_{\mathcal{F}_{n-1}} \|V_i(P)\| \, |\Gamma_{P,n-1}| & \sup_{z \in \Gamma_{P,n-1}} \sum_{j=1}^{\infty} \left\| \frac{1}{H_{P,\Xi_{n-1}} - z} \left[-g\phi^*|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - z} \right]^j \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \\
&\le \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| + C \frac{|g|^{\delta}}{\Lambda \gamma^n} \qquad (77)
\end{aligned}
$$

where we have used the bound in (41), the inequality in (46), and the gap estimate given in Theorem 3.6. Using the same ingredients, we estimate

$$
\left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,n-1} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \qquad (78)
$$

by expanding the spectral projection on the right, i.e.,

$$
\begin{aligned}
(78) \leq & \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \\
& + C \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} \right\|_{\mathcal{F}_{n-1}} |\Gamma_{P,n-1}| \sup_{z \in \Gamma_{P,n-1}} \sum_{j=1}^{\infty} \left\| \frac{1}{H_{P,\Xi_{n-1}} - z} \left[-g \Phi|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - z} \right]^j \right\|_{\mathcal{F}_{n-1}} \|V_i(P)\| \\
& \leq \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| + C \frac{|g|^{\delta}}{\Lambda\gamma^n} \qquad (79)
\end{aligned}
$$

where $Q^{\perp}_{P,\Xi_{n-1}} \equiv Q^{\perp}_{P,l}$, for some $l \leq N$ specified in (40). Next, we study

$$
\left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \qquad (80)
$$

by applying the resolvent formula

$$
\begin{aligned}
(80) \leq & \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \\
& + \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,n-1} - E_{P,n-1}} g\phi^*|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| . \qquad (81)
\end{aligned}
$$

In order to estimate (81) we make use of the following intermediate steps:

- $\left\| Q^{\perp}_{P,n-1} \left(\frac{1}{H_{P,n-1} - E_{P,n-1}} \right) \right\|_{\mathcal{F}_{n-1}} \leq \frac{C}{\Lambda\gamma^n}$,
- $$
\begin{aligned}
& \left\| g\phi^*|^{\Xi_{n-1}}_{\Lambda\gamma^{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \\
& \quad = |g| \left(\int_{\Lambda\gamma^{n-1}}^{\Xi_{n-1}} dk\, \rho(k)^2 \right)^{1/2} \left\| \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \\
& \quad \leq C|g| \Xi_{n-1} \frac{1}{\Xi_{n-1}}
\end{aligned}
$$

  following from

$$
\left\| Q^{\perp}_{P,\Xi_{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} \right\|_{\mathcal{F}|^{\Lambda}_{\Xi_{n-1}}} \leq \frac{C}{\Xi_{n-1}} = C \max\left(\frac{g^{\epsilon}}{\Lambda\gamma^n}; \frac{1}{\Lambda} \right) \qquad (82)
$$

  that holds because of Theorem 3.6 and inequality (i) in Lemma 3.1.

This implies

$$
(80) \leq \left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| + C \frac{|g|}{\Lambda\gamma^n}. \qquad (83)
$$

Next we consider

$$\left\| Q^{\perp}_{P,n-1} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \tag{84}$$

and re-expand the first spectral projection. Hence, by using (41) and (82) we can conclude that

$$(84) \leq \left\| Q^{\perp}_{P,\Xi_{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| + C \frac{|g|^{\delta}}{\Lambda \gamma^n}. \tag{85}$$

As a last step, for the first term on the right-hand side of (85) we have to regard two cases:

1. Case $\Xi_{n-1} < \Lambda$. In this case we exploit

$$\left\| Q^{\perp}_{P,\Xi_{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} \right\|_{\mathcal{F}|^{\Lambda}_{\Xi_{n-1}}} \leq \frac{g^{\epsilon} C}{\Lambda \gamma^n}$$

2. Case $\Xi_{n-1} = \Lambda$. In this case we have

$$Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} = \frac{P_i}{\sqrt{P^2 + m^2}} Q^{\perp}_{P,\Xi_{n-1}} \widehat{\Psi}_{P,\Xi_{n-1}} = 0.$$

For both cases the estimate

$$\left\| Q^{\perp}_{P,\Xi_{n-1}} \frac{1}{H_{P,\Xi_{n-1}} - E_{P,n-1}} Q^{\perp}_{P,\Xi_{n-1}} V_i(P) \widehat{\Psi}_{P,\Xi_{n-1}} \right\| \leq \frac{C g^{\epsilon}}{\Lambda \gamma^n}$$

holds true.

Choosing $\epsilon = \frac{1}{2}$ and collecting all the remainders the bound in (76) is seen to be true. Hence, we have also proven the inequality in (55). This concludes the proof of the bound in (56). □

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Relation between the Resonance and the Scattering Matrix in the massless Spin-Boson Model

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Abstract

We establish the precise relation between the integral kernel of the scattering matrix and the resonance in the massless Spin-Boson model which describes the interaction of a two-level quantum system with a second-quantized scalar field. For this purpose, we derive an explicit formula for the two-body scattering matrix. We impose an ultraviolet cut-off and assume a slightly less singular behavior of the boson form factor of the relativistic scalar field but no infrared cut-off. The purpose of this work is to bring together scattering and resonance theory and arrive at a similar result as provided by Simon in [39], where it was shown that the singularities of the meromorphic continuation of the integral kernel of the scattering matrix are located precisely at the resonance energies. The corresponding problem has been open in quantum field theory ever since. To the best of our knowledge, the presented formula provides the first rigorous connection between resonance and scattering theory in the sense of [39] in a model of quantum field theory.

1 Introduction

In this paper, we analyze the massless Spin-Boson model which is a non-trivial model of quantum field theory. It can be seen as a model of a two-level atom interacting with its second-quantized scalar field, and hence, provides a widely employed model for quantum optics which gives insights into scattering processes between photons and atoms. The unperturbed energies of the two-level atom shall be denoted by real numbers $0 = e_0 < e_1$. It is well-known that after switching on the interaction with a massless scalar field, which may induce transitions between the atom levels, the free ground state energy e_0 is shifted to the interacting ground state energy λ_0 while the free excited state with energy e_1 turns into a resonance with complex "energy" λ_1.

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One of the main mathematical difficulties in the study of the massless Spin-Boson model is the absence of a spectral gap which does not allow a straight-forward application of regular perturbation theory. Several techniques have been developed to overcome this difficulty. There are two methods that rigorously address this problem: The so-called renormalization group (see e.g. [8, 10, 9, 6, 11, 2, 26, 27, 38, 21, 15]) which was the first one used to construct resonances in models of quantum field theory, and furthermore, the so-called multiscale method which was developed in [33, 34, 4, 5] and also successfully applied in various models of quantum field theory. In both cases, a family of spectrally dilated Hamiltonians is analyzed since this allows for complex eigenvalues. Our work draws from the results obtained in a previous article [14] which is build on the latter technique mentioned above. Beyond the construction, we obtained several spectral estimates and analyticity properties in [14] which are crucial ingredients for this work.

In addition to the resonance theory, also the scattering theory is well-established in various models of quantum field theory, e.g., in [23, 22, 16, 25, 24], and in particular in the massless Spin-Boson model, e.g., in [17, 18, 19, 20, 12]. The purpose of this work is to bring these two well-developed fields together and to arrive at a similar result as provided by Simon in [39]. Therein, it was shown that the singularities of the meromorphic continuation of the integral kernel of the scattering matrix are located precisely at the resonance energies. To the best of our knowledge, this question has not yet been addressed in models of quantum field theory, which is most probably due to the fact that quantum field models involve new subtleties as compared to the quantum mechanical ones. These can however be addressed with the recently developed methods of multiscale analysis and spectral renormalization (while we rely on the former in this work). We provide a representation of the scattering matrix in terms of an expectation value of the resolvent of a spectrally dilated Hamiltonian; see Theorem 2.2 below. The relation of the scattering matrix and the resonance can then be read of this formula; see Eqs. (2.3) and (2.4) below. Loosely put, our results imply that, for the photon momenta $|k'|$ in a neighborhood of $\operatorname{Re}\lambda_1 - \lambda_0$, the leading order (in g for small g) of the integral kernel of the transition matrix fulfills

$$|T(k,k')|^2 \sim \frac{E_1^2 g^4}{(|k'| + \lambda_0 - \operatorname{Re}\lambda_1)^2 + g^4 E_1^2}, \tag{1.1}$$

where we define

$$E_1 := g^{-2} \operatorname{Im}\lambda_1, \tag{1.2}$$

and it turns out that there are constant numbers $E_I < 0$, $a > 0$ and a uniformly bounded function $\Delta \equiv \Delta(g)$ such that $E_1 = E_I + g^a \Delta$. Heuristically, for an experiment in which a two-level atom is irradiated with monochromatic incoming light quanta of momentum $k' \in \mathbb{R}^3$, the relation (1.1) states that the intensity of the outgoing light quanta with momentum $k \in \mathbb{R}^3$ is proportional to $|T(k,k')|^2$, which is given as a Lorentzian function with maximum at $|k'| = \operatorname{Re}\lambda_1 - \lambda_0$ and width $2\operatorname{Im}\lambda_1$. This relation is already found as folklore knowledge in physics text-books. In this work we give a rigorous derivation in the model at hand. On the other hand, the relation between the imaginary value of the resonance and the decay rate of the unstable excited state was established rigorously in several articles [1, 29, 37, 13].

In [7], a rigorous mathematical justification of Bohr's frequency condition is derived, using an expansion of the scattering amplitudes with respect to powers the finestructur constant for the Pauli-Fierz model. In particular, they calculate the leading order term and provide an algorithm for computing the other terms. In [12], the photoelectric effect is studied for a model of an atom with a single bound state, coupled to the quantized electromagnetic field. In their work, they use similar techniques for estimating time evolution as the ones presented in this manuscript.

1.1 The Spin-Boson model

In this section we introduce the considered model and state preliminary definitions and well-known tools and facts from which we start our analysis. If the reader is already familiar with the introductory Sections 1.1 until 1.2 of [14], these subsections can be skipped. The notation is identical and these subsections are only given for the purpose of self-containedness.

The non-interacting Spin-Boson Hamiltonian is defined as

$$H_0 := K + H_f, \qquad K := \begin{pmatrix} e_1 & 0 \\ 0 & e_0 \end{pmatrix}, \qquad H_f := \int \mathrm{d}^3k\, \omega(k) a(k)^* a(k). \tag{1.3}$$

We regard K as an idealized free Hamiltonian of a two-level atom. As already stated in the introduction, its two energy levels are denoted by the real numbers $0 = e_0 < e_1$. Furthermore, H_f denotes the free Hamiltonian of a massless scalar field having dispersion relation $\omega(k) = |k|$, and a, a^* are the annihilation and creation operators on the standard Fock space which will be defined in (1.12) and (1.13) below. In the following we will sometimes call K the atomic part, and H_f the free field part of the Hamiltonian. The sum of the free two-level atom Hamiltonian K and the free field Hamiltonian H_f will simply be referred to as the "free Hamiltonian" H_0. The interaction term reads

$$V := \sigma_1 \otimes (a(f) + a(f)^*), \qquad \sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1.4}$$

where the boson form factor is given by

$$f : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}, \qquad k \mapsto e^{-\frac{k^2}{\Lambda^2}} |k|^{-\frac{1}{2}+\mu}. \tag{1.5}$$

Note that the relativistic form factor of a scalar field should rather be $f(k) = (2\pi)^{-\frac{3}{2}}(2|k|)^{-\frac{1}{2}}$, which however renders the model ill-defined due to the fact that such an f would not be square integrable. This is referred to as ultraviolet divergence. In our case, the gaussian factor in (1.5) acts as an ultraviolet cut-off for $\Lambda > 0$ being the ultraviolet cut-off parameter and in addition the fixed number

$$\mu \in (0, 1/2) \tag{1.6}$$

implies a regularization of the infrared singularity at $k = 0$ which is a technical assumption chosen for this work to keep the proofs more tractable. With additional work, one can also treat the case $\mu = 0$ with methods described in [3]. The missing factor of $2^{-\frac{1}{2}}(2\pi)^{-\frac{3}{2}}$ will be absorbed in the coupling constant g in our notation. Note that the form factor f only depends on the radial part of k. To emphasize this, we often write $f(k) \equiv f(|k|)$.

The full Spin-Boson Hamiltonian is then defined as

$$H := H_0 + gV \tag{1.7}$$

for some coupling constant $g > 0$ on the Hilbert space

$$\mathcal{H} := \mathcal{K} \otimes \mathcal{F}[\mathfrak{h}], \qquad \mathcal{K} := \mathbb{C}^2, \tag{1.8}$$

where

$$\mathcal{F}[\mathfrak{h}] := \bigoplus_{n=0}^{\infty} \mathcal{F}_n[\mathfrak{h}], \qquad \mathcal{F}_n[\mathfrak{h}] := \mathfrak{h}^{\odot n}, \qquad \mathfrak{h} := L^2(\mathbb{R}^3, \mathbb{C}) \tag{1.9}$$

denotes the standard bosonic Fock space, and superscript $\odot n$ denotes the n-th symmetric tensor product, where by convention $\mathfrak{h}^{\odot 0} \equiv \mathbb{C}$. Note that we identify $K \equiv K \otimes 1_{\mathcal{F}[\mathfrak{h}]}$ and $H_f \equiv 1_{\mathcal{K}} \otimes H_f$ in our notation (see Remark 1.2 below).

Due to the direct sum, an element $\Psi \in \mathcal{F}[\mathfrak{h}]$ can be represented as a family $(\psi^{(n)})_{n\in\mathbb{N}_0}$ of wave functions $\psi^{(n)} \in \mathfrak{h}^{\odot n}$. The state Ψ with $\psi^{(0)} = 1$ and $\psi^{(n)} = 0$ for all $n \geq 1$ is called the vacuum and is denoted by

$$\Omega := (1, 0, 0, \dots) \in \mathcal{F}[\mathfrak{h}]. \tag{1.10}$$

We define

$$\mathcal{F}_0 := \left\{ \Psi = (\psi^{(n)})_{n\in\mathbb{N}_0} \in \mathcal{F}[\mathfrak{h}] \,\middle|\, \exists N \in \mathbb{N}_0 : \psi^{(n)} = 0 \,\forall n \geq N, \forall n \in \mathbb{N} : \psi^{(n)} \in S(\mathbb{R}^{3n}, \mathbb{C}) \right\}, \tag{1.11}$$

where $S(\mathbb{R}^{3n}, \mathbb{C})$ denotes the Schwartz space of infinitely differentiable functions with rapid decay.

Then, for any $h \in \mathfrak{h}$, we define the operator $a(h) : \mathcal{F}_0 \to \mathcal{F}_0$ by

$$\left(a(h)\Psi\right)^{(n)}(k_1, ..., k_n) = \sqrt{n+1} \int \mathrm{d}^3k \, \overline{h(k)} \psi^{(n+1)}(k, k_1, ..., k_n) \tag{1.12}$$

and $a(h)\Omega = 0$. The operator $a(h)$ is closable and, using a slight abuse of notation, we denote its closure by the same symbol $a(h)$ in the following. The operator $a(h)$ is called the annihilation operator. The creation operator is defined as the adjoint of $a(h)$ and we denote it by $a(h)^*$. For $\Psi = (\psi^{(n)})_{n\in\mathbb{N}_0} \in \mathcal{F}_0$, we find that

$$(a(h)^*\Psi)^{(n)}(k_1,...,k_n) = \frac{1}{\sqrt{n}}\sum_{i=1}^{n} h(k_i)\psi^{(n-1)}(k_1,...,\tilde{k}_i,...,k_n), \tag{1.13}$$

where the notation $\tilde{\cdot}$ means that the corresponding variable is omitted.

Occasionally, we shall also use the physics notation and define the point-wise creation and annihilation operators. The action of the latter in the n boson sector is to be understood as:

$$(a(k)\Psi)^{(n)}(k_1,...,k_n) = \sqrt{n+1}\psi^{(n+1)}(k,k_1,...,k_n), \tag{1.14}$$

for $\Psi = (\psi^{(n)})_{n\in\mathbb{N}_0} \in \mathcal{F}_0$. The operator $a(k)$ is not closable. The point-wise creation operator $a(k)^*$ is only defined as a quadratic form on $\mathcal{F}_0$ in the following sense:

$$\langle\Phi, a(k)^*\Psi\rangle = \langle a(k)\Phi, \Psi\rangle, \qquad \forall\Phi,\Psi\in\mathcal{F}_0. \tag{1.15}$$

Moreover, we define quadratic forms:

$$\mathcal{F}_0\times\mathcal{F}_0\to\mathbb{C}, \quad (\Phi,\Psi)\mapsto \int \mathrm{d}^3k\,\overline{h(k)}\,\langle\Phi, a(k)\Psi\rangle \tag{1.16}$$

and

$$\mathcal{F}_0\times\mathcal{F}_0\to\mathbb{C}, \quad (\Phi,\Psi)\mapsto \int \mathrm{d}^3k\,h(k)\,\langle\Phi, a(k)^*\Psi\rangle\,. \tag{1.17}$$

It is not difficult to see that these quantities are equal to $\langle\Phi, a(h)\Psi\rangle$ and $\langle\Phi, a(h)^*\Psi\rangle$, respectively. The point-wise creation operator $a(k)^*$ is not defined as an operator but, formally, we can express it in the following way:

$$(a(k)^*\Psi)^{(n)}(k_1,...,k_n) = \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\delta^{(3)}(k-k_i)\psi^{(n-1)}(k_1,...,\tilde{k}_i,...,k_n). \tag{1.18}$$

This is the usual formula that physicists use. Here, δ denotes the Dirac's delta tempered distribution acting on the Schwartz space of test functions. Note that a and a^* fulfill the canonical commutation relations:

$$\forall h,l\in\mathfrak{h}, \qquad [a(h),a^*(l)] = \langle h,l\rangle_2\,, \qquad [a(h),a(l)] = 0, \qquad [a^*(h),a^*(l)] = 0. \tag{1.19}$$

Let us recall some well-known facts about the introduced model. Clearly, K is self-adjoint on $\mathcal{K}$ and its spectrum consists of two eigenvalues e_0 and e_1. The corresponding eigenvectors are

$$\varphi_0 = (0,1)^T \qquad \text{and} \qquad \varphi_1 = (1,0)^T \qquad \text{with} \qquad K\varphi_i = e_i\varphi_i, \quad i=0,1. \tag{1.20}$$

Moreover, H_f is self-adjoint on its natural domain $\mathcal{D}(H_f) \subset \mathcal{F}[\mathfrak{h}]$ and its spectrum $\sigma(H_f) = [0,\infty)$ is absolutely continuous (see [36]). Consequently, the spectrum of H_0 is given by $\sigma(H_0) = [e_0,\infty)$, and e_0, e_1 are eigenvalues embedded in the absolutely continuous part of the spectrum of H_0 (see [35]).

Finally, also the self-adjointness of the full Hamiltonian H is well-known (see, e.g., [31]) and it can be shown using the standard estimate in Lemma A.1.

Proposition 1.1. *The operator gV is relatively bounded by H_0 with infinitesimal bound and, consequently, H is self-adjoint and bounded below on the domain*

$$\mathcal{D}(H) = D(H_0) = \mathcal{K} \otimes \mathcal{D}(H_f), \tag{1.21}$$

i.e., there is a constant $b \in \mathbb{R}$ such that

$$b \leq H. \tag{1.22}$$

Remark 1.2. *In this work we omit spelling out identity operators whenever unambiguous. For every vector spaces V_1, V_2 and operators A_1 and A_2 defined on V_1 and V_2, respectively, we identify*

$$A_1 \equiv A_1 \otimes \mathbb{1}_{V_2}, \qquad A_2 \equiv \mathbb{1}_{V_1} \otimes A_2. \tag{1.23}$$

In order to simplify our notation further, and whenever unambiguous, we do not utilize specific notations for every inner product or norm that we employ.

1.2 Access to the resonance: Complex dilation

It is known (e.g., [31]) that the only eigenvalue in the spectrum of H is

$$\lambda_0 := \inf \sigma(H) \tag{1.24}$$

while the rest of the spectrum is absolutely continuous. This implies that there is no stable excited state in the massless Spin-Boson model. Heuristically, the reason for this is that the atomic energy of the excited state e_1 turns into what can be seen as a complex "energy" λ_1 with strictly negative imaginary part once the interaction is switched on (see e.g. [4, 5]). This complex energy λ_1 is referred to as resonance energy and its imaginary part is responsible for the decay of the excited state (see e.g. [1, 29]).

Note that the ground state Ψ_{λ_0} of H corresponding to ground state energy λ_0, i.e.,

$$H\Psi_{\lambda_0} = \lambda_0 \Psi_{\lambda_0}, \tag{1.25}$$

has already been constructed, e.g., in [31, Theorem 1], [28, Theorem 1] and [3, Theorem 3.5]. Since H on $\mathcal{H}$ is a self-adjoint operator, λ_1 should rather be thought of as a complex eigenvalue of H on a bigger space than $\mathcal{H}$. This prevents us from being able to calculate the resonance energy directly by regular perturbation theory on $\mathcal{H}$. The standard way to nevertheless get access to such a resonance without leaving the underlying Hilbert space is the method of complex dilation which will be introduced next. We start by defining a family of unitary operators on $\mathcal{H}$ indexed by $\theta \in \mathbb{R}$.

Definition 1.3. *For $\theta \in \mathbb{R}$, we define the unitary transformation*

$$u_\theta : \mathfrak{h} \to \mathfrak{h}, \qquad \psi(k) \mapsto e^{-\frac{3\theta}{2}} \psi(e^{-\theta} k). \tag{1.26}$$

Similarly, we define its canonical lift $U_\theta : \mathcal{F}[\mathfrak{h}] \to \mathcal{F}[\mathfrak{h}]$ by the lift condition $U_\theta a(h)^* U_\theta^{-1} = a(u_\theta h)^*$, $h \in \mathfrak{h}$, and $U_\theta \Omega = \Omega$. This defines U_θ uniquely up to a phase which we choose to equal one. With slight abuse of notation, we also denote $\mathbb{1}_\mathcal{K} \otimes U_\theta$ on $\mathcal{H}$ by the same symbol U_θ.

Thereby, we define the family of transformed Hamiltonians, for $\theta \in \mathbb{R}$,

$$H^\theta := U_\theta H U_\theta^{-1} = K + H_f^\theta + gV^\theta, \tag{1.27}$$

where

$$H_f^\theta := \int \mathrm{d}^3k \, \omega^\theta(k) a^*(k) a(k), \qquad V^\theta := \sigma_1 \otimes \left(a(\overline{f^\theta}) + a(f^\theta)^* \right) \tag{1.28}$$

and

$$\omega^\theta(k) := e^{-\theta}|k|, \qquad f^\theta : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}, \quad k \mapsto e^{-\theta(1+\mu)} e^{-e^{2\theta}\frac{k^2}{\Lambda^2}} |k|^{-\frac{1}{2}+\mu}. \tag{1.29}$$

Eqs. (1.29), (1.28) and the right hand side of Eq. (1.27) can be defined for complex θ. If $|\theta|$ is small enough, $K + H_f^\theta + gV^\theta$ is a closed (non self-adjoint) operator. However, the middle term in Eq. (1.27) is not necessarily correct because although U_θ can be defined for complex θ, it turns out to be an unbounded operator, and $U_\theta H U_\theta^{-1}$ might not be densely defined.

We say that Ψ is an analytic vector if the map $\theta \mapsto \Psi^\theta := U_\theta \Psi$ has an analytic continuation from an open connected set in the real line to a (connected) domain in the complex plane. In general we will not specify their domains of analyticity (it will be clear from the context). It is well-known that there is a dense set of entire vectors (they are analytic in $\mathbb{C}$). This result has been proven in a variety of similar models, for example, in [4, 32]. For the sake of completeness, we provide a proof in Appendix B. Furthermore, we define the open disc

$$D(x, r) := \{z \in \mathbb{C} : |z - x| < r\} \qquad x \in \mathbb{C}, r > 0, \tag{1.30}$$

and note that for $\theta \in D(0, \pi/16)$ we have

$$\left\| V^\theta \left(H_0 + 1\right)^{-\frac{1}{2}} \right\| \le \left\| f^\theta \right\|_2 + 2 \left\| f^\theta / \sqrt{\omega} \right\|_2 \tag{1.31}$$

which is guaranteed by the standard estimate (A.4) given in Appendix A, since (1.29) together with the special choice $\theta \in D(0, \pi/16)$ imply that $f^\theta, f^\theta/\sqrt{\omega} \in \mathfrak{h}$. Hence, for $\theta \in D(0, \pi/16)$ the operators H^θ are densely defined and closed. Moreover, the analytic properties of this family of operators in g and θ are known:

Lemma 1.4. *The family* $\left\{H^\theta\right\}_{\theta \in \mathbb{R}}$ *of unitary equivalent, self-adjoint operators with* $\mathcal{D}(H^\theta) = \mathcal{D}(H)$ *extends to an analytic family of type A for* $\theta \in D(0, \pi/16)$.

The above result was proven for the Pauli-Fierz model in [4, Theorem 4.4], and with small effort that proof can be adapted to our setting.

Lemma 1.5. *Let* $\theta \in \mathbb{C}$. *Then,* $\sigma(H_0^\theta) = \left\{ e_i + e^{-\theta} r : r \ge 0, i = 0, 1 \right\}$.

We provide a proof in Appendix B. For sufficiently small coupling constants and for $\theta \in \mathcal{S}$, where $\mathcal{S}$ is the subset of the complex plane defined in Eq. (3.2) below, it has been shown that H^θ has two non-degenerate eigenvalues λ_0^θ and λ_1^θ with corresponding rank one projectors denoted by P_0^θ and P_1^θ, respectively; see, e.g., [14, Proposition 2.1]. Note that there the θ-dependence was omitted in the notation. For convenience of the reader, we make it explicit in this paper. The corresponding dilated eigenstates can, therefore, be written as

$$\Psi_{\lambda_i}^\theta := P_i^\theta \varphi_i \otimes \Omega, \qquad i = 0, 1, \tag{1.32}$$

where the eigenstates φ_i of the free atomic system are given in (1.20), and Ω is the bosonic vacuum defined in (1.10). In our notation $\Psi_{\lambda_i}^\theta$ is not necessarily normalized. We know from [14, Theorem 2.3] that the eigenvalues λ_i^θ are independent of θ as long as θ belongs to the set $\mathcal{S}$, and therefore, we suppress it in our notation writing $\lambda_i^\theta \equiv \lambda_i$. Note that this is not true for the eigenstates $\Psi_{\lambda_i}^\theta$. In [14] (as well as in Eq. (3.2) below) we choose an open connected set $\mathcal{S}$ that does not include 0 (the imaginary parts of the points in this set are bounded from below by a fixed positive constant). We chose such a set in order to have a single set $\mathcal{S}$ for the cases $i = 0$ and $i = 1$, because we want to keep our notation as simple as possible (otherwise a two cases formulation would propagate all over our papers). However, the fact that 0 is not contained in $\mathcal{S}$ is only necessary for the case $i = 1$ (the resonance - due to the self-adjointness of H the state $\Psi_{\lambda_1}^\theta$ can not even exist for $\theta = 0$). For the case $i = 0$ (the ground state) we can choose instead a connected open set containing 0. In this set, it is still valid that λ_0^θ does not depend on θ and, therefore, it equals the ground state energy, and $\Psi_{\lambda_0}^{\theta=0} = \Psi_{\lambda_0}$ - as introduced above. This is explained in [14, Remark 2.4].

1.3 Scattering theory

Finally, we give a short review of scattering theory which will be necessary to state the main results in Section 2.

The first obstacle in formulating a scattering theory of a second-quantized system lies in the definition of the wave operators. Unlike in first-quantized quantum theory, where one defines the scattering operator to be $S := \Omega_+^* \Omega_-$ with the wave operators $\Omega_\pm$ given by the strong limits $\Omega_\pm := s\text{-}\lim_{t\to\pm\infty} e^{itH} e^{-itH_0}$, in quantum field theory, the corresponding wave operators do not exist in a straight forward sense. Instead, one establishes the existence of the asymptotic annihilation and creation operators first, which can then be used to define the wave operators.

Definition 1.6 (Basic components of scattering theory)**.** *We denote the dense subspace of compactly supported, smooth, and complex-valued functions on $\mathbb{R}^3 \setminus \{0\}$ in $\mathfrak{h}$ by*

$$\mathfrak{h}_0 := C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}) \subset \mathfrak{h}. \tag{1.33}$$

Furthermore, we define the following objects:

(i) For $h \in \mathfrak{h}_0$ and $\Psi \in \mathcal{K} \otimes \mathcal{D}(H_f^{1/2})$, the asymptotic annihilation operators

$$a_\pm(h)\Psi := \lim_{t\to\pm\infty} a_t(h)\Psi, \quad a_t(h) := e^{itH}a(h_t)e^{-itH}, \quad h_t(k) := h(k)e^{-it\omega(k)}. \tag{1.34}$$

The existence of this limit is proven in Lemma 4.1 (i) below. Moreover, we define the asymptotic creation operators $a_\pm^*(h)$ as the respective adjoints.

(ii) The asymptotic Hilbert spaces

$$\mathcal{H}^\pm := \mathcal{K}^\pm \otimes \mathcal{F}[\mathfrak{h}] \quad \textit{where} \quad \mathcal{K}^\pm := \{\Psi \in \mathcal{H} : a_\pm(h)\Psi = 0 \ \ \forall h \in \mathfrak{h}_0\}. \tag{1.35}$$

(iii) The wave operators

$$\Omega_\pm : \mathcal{H}^\pm \to \mathcal{H} \tag{1.36}$$
$$\Omega_\pm \Psi \otimes a^*(h_1)...a^*(h_n)\Omega := a_\pm^*(h_1)...a_\pm^*(h_n)\Psi, \quad h_1,...,h_n \in \mathfrak{h}_0, \quad \Psi \in \mathcal{K}^\pm.$$

(iv) The scattering operator $S := \Omega_+^*\Omega_-$.

The limit operators $a_\pm$ and $a_\pm^*$ are called asymptotic outgoing/ingoing annihilation and creation operators. The existence of the limits in (1.34), their properties, especially that $\Psi_{\lambda_0} \in \mathcal{K}^\pm$ and $\Omega_\pm$ are well-defined, are well-known facts (see e.g. [23, 22, 16, 25, 24, 17, 18, 19, 20, 12]). For the convenience of the reader, Lemma 4.1 collects all relevant facts and we provide simplified proofs for our setting in Appendix C. We can thus define the following two-body scattering matrix coefficients:

$$S(h,l) = \|\Psi_{\lambda_0}\|^{-2} \langle a_+^*(h)\Psi_{\lambda_0}, a_-^*(l)\Psi_{\lambda_0}\rangle, \qquad \forall h,l \in \mathfrak{h}_0, \tag{1.37}$$

where the factor $\|\Psi_{\lambda_0}\|^{-2}$ appears due to the fact that, as already mentioned above, in our notation, the ground state Ψ_{λ_0} is not necessarily normalized. In addition, it will be convenient to work with the corresponding two-body transition matrix coefficients given by

$$T(h,l) = S(h,l) - \langle h,l\rangle_2 \qquad \forall h,l \in \mathfrak{h}_0. \tag{1.38}$$

These matrix coefficients carry a ready physical interpretation as transition amplitudes of the scattering process in which an incoming boson with wave function l is scattered at the two-level atom into an outgoing boson with wave function h. Notice that the transition matrix coefficients of multi-photon processes can be defined likewise but in this work we focus on one-photon processes only.

It has been shown in [31] that the spectrum of H contains only one eigenvalue λ_0 (and it is non-degenerate), namely the ground state energy, and the rest of the spectrum of H is absolutely continuous. In case that asymptotic completeness holds, i.e.

$$\mathcal{K}^\pm = \mathrm{Ran}\,(\chi_{\mathrm{pp}}(H)), \tag{1.39}$$

all one-boson processes are of the form (1.37). Here, $\operatorname{Ran}(\chi_{\mathrm{pp}}(H))$ denotes the states associated with pure points in the spectrum of H.

Asymptotic completeness has actually been proven in [17, 18, 19] for the Hamiltonian H defined in (1.7), however, with coupling functions $f \in C_c^3(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})$, i.e., the functions that are three times continuously differentiable and have compact support. In our case, we need an analytic continuation of our Hamiltonian in order to study resonances. This implies that the coupling function f cannot be compactly supported (see (1.5)), however it belongs to the Schwartz space. We expect asymptotic completeness also to hold in our case, although our results do not depend on it.

2 Main result

We are now able to state our main results. The corresponding proofs will be provided in Section 4 after we review a list of necessary results of a previous work [14] in Section 3.

First, we state a definition that we use for our main result

Definition 2.1. *Using solid angles* $\mathrm{d}\Sigma, \mathrm{d}\Sigma'$*, we define, for all* $h, l \in \mathfrak{h}_0$,

$$G : \mathbb{R} \to \mathbb{C}, \qquad r \mapsto G(r) := \begin{cases} \int \mathrm{d}\Sigma \mathrm{d}\Sigma' \, r^4 \overline{h(r,\Sigma)} l(r,\Sigma') f(r)^2 & \textit{for} \quad r \geq 0 \\ 0 & \textit{for} \quad r < 0. \end{cases} \tag{2.1}$$

We recall the definition $E_1 = g^{-2} \operatorname{Im} \lambda_1$ given in (1.2). It follows from Eqs. (3.11) and (3.12) below that $E_1 = E_I + g^a \Delta$ where $a > 0$, $\Delta \equiv \Delta(g)$ is uniformly bounded and $E_I < 0$ is the constant defined in (3.11). This implies that

$$E_1 \leq -\boldsymbol{c} < 0, \tag{2.2}$$

for some constant $\boldsymbol{c}$ that does not depend on g (for small enough g).

Our main result provides a relation between the scattering matrix element and the complex dilated resolvent of the Hamiltonian.

Theorem 2.2 (Scattering formula)**.** *There is a constant* $\boldsymbol{g} > 0$ *such that for every* $g \in (0, \boldsymbol{g}]$*,* θ *in the set* $\mathcal{S}$ *defined in* (3.2) *below, and for all* $h, l \in \mathfrak{h}_0$*, the two-body transition matrix coefficients are given by*

$$T(h,l) = T_P(h,l) + R(h,l), \tag{2.3}$$

where

$$\begin{aligned} T_P(h,l) :=& 4\pi i g^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \int \mathrm{d}r \, G(r) \left(\frac{\operatorname{Re}\lambda_1 - \lambda_0}{(r + \lambda_0 - \lambda_1)(r - \lambda_0 + \overline{\lambda_1})} \right) \\ =& M \int \mathrm{d}r \, G(r) \Big(\frac{E_1 g^2}{(r + \lambda_0 - \operatorname{Re}\lambda_1 - i g^2 E_1)(r - \lambda_0 + \overline{\lambda_1})} \Big), \end{aligned} \tag{2.4}$$

and there is a constant $C(h,l)$ (that does not depend on g) such that

$$|R(h,l)| \leq C(h,l) g^3 |\log g|. \tag{2.5}$$

Here, we use the notation

$$M := 4\pi i (\operatorname{Re}\lambda_1 - \lambda_0) E_1^{-1} \left\| \Psi_{\lambda_0} \right\|^{-2}. \tag{2.6}$$

$T_P(h,l)$ is the leading term in terms of powers of g for small g, and $R(h,l)$ is regarded as the error term. This is justified by Remark 2.3 below.

Our proof permits us to find an explicit formula for the dependence of $C(h,l)$ on h and l, see Remark 4.16 below.

Remark 2.3. *The scattering processes described by the transition matrix in* (2.3) *clearly depend on the incoming and outgoing photon states, l and h. This is well understood from the physics as well as the mathematics perspectives. For example, it can be read from* (2.1) *that if l is supported in a ball of radius t and h is supported in its complement, then the principal term $T_P(h,l)$ vanishes and only higher order terms (with respect to powers of g) contribute to the scattering process. The quantity $T_P(h,l)$ is the only one that might produce scattering processes of order g^2 since the remainder is of order $g^3|\log g|$. If an experiment is appropriately prepared, then such an scattering process will be observed and the term describing this is $T_P(h,l)$. This justifies why we call it the leading order (or principal) term. In Appendix D give an example of a large class of functions h and l that make $T_P(h,l)$ larger or equal than a strictly positive constant times g^2. In particular, we prove that this happens when the corresponding function G is positive and strictly positive at* $\operatorname{Re}\lambda_1 - \lambda_0$.

Remark 2.4. *By Eqs.* (2.4) *and* (2.1), *we can express the principal term $T_P(h,l)$ in terms of an integral kernel:*

$$T_P(h,l) = \int \mathrm{d}^3k \mathrm{d}^3k' \, \overline{h(k)} l(k') \delta(|k| - |k'|) T_P(k,k'), \tag{2.7}$$

where

$$T_P(k,k') = M f(k) f(k') \left(\frac{E_1 g^2}{\left(|k'| + \lambda_0 - \operatorname{Re}\lambda_1 - i g^2 E_1\right)\left(|k'| - \lambda_0 + \overline{\lambda_1}\right)} \right). \tag{2.8}$$

Eq. (2.7) *is important, because it allows us to calculate the leading order of the scattering cross section. It is proportional to the modulus squared of $T_P(k,k')$:*

$$|T_P(k,k')|^2 = \left(\frac{|M|^2 |f(k)|^2 |f(k')|^2}{||k'| - \lambda_0 + \overline{\lambda_1}|^2} \right) \frac{E_1^2 g^4}{(|k'| + \lambda_0 - \operatorname{Re}\lambda_1)^2 + g^4 E_1^2}. \tag{2.9}$$

For momenta $|k'|$ in a neighborhood of $\operatorname{Re}\lambda_1 - \lambda_0$, *the behavior in the expression above is dominated by the Lorentzian function. As expected, there is a maximum when the energy of the incoming photons is close to the difference of the resonance and the ground state energies of the system and the width of this peak is controlled by the imaginary part of the resonance* $\operatorname{Im}\lambda_1$.

Note that the Dirac's delta distribution in (2.7) is to be understood as the expression in (2.4). Notice that (2.8) is not defined for $k = 0$ or $k' = 0$. However, since we take $h, l \in \mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})$, the expression (2.7) is well-defined. Similar distribution kernels in a related model have been studied in [12, 7].

Remark 2.5. *In this work we denote by C any generic (indeterminate) constant that might change from line to line. This constants do not depend on the coupling constant and the auxiliary parameter n introduced in Section 3.2.*

3 Known results on spectral properties and resolvent estimates

In this section we present results about the spectrum of the dilated Spin-Boson Hamiltonian and resolvent estimates proven in our previous paper [14]. Here, we do not repeat proofs but give precise references for them. We collect only properties and estimates for the model under consideration that are necessary for the proofs of our main theorems.

Throughout this paper we address the case of small coupling, i.e., we assume the coupling constant g to be sufficiently small. The restrictions on the coupling constant only stem from the requirements needed to prove the results reviewed in this section, i.e., the ones considered in [14]. We do not explicitly specify how small the coupling constant must be but give precise references from which such bounds can be inferred. This issue is addressed by the next definition:

Definition 3.1 (Coupling Constant)**.** *Throughout this work we assume that $g \leq \boldsymbol{g}$, where $0 < \boldsymbol{g}$ satisfies Definition 4.3 and Eq. (5.58) in [14], the Fermi-golden rule (see Eqs.* (3.12) *and* (3.13) *below) and Eq.* (3.28) *below.*

We denote the imaginary part of the dilation parameter θ by

$$\nu := \operatorname{Im} \theta \tag{3.1}$$

and assume that θ belongs to the set

$$\mathcal{S} := \Big\{ \theta \in \mathbb{C} : -10^{-3} < \operatorname{Re} \theta < 10^{-3} \text{ and } \boldsymbol{\nu} < \operatorname{Im} \theta < \pi/16 \Big\}, \tag{3.2}$$

where $\boldsymbol{\nu} \in (0, \pi/16)$ is a fixed number (see [14, Definition 1.4]).

3.1 Spectral estimates

We know from [14, Proposition 2.1] that the Hamiltonian H^θ has two eigenvalues λ_0 and λ_1 in small neighborhoods of e_0 and e_1, respectively. Loosely put, e_0 turns into the ground state λ_0 and e_1 tuns into the resonance λ_1 once the interaction is tuned on. Both λ_0 and λ_1 do not depend on θ provided that $\theta \in \mathcal{S}$ and in the case of λ_0 we can take θ in a neighborhood of 0 and, therefore, infer that λ_0 is real and gives the ground state energy. This is proven in [14, Theorem 2.3] and [14, Remark 2.4].

In [14, Theorem 2.7], we give a very sharp estimation of the location of the spectrum of H^θ. We prove, among other things that, locally, in neighborhoods of λ_0 and λ_1, its spectrum is contained in cones with vertices at λ_0 and λ_1. To make this statement more precise we need to introduce some more concepts and notation. There are two auxiliary parameters that play an important role in our constructions:

$$\rho_0 \in (0,1), \qquad \rho \in (0, \min e_1/4), \tag{3.3}$$

which also satisfy the conditions in (3.31) below. In order to specify the spectral properties of H^θ we define some regions in the complex plane:

Definition 3.2. *For fixed $\theta \in \mathcal{S}$, we set $\delta = e_1 - e_0 = e_1$ and define the regions*

$$A := A_1 \cup A_2 \cup A_3, \tag{3.4}$$

where

$$A_1 := \{z \in \mathbb{C} : \operatorname{Re} z < e_0 - \delta/2\} \tag{3.5}$$

$$A_2 := \left\{z \in \mathbb{C} : \operatorname{Im} z > \frac{1}{8}\delta \sin(\nu)\right\} \tag{3.6}$$

$$A_3 := \{z \in \mathbb{C} : \operatorname{Re} z > e_1 + \delta/2, \operatorname{Im} z \geq -\sin(\nu/2)\,(\operatorname{Re}(z) - (e_1 + \delta/2))\}\,, \tag{3.7}$$

and for $i = 0, 1$, we define

$$B_i^{(1)} := \left\{z \in \mathbb{C} : |\operatorname{Re} z - e_i| \leq \frac{1}{2}\delta, -\frac{1}{2}\rho_1 \sin(\nu) \leq \operatorname{Im} z \leq \frac{1}{8}\delta \sin(\nu)\right\}. \tag{3.8}$$

These regions are depicted in Figure 1.

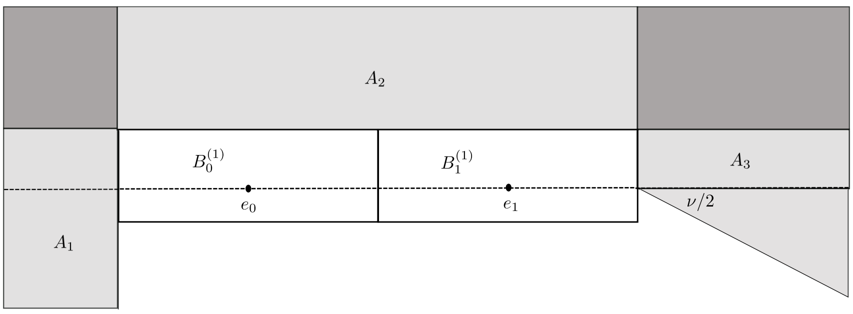

Figure 1: An illustration of the subsets of the complex plane introduced in Definition 3.2.

For a fixed $m \in \mathbb{N}$, $m \geq 4$, we define the cone

$$\mathcal{C}_m(z) := \left\{z + xe^{-i\alpha} : x \geq 0, |\alpha - \nu| \leq \nu/m\right\}. \tag{3.9}$$

It follows from the induction scheme in [14, Section 4] that $\lambda_i \in B_i^{(1)}$, and moreover, [14, Theorem 2.7] together with [14, Lemma 3.13] yields

$$\sigma(H^\theta) \subset \mathbb{C} \setminus \Big[A \cup (B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0)) \cup (B_1^{(1)} \setminus \mathcal{C}_m(\lambda_1)) \Big]. \tag{3.10}$$

As we mention above, we have $\lambda_0 \in \mathbb{R}$. The imaginary part of λ_1 can be also estimated (see [14, Remark 2.2] – Fermi golden rule): Recalling (1.5), we define

$$E_I := -4\pi^2 (e_1 - e_0)^2 |f(e_1 - e_0)|^2. \tag{3.11}$$

Then, for g small enough, there are constants $C, a > 0$ such that

$$\Big| \mathrm{Im}\, \lambda_1 - g^2 E_I \Big| \le g^{2+a} C. \tag{3.12}$$

This implies that, for g small enough, there is constant $\boldsymbol{c} > 0$ such that

$$\mathrm{Im}\, \lambda_1 < -g^2 \boldsymbol{c} < 0. \tag{3.13}$$

3.2 Auxiliary (infrared cut-off) Hamiltonians

Some of the bounds in Section 4 employ a certain approximation of the Hamiltonian H^θ by Hamiltonians with infrared cut-offs. The strategy will be the following: A mathematical expression that depends on H^θ is replaced by a corresponding one that depends on a particular infrared cut-off Hamiltonian. We then analyze the infrared cut-off expression and estimate the difference between both expressions. The construction of a sequence of infrared cut-off Hamiltonians $(H^{(n),\theta})$ such that, as n tends to infinity, the cut-off is removed is called multiscale analysis. In [14], we present the full details of this method and derive several results. Here, we only use some of those results and only present the notation necessary to review this part of [14]. The infrared cut-off Hamiltonians $H^{(n),\theta}$ are parametrized by a sequence of numbers (see also (3.3) and (3.31))

$$\rho_n := \rho_0 \rho^n, \tag{3.14}$$

where the Hamiltonians $H^{(n),\theta}$ are defined by

$$H^{(n),\theta} := K + H_f^{(n),\theta} + gV^{(n),\theta} =: H_0^{(n),\theta} + gV^{(n),\theta} \tag{3.15}$$

$$H_f^{(n),\theta} := \int_{\mathbb{R}^3 \setminus \mathcal{B}_{\rho_n}} \mathrm{d}^3k\, \omega^\theta(k) a^*(k) a(k), \quad \omega^\theta(k) = e^{-\theta}|k| \tag{3.16}$$

$$V^{(n),\theta} := \sigma_1 \otimes \int_{\mathbb{R}^3 \setminus \mathcal{B}_{\rho_n}} \mathrm{d}^3k \, \Big(f^\theta(k) a(k) + f^{\theta}(k) a^*(k) \Big), \tag{3.17}$$

$$f^\theta : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}, \quad k \mapsto e^{-\theta(1+\mu)} e^{-e^{2\theta} \frac{k^2}{\Lambda^2}} |k|^{-\frac{1}{2}+\mu}, \tag{3.18}$$

on the Hilbert space

$$\mathcal{H}^{(n)} := \mathcal{K} \otimes \mathcal{F}[\mathfrak{h}^{(n)}], \quad \mathfrak{h}^{(n)} := L^2(\mathbb{R}^3 \setminus \mathcal{B}_{\rho_n}, \mathbb{C}), \quad \mathcal{B}_{\rho_n} := \Big\{ x \in \mathbb{R}^3 : |x| < \rho_n \Big\}. \tag{3.19}$$

Additionally, we define

$$\tilde{H}^{(n),\theta} := H_0^\theta + gV^{(n),\theta} \tag{3.20}$$

and fix the Hilbert spaces

$$\mathfrak{h}^{(n,\infty)} := L^2(\mathcal{B}_{\rho_n}) \quad \text{and} \quad \mathcal{F}[\mathfrak{h}^{(n,\infty)}], \tag{3.21}$$

defined as in (1.9) with $\mathfrak{h}^{(n,\infty)}$ instead of $\mathfrak{h}$, with vacuum states $\Omega^{(n,\infty)}$ and corresponding orthogonal projections $P_{\Omega^{(n,\infty)}}$. Note that $\mathcal{H} \equiv \mathcal{H}^{(n)} \otimes \mathcal{F}[\mathfrak{h}^{(n,\infty)}]$.

In [14, Proposition 2.1] and [14, Theorem 4.5], we prove that, for each $n \in \mathbb{N}$, $H^{(n),\theta}$ has isolated eigenvalues $\lambda_i^{(n)}$ in certain neighborhoods of e_i, for $i \in \{0,1\}$, respectively. The fact that these eigenvalues are isolated permits us to define their corresponding Riesz projections which are denoted by

$$P_i^{(n)} \equiv P_i^{(n),\theta}. \tag{3.22}$$

In [14, Proposition 2.1], we prove that this sequence of projections converges to the projection associated to the eigenvalue λ_i, i.e.,

$$P_i^\theta \equiv P_i = \lim_{n\to\infty} P_i^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}}, \tag{3.23}$$

and that the latter is analytic with respect to θ (see [14, Theorem 2.3]). Furthermore, it follows from [14, Remark 5.11] that

$$\left\| P_i^\theta - P_i^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}} \right\| \le 2\frac{g}{\rho}\rho_n^{\mu/2} \le \rho_n^{\mu/2}. \tag{3.24}$$

This together with [14, Lemma 3.6] implies that there is a constant C such that

$$\left\| P_i^\theta - P_{\varphi_i} \otimes P_\Omega \right\| \le Cg, \tag{3.25}$$

and in addition, we know from [14, Lemma 4.7] that

$$\left\| P_i^{(n),\theta} \right\| \le 3, \tag{3.26}$$

for every $n \in \mathbb{N}$. Finally, [14, Lemma 5.1] yields that for all $n \in \mathbb{N}$

$$|\lambda_i - \lambda_i^{(n)}| \le 2g\rho_n^{1+\mu/2}. \tag{3.27}$$

This together with [14, Lemma 3.10], which states that there is a constant C such that $|e_i - \lambda_i^{(1)}| < Cg$, proves that there is a constant C such that, for every $n \in \mathbb{N}$ and for g sufficiently small, we have

$$|\lambda_i^{(n)} - e_i| \le Cg \le 10^{-3}e_1, \qquad |\lambda_i - e_i| \le Cg \le 10^{-3}e_1. \tag{3.28}$$

3.3 Resolvent estimates

In [14], we derive bounds for the resolvent of H^θ in $\Big[A \cup (B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0)) \cup (B_1^{(1)} \setminus \mathcal{C}_m(\lambda_1))\Big]$, see (3.10). The region A is far away from the spectrum, and therefore, resolvent estimates in this region are easy. In [14, Theorem 3.2], we prove that there is a constant C such that

$$\Big\| \frac{1}{H^\theta - z} \Big\| \leq C \frac{1}{|z - e_1|}, \qquad \forall z \in A. \tag{3.29}$$

Resolvent estimates in the regions $B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0)$ and $B_1^{(1)} \setminus \mathcal{C}_m(\lambda_1)$ are much more complicated because these regions share boundaries with the spectrum.

In [14, Theorem 5.5], we prove that, for $i \in \{0,1\}$, $B_i^{(1)} \setminus \mathcal{C}_m \Big(\lambda_i^{(n)} + (1/4)\rho_n e^{-i\nu} \Big) \setminus \{\lambda_i^{(n)}\}$ is contained in the resolvent set of $H^{(n),\theta}$ and that there is a constant $\boldsymbol{C}$ such that

$$\Big\| \frac{1}{H^{(n),\theta} - z} \overline{P_i^{(n),\theta}} \Big\| \leq \boldsymbol{C}^{n+1} \frac{1}{\mathrm{dist}(z, \mathcal{C}_m(\lambda_i^{(n)} + (1/4)\rho_n e^{-i\nu}))}, \tag{3.30}$$

for every $z \in B_i^{(1)} \setminus \mathcal{C}_m \Big(\lambda_i^{(n)} + (1/4)\rho_n e^{-i\nu} \Big)$, where $\overline{P_i^{(n),\theta}} = 1 - P_i^{(n),\theta}$. Here, the symbol dist denotes the Euclidean distance in $\mathbb{C}$. In [14], we select the auxiliary numbers ρ and ρ_0 satisfying $\boldsymbol{C}^8 \rho_0^\mu \leq 1$, and $\boldsymbol{C}^4 \rho^\mu \leq 1/4$. In this paper we assume the stronger conditions

$$\boldsymbol{C}^8 \rho_0^\mu \leq 1, \qquad \boldsymbol{C}^8 \rho^\mu \leq 1/4, \qquad \text{(and hence} \qquad \boldsymbol{C} \rho^{\frac{1}{2}\iota(1+\mu/4)} \leq 1), \tag{3.31}$$

where

$$\iota = \frac{\mu/4}{(1+\mu/4)} \in (0,1). \tag{3.32}$$

The constant $\boldsymbol{C}$ is larger that 10^6, it is specified in Definition 4.1 and Eq. (5.58) in [14], however, its precise form is not relevant in this paper (in [14], we do not intend to calculate optimal constants, because this would make the work harder to read). From the inequalities above and Eq. (3.3) we obtain that, for very $n \in \mathbb{N}$:

$$\rho_n \leq 10^{-6} e_1. \tag{3.33}$$

Finally, we prove in [14, Theorem 5.9] that the set $\in B_i^{(1)} \setminus \mathcal{C}_m(\lambda_i^{(n)} - e^{-i\nu}\rho_n^{1+\mu/4})$ is contained in the resolvent set of both H^θ and $\tilde{H}^{(n),\theta}$ and for all z in this set there is a constant C such that:

$$\Big\| \frac{1}{H^\theta - z} - \frac{1}{\tilde{H}^{(n),\theta} - z} \Big\| \leq gC\mathbf{C}^{2n+2} \frac{1}{\rho_n} \rho_n^{\frac{\mu}{2}} \leq gC \frac{1}{\rho_n} \rho_n^{\frac{\mu}{4}}, \tag{3.34}$$

where we use (3.31). Notice that Eq. (3.30) implies that there is a constant C such that

$$\Big\| \frac{1}{H^{(n),\theta} - z} \overline{P_i^{(n),\theta}} \Big\| \leq C\boldsymbol{C}^{n+1} \frac{1}{\rho_n}, \tag{3.35}$$

for every $z \in B_i^{(1)} \backslash \mathcal{C}_m(\lambda_i^{(n)})$. Moreover, [14, Theorem 2.6] implies that there is a constant C such that

$$\left\| \frac{1}{H^\theta - z} \right\| \le C \boldsymbol{C}^{n+1} \frac{1}{\rho_n^{1+\mu/4}}, \tag{3.36}$$

for every $z \in B_i^{(1)} \setminus \mathcal{C}_m(\lambda_i^{(n)} - \rho_n^{1+\mu/4} e^{-i\nu})$ and

$$\left\| \frac{1}{H^\theta - z} \right\| \le C \boldsymbol{C}^{n+1} \frac{1}{\operatorname{dist}\Big(z, \mathcal{C}_m(\lambda_i)\Big)}, \tag{3.37}$$

for every $z \in B_i^{(1)} \setminus \mathcal{C}_m(\lambda_i - 2\rho_n^{1+\mu/4} e^{-i\nu})$.

4 Proof of the main result

In the remainder of this work we provide the proofs of the main result Theorem 2.2. This section has three parts: In Section 4.1, we derive a preliminary formula for the scattering matrix coefficients (see Theorem 4.3 below). This formula together with several technical ingredients provided in Sections 4.2 and 4.3 will pave the way for the proofs of the main results given in Section 4.4.

4.1 Preliminary scattering formula

In Theorem 4.3 below we derive a preliminary formula for scattering processes with one incoming and outgoing asymptotic photon. A related formula was already employed in [30]. In order to derive it rigorously we need several properties of the asymptotic creation and annihilation operators. The necessary properties are collected in Lemma 4.1. They have already been proven for a range of models in several works [23, 22, 16, 25, 24, 17, 18, 19, 20, 12]. For convenience of the reader we provide a self-contained proof of Lemma 4.1 in the Appendix C.

Lemma 4.1. *Let $\Psi \in \mathcal{K} \otimes D(H_f^{1/2})$ and $h, l \in \mathfrak{h}_0$. The asymptotic creation and annihilation operators $a_\pm^*, a_\pm$ defined in Definition 1.6 have the following properties:*

(i) The limits $a_\pm^\#(h)\Psi = \lim_{t\to\pm\infty} a_t^\#(h)\Psi$ exist, where $a^\#$ stands for a or a^*.

(ii) The next equalities holds true:

$$a_+(h)\Psi = a(h)\Psi - ig \int_0^\infty \mathrm{d}s\, e^{isH} \langle h_s, f\rangle_2\, \sigma_1 e^{-isH} \Psi, \tag{4.1}$$

$$a_-(h)\Psi = a(h)\Psi + ig \int_{-\infty}^0 \mathrm{d}s\, e^{isH} \langle h_s, f\rangle_2\, \sigma_1 e^{-isH} \Psi. \tag{4.2}$$

We point out to the reader that the integrals above are convergent since it can be shown by integration by parts that there is constant C such that $|\langle h_s, f\rangle_2| \le C/(1+s^2)$ for $s \in \mathbb{R}$ (see (C.7) below).

(iii) The following pull-through formula holds true:

$$e^{-isH}a_-(h)^*\Psi = a_-(h_s)^*e^{-isH}\Psi. \tag{4.3}$$

(iv) The equality $a_\pm(h)\Psi_{\lambda_0} = 0$ *holds true, i.e.,* $\Psi_{\lambda_0} \in \mathcal{K}^\pm$.

(v) The following commutation relation holds: $\langle a_\pm(h)^*\Psi_{\lambda_0}, a_\pm(l)^*\Psi_{\lambda_0}\rangle = \langle h,l\rangle_2 \|\Psi_{\lambda_0}\|^2$.

(vi) There is a finite constant $C(h) > 0$ *such that for all* $t \in \mathbb{R}$

$$\left\|a_t(h)^*(H_f+1)^{-\frac{1}{2}}\right\|, \left\|a_t(h)(H_f+1)^{-\frac{1}{2}}\right\| \leq C(h). \tag{4.4}$$

Definition 4.2. *Let* $S(\mathbb{R},\mathbb{C})$ *denote the Schwartz space of functions with rapid decay. For all* $u \in S(\mathbb{R},\mathbb{C})$*, we define the Fourier transform of a function and its inverse*

$$\mathfrak{F}[u](x) := \int_{\mathbb{R}} \mathrm{d}s\, u(s)e^{-isx}, \qquad \mathfrak{F}^{-1}[u](x) := (2\pi)^{-1}\int_{\mathbb{R}} \mathrm{d}s\, u(s)e^{isx}. \tag{4.5}$$

Note the factor $(2\pi)^{-1}$ *which is not the normalization factor of the standard definition of the inverse Fourier transform. However, it is convenient in our setting (see e.g. [35]).*

Theorem 4.3 (Preliminary Scattering Formula)**.** *For* $h,l \in \mathfrak{h}_0$*, the two-body transition matrix coefficient* $T(h,l)$ *defined in* (1.38) *fulfills*

$$T(h,l) = \lim_{t\to-\infty}\int \mathrm{d}^3k\mathrm{d}^3k'\,\overline{h(k)}l(k')\delta(\omega(k)-\omega(k'))T_t(k,k') \tag{4.6}$$

for the integral kernel

$$T_t(k,k') = -2\pi i g f(k)\,\|\Psi_{\lambda_0}\|^{-2}\,\langle\sigma_1\Psi_{\lambda_0}, a_t(k')^*\Psi_{\lambda_0}\rangle. \tag{4.7}$$

The integral in (4.6) is to be understood as

$$T(h,l) = -2\pi i g\,\|\Psi_{\lambda_0}\|^{-2}\left\langle\sigma_1\Psi_{\lambda_0}, a_-(W)^*\Psi_{\lambda_0}\right\rangle \tag{4.8}$$

for $W \in \mathfrak{h}_0$ given by

$$\mathbb{R}^3 \ni k \mapsto W(k) := |k|^2 l(k)\int \mathrm{d}\Sigma\,\overline{h(|k|,\Sigma)}f(|k|,\Sigma) \tag{4.9}$$

using spherical coordinates $k = (|k|,\Sigma)$ with Σ being the solid angle.

Proof. Let $h,l \in \mathfrak{h}_0$. Thanks to Lemma 4.1 (i) and the fact that the ground state Ψ_{λ_0} lies in $\mathcal{D}(H) = \mathcal{K}\otimes\mathcal{D}(H_f)$, c.f. [31, Theorem 1] and Proposition 1.1, the transmission matrix coefficient given in (1.38), i.e.,

$$T(h,l) = S(h,l) - \langle h,l\rangle_2 = \|\Psi_{\lambda_0}\|^{-2}\,\langle a_+(h)^*\Psi_{\lambda_0}, a_-(l)^*\Psi_{\lambda_0}\rangle - \langle h,l\rangle_2 \tag{4.10}$$

is well-defined. Lemma 4.1 (iv) and (v) implies that

$$(4.10) = \|\Psi_{\lambda_0}\|^{-2} \langle [a_+(h)^* - a_-(h)^*]\Psi_{\lambda_0}, a_-(l)^*\Psi_{\lambda_0}\rangle. \tag{4.11}$$

Using Lemma 4.1 (ii), we obtain

$$(4.10) = -ig\,\|\Psi_{\lambda_0}\|^{-2} \int_{-\infty}^{\infty} \mathrm{d}s \langle \Psi_{\lambda_0}, e^{isH}\sigma_1 e^{-isH} a_-(l)^*\Psi_{\lambda_0}\rangle \langle h_s, f\rangle_2. \tag{4.12}$$

Finally, we use Lemma 4.1 (iii) to get

$$\begin{aligned}(4.10) &= -ig\,\|\Psi_{\lambda_0}\|^{-2} \int_{-\infty}^{\infty} \mathrm{d}s \left\langle e^{-isH}\Psi_{\lambda_0}, \sigma_1 a_-(l_s)^* e^{-isH}\Psi_{\lambda_0}\right\rangle \langle h_s, f\rangle_2 \\ &= -ig\,\|\Psi_{\lambda_0}\|^{-2} \int_{-\infty}^{\infty} \mathrm{d}s \,\langle \sigma_1\Psi_{\lambda_0}, a_-(l_s)^*\Psi_{\lambda_0}\rangle \langle h_s, f\rangle_2. \end{aligned} \tag{4.13}$$

We insert the definition of the asymptotic creation operator in (1.34) to find

$$(4.10) = -ig\,\|\Psi_{\lambda_0}\|^{-2} \int_{-\infty}^{\infty} \mathrm{d}s \lim_{t\to-\infty} \langle \sigma_1\Psi_{\lambda_0}, a_t(l_s)^*\Psi_{\lambda_0}\rangle \langle h_s, f\rangle_2. \tag{4.14}$$

Next, it is possible to interchange the ds integral and the limit $t \to -\infty$. This can be seen as follows. A two-fold partial integration implies that there is a constant C such that, for all $s \in \mathbb{R}$, we get

$$|\langle h_s, f\rangle_2| \le C\frac{1}{1+|s|^2}. \tag{4.15}$$

By applying Lemma 4.1 (vi), we infer that there is a finite constant $C_{(4.16)}(l) > 0$ such that for all $s \in \mathbb{R}$

$$\begin{aligned}|\langle \sigma_1\Psi_{\lambda_0}, a_t(l_s)^*\Psi_{\lambda_0}\rangle| &\le \|\sigma_1\Psi_{\lambda_0}\|\,\|a_t(l_s)^*(H_f+1)^{-\frac{1}{2}}\|\,\|(H_f+1)^{\frac{1}{2}}\Psi_{\lambda_0}\| \\ &\le C_{(4.16)}(l)\|\Psi_{\lambda_0}\|\|\Psi_{\lambda_0}\|_{H_f} \end{aligned} \tag{4.16}$$

holds true. Both estimates, (4.15) and (4.16), give an integrable bound of the ds-integrand in (4.14) that is uniform in t. Hence, by dominated convergence, we have the equality

$$\begin{aligned}(4.10) &= -ig\,\|\Psi_{\lambda_0}\|^{-2} \lim_{t\to-\infty} \int_{-\infty}^{\infty} \mathrm{d}s \,\langle \sigma_1\Psi_{\lambda_0}, a_t(l_s)^*\Psi_{\lambda_0}\rangle \langle h_s, f\rangle_2 \\ &= -ig\,\|\Psi_{\lambda_0}\|^{-2} \lim_{t\to-\infty} e^{-it\lambda_0} \int_{-\infty}^{\infty} \mathrm{d}s \left\langle e^{-itH}\sigma_1\Psi_{\lambda_0}, a(l_{s+t})^*\Psi_{\lambda_0}\right\rangle \langle h_s, f\rangle_2, \end{aligned} \tag{4.17}$$

where in the last step we have inserted definition (1.34) and exploited the ground state property (1.25).

In order to rewrite this integral in form of (4.6)-(4.7), or more precisely, (4.8)-(4.9), we shall use the following approximation argument. Let

$$\mathcal{H}_0 := \mathcal{K} \otimes \mathcal{F}_{\mathrm{fin}}[\mathfrak{h}_0] \tag{4.18}$$

be the set of states with only finitely many bosons, i.e.,

$$\mathcal{F}_{\text{fin}}[\mathfrak{h}_0] := \Big\{\Psi = (\psi^{(n)})_{n\in\mathbb{N}_0} \in \mathcal{F}[\mathfrak{h}] \,\big|\, \exists N \in \mathbb{N}_0 : \psi^{(n)} = 0 \,\forall n \geq N, \quad \forall n \in \mathbb{N} : \psi^{(n)} \in C_c^\infty(\mathbb{R}^{3n} \setminus \{0\}, \mathbb{C})\Big\}. \tag{4.19}$$

Note that $\mathcal{H}_0$ is a dense subset of $\mathcal{H}$ with respect to the norm in $\mathcal{H}$ and it is dense in the domain of H_f with respect to the graph norm of the operator H_f defined by $\|\cdot\|_{H_f} := \|H_f\cdot\| + \|\cdot\|$. Hence, for $t \in \mathbb{R}$, there are sequences $(\Psi_m)_{m\in\mathbb{N}}$, $(\Phi_m^t)_{m\in\mathbb{N}}$ in $\mathcal{H}_0$ with $\|\Psi_m - \Psi_{\lambda_0}\|_{H_f} \to 0$, as $m \to \infty$, and $\left\|\Phi_m^t - e^{-itH}\sigma_1\Psi_{\lambda_0}\right\| \to 0$, as $m \to \infty$. Then, Lemma A.1, applied in the same fashion as in (4.16), implies that

$$\lim_{m\to\infty} \left\langle \Phi_m^t, a(l_{s+t})^*\Psi_m \right\rangle = \left\langle e^{-itH}\sigma_1\Psi_{\lambda_0}, a(l_{s+t})^*\Psi_{\lambda_0} \right\rangle, \tag{4.20}$$

uniformly in s. Thanks to the bound (4.15), we may apply dominated convergence theorem to conclude that

$$\lim_{m\to\infty} \int_{-\infty}^{\infty} \mathrm{d}s \left\langle \Phi_m^t, a(l_{s+t})^*\Psi_m \right\rangle \langle h_s, f\rangle_2 = \int_{-\infty}^{\infty} \mathrm{d}s \left\langle e^{-itH}\sigma_1\Psi_{\lambda_0}, a(l_{s+t})^*\Psi_{\lambda_0} \right\rangle \langle h_s, f\rangle_2. \tag{4.21}$$

Now, we study the integrals in the left hand side of Eq. (4.21). The advantage of the sequences $(\Psi_m)_{m\in\mathbb{N}}$, $(\Phi_m^t)_{m\in\mathbb{N}}$ is that they allow to use point-wise annihilation operators in the following manner:

$$\begin{aligned} &\int_{-\infty}^{\infty} \mathrm{d}s \left\langle \Phi_m^t, a(l_{s+t})^*\Psi_m \right\rangle \langle h_s, f\rangle_2 \qquad (4.22)\\ &= \int_{-\infty}^{\infty} \mathrm{d}s \int d^3k' e^{-is\omega(k')} e^{-it\omega(k')} l(k') \left\langle a(k')\Phi_m^t, \Psi_m \right\rangle \int \mathrm{d}^3k\, \overline{h(k)} f(k) e^{is\omega(k)}\\ &= \int_{-\infty}^{\infty} ds \Big[\Big(\int_{-\infty}^{\infty} \mathrm{d}r\, e^{isr}\Theta(r)u(r)\Big)\Big(\int_{-\infty}^{\infty} \mathrm{d}r'\, e^{-isr'}\Theta(r')v_m^t(r')\Big)\Big], \end{aligned}$$

where Θ is the Heaviside function and we use spherical coordinates and the abbreviations

$$u(r) := r^2 \int \mathrm{d}\Sigma\, \overline{h(r,\Sigma)} f(r,\Sigma) \quad \text{and} \quad v_m^t(r') := e^{-itr'} r'^2 \int \mathrm{d}\Sigma'\, l(r',\Sigma') \left\langle a(r',\Sigma')\Phi_m^t, \Psi_m \right\rangle.$$

By definition, v_m^t and u belong to $C_c^\infty(\mathbb{R} \setminus \{0\})$ so that the integrals with respect to r and r' above can be regarded as Fourier transform, introduced in Definition 4.2, i.e.,

$$(4.22) = \int_{-\infty}^{\infty} \mathrm{d}s\, \overline{\mathfrak{F}\left[\overline{\Theta u}\right]}(s) \mathfrak{F}\left[\Theta v_m^t\right](s) \tag{4.23}$$

holds true. Plancherel's identity yields for all $t \in \mathbb{R}$

$$\begin{aligned} (4.22) &= 2\pi \int_{-\infty}^{\infty} dr'\, \Theta u \Theta v_m^t(r')\\ &= 2\pi \int_0^{\infty} dr'\, r'^2 \int \mathrm{d}\Sigma\, \overline{h(r',\Sigma)} f(r',\Sigma) e^{-itr'} r'^2 \int \mathrm{d}\Sigma'\, l(r',\Sigma') \left\langle a(r',\Sigma')\Phi_m^t, \Psi_m \right\rangle\\ &= 2\pi \left\langle a(W_t)\Phi_m^t, \Psi_m \right\rangle = 2\pi \left\langle \Phi_m^t, a(W_t)^*\Psi_m \right\rangle \end{aligned} \tag{4.24}$$

where we have used the definition of W in (4.9) and the definition (1.34), in particular, the notation $W_t(k) = W(k)e^{-it\omega(k)}$. Using Lemma A.1, applied in the same fashion as in (4.16), allows to carry out the limit $m \to \infty$ which results in

$$(4.21) = \lim_{m\to\infty} (4.24) = 2\pi \left\langle e^{-itH}\sigma_1\Psi_{\lambda_0},\ a(W_t)^*\Psi_{\lambda_0}\right\rangle . \tag{4.25}$$

This together with (4.17) and Lemma 4.1 guarantees

$$(4.10) = -ig \left\|\Psi_{\lambda_0}\right\|^{-2} \lim_{t\to-\infty} e^{-it\lambda_0} 2\pi \left\langle e^{-itH}\sigma_1\Psi_{\lambda_0}, a(W_t)^*\Psi_{\lambda_0}\right\rangle \tag{4.26}$$

$$= -2\pi ig \left\|\Psi_{\lambda_0}\right\|^{-2} \lim_{t\to-\infty} \left\langle \sigma_1\Psi_{\lambda_0}, a_t(W)^*\Psi_{\lambda_0}\right\rangle \tag{4.27}$$

$$= -2\pi ig \left\|\Psi_{\lambda_0}\right\|^{-2} \left\langle \sigma_1\Psi_{\lambda_0}, a_-(W)^*\Psi_{\lambda_0}\right\rangle , \tag{4.28}$$

which concludes the proof. □

4.2 Technical ingredients

Here, we derive some technical results which will be applied in the proof of the main results in Section 4.4. The statements in this section will mostly be formulated without motivation, however, their importance will become clear later in the proofs of the main results.

4.2.1 General results

Lemma 4.4. *For $n \in \mathbb{N}$ and $\theta \in \mathcal{S}$, we have*

$$P_0^{(n),\theta}\sigma_1 P_0^{(n),\theta} = 0. \tag{4.29}$$

The statement has already been proven in [3, Lemma 2.1].

Next, we prove a representation formula of the evolution operator similar to the Laplace transform representation (see, e.g., [4]).

Lemma 4.5. *For $\epsilon > 0$ and sufficiently large $R > 0$, we consider the concatenated contour $\Gamma(\epsilon, R) := \Gamma_-(\epsilon, R) \cup \Gamma_c(\epsilon) \cup \Gamma_d(R)$ (see Figure 2), where*

$$\begin{aligned}
\Gamma_-(\epsilon, R) &:= [-R, \lambda_0 - \epsilon] \cup [\lambda_0 + \epsilon, R],\\
\Gamma_d(R) &:= \left\{-R - ue^{i\frac{\nu}{4}} : u \geq 0\right\} \cup \left\{R + ue^{-i\frac{\nu}{4}} : u \geq 0\right\},\\
\Gamma_c(\epsilon) &:= \left\{\lambda_0 - \epsilon e^{-it} : t \in [0, \pi]\right\}.
\end{aligned} \tag{4.30}$$

The orientations of the contours in (4.30) are given by the arrows depicted in Figure 2. Then, for all analytic vectors $\phi, \psi \in \mathcal{H}$ (analytic in a – connected – domain containing 0) and $t > 0$ the following identity holds true:

$$\left\langle \phi, e^{-itH}\psi\right\rangle = \frac{1}{2\pi i}\int_{\Gamma(\epsilon,R)} \mathrm{d}z\, e^{-itz} \left\langle \psi^{\overline{\theta}}, \left(H^\theta - z\right)^{-1}\phi^\theta\right\rangle . \tag{4.31}$$

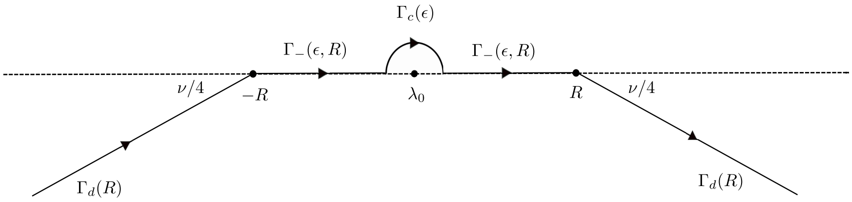

Figure 2: An illustration of the contour $\Gamma(\epsilon, R) := \Gamma_-(\epsilon, R) \cup \Gamma_c(\epsilon) \cup \Gamma_d(R)$.

Proof. Let $t > 0$ and $\epsilon > 0$. We define a contour $\hat{\Gamma}(\epsilon) := \mathbb{R} + i\epsilon$ with a mathematical negative orientation if the contour were closed in the lower complex plane. As an application of the residue theorem closing the contour in the lower complex plane, we observe for all $E \in \mathbb{R}$

$$\frac{1}{2\pi i} \int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z \, \frac{e^{-itz}}{it(E-z)^2} = e^{-itE} \tag{4.32}$$

holds true. Thanks to the spectral theorem we may write for all $\psi \in \mathcal{H}$

$$\left\langle \psi, e^{-itH} \psi \right\rangle = \int_{\sigma(H)} \langle \psi, \mathrm{d}P_E \psi \rangle \, e^{-itE} = \frac{1}{2\pi i} \int_{\sigma(H)} \int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z \, \langle \psi, dP_E \psi \rangle \, \frac{e^{-itz}}{it(E-z)^2}. \tag{4.33}$$

Next, we may interchange the order of the integrals by the Fubini-Tonelli Theorem since the following integral is finite:

$$\int_{\sigma(H)} \langle \psi, dP_E \psi \rangle \int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z \left| \frac{e^{-itz}}{it(E-z)^2} \right| \leq \frac{e^{t\epsilon}}{t} \int_{\sigma(H)} \langle \psi, dP_E \psi \rangle \int_{-\infty}^{\infty} dx \, |x - i\epsilon|^{-2} < \infty. \tag{4.34}$$

Hence, after the interchange we may apply the spectral theorem again to find

$$(4.33) = \frac{1}{2\pi i} \int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z \int_{\sigma(H)} \langle \psi, dP_E \psi \rangle \, \frac{e^{-itz}}{it(E-z)^2} = \frac{1}{2\pi i} \int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z \, \frac{e^{-itz}}{it} \left\langle \psi, \frac{1}{(H-z)^2} \psi \right\rangle. \tag{4.35}$$

Exploiting the polarization identities we recover for all $\psi, \phi \in \mathcal{H}$ the identity

$$\left\langle \psi, e^{-itH} \phi \right\rangle = \frac{1}{2\pi i} \int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z \, \frac{e^{-itz}}{it} \left\langle \psi, \frac{1}{(H-z)^2} \phi \right\rangle. \tag{4.36}$$

The fact that the family H^θ is an analytic family of type A implies that the operator valued function

$$\theta \mapsto \frac{1}{H^\theta - z} \tag{4.37}$$

is analytic for all z in the resolvent set of H^θ. A detailed and self-contained exposition of this topic is presented in [14, Section 7]. It is straight forward to prove that for real θ

$$\frac{1}{H^\theta - z} = U^\theta \frac{1}{H-z}(U^\theta)^{-1}. \tag{4.38}$$

For complex θ, however, this expression is not necessarily correct (due to a problem of domains of unbounded operators). Nevertheless, Eqs. (4.37) and (4.38) imply that the function

$$\theta \mapsto \left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)^2}\phi^\theta \right\rangle, \tag{4.39}$$

where $\phi^\theta = U^\theta \phi$, $\psi^{\overline{\theta}} = U^{\overline{\theta}}\psi$, is analytic and it coincides with $\left\langle \psi, \frac{1}{(H-z)^2}\phi \right\rangle$ for real θ, because in this case U^θ is unitary. Hence, we conclude that

$$\left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)^2}\phi^\theta \right\rangle = \left\langle \psi, \frac{1}{(H-z)^2}\phi \right\rangle \tag{4.40}$$

for every θ in a connected (open) domain containing 0 such that (4.39) is analytic in this domain. We obtain:

$$(4.36) = \frac{1}{2\pi i}\int_{\hat{\Gamma}(\epsilon)} \mathrm{d}z\, \frac{e^{-itz}}{it} \left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)^2}\phi^\theta \right\rangle \tag{4.41}$$

Eqs. (3.10) and (3.13) imply that the only spectral point of H^θ on the real line is λ_0^θ and all other spectral points have strictly negative imaginary part. Therefore, the operator valued function

$$A \cup \mathbb{C}^+ \ni z \mapsto \frac{1}{H^\theta - z}, \tag{4.42}$$

where $\mathbb{C}^+ = \{x + iy | x \in \mathbb{R}, y > 0\}$, is analytic. Moreover, for $R \geq e_1 + \delta = 2e_1$, $\Gamma_d(R)$ is contained in the region A, and hence, it follows from (3.29) that there is a constant C such that

$$\left\| \frac{1}{H^\theta - z} \right\| \leq \frac{C}{|z - e_1|} \qquad \forall z \in \Gamma_d. \tag{4.43}$$

Due to the analyticity, we may deform the integration contour from $\hat{\Gamma}(\epsilon)$ to $\Gamma(\epsilon, R)$ which gives:

$$(4.41) = \frac{1}{2\pi i}\int_{\Gamma(\epsilon,R)} \mathrm{d}z\, \frac{e^{-itz}}{it} \left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)^2}\phi^\theta \right\rangle. \tag{4.44}$$

Now we observe that the integrand on the right-hand side features an exponential decay for large $|\operatorname{Re} z|$ thanks to the factor e^{-itz} in the integrand and the definition of $\Gamma_d(\epsilon, R)$.

In particular, the decay in $|z|$ provided by the resolvent, i.e., bound (4.43), is not necessary anymore to make the integral converge. We may therefore perform an integration by parts. Note that, for z in $A \cup \mathbb{C}^+$, we have

$$\frac{d}{dz}\left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)}\phi^\theta \right\rangle = \left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)^2}\phi^\theta \right\rangle \tag{4.45}$$

which is implied by the resolvent identity

$$\left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - (z+u))}\phi^\theta \right\rangle - \left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - z)}\phi^\theta \right\rangle = \left\langle \psi^{\overline{\theta}}, \frac{1}{(H^\theta - (z+u))} u \frac{1}{(H^\theta - z)}\phi^\theta \right\rangle . \tag{4.46}$$

Moreover, the boundary terms of the partial integration resulting from the piece-wise concatenation of contours, i.e., $\Gamma(\epsilon, R) = \Gamma_-(\epsilon, R) \cup \Gamma_c(\epsilon) \cup \Gamma_d(R)$, cancel and the ones at $|\operatorname{Re} z| \to \infty$ vanish because of the exponential decay. In conclusion, the identity

$$(4.41) = \frac{1}{2\pi i}\int_{\Gamma(\epsilon,R)} \mathrm{d}z\, e^{-itz} \left\langle \psi^{\overline{\theta}}, \frac{1}{H^\theta - z}\phi^\theta \right\rangle \tag{4.47}$$

holds true which proves the claim. □

4.3 Key ingredients

The next definition is motivated by a simple geometric argument which we give in the following for the convenience of the reader: take a cone of the form $\mathcal{C}_m(\lambda_0^{(n)} - xe^{-i\nu})$, $x > 0$, where m is a fixed (arbitrary) number greater or equal than 4. Although m is arbitrary, our estimates and constants depend on it. The distance between the vertex of the cone and the intersection of the line $\lambda_0^{(n)} - ix\sin(\nu) + \mathbb{R}$ with the cone is

$$\sqrt{\Big(\frac{2x\sin(\nu)}{\tan\left((1-1/m)\nu\right)}\Big)^2 + (2x\sin(\nu))^2} \le 4x\frac{\sin(\nu)}{\sin\left((1-1/m)\nu\right)} \le 8x.$$

To obtain the last inequality we use the sum of angles formula for $\sin(\nu)$, writing $\nu = (\nu - \nu/m) + \nu/m$. Then, we have that the distance between $\lambda_0^{(n)}$ and the line segment described above is smaller than $8x$.

Definition 4.6. *For every $n \in \mathbb{N}$, we define*

$$\epsilon_n := 20\rho_n^{1+\mu/4}. \tag{4.48}$$

It follows from (3.33) *and* (3.28) *that for every $n \in \mathbb{N}$*

$$D(\lambda_0, 2\epsilon_n) \subset B_0^{(1)}. \tag{4.49}$$

The geometric argument given above together with $|\lambda_0^{(n)} - \lambda_0| \le 10^{-2}\rho_n^{1+\mu/2}$ (see Definition 3.1 and (3.27)*) yields that, for all $n \in \mathbb{N}$ and a fixed (arbitrary) $m \ge 4$,*

$$\mathcal{C}_m(\lambda_0^{(n)} - 2\rho_n^{1+\mu/4}e^{-i\nu}) \cap \left(\overline{\mathbb{C}^+} + \lambda_0^{(n)} - i2\sin(\nu)\rho_n^{1+\mu/4}\right) \subset D(\lambda_0, \epsilon_n) \subset D(\lambda_0, 2\epsilon_n) \subset B_0^{(1)} \tag{4.50}$$

and

$$\mathcal{C}_m(\lambda_0 - 2\rho_n^{1+\mu/4}e^{-i\nu}) \cap \left(\overline{\mathbb{C}^+} + \lambda_0 - i2\sin(\nu)\rho_n^{1+\mu/4}\right) \subset D(\lambda_0, \epsilon_n) \subset D(\lambda_0, 2\epsilon_n) \subset B_0^{(1)}. \tag{4.51}$$

Note that (3.27) *and the fact that* $\lambda_0 \in \mathbb{R}$ *imply that*

$$\operatorname{Im}\lambda_0^{(n)} - 2\sin(\nu)\rho_n^{1+\mu/4} \le 2g\rho_n^{1+\mu/2} - 2\sin(\nu)\rho_n^{1+\mu/4} < 0, \qquad \forall n \in \mathbb{N}, \tag{4.52}$$

for small enough g *(see Definition 4.3 in [14]). Eq.* (4.50) *implies that for every* $n \in \mathbb{N}$

$$\Gamma_c(\epsilon_n) \subset B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0^{(n)} - 2\rho_n^{1+\mu/4}e^{-i\nu}). \tag{4.53}$$

Lemma 4.7. *For all* $n \in \mathbb{N}$*, a fixed (arbitrary)* $m \ge 4$ *and* $\theta \in \mathcal{S}$*, there is a constant* C *(that depends on* m*) such that*

$$\left\| \frac{1}{H^\theta - z}\sigma_1 \Psi^\theta_{\lambda_0} \right\| \le C\boldsymbol{C}^{n+1}\frac{1}{\rho_n}, \tag{4.54}$$

for every $z \in B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0^{(n)} - \rho_n^{1+\mu/4}e^{-i\nu})$*, and hence, for every* $z \in B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0 - 2\rho_n^{1+\mu/4}e^{-i\nu})$*, see [14, Theorem 5.10].*

Proof. We take $z \in B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0^{(n)} - \rho_n^{1+\mu/4}e^{-i\nu})$ and recall the definition $\Psi^\theta_{\lambda_0} = P_0^\theta \varphi_0 \otimes \Omega$. Then, Eq. (3.24) yields

$$\|\Psi^\theta_{\lambda_0} - P_0^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}}\varphi_0 \otimes \Omega\| \le \rho_n^{\mu/2}. \tag{4.55}$$

This together with Eqs. (3.34), (3.36), (3.31) and (3.26) implies that there is a constant C such that (we use a telescopic sum argument)

$$\begin{aligned}
&\left\| \frac{1}{H^\theta - z}\sigma_1 \Psi^\theta_{\lambda_0} - \frac{1}{\tilde{H}^{(n),\theta} - z}\sigma_1 P_0^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}}\varphi_0 \otimes \Omega \right\| \\
&\le \left\| \frac{1}{H^\theta - z} - \frac{1}{\tilde{H}^{(n),\theta} - z} \right\| \left\| P_0^{(n),\theta} \right\| + \left\| \frac{1}{H^\theta - z} \right\| \left\| \Psi^\theta_{\lambda_0} - P_0^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}}\varphi_0 \otimes \Omega \right\| \\
&\le C\boldsymbol{C}^{n+1}\frac{1}{\rho_n}.
\end{aligned} \tag{4.56}$$

The fact (see Remark (1.2)) that

$$\Big(\frac{1}{\tilde{H}^{(n),\theta} - z}\sigma_1\Big)\Big(P_0^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}}\Big)\varphi_0 \otimes \Omega = \Big(\big(\frac{1}{H^{(n),\theta} - z}\sigma_1\big) \otimes P_{\Omega^{(n,\infty)}}\Big)P_0^{(n),\theta}\varphi_0 \otimes \Omega \tag{4.57}$$

guarantees that there is a constant C such that

$$\left\| \frac{1}{\tilde{H}^{(n),\theta} - z}\sigma_1 P_0^{(n),\theta} \otimes P_{\Omega^{(n,\infty)}}\varphi_0 \otimes \Omega \right\| \le \left\| \Big(\overline{P_0^{(n),\theta}} \frac{1}{H^{(n),\theta} - z}\Big) \otimes P_{\Omega^{(n,\infty)}} \right\| \le C\frac{\boldsymbol{C}^{n+1}}{\rho_n}. \tag{4.58}$$

Here, we use Eqs. (3.35), (3.26) and Lemma 4.4. $\square$

Remark 4.8. *Set* $c \equiv c_g := \mathrm{Im}\lambda_1$*. Notice that there is a strictly positive constant* $\boldsymbol{c}$ *(independent of* g*) with* $c_g \leq -g^2\boldsymbol{c}$*, for small enough* g *(see* (3.13)*). Then, for all real numbers* $b > a$ *and every* $x \in \{0, 1\}$*,*

$$\int_a^b \mathrm{d}r \, \frac{1}{|r - \lambda_1|^{1+x}} = \int_a^b \mathrm{d}r \, \frac{1}{g^{2(1+x)}} \frac{1}{((r - \mathrm{Re}\lambda_1)/g^2)^2 + (c/g^2)^2)^{(1+x)/2}} \tag{4.59}$$
$$\leq \frac{1}{g^{2x}} \int_{(a-\mathrm{Re}\lambda_1)/g^2}^{(b-\mathrm{Re}\lambda_1)/g^2} \mathrm{d}y \, \frac{1}{(y^2 + \boldsymbol{c}^2)^{(1+x)/2}}$$
$$\leq 2\frac{1}{g^{2x}} \int_0^1 \mathrm{d}\tau \, \frac{1}{\boldsymbol{c}^{1+x}} + 2\frac{1}{g^{2x}} \int_1^{1+|b-\mathrm{Re}\lambda_1|/g^2+|a-\mathrm{Re}\lambda_1|/g^2} \mathrm{d}\tau \, \frac{1}{\tau^{1+x}}$$
$$\leq C \begin{cases} \frac{1}{g^2}, & \text{if } x = 1, \\ |\log(g)|, & \text{if } x = 0, \end{cases}$$

where C *does not depend on* g *(for small enough* g*).*

Lemma 4.9. *Set* $\mathcal{L} := B_1^{(1)} \cap \mathbb{R}$*. Then, for* $g > 0$ *sufficiently small and* $\theta \in \mathcal{S}$*,*

$$\int_{\mathcal{L}} \mathrm{d}r \, \left\| \frac{1}{H^\theta - r} \sigma_1 \Psi_{\lambda_0}^\theta \right\| \leq C |\log g|, \tag{4.60}$$

where C *is a constant that does not depend on* g*.*

Proof. Let $\boldsymbol{c}$ be the constant introduced in (2.2), see Remark 4.8. The vertex of the cone $\mathcal{C}_m(\lambda_1 - 2\rho_n^{1+\mu/4} e^{-i\nu})$ belongs to the lower (open) half space of the complex plane if

$$-g^2\boldsymbol{c} + 2\rho_n^{1+\mu/4} \sin(\nu) < 0.$$

This is fulfilled if

$$n > \log\Big(\frac{g^2\boldsymbol{c}}{2\sin(\nu)\rho_0^{1+\mu/4}} \Big) \frac{1}{(1 + \mu/4)\log(\rho)}.$$

We fix $n_0 > 0$ to be the smallest integer number satisfying this inequality. Then

$$n_0 \leq \log\Big(\frac{g^2\boldsymbol{c}}{2\sin(\nu)\rho_0^{1+\mu/4}} \Big) \frac{1}{(1 + \mu/4)\log(\rho)} + 1. \tag{4.61}$$

For such n_0, the cone $\mathcal{C}_m(\lambda_1 - 2\rho_{n_0}^{1+\mu/4} e^{-i\nu})$ belongs to the lower (open) half space of the complex plane and, therefore, $\mathcal{L}$ is contained in the complement of this cone. This allows us to use (3.37) and estimate

$$\left\| \frac{1}{H^\theta - r} \right\| \leq C\boldsymbol{C}^{n_0+1} \frac{1}{\mathrm{dist}(r, \mathcal{C}_m(\lambda_1))}, \tag{4.62}$$

for every $r \in \mathcal{L}$. Eq. (4.61) implies that

$$\boldsymbol{C}^{n_0} \leq \boldsymbol{C} \exp\Big[-\log\Big(\frac{g^2\boldsymbol{c}}{2\sin(\nu)\rho_0^{1+\mu/4}} \Big) \Big]^{-\frac{\log(\boldsymbol{C})}{(1+\mu/4)\log(\rho)}} = \boldsymbol{C} \Big(\frac{2\sin(\nu)\rho_0^{1+\mu/4}}{g^2\boldsymbol{c}} \Big)^{-\frac{\log(\boldsymbol{C})}{(1+\mu/4)\log(\rho)}}$$
$$\leq C g^{-\iota}, \tag{4.63}$$

where we use that $\boldsymbol{C}\rho^{\frac{1}{2}\iota(1+\mu/4)} \leq 1$, see (3.31). This together with (3.37) lead us to

$$\Big\|\frac{1}{H^\theta - r}\Big\| \leq Cg^{-\iota}\frac{1}{\operatorname{dist}(r, \mathcal{C}_m(\lambda_1))}, \qquad \forall r \in \mathcal{L}. \tag{4.64}$$

It is geometrically clear, because $\mathrm{Im}\lambda_1 < -g^2\boldsymbol{c} < 0$ - see (3.13), that there is a constant C (that depends on $\boldsymbol{\nu}$ and m, but not on g) such that, for every $r \in \mathcal{L}$,

$$|r - \lambda_1| \leq C\operatorname{dist}(r, \mathcal{C}_m(\lambda_1)). \tag{4.65}$$

Eqs. (4.64) and (4.65) yield

$$\Big\|\frac{1}{H^\theta - r}\Big\| \leq Cg^{-\iota}\frac{1}{|r - \lambda_1|}. \tag{4.66}$$

Moreover, we observe from (3.25) that

$$\Big\|\overline{P_1^\theta}\sigma_1\Psi_{\lambda_0}^\theta\Big\| = \Big\|(1 - P_1^\theta)\sigma_1 P_0^\theta\varphi_0 \otimes \Omega\Big\| \leq \|(1 - P_{\varphi_1} \otimes P_\Omega)\varphi_1 \otimes \Omega\| + Cg = Cg. \tag{4.67}$$

Inserting $P_1^\theta + \overline{P_1^\theta} = 1$ in the left hand side of (4.60) and using (4.66), we find

$$\Big\|\frac{1}{H^\theta - r}\sigma_1\Psi_{\lambda_0}^\theta\Big\| \leq C\left(\frac{1}{|\lambda_1 - r|} + g\Big\|\frac{1}{H^\theta - r}\Big\|\right). \tag{4.68}$$

This together with $\iota \in (0,1)$ and (4.66) yields that

$$\Big\|\frac{1}{H^\theta - r}\sigma_1\Psi_{\lambda_0}^\theta\Big\| \leq C\frac{1}{|\lambda_1 - r|}. \tag{4.69}$$

From (4.69) and Remark 4.8, we obtain

$$\int_{\mathcal{L}} \mathrm{d}r\, \Big\|\frac{1}{H^\theta - r}\sigma_1\Psi_{\lambda_0}^\theta\Big\| \leq C\int_{\mathcal{L}} \frac{1}{|r - \lambda_1|} \leq C|\log g|. \tag{4.70}$$

□

Lemma 4.10. *For every bounded measurable function h, there is a constant C such that for all natural numbers $n \in \mathbb{N}$ and $\theta \in \mathcal{S}$*

$$\int_{\left((B_0^{(1)} \cup B_1^{(1)}) \cap \mathbb{R}\right) \setminus (\lambda_0 - \epsilon_n, \lambda_0 + \epsilon_n)} dz|h(z)|\Big\|\frac{1}{H^\theta - z}\sigma_1\Psi_{\lambda_0}^\theta\Big\| \leq C|\log g|\|h\|_\infty, \tag{4.71}$$

where $\|h\|_\infty$ denotes the supremum of $|h|$.

Proof. We set

$$\tilde{h}(z) = |h(z)|\Big\|\frac{1}{H^\theta - z}\sigma_1\Psi_{\lambda_0}^\theta\Big\|. \tag{4.72}$$

For any natural number $l \geq 2$, we set $I_l := B_0^{(1)} \cap [\lambda_0 - \epsilon_{l-1}, \lambda_0 + \epsilon_{l-1}] \setminus (\lambda_0 - \epsilon_l, \lambda_0 + \epsilon_l)$. We define $I_1 := \mathbb{R} \cap B_0^{(1)} \setminus I_2$. Then, we compute

$$\int_{(\mathbb{R}\cap B_0^{(1)})\setminus(\lambda_0-\epsilon_n,\lambda_0+\epsilon_n)} dz\, \tilde{h}(z) = \sum_{l=1}^{n} \int_{I_l} dz\, \tilde{h}(z). \tag{4.73}$$

Using Definition 4.6 and Lemma 4.7, we obtain that there is a constant C such that

$$\begin{aligned}\sum_{l=1}^{n} \int_{I_l} dz\, \tilde{h}(z) &\leq C \sum_{l=2}^{n} \boldsymbol{C}^{l+1} \frac{\epsilon_{l-1}}{\rho_l} \|h\|_\infty + C\|h\|_\infty \qquad (4.74)\\ &\leq C\frac{1}{\rho} \sum_{l=2}^{n} \boldsymbol{C}^{l+1} \rho_{l-1}^{\mu/4} \|h\|_\infty + C\|h\|_\infty \leq C\|h\|_\infty,\end{aligned}$$

where we use (3.31). Eq. (4.74) and Lemma 4.9 imply (4.71). □

Lemma 4.11. *For every bounded measurable function h, there is a constant C such that for all natural numbers $n \in \mathbb{N}$ and $\theta \in \mathcal{S}$*

$$\int_{\Gamma_c(\epsilon_n)} dz |h(z)| \Big\| \frac{1}{H^\theta - z} \sigma_1 \Psi_{\lambda_0}^\theta \Big\| \leq \rho_n^{\mu/8} C \sup_{z\in\Gamma_c(\epsilon_n)} \{|h(z)|\}. \tag{4.75}$$

Proof. This is a direct consequence of Lemma 4.7 and (3.31). □

Lemma 4.12. *There is a constant C such that (for $s > 0$)*

$$\Big| \int_{\Gamma_d(R)\cup\Gamma_-(\epsilon_n,R)\setminus\Big(\big(B_0^{(1)}\cup B_1^{(1)}\big)\cap\mathbb{R}\Big)} \mathrm{d}z\, e^{-isz} \Big\langle \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \Big(H^\theta - z\Big)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \Big\rangle \Big| \leq Cg\frac{1}{s}. \tag{4.76}$$

Proof. After an integration by parts, we obtain

$$\begin{aligned}&\Big| \int_{\Gamma_d(R)\cup\Gamma_-(\epsilon_n,R)\setminus\Big(\big(B_0^{(1)}\cup B_1^{(1)}\big)\cap\mathbb{R}\Big)} \mathrm{d}z\, e^{-isz} \Big\langle \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \Big(H^\theta - z\Big)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \Big\rangle \Big| \\ \leq &\frac{1}{s} \int_{\Gamma_d(R)\cup\Gamma_-(\epsilon_n,R)\setminus\Big(\big(B_0^{(1)}\cup B_1^{(1)}\big)\cap\mathbb{R}\Big)} \mathrm{d}z \Big| \Big\langle \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \Big(H^\theta - z\Big)^{-2} \sigma_1 \Psi_{\lambda_0}^\theta \Big\rangle \Big| \\ &+ \frac{1}{s} \sum_{z\in\{e_1+\delta/2, e_0-\delta/2\}} \Big| \Big\langle \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \Big(H^\theta - z\Big)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \Big\rangle \Big|. \qquad (4.77)\end{aligned}$$

Now, we recall (4.67)

$$\Big\| \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \Big\| = \Big\| \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} - \overline{P_{\varphi_1}} \otimes P_\Omega \sigma_1 \varphi_0 \otimes \Omega \Big\| \leq Cg, \tag{4.78}$$

where we use Eq. (3.25) and $\sigma_1\varphi_0 = \varphi_1$. Eq (4.76) is a direct consequence of (4.77), (4.78) and (3.29). □

Lemma 4.13. *For real numbers $0 < q \leq e^{-1} < 1 < Q < \infty$ and $\theta \in \mathcal{S}$, the term (recall* (2.1)*)*

$$R_1(q,Q) := \int_q^Q \mathrm{d}s \int dr\, G(r) e^{is(r+\lambda_0)} \times \int_{\Gamma(\epsilon_n,R)} \mathrm{d}z\, e^{-isz} \left\langle \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle \tag{4.79}$$

fulfills

$$|R_1(q,Q)| \leq Cg\left(|\log(q)| + |\log(g)|\right). \tag{4.80}$$

Notice that $R_1(q,Q)$ does not depend on ϵ_n and R, because a change in ϵ_n and R implies a change in the contour of integration of the analytic function above.

Proof. First, we recall that (see (4.78))

$$\left\| \overline{P_1^{\overline{\theta}}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\| \leq Cg. \tag{4.81}$$

A two-fold integration by parts together with the fact $G \in C_c^\infty(\mathbb{R} \setminus \{0\}, \mathbb{C})$ (recall (2.1)) shows that there is a constant C such that

$$\left| \int dr\, G(r) e^{is(r+\lambda_0)} \right| \leq \frac{C}{1+s^2}, \qquad \forall s \in \mathbb{R}. \tag{4.82}$$

Lemmas 4.10, 4.11 and 4.12, an Eq. (4.81) imply that

$$|R_1(q,Q)| \leq Cg \int_q^Q ds \frac{1}{s^2+1} \Big(\frac{1}{s} + e^{\epsilon_n Q} \rho_n^{\mu/8} + |\log g| \Big). \tag{4.83}$$

Since $R_1(q,Q)$ does not depend on n, we can take n to infinity and obtain the bound

$$|R_1(q,Q)| \leq Cg \int_q^Q ds \frac{1}{s^2+1} \Big(\frac{1}{s} + |\log g| \Big). \tag{4.84}$$

Eq. (4.84) and the condition $0 < q < e^{-1}$ imply (4.80). Notice that

$$\int_q^Q ds \frac{1}{(s^2+1)s} \leq \int_q^1 \frac{1}{s} + \int_1^\infty \frac{1}{s^2+1} \leq C|\log(q)|, \tag{4.85}$$

since $\int_1^\infty \frac{1}{s^2+1}$ is a constant and $|\log(q)| \geq 1$. □

Lemma 4.14. *For real numbers $0 < q < 1 < Q < \infty$ and $\theta \in \mathcal{S}$, the term*

$$P_1(q,Q) = \int_q^Q \mathrm{d}s \int dr\, G(r) e^{is(r+\lambda_0)} \times \int_{\Gamma(\epsilon_n,R)} \mathrm{d}z\, e^{-isz} \left\langle P_1^{\overline{\theta}} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle. \tag{4.86}$$

fulfills

$$P_1(q,Q) = -2\pi \int \mathrm{d}r\, G(r) \frac{1}{r+\lambda_0-\lambda_1} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle + R_2(q,Q), \tag{4.87}$$

where

$$|R_2(q,Q)| \leq C\Big(q + \frac{1}{Qg^2}\Big). \tag{4.88}$$

Notice that $P_1(q,Q)$ does not depend on ϵ_n and R, because a change in ϵ_n and R implies a change in the contour of integration of the analytic function above.

Proof. We have that

$$P_1(q,Q) = \int_q^Q \mathrm{d}s \int dr\, G(r) e^{is(r+\lambda_0)} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle \int_{\Gamma(\epsilon_n,R)} \mathrm{d}z\, \frac{e^{-isz}}{\lambda_1 - z}. \tag{4.89}$$

The residue theorem together with methods of complex analysis provides

$$\int_{\Gamma(\epsilon_n,R)} \mathrm{d}z\, \frac{e^{-isz}}{\lambda_1 - z} = 2\pi i e^{-is\lambda_1}, \tag{4.90}$$

and hence, we obtain

$$\begin{aligned} P_1(q,Q) &= 2\pi i \int_q^Q \mathrm{d}s \int dr\, G(r) e^{is(r+\lambda_0-\lambda_1)} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle \\ &= 2\pi \int \mathrm{d}r\, G(r) (e^{iQ(r+\lambda_0-\lambda_1)} - e^{iq(r+\lambda_0-\lambda_1)}) \frac{1}{r+\lambda_0-\lambda_1} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle \\ &= -2\pi \int \mathrm{d}r\, G(r) \frac{1}{r+\lambda_0-\lambda_1} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle + r_1(Q) + r_2(q), \end{aligned} \tag{4.91}$$

where

$$r_1(Q) := 2\pi \int \mathrm{d}r\, G(r) e^{iQ(r+\lambda_0-\lambda_1)} \frac{1}{r+\lambda_0-\lambda_1} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle \tag{4.92}$$

and

$$r_2(q) := 2\pi \int \mathrm{d}r\, G(r) (1 - e^{iq(r+\lambda_0-\lambda_1)}) \frac{1}{r+\lambda_0-\lambda_1} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle. \tag{4.93}$$

It follows from

$$|1 - e^{iq(r+\lambda_0-\lambda_1)}| \leq |q(r+\lambda_0-\lambda_1)|, \tag{4.94}$$

that there is a constant C such that $|r_2(q)| \leq Cq$. Applying the integration by parts formula in Eq. (4.92), we obtain a factor $\frac{1}{Q}$ and the derivative of $G(r)\frac{1}{(r+\lambda_0-\lambda_1)}$. We obtain

$$\begin{aligned} |r_1(Q)| &\leq C\frac{1}{Q} \int \mathrm{d}r \Big(|G(r)| \frac{1}{|r+\lambda_0-\lambda_1|^2} + |\frac{d}{dr} G(r)| \frac{1}{|r+\lambda_0-\lambda_1|} \Big) | \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1 \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle | \\ &\leq C\frac{1}{Q}(\frac{1}{g^2} + |\log(g)|) \leq C\frac{1}{Qg^2}, \end{aligned} \tag{4.95}$$

where we use (4.59), with $x = 1$ and $x = 0$, and $r + \lambda_0$ instead of r. □

Lemma 4.15. *For real numbers $0 < q < 1 < Q < \infty$ and $\theta \in \mathcal{S}$, we define the term*

$$\widetilde{P}_1(q,Q) := \int_q^Q \mathrm{d}s \int dr\, G(r) e^{is(r-\lambda_0)} \times \int_{\widetilde{\Gamma}(\epsilon_n,R)} \mathrm{d}z\, e^{isz} \left\langle P_1^\theta \sigma_1 \Psi_{\lambda_0}^\theta, \left(H^{\overline{\theta}} - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\rangle, \tag{4.96}$$

where $\widetilde{\Gamma}(\epsilon_n, R)$ is a positively oriented curve obtained by conjugating the elements of $\Gamma(\epsilon_n, R)$. It follows that

$$\widetilde{P}_1(q,Q) = 2\pi \int \mathrm{d}r\, G(r) \frac{1}{r - \lambda_0 + \overline{\lambda_1}} \left\langle P_1^\theta \sigma_1 \Psi_{\lambda_0}^\theta, \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\rangle + \widetilde{R}_2(q,Q), \tag{4.97}$$

where

$$|\widetilde{R}_2(q,Q)| \leq C\Big(q + \frac{1}{Qg^2}\Big). \tag{4.98}$$

Proof. This proof is very similar to the proof of Lemma 4.14: We have that

$$\widetilde{P}_1(q,Q) = -2\pi i \int_q^Q \mathrm{d}s \int dr\, G(r) e^{is(r-\lambda_0+\overline{\lambda_1})} \left\langle P_1^\theta \sigma_1 \Psi_{\lambda_0}^\theta, \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\rangle \tag{4.99}$$

and hence, we infer

$$\begin{aligned} P_1(q,Q) =& -2\pi \int \mathrm{d}r\, G(r)(e^{iQ(r-\lambda_0+\overline{\lambda_1})} - e^{iq(r-\lambda_0+\overline{\lambda_1})}) \frac{1}{r - \lambda_0 + \overline{\lambda_1}} \left\langle P_1^\theta \sigma_1 \Psi_{\lambda_0}^\theta, \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\rangle \\ =& 2\pi \int \mathrm{d}r\, G(r) \frac{1}{r - \lambda_0 + \overline{\lambda_1}} \left\langle P_1^\theta \sigma_1 \Psi_{\lambda_0}^\theta, \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\rangle + \widetilde{R}_2(q,Q). \end{aligned} \tag{4.100}$$

We conclude the proof as in the proof of Lemma 4.14. □

4.4 Proof of Theorem 2.2

In this section, we give the proof of the main theorem based on the previous results.

Proof of Theorem 2.2. Let $h, l \in \mathfrak{h}_0$; c.f. (1.33). Recall the definition of W given in (4.9) and the form factor f in (1.5). Since $f \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})$ we find

$$hf, lf, W \in \mathfrak{h}_0. \tag{4.101}$$

Theorem 4.3, i.e., equation (4.8), together with Lemma 4.1 (iv) yields

$$T(h,l) = -2\pi i g \left\|\Psi_{\lambda_0}\right\|^{-2} \langle a_-(W)\sigma_1 \Psi_{\lambda_0}, \Psi_{\lambda_0}\rangle = -2\pi i g \left\|\Psi_{\lambda_0}\right\|^{-2} \langle [a_-(W), \sigma_1]\Psi_{\lambda_0}, \Psi_{\lambda_0}\rangle, \tag{4.102}$$

and furthermore, recalling $\omega(k) = |k|$, equation (4.2) in Lemma 4.1 (ii) implies

$$\begin{aligned} T(h,l) &= 2\pi(ig)^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \int_{-\infty}^{0} \mathrm{d}s\, \overline{\langle W_s, f\rangle_2} \left\langle \left[e^{isH}\sigma_1 e^{-isH}, \sigma_1\right] \Psi_{\lambda_0}, \Psi_{\lambda_0}\right\rangle \\ &= 2\pi g^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \int_{0}^{\infty} \mathrm{d}s\, \langle f, W_{-s}\rangle_2 \left\langle \left[e^{-isH}\sigma_1 e^{isH}, \sigma_1\right] \Psi_{\lambda_0}, \Psi_{\lambda_0}\right\rangle \\ &= 2\pi g^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \left(T^{(1)} - T^{(2)}\right), \end{aligned} \tag{4.103}$$

where we used the abbreviations

$$T^{(j)} := T^{(j)}(0,\infty) \tag{4.104}$$

for $j = 1, 2$ with

$$\begin{aligned} T^{(1)}(q,Q) &:= \int_q^Q \mathrm{d}s \int \mathrm{d}^3k\, W(k) f(k) e^{is(|k|+\lambda_0)} \left\langle \sigma_1\Psi_{\lambda_0}, e^{-isH}\sigma_1\Psi_{\lambda_0}\right\rangle \\ &= \int_q^Q \mathrm{d}s \int \mathrm{d}r G(r) e^{is(r+\lambda_0)} \left\langle \sigma_1\Psi_{\lambda_0}, e^{-isH}\sigma_1\Psi_{\lambda_0}\right\rangle \end{aligned} \tag{4.105}$$

and

$$T^{(2)}(q,Q) := \int_q^Q \mathrm{d}s \int \mathrm{d}r G(r) e^{is(r-\lambda_0)} \left\langle \sigma_1\Psi_{\lambda_0}, e^{isH}\sigma_1\Psi_{\lambda_0}\right\rangle. \tag{4.106}$$

We recall the definitions (4.9) and (2.1):

$$W(k) = |k|^2 l(k) \int \mathrm{d}\Sigma\, \overline{h(|k|,\Sigma)} f(|k|,\Sigma), \qquad G(r) = \int \mathrm{d}\Sigma \mathrm{d}\Sigma'\, r^4 \overline{h(r,\Sigma)} l(r,\Sigma') f(r)^2. \tag{4.107}$$

We observe that there is a constant C such that

$$|T^{(i)}(q,Q) - T^{(i)}(0,Q)| \le Cq. \tag{4.108}$$

We start with analyzing the term $T^{(1)}(q,Q)$. Lemma 4.5 together with the identity $P_1^{\overline{\theta}} + \overline{P_1^{\overline{\theta}}} = 1$ allows us to write this term as

$$T^{(1)}(q,Q) = \frac{1}{2\pi i} P_1(q,Q) + \frac{1}{2\pi i} R_1(q,Q) \tag{4.109}$$

for all $0 < q < Q < \infty$. Here, $P_1(q,Q)$ and $R_1(q,Q)$ are defined in (4.86) and (4.79), respectively. Moreover, Lemma 4.14 implies

$$\begin{aligned} T^{(1)}(q,Q) = &-2\pi \frac{1}{2\pi i} \int \mathrm{d}r\, G(r) \frac{1}{r+\lambda_0-\lambda_1} \left\langle \sigma_1\Psi_{\lambda_0}^{\overline{\theta}}, P_1^{\theta}\sigma_1\Psi_{\lambda_0}^{\theta}\right\rangle \\ &+ \frac{1}{2\pi i}\Big(R_1(q,Q) + R_2(q,Q)\Big), \end{aligned} \tag{4.110}$$

where Lemmas 4.13 and 4.14 provide the estimates:

$$|R_1(q,Q)| \leq Cg\left(|\log(q)| + |\log(g)|\right), \qquad |R_2(q,Q)| \leq C(q + \frac{1}{g^2 Q}) \tag{4.111}$$

for $0 < q \leq e^{-1} < 1 < Q$. As explained in Lemmas 4.13 and 4.14, the terms $P_1(q,Q)$ and $R_1(q,Q)$ do not depend on n and R because both are given by contour integrals of analytic functions and a change of these parameters signifies a change in the contour of integration only. Taking the limit Q to infinity and $q = g$, we obtain from Eqs. (4.108), (4.110) and (4.111):

$$T^{(1)}(0,\infty) = i\int \mathrm{d}r\, G(r)\frac{1}{r+\lambda_0-\lambda_1}\left\langle \sigma_1\Psi^{\overline{\theta}}_{\lambda_0}, P^{\theta}_1\sigma_1\Psi^{\theta}_{\lambda_0}\right\rangle + R_3 \tag{4.112}$$

and that there is a constant C such that

$$|R_3| \leq C|\log(g)|. \tag{4.113}$$

The term $T^{(2)}(0,\infty)$ can be inferred by repeating the calculation with θ replaced by $\overline{\theta}$ and reflecting the path of integration $\Gamma(\epsilon, R)$ on the real axis when applying Lemma 4.5. In this case one has to consider the Hamiltonian $H^{\overline{\theta}}$. Notice that in this case the factor $\frac{1}{2\pi i}$ in Eq. (4.31) is substituted by $-\frac{1}{2\pi i}$, which is produced from the change of orientation of the integration curve. Due to the similarity of the calculation, we omit the proof and only state the result (it follows from Lemma 4.15 and similar computations)

$$T^{(2)}(0,\infty) = \frac{-1}{2\pi i}2\pi\int \mathrm{d}r\, G(r)\frac{1}{r-\lambda_0+\overline{\lambda_1}}\left\langle \sigma_1\Psi^{\theta}_{\lambda_0}, P^{\overline{\theta}}_1\sigma_1\Psi^{\overline{\theta}}_{\lambda_0}\right\rangle + R_4 \tag{4.114}$$

and that there is a constant C such that

$$|R_4| \leq C|\log(g)|. \tag{4.115}$$

The identities (4.103), (4.112) and (4.114), together with (4.113), (4.115) and (3.25) imply

$$\begin{aligned} T(h,l) &= 2\pi g^2\left\|\Psi_{\lambda_0}\right\|^{-2}\left(T^{(1)} - T^{(2)}\right) + R \qquad (4.116)\\ &= 2\pi i g^2\left\|\Psi_{\lambda_0}\right\|^{-2}\int \mathrm{d}r\, G(r)\Big(\frac{1}{r+\lambda_0-\lambda_1} - \frac{1}{r-\lambda_0+\overline{\lambda_1}}\Big) + R\\ &= 4\pi i g^2\left\|\Psi_{\lambda_0}\right\|^{-2}\int \mathrm{d}r\, G(r)\Big(\frac{\operatorname{Re}\lambda_1-\lambda_0}{(r+\lambda_0-\lambda_1)(r-\lambda_0+\overline{\lambda_1})}\Big) + R, \end{aligned}$$

where $|R| \leq C|\log(g)|$. □

Remark 4.16. *The constant $C(h,l)$ in Theorem 2.2 depends on h and l. From our methods, this dependence can be made explicit. However, for the sake of simplicity and clarity we do not present this analysis in this paper, but indicate instead how to do it. The key ingredients are Eqs.* (4.82) *and* (4.93) *(notice that* (4.92) *does not play a role* *because the corresponding term vanishes when Q tends to infinity). These terms give a contribution of the form*

$$C\int dr\Big[|G(r)|+\Big|\frac{d}{dr}G(r)\Big|+\Big|\frac{d^2}{dr^2}G(r)\Big|\Big], \tag{4.117}$$

for a constant C that does not depend on h and l. Moreover, with respect to (4.82)*, a minor change in the proof of Lemma 4.13 would make the second derivative term unnecessary because we have an extra factor of the form s^{-1} in* (4.76)*. This is essentially the only necessary contribution that comes from h and l. However, in order to simplify our final formula, we substituted the inner products in Eqs.* (4.112) *and* (4.114) *by the constant* 1 *(using* (3.25)*). This produces (explicit) error terms that contribute differently as* (4.117)*, as we can see from our arguments below* (4.115)*.*

A Standard Estimates

In the following we shall use the well-known standard inequalities

$$\begin{aligned}\|a(h)\Psi\| &\le \|h/\sqrt{\omega}\|_2\,\|H_f^{1/2}\Psi\|\\ \|a(h)^*\Psi\| &\le \|h/\sqrt{\omega}\|_2\,\|H_f^{1/2}\Psi\|+\|h\|_2\,\|\Psi\|\end{aligned} \tag{A.1}$$

which hold for all $h, h/\sqrt{\omega}\in\mathfrak{h}$ and $\Psi\in\mathcal{H}$ such that the left- and right-hand side are well-defined; see [40, Eq. (13.70)].

Lemma A.1. *Let $h, h/\sqrt{\omega}\in\mathfrak{h}$. Then, we have the following estimates:*

$$\Big\|a(h)^*(H_f+1)^{-\frac12}\Big\| \le \|h\|_2+\|h/\sqrt{\omega}\|_2\,, \tag{A.2}$$

$$\Big\|a(h)(H_f+1)^{-\frac12}\Big\| \le \|h/\sqrt{\omega}\|_2\,, \tag{A.3}$$

$$\Big\|V\,(H_f+1)^{-\frac12}\Big\| \le \|f\|_2+2\,\|f/\sqrt{\omega}\|_2\,. \tag{A.4}$$

Proof. Let $\Psi\in\mathcal{F}[\mathfrak{h}]$ with $\|\Psi\|_{\mathcal{H}}=1$. Applying (A.1) and the spectral theorem, we find

$$\begin{aligned}\|a(h)^*(H_f+1)^{-\frac12}\Psi\| &\le \|h\|_2\|(H_f+1)^{-\frac12}\Psi\|+\|h/\sqrt{\omega}\|_2\|H_f^{\frac12}(H_f+1)^{-\frac12}\Psi\|\\ &\le \|h\|_2+\|h/\sqrt{\omega}\|_2,\end{aligned} \tag{A.5}$$

$$\|a(h)(H_f+1)^{-\frac12}\Psi\| \le \|h/\sqrt{\omega}\|_2\|H_f^{\frac12}(H_f+1)^{-\frac12}\Psi\| \le \|h/\sqrt{\omega}\|_2. \tag{A.6}$$

The inequality (A.4) is implied by the boundedness of σ_1 and the triangle inequality:

$$\begin{aligned}\Big\|V\,(H_f+1)^{-\frac12}\Big\| &\le \Big\|\sigma_1\otimes a(f)\,(H_f+1)^{-\frac12}\Big\|+\Big\|\sigma_1\otimes a(f)^*\,(H_f+1)^{-\frac12}\Big\|\\ &\le \Big\|a(f)\,(H_f+1)^{-\frac12}\Big\|+\Big\|a(f)^*\,(H_f+1)^{-\frac12}\Big\| \le \|f\|_2+2\,\|f/\sqrt{\omega}\|_2\,.\end{aligned} \tag{A.7}$$

This completes the proof. □

34

As preparation of the proof of Lemma 4.1 (in Appendix C below) we recall that the Hamiltonians H, c.f. (1.7), as well as H_f, c.f. (1.3), are self-adjoint on the common domain $D(H) = \mathcal{K} \otimes \mathcal{D}(H_f)$ and bounded below by the constant $b \in \mathbb{R}$; c.f. Proposition 1.1 and (1.22). By spectral calculus we can define the operators $H_f^{1/2}$, $(H - b + 1)^{1/2}$ and $(H_f + 1)^{-1/2}$, $(H - b + 1)^{-1/2}$ which are closed and densely defined and the latter two are even bounded by 1. For the proof Lemma 4.1 we shall need the following lemma.

Lemma A.2. *The following operators are bounded:*

$$H_f^{\frac{1}{2}}(H - b + 1)^{-\frac{1}{2}}, \tag{A.8}$$

$$(H - b + 1)^{\frac{1}{2}}(H_f + 1)^{-\frac{1}{2}}. \tag{A.9}$$

Proof. Let $\Psi \in \mathcal{H}$ with $\|\Psi\| = 1$. The boundedness of (A.8) follows from the equality

$$\begin{aligned}\|H_f^{\frac{1}{2}}(H - b + 1)^{-\frac{1}{2}}\Psi\|^2 &= \langle (H - b + 1)^{-\frac{1}{2}}\Psi, H_f(H - b + 1)^{-\frac{1}{2}}\Psi\rangle \\ &= \langle (H - b + 1)^{-\frac{1}{2}}\Psi, (H - K - gV)(H - b + 1)^{-\frac{1}{2}}\Psi\rangle \end{aligned} \tag{A.10}$$

and the fact that K is bounded by $|e_1|$ and that for all $\epsilon > 0$

$$\begin{aligned}&|\langle (H - b + 1)^{-\frac{1}{2}}\Psi, gV(H - b + 1)^{-\frac{1}{2}}\Psi\rangle| \leq \|(H - b + 1)^{-\frac{1}{2}}\Psi\| \, \|gV(H - b + 1)^{-\frac{1}{2}}\Psi\| \\ &\leq \frac{g}{\epsilon} 2\|f/\sqrt{\omega}\|_2 \, \epsilon \|H_f^{\frac{1}{2}}(H - b + 1)^{-\frac{1}{2}}\Psi\| + \|f\|_2 \|\Psi\| \\ &\leq \left(\frac{g}{\epsilon} 2\|f/\sqrt{\omega}\|_2\right)^2 + \epsilon^2 \|H_f^{\frac{1}{2}}(H - b + 1)^{-\frac{1}{2}}\Psi\|^2 + \|f\|_2 \end{aligned} \tag{A.11}$$

holds, which is a consequence of (A.1). Choosing $0 < \epsilon < 1$ an explicit bound is

$$\|H_f^{\frac{1}{2}}(H - b + 1)^{-\frac{1}{2}}\Psi\|^2 \leq \frac{1 + |e_1| + (\frac{g}{\epsilon} 2\|f/\sqrt{\omega}\|_2)^2 + \|f\|_2}{1 - \epsilon^2} < \infty. \tag{A.12}$$

The boundedness of (A.9) is implied by

$$\|(H - b + 1)^{\frac{1}{2}}(H_f + 1)^{-\frac{1}{2}}\Psi\|^2 = \langle (H_f + 1)^{-\frac{1}{2}}\Psi, (K + H_f + gV - b + 1)(H_f + 1)^{-\frac{1}{2}}\Psi\rangle \tag{A.13}$$

and, again as a consequence of (A.1),

$$\begin{aligned}|\langle (H_f + 1)^{-\frac{1}{2}}\Psi, gV(H_f + 1)^{-\frac{1}{2}}\Psi\rangle| &\leq g2\|f/\sqrt{\omega}\|_2 \, \|H_f^{\frac{1}{2}}(H_f + 1)^{-\frac{1}{2}}\Psi\| + \|f\|_2 \\ &\leq \|f\|_2 + 2\|f/\sqrt{\omega}\|_2. \end{aligned} \tag{A.14}$$

□

B Proofs for Section 1.2

It is well-known that there is a dense domain of analytic vectors; for example

$$\mathcal{D} = \left\{ \chi_{[-R,R]}(A)\Psi : \Psi \in \mathcal{H}, R > 0 \right\}$$

with A being the generator of U_θ and χ the corresponding spectral projection (c.f. [4, 32]).

Proof of Lemma 1.5. Let $\theta \in \mathbb{C}$. Definition in (1.3) implies that $H_0^\theta = K \otimes \mathbb{1}_{\mathcal{F}[\mathfrak{h}]} + \mathbb{1}_{\mathcal{K}} \otimes H_f^\theta$ is a sum of commuting self-adjoint operators and $\sigma(K) = \{e_0, e_1\}$. As shown in [36], we have $\sigma(H_f) = \mathbb{R}_0^+$ and it follows from the definition of $H_f^\theta = e^{-\theta} H_f$ in (1.28) that $\sigma(H_f^\theta) = \left\{ e^{-\theta} r : r \geq 0 \right\}$. The claim then follows from the spectral theorem for two commuting normal operators. □

C Asymptotic creation/annihilation operators

Proof of Lemma 4.1. Let $h, l \in \mathfrak{h}_0$ and $\Psi \in \mathcal{K} \otimes \mathcal{D}(H_f^{1/2})$. Thanks to Lemma A.2 we have $\mathcal{K} \otimes \mathcal{D}(H_f^{\frac{1}{2}}) = \mathcal{D}((H - b + 1)^{\frac{1}{2}})$. We prove claims (i)-(vi) separately:

(ii) The subspace of $\mathcal{H}_0$, defined in (4.18), is dense in the domain of $(H - b + 1)^{1/2}$ w.r.t. the graph norm $\| \cdot \|_{(H-b+1)^{1/2}}$ of $(H - b + 1)^{\frac{1}{2}}$ so that there is a sequence $(\Psi_n)_{n \in \mathbb{N}}$ in $\mathcal{K} \otimes \mathcal{F}_{\text{fin}}[\mathfrak{h}_0]$ with $\Psi_n \to \Psi$ in this norm as $n \to \infty$. For all $n \in \mathbb{N}$, the definition in (1.34) together with the group properties $(e^{-itH})_{t \in \mathbb{R}}$, in particularly, the strong continuous differentiability on $D(H)$, justify

$$\begin{aligned} a_t(h)\Psi_n = e^{itH} a(h_t) e^{-itH} &= a(h)\Psi_n + \int_0^t ds \, \frac{d}{ds} e^{isH} a(h_s) e^{-isH} \Psi_n \\ &= a(h)\Psi_n - ig \int_0^t ds \, \langle h_s, f \rangle_2 e^{isH} \sigma_1 e^{-isH} \Psi_n, \end{aligned} \tag{C.1}$$

where the last integrand was computed by observing the CCR (c.f. (1.19))

$$[V, a(h_s)] = \sigma_1 \otimes [a(f) + a(f)^*, a(h_s)] = -\sigma_1 \langle h_s, f \rangle_2 . \tag{C.2}$$

We may now take the limit $n \to \infty$ of identity (C.1) and find

$$a_t(h)\Psi = a(h)\Psi - ig \int_0^t ds \, \langle h_s, f \rangle_2 \, e^{isH} \sigma_1 e^{-isH} \Psi \tag{C.3}$$

because of the following two ingredients: First, by definition (1.34), the standard estimate (A.1) and Lemma A.2, for all $m \in \mathfrak{h}_0$, there is a finite constant $C_{(\text{C.4})}$ such that

$$\begin{aligned} \|a_t(m)(\Psi - \Psi_n)\| &= \|a(m_t)(H - b + 1)^{-\frac{1}{2}} e^{-itH} (H - b + 1)^{\frac{1}{2}} (\Psi - \Psi_n)\| \\ &\leq \|m/\sqrt{\omega}\|_2 \, \|H_f^{\frac{1}{2}} (H - b + 1)^{-\frac{1}{2}}\| \, \|(H - b + 1)^{\frac{1}{2}} (\Psi - \Psi_n)\| \\ &= C_{(\text{C.4})} \|\Psi - \Psi_n\|_{(H-b+1)^{1/2}}, \end{aligned} \tag{C.4}$$

and likewise

$$\begin{aligned}\|a(m)(\Psi-\Psi_n)\| &= \|a(m)(H-b+1)^{-\frac{1}{2}}(H-b+1)^{\frac{1}{2}}(\Psi-\Psi_n)\| \\ &\le \|m/\sqrt{\omega}\|_2\,\|H_f^{\frac{1}{2}}(H-b+1)^{-\frac{1}{2}}\|\,\|(H-b+1)^{\frac{1}{2}}(\Psi-\Psi_n)\| \\ &= C_{(\mathrm{C}.4)}\|\Psi-\Psi_n\|_{(H-b+1)^{1/2}}. \end{aligned} \tag{C.5}$$

Second, the integrand in (C.1) is continuous in s and, for sufficiently large n, fulfills an n-independent bound

$$\|e^{isH}\sigma_1 e^{-isH}(\Psi-\Psi_n)\| \le \|\sigma_1\|\,\|\Psi-\Psi_n\| \le 1 \tag{C.6}$$

so dominated convergence can be applied to interchanging the integral and the $n\to\infty$ limit to prove (C.3).

Finally, a stationary phase argument in $\omega(k)=|k|$ as well as the facts that $h\in\mathfrak{h}_0$ and $f\in\mathcal{C}^\infty(\mathbb{R}\setminus\{0\})$, c.f. (1.5), provide the estimate

$$\langle h_s, f\rangle = C\frac{1}{1+|s|^2} \tag{C.7}$$

for all $s\in\mathbb{R}$, thanks to a two-fold partial integration. Hence, me way finally carry out the limit $t\to\pm\infty$ to find

$$a_\pm(h)\Psi = \lim_{t\to\pm\infty} a_t(h)\Psi = a(h)\Psi - ig\int_0^{\pm\infty} ds\,\langle h_s, f\rangle_2 e^{isH}\sigma_1 e^{-isH}\Psi \tag{C.8}$$

as the indefinite integral exists thanks to (C.7) and the continuity of the integrand in s. We omit the proof for the asymptotic creation operator $a_\pm^*$ as the argument is almost the same.

(i) This follows from (ii).

(iii) Next, we calculate

$$\begin{aligned} e^{-isH}a_-(h)^*\psi &= \lim_{t\to-\infty} e^{-isH}e^{itH}a(h_t)^*e^{-itH}\psi \\ &= \lim_{t\to-\infty} e^{i(t-s)H}a(h_{(t-s)+s})^*e^{-i(t-s)H}e^{-isH}\psi \\ &= \lim_{t'\to-\infty} e^{it'H}a(h_{t'+s})^*e^{-it'H}e^{-isH}\psi = a_-(h_s)^*e^{-isH}\psi \end{aligned} \tag{C.9}$$

which proves the pull-through formula in (iii).

(iv) First, for all $t\in\mathbb{R}$ we observe

$$\|a_t(h)\Psi_{\lambda_0}\| = \|e^{itH}a(h_t)e^{-itH}\Psi_{\lambda_0}\| = \|a(h_t)\Psi_{\lambda_0}\| \tag{C.10}$$

due to the ground state property in (1.25). Second, for $\Psi = \Psi_{\lambda_0} \in \mathcal{D}(H) \subset \mathcal{K} \otimes \mathcal{D}(H_f^{1/2})$, we employ the same sequence $(\Psi_n)_{n\in\mathbb{N}}$ as in (ii) to compute

$$\|a(h_t)\Psi_n\|^2 = \sum_{l\in\mathbb{N}} \sqrt{l+1} \int d^3k_1 \dots d^3k_l \left| \int d^3k\, e^{it\omega(k)} \overline{h(k)} \psi_n^{(l+1)}(k, k_1, \dots, k_l) \right|^2, \tag{C.11}$$

where we used the Fock vector representation $\Psi_n = (\psi_n^{(l)})_{l\in\mathbb{N}_0}$. We observe that $\Psi_n \in \mathcal{H}_0$ implies $\psi_n^{(l)} \in \mathcal{K} \otimes C_0^\infty(\mathbb{R}^{3l} \setminus \{0\})$ and, by definition of $\mathcal{H}_0$, c.f. (4.18), there is a constant L such that $\psi_n^{(l)} = 0$ for $l \geq L$. A stationary phase argument in $\omega(k) = |k|$ and a partial integration in k gives

$$\begin{aligned} &\left| \int d^3k\, e^{it\omega(k)} \overline{h(k)} \psi_n^{(l+1)}(k, k_1, \dots, k_l) \right| \\ &\leq \frac{1}{t} \int d^3k\, |k|^{-2} |\partial_{|k|} (|k|^2 \overline{h(|k|, \Sigma)} \psi_n^{(l+1)}(|k|, \Sigma, |k_1|, \Sigma_1, \dots, |k_l|, \Sigma_l))|, \end{aligned} \tag{C.12}$$

where we use spherical coordinates $k = (|k|, \Sigma)$ and $k_i = (|k_i|, \Sigma_i)$. Here, Σ and Σ_i denote the solid angles. Then, we find

$$\begin{aligned} \text{(C.11)} \leq &\frac{1}{t} \sum_{0\leq l<L} \sqrt{l+1} \int d^3k_1 \dots d^3k_l \qquad \text{(C.13)} \\ &\times \left(\int d^3k\, |k|^{-2} |\partial_{|k|} (|k|^2 \overline{h(|k|, \Sigma)} \Psi_n^{(l+1)}(|k|, \Sigma, |k_1|, \Sigma_1, \dots, |k_l|, \Sigma_l)| \right)^2 \end{aligned}$$

which converges to zero for $t \to \pm\infty$. In conclusion, for all $n \in \mathbb{R}$ we have

$$\lim_{t\to\pm\infty} a(h_t)\Psi_n = 0. \tag{C.14}$$

Moreover, there is a t-independent, finite constant $C_{(C.15)}(h)$ such that

$$\begin{aligned} \|a_t(h)(\Psi_{\lambda_0} - \Psi_n)\| &= \|e^{itH} a(h_t) e^{-itH} (\Psi_{\lambda_0} - \Psi_n)\| \\ &= \|a(h_t)(H - b + 1)^{-\frac{1}{2}} e^{-itH} (H - b + 1)^{\frac{1}{2}} (\Psi - \Psi_n)\| \\ &\leq \||h|/\sqrt{\omega}\|_2 \, \|H_f^{\frac{1}{2}} (H - b + 1)^{-\frac{1}{2}}\| \|\Psi - \Psi_n\|_{(H-b+1)^{1/2}} \\ &= C_{(C.15)}(h) \|\Psi - \Psi_n\|_{(H-b+1)^{1/2}} \end{aligned} \tag{C.15}$$

and

$$\begin{aligned} \|a_\pm(h)\Psi_{\lambda_0}\| &\leq \lim_{t\to\pm\infty} (\|a_t(h)(\Psi_{\lambda_0} - \Psi_n)\| + \|a_t(h)\Psi_n\|) \\ &\leq C_{(C.15)}(h) \|\Psi - \Psi_n\|_{(H-b+1)^{1/2}} \end{aligned} \tag{C.16}$$

holds true for all $n \in \mathbb{N}$, where we have use the standard inequalities (A.1), Lemma A.2 and (C.14). Taking the limit $n \to \infty$ proves the claim (iv).

(v) We consider the same sequence $(\Psi_n)_{n\in\mathbb{N}}$ as in (iv) and, for all $n \in \mathbb{N}$, we observe that, by (i) and definition in (1.34), it holds

$$\langle a(h)^*_\pm \Psi_{\lambda_0}, a(l)^*_\pm \Psi_{\lambda_0}\rangle = \lim_{t\to\pm\infty} \langle a(h_t)^* \Psi_{\lambda_0}, a(l_t)^* \Psi_{\lambda_0}\rangle. \tag{C.17}$$

Furthermore, using the CCR in (1.19), we find for all $n \in \mathbb{N}$ that

$$\begin{aligned} &\langle a(h_t)^* \Psi_{\lambda_0}, a(l_t)^* \Psi_n\rangle = \langle \Psi_{\lambda_0}, a(h_t) a(l_t)^* \Psi_n\rangle \\ &= \langle \Psi_{\lambda_0}, (a(l_t)^* a(h_t) + [a(h_t), a(l_t)^*])\, \Psi_n\rangle = \langle a(l_t)\Psi_{\lambda_0}, a(h_t)\Psi_n\rangle + \langle \Psi_{\lambda_0}, \Psi_n\rangle\, \langle h, l\rangle_2 \end{aligned} \tag{C.18}$$

holds. We may control the limit $n \to \infty$ of this identity by

$$\begin{aligned} &|\langle a(h_t)^* \Psi_{\lambda_0}, a(l_t)^* (\Psi_{\lambda_0} - \Psi_n)\rangle| \le \|a(h_t)^* \Psi_{\lambda_0}\|\, \|a(l_t)^*(\Psi_{\lambda_0} - \Psi_n)\| \\ &\le (\|h\|_2 + \|h/\sqrt{\omega}\|_2)\|\Psi_{\lambda_0}\|_{(H-b+1)^{1/2}} (\|l\|_2 + \|l/\sqrt{\omega}\|_2)\|\Psi_{\lambda_0} - \Psi_n\|_{(H-b+1)^{1/2}}, \end{aligned} \tag{C.19}$$

and likewise,

$$\begin{aligned} &|\langle a(l_t) \Psi_{\lambda_0}, a(h_t) (\Psi_{\lambda_0} - \Psi_n)\rangle| \le \|a(l_t) \Psi_{\lambda_0}\|\, \|a(h_t)(\Psi_{\lambda_0} - \Psi_n)\| \\ &\le (\|l\|_2 + \|l/\sqrt{\omega}\|_2)\|\Psi_{\lambda_0}\|_{(H-b+1)^{1/2}} (\|h\|_2 + \|h/\sqrt{\omega}\|_2)\|\Psi_{\lambda_0} - \Psi_n\|_{(H-b+1)^{1/2}}, \end{aligned} \tag{C.20}$$

which are ensured by the standard estimates (A.1) and Lemma A.2. These bounds allow to take the limit $n \to \infty$ of identity (C.19) which yields

$$\langle a(h_t)^* \Psi_{\lambda_0}, a(l_t)^* \Psi_{\lambda_0}\rangle = \langle a(l_t)\Psi_{\lambda_0}, a(h_t)\Psi_{\lambda_0}\rangle + \langle \Psi_{\lambda_0}, \Psi_{\lambda_0}\rangle\, \langle h, l\rangle_2$$

Finally, recalling (C.17) and exploiting (iv) that states $a_\pm(h)\Psi_{\lambda_0} = 0$, we find

$$\langle a(h)^*_\pm \Psi_{\lambda_0}, a(l)^*_\pm \Psi_{\lambda_0}\rangle = \lim_{t\to\pm\infty} \langle a(h_t)^* \Psi_{\lambda_0} a(l_t)^* \Psi_{\lambda_0}\rangle = \langle \Psi_{\lambda_0}, \Psi_{\lambda_0}\rangle\, \langle h, l\rangle_2$$

which concludes the proof of (v).

(vi) Let $t \in \mathbb{R}$. Thanks to the standard estimate (A.1), we find

$$\begin{aligned} &\|a_t(h)(H_f+1)^{-\frac{1}{2}}\| = \|e^{itH} a(h_t)(H-b+1)^{-\frac{1}{2}} e^{-itH} (H-b+1)^{\frac{1}{2}} (H_f+1)^{-\frac{1}{2}}\| \\ &\le \|a(h_t)(H-b+1)^{-\frac{1}{2}}\|\, \|(H-b+1)^{\frac{1}{2}}(H_f+1)^{-\frac{1}{2}}\| \\ &\le \|h/\sqrt{\omega}\|_2\, \|H_f^{\frac{1}{2}}(H-b+1)^{-\frac{1}{2}}\|\, \|(H-b+1)^{\frac{1}{2}}(H_f+1)^{-\frac{1}{2}}\|. \end{aligned} \tag{C.21}$$

Lemma A.2 ensures that the right-hand side of (C.21) is bounded by a finite constant $C(h)$ which depends only on h. This proves the first inequality of (vi). The proof of the second is omitted here as it is almost identical.

□

D The principle term $T_p(h,l)$

In the section, we prove that if $G \equiv G(h,l)$ is positive and strictly positive at $\mathrm{Re}\,\lambda_1 - \lambda_0$ then the absolute of the principal term $T_P(h,l)$ can be bounded by a strictly positive constant times g^2.

Lemma D.1. *Suppose that $G \equiv G(h,l)$ is positive and strictly positive at $\mathrm{Re}\,\lambda_1 - \lambda_0$, then, for small enough g (depending on G), there is a constant $C(h,l) > 0$ (independent of g) such that*

$$|T_P(h,l)| \geq C(h,l)g^2. \tag{D.1}$$

Proof. We set

$$I := \int \mathrm{d}r \frac{G(r)}{(r+\lambda_0 - \mathrm{Re}\,\lambda_1 - ig^2E_1)(r - \lambda_0 + \overline{\lambda_1})}, \tag{D.2}$$

and take small enough g. Recalling (2.4), we observe that

$$T_P(h,l) = g^2 E_1 M I. \tag{D.3}$$

We recall from the discussion below Definition 2.1 that $E_1 = E_I + g^a\Delta$, where $a > 0$, $\Delta \equiv \Delta(g)$ is uniformly bounded and E_I is a strictly negative constant that does not depend on g, see (3.11). Additionally, it follows from (3.25) together with $\|\varphi_0 \otimes \Omega\| = 1$ that $\|\Psi_{\lambda_0}\| \geq C > 0$, for some constant C that does not depend on g. Moreover, we conclude from (3.28) that $\mathrm{Re}\,\lambda_1 - \lambda_0 \geq C > 0$ for some constant C (independent of g). Consequently, (2.6) guarantees that there is a constant C (independent of g) such that $|M| \geq C > 0$.

This together with (D.3) implies that it suffices to show that there is a constant $C(h,l) > 0$ such that

$$|I| \geq C(h,l), \tag{D.4}$$

in order to conclude (D.1).

For $\alpha \equiv \alpha_g := \mathrm{Re}\,\lambda_1 - \lambda_0$ and recalling (1.2), we observe

$$I = \int \mathrm{d}r \frac{G(r)}{(r-\alpha-ig^2E_1)(r+\alpha-ig^2E_1)} = \int \mathrm{d}r \frac{G(r)\,(r^2-\alpha^2-g^4E_1^2+2ig^2E_1 r)}{(r^2-\alpha^2-g^4E_1^2)^2+4g^4E_1^2r^2}. \tag{D.5}$$

Let $c > 0$ be such that G is supported in the complement of the ball or radius c and center 0. Then, we have

$$|\,\mathrm{Im}(I)| \geq |E_1| \int \mathrm{d}r G(r) \frac{2g^2 r}{(r^2-\alpha^2-g^4E_1^2)^2+4g^4E_1^2c^2}. \tag{D.6}$$

Substituting $s = r^2$, yields

$$|\operatorname{Im}(I)| \geq |E_1| \int \mathrm{d}s G(\sqrt{s}) \frac{g^2}{(s - \alpha^2 - g^4 E_1^2)^2 + 4g^4 E_1^2 c^2}. \tag{D.7}$$

Since $G(\alpha) \neq 0$, then for small enough g there is a constant r_0, that does not depend on g and a constant $C > 0$ (independent of g) such that $G(\sqrt{s}) \geq C$, for every $s \in [\alpha^2 + g^4 E_1^2 - r_0, -\alpha^2 - g^4 E_1^2 + r_0]$. We apply the change of variables $u = s - \alpha^2 - g^4 E_1^2$ and obtain

$$|\operatorname{Im}(I)| \geq C|E_1| \int_{-r_0}^{r_0} \mathrm{d}s \frac{g^2}{s^2 + 4g^4 E_1^2 c^2}. \tag{D.8}$$

Finally, we change to the variable $\tau = s/g^2$ to obtain:

$$|\operatorname{Im}(I)| \geq C|E_1| \int_{-r_0/g^2}^{r_0/g^2} \mathrm{d}\tau \frac{1}{\tau^2 + 4E_1^2 c^2} \geq C|E_1|, \tag{D.9}$$

for small enough g (depending on G). □

List of main notations

In this section we provide of list of main notations and their place of definition used in this

Symbol	Place of definition
E_1	below (1.1)
H_0, K, H_f	(1.3)
e_0, e_1	below (1.3)
ω	below (1.3)
V, σ_1	(1.4)
f	(1.5)
μ	(1.6)
H	(1.7)
g	below (1.7), see also Definition 3.1, (3.31) and Definition 4.3 in [14]
$\mathcal{H}$, $\mathcal{K}$	(1.8)
$\mathcal{F}[\mathfrak{h}]$, $\mathfrak{h}$	(1.9)
$\odot$	below (1.9)
Ω	(1.10)
$\mathcal{F}_0$	(1.11)
$S(\mathbb{R}^3, \mathbb{C})$	below (1.11)
$a(h)$	(1.12)
$a(h)^*$	(1.13)
$a(k)$	(1.14)
$a(k)^*$	(1.15)

φ_0, φ_1	(1.20)
$\mathcal{D}(\bullet)$	below (1.20)
$\sigma(\bullet)$	below (1.20)
θ, u_θ, U_θ	Definition 1.3
H^θ	(1.27)
H_f^θ, V^θ	(1.28)
ω^θ, f^θ	(1.29)
$D(\bullet, \bullet)$	(1.30)
λ_0, λ_1	below Lemma 1.5
Ψ_{λ_0}, Ψ_{λ_1}	(1.32)
$\mathfrak{h}_0$	(1.33)
$a_\pm(h)$	(1.34)
$a_\pm(h)^*$	below (1.34)
$\mathcal{K}^\pm$, $\mathcal{H}^\pm$	(1.35)
$\Omega_\pm$	(1.36)
$S(h,l)$	(1.37)
$T(h,l)$	(1.38)
G	(2.1)
ι	(3.31) and (3.32)
$T_P(h,l)$	(2.4)
$R(h,l)$	(2.5)
ν	(3.1)
$\mathcal{S}$	(3.2)
$\boldsymbol{\nu}$	below (3.2)
ρ_0, ρ	(3.3) and (3.31)
A	(3.4)
$B_0^{(1)}$, $B_1^{(1)}$	(3.8)
$\mathcal{C}_m(z)$	(3.9)
E_I	(3.11)
ρ_n	(3.14)
$H^{(n),\theta}$	(3.15)
$H_f^{(n),\theta}$	(3.16)
$V^{(n),\theta}$	(3.17)
$\mathcal{H}^{(n)}$, $\mathfrak{h}^{(n)}$	(3.19)
$\tilde{H}^{(n)}$	(3.20)
$\mathfrak{h}^{(n,\infty)}$	(3.21)
$\Omega^{(n,\infty)}$, $P_{\Omega^{(n,\infty)}}$	below (3.21)
$\lambda_0^{(n)}$, $\lambda_1^{(n)}$	above (3.22)
$P_0^{(n),\theta}$, $P_1^{(n),\theta}$	(3.22)
P_0^θ, P_1^θ	(3.23)
$\boldsymbol{C}$	below (3.32)
$\mathfrak{F}$, $\mathfrak{F}^{-1}$	Definition 4.2

W	(4.9)
Σ	below (4.9)
$\mathcal{H}_0$	(4.18)
$\mathcal{F}_{\text{fin}}[\mathfrak{h}_0]$	(4.19)
$\|\bullet\|_\bullet$	below (4.19)
$\Gamma(\epsilon, R)$	above (4.30)
$\Gamma_-(\epsilon, R)$	(4.30)
$\Gamma_d(R)$	(4.30)
$\Gamma_c(\epsilon)$	(4.30)
ϵ_n	(4.48)
$R_1(q, Q)$	(4.79)
$P_1(q, Q)$	(4.86)
$\tilde{P}_1(q, Q)$	(4.96)

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One-Boson Scattering Processes in the Massless Spin-Boson Model – A Non-Perturbative Formula

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Abstract

In scattering experiments, physicists observe so-called resonances as peaks at certain energy values in the measured scattering cross sections per solid angle. These peaks are usually associate with certain scattering processes, e.g., emission, absorption, or excitation of certain particles and systems. On the other hand, mathematicians define resonances as poles of an analytic continuation of the resolvent operator through complex dilations. A major challenge is to relate these scattering and resonance theoretical notions, e.g., to prove that the poles of the resolvent operator induce the above mentioned peaks in the scattering matrix. In the case of quantum mechanics, this problem was addressed in numerous works that culminated in Simon's seminal paper [33] in which a general solution was presented for a large class of pair potentials. However, in quantum field theory the analogous problem has been open for several decades despite the fact that scattering and resonance theories have been well-developed for many models. In certain regimes these models describe very fundamental phenomena, such as emission and absorption of photons by atoms, from which quantum mechanics originated. In this work we present a first non-perturbative formula that relates the scattering matrix to the resolvent operator in the massless Spin-Boson model. This result can be seen as a major progress compared to our previous works [14] and [12] in which we only managed to derive a perturbative formula.

Keywords: Scattering Theory; Resonance Theory; Spin-Boson Model; Multiscale Analysis

1 Introduction

In this work we analyze the massless Spin-Boson model which describes a two-level atom interacting with a second-quantized massless scalar field. We derive a non-perturbative expression of the scattering matrix in terms of the resolvent operator for one-boson

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processes, and thus, prove an analogous result that was obtained by Simon in [33] for the N-body Schrödinger operator in this particular model of quantum field theory. More precisely, we show that the pole of a meromorphic continuation of the integral kernel of the scattering matrix is located precisely at the resonance energy. The objective in this result is to contribute to the understanding of the relation between resonance and scattering theory. In our previous works [14] and [12], we were already able to derive perturbative results of this kind in case of the massless and massive Spin-Boson models, respectively. However, both results are only given in leading order with respect to the coupling constant. The present work can be seen as a major improvement of these pertubative results because it provides a closed and non-perturbative formula that connects the integral kernel of the scattering matrix elements for one-boson processes in terms of the dilated resolvent.

Our results are based on the well-established fields of scattering and resonance theories and the numerous works in the classical literature of which we want to give a short overview here. Resonance theory, in the realm of quantum field theory, has been developed in a variety of models; see, e.g., [6, 8, 7, 4, 9, 1, 26, 27, 32, 21, 15, 28, 29, 2, 3, 13]. In these works, several techniques have been invented for massless models of quantum field theory in order to cope with the absence of a spectral gap. Scattering theory has also been developed in various models of quantum field theory (see, e.g., [23, 22, 16, 25, 24]) and in particular in the massless Spin-Boson model (see, e.g., [17, 18, 19, 20, 10, 14, 12]). In [5], a rigorous mathematical justification of Bohr's frequency condition was derived using an expansion of the scattering amplitudes with respect to powers of the fine structure constant for the Pauli-Fierz model. In [10], the photoelectric effect has been studied for a model of an atom with a single bound state, coupled to the quantized electromagnetic field. A related problem is studying the time-evolution in models of quantum field theory. In [11], this question has been addressed for the Spin-Boson model. A good overview has been given in [34].

This work heavily relies on the multiscale analysis carried out in [13] as well as on the results in [14]. We de not repeat any of those proofs here but rather focus on the core argument to derive the above mentioned non-perturbative formula. However, throughout this work, we give precise references to any of the utilized theorems and lemmas which also contain all technical details.

1.1 The Spin-Boson model

In this section we introduce the considered model and state preliminary definitions, well-known tools and facts from which we start our analysis. If the reader is already familiar with the introductory Sections 1.1 until 1.3 of [13], these subsections can be skipped.

The non-interacting Spin-Boson Hamiltonian is defined as

$$H_0 := K + H_f, \qquad K := \begin{pmatrix} e_1 & 0 \\ 0 & e_0 \end{pmatrix}, \qquad H_f := \int \mathrm{d}^3k\, \omega(k) a(k)^* a(k). \tag{1.1}$$

We regard K as an idealized free Hamiltonian of a two-level atom. As already stated in the introduction, its two energy levels are denoted by the real numbers $0 = e_0 < e_1$.

Furthermore, H_f denotes the free Hamiltonian of a massless scalar field having dispersion relation $\omega(k) = |k|$, and a, a^* are the annihilation and creation operators on the standard Fock space. For a precise defintion we refer to [14, Section 1.1]. Below, we sometimes call K the atomic part, and H_f the free field part of the Hamiltonian. The sum of the free two-level atom Hamiltonian K and the free field Hamiltonian H_f is named "free Hamiltonian" H_0. The interaction term reads

$$V := \sigma_1 \otimes (a(f) + a(f)^*), \qquad \sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1.2}$$

where the boson form factor is given by

$$f : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}, \qquad k \mapsto e^{-\frac{k^2}{\Lambda^2}} |k|^{-\frac{1}{2}+\mu}. \tag{1.3}$$

In our case, the gaussian factor in (1.3) acts as an ultraviolet cut-off for $\Lambda > 0$ being the ultraviolet cut-off parameter and in addition the fixed number

$$\mu \in (0, 1/2) \tag{1.4}$$

yields a regularization of the infrared singularity at $k = 0$ which is a technical assumption chosen such that we can apply the results obtained in [13]. Note that the form factor f only depends on the radial part of k. To emphasize this, we often write $f(k) \equiv f(|k|)$.

The full Spin-Boson Hamiltonian is then defined as

$$H := H_0 + gV \tag{1.5}$$

for some coupling constant $g > 0$ on the Hilbert space

$$\mathcal{H} := \mathcal{K} \otimes \mathcal{F}[\mathfrak{h}], \qquad \mathcal{K} := \mathbb{C}^2, \tag{1.6}$$

where

$$\mathcal{F}[\mathfrak{h}] := \bigoplus_{n=0}^{\infty} \mathcal{F}_n[\mathfrak{h}], \qquad \mathcal{F}_n[\mathfrak{h}] := \mathfrak{h}^{\odot n}, \qquad \mathfrak{h} := L^2(\mathbb{R}^3, \mathbb{C}) \tag{1.7}$$

denotes the standard bosonic Fock space, and superscript $\odot n$ denotes the n-th symmetric tensor product, where by convention $\mathfrak{h}^{\odot 0} \equiv \mathbb{C}$. Note that we identify $K \equiv K \otimes 1_{\mathcal{F}[\mathfrak{h}]}$ and $H_f \equiv 1_{\mathcal{K}} \otimes H_f$ in our notation (see Notation 1.1 below).

An element $\Psi \in \mathcal{F}[\mathfrak{h}]$ can be represented as a sequence $(\psi^{(n)})_{n\in\mathbb{N}_0}$ of wave functions $\psi^{(n)} \in \mathfrak{h}^{\odot n}$. The state Ψ with $\psi^{(0)} = 1$ and $\psi^{(n)} = 0$ for all $n \geq 1$ is called the vacuum and is denoted by

$$\Omega := (1, 0, 0, \dots) \in \mathcal{F}[\mathfrak{h}]. \tag{1.8}$$

Note that a and a^* fulfill the canonical commutation relations:

$$\forall h, l \in \mathfrak{h}, \qquad [a(h), a^*(l)] = \langle h, l \rangle_2, \qquad [a(h), a(l)] = 0, \qquad [a^*(h), a^*(l)] = 0. \tag{1.9}$$

Let us recall some well-known facts about the introduced model. It is well-known that K, H_f, H_0, H are self-adjoint and bounded below on the domains $\mathcal{K}, \mathcal{D}(H_f), \mathcal{D}(H_0), \mathcal{D}(H)$, respectively (see, e.g., [14, Proposition 1.1]). The spectrum of K consists of two eigenvalues e_0 and e_1 and the corresponding eigenvectors are

$$\varphi_0 = (0,1)^T \qquad \text{and} \qquad \varphi_1 = (1,0)^T \qquad \text{with} \qquad K\varphi_i = e_i\varphi_i, \quad i = 0,1. \tag{1.10}$$

The spectrum of H_f is $\sigma(H_f) = [0,\infty)$ and it is absolutely continuous (see [31]). Consequently, the spectrum of H_0 is given by $\sigma(H_0) = [e_0,\infty)$, and e_0, e_1 are eigenvalues embedded in the absolutely continuous part of the spectrum of H_0 (see [30]).

Notation 1.1. *In this work we omit spelling out identity operators whenever unambiguous. For every vector spaces V_1, V_2 and operators A_1 and A_2 defined on V_1 and V_2, respectively, we identify*

$$A_1 \equiv A_1 \otimes \mathbb{1}_{V_2}, \qquad\qquad A_2 \equiv \mathbb{1}_{V_1} \otimes A_2. \tag{1.11}$$

In order to simplify our notation further, and whenever unambiguous, we do not utilize specific notations for every inner product or norm that we employ.

1.2 Complex dilation

In this section we shortly introduce the method of complex dilation which is a key tool for proving our main result. For a more detailed presentation we refer to [14, Section 1.2]. We start by defining a family of unitary operators on $\mathcal{H}$ indexed by $\theta \in \mathbb{R}$.

Definition 1.2. *For $\theta \in \mathbb{R}$, we define the unitary transformation*

$$u_\theta : \mathfrak{h} \to \mathfrak{h}, \qquad \psi(k) \mapsto e^{-\frac{3\theta}{2}}\psi(e^{-\theta}k). \tag{1.12}$$

Similarly, we define its canonical lift $U_\theta : \mathcal{F}[\mathfrak{h}] \to \mathcal{F}[\mathfrak{h}]$ by the lift condition $U_\theta a(h)^* U_\theta^{-1} = a(u_\theta h)^*$, $h \in \mathfrak{h}$, and $U_\theta\Omega = \Omega$. This defines U_θ uniquely. With slight abuse of notation, we also denote $\mathbb{1}_{\mathcal{K}} \otimes U_\theta$ on $\mathcal{H}$ by the same symbol U_θ.

We say that $\Psi \in \mathcal{F}[\mathfrak{h}]$ is an analytic vector if the map $\theta \mapsto \Psi^\theta := U_\theta\Psi$ has an analytic continuation from an open connected set in the real line to a (connected) domain in the complex plane.

We define the family of transformed Hamiltonians, for $\theta \in \mathbb{R}$,

$$H^\theta := U_\theta H U_\theta^{-1} = K + H_f^\theta + gV^\theta, \tag{1.13}$$

where

$$H_f^\theta := \int \mathrm{d}^3k\, \omega^\theta(k) a^*(k) a(k), \qquad V^\theta := \sigma_1 \otimes \left(a(f^{\overline{\theta}}) + a(f^\theta)^* \right) \tag{1.14}$$

and

$$\omega^\theta(k) := e^{-\theta}|k|, \qquad f^\theta : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}, \quad k \mapsto e^{-\theta(1+\mu)} e^{-e^{2\theta}\frac{k^2}{\Lambda^2}} |k|^{-\frac{1}{2}+\mu}. \tag{1.15}$$

Eqs. (1.15), (1.14) and the right-hand side of (1.13) can be defined for complex θ (see, e.g., [14, Lemma 1.4]). For sufficiently small coupling constants and $\theta \in \mathcal{S}$, where $\mathcal{S}$ is a suitable subset of the complex plane defined in (A.3) below, it has been shown that H^θ has two non-degenerate eigenvalues λ_0^θ and λ_1^θ with corresponding rank one projectors denoted by P_0^θ and P_1^θ, respectively; see, e.g., [13, Proposition 2.1]. Note that there the θ-dependence was omitted in the notation. For convenience of the reader, we make it explicit in this paper. The corresponding dilated eigenstates can, therefore, be written as

$$\Psi_{\lambda_i}^\theta := P_i^\theta \varphi_i \otimes \Omega, \qquad i = 0, 1. \tag{1.16}$$

where the eigenstates φ_i of the free atomic system are given in (1.10), and Ω is the bosonic vacuum defined in (1.8). In our notation $\Psi_{\lambda_i}^\theta$ is not necessarily normalized. We know from [13, Theorem 2.3] that the eigenvalues λ_i^θ are independent of θ as long as θ belongs to $\mathcal{S}$ and, therefore, we suppress it in our notation writing $\lambda_i^\theta \equiv \lambda_i$. In the case that $i = 1$, it is necessary that 0 does not belong to $\mathcal{S}$. This is not required if $i = 0$, and in this situation we extend the set $\mathcal{S}$, with the same notation, to an open connected set that contains 0 (see [13, Definition 1.4 and Remark 2.4]). From this, it is easy to see that $\Psi_{\lambda_0}^{\theta=0} = \Psi_{\lambda_0}$ - as introduced above.

1.3 Scattering theory

Finally, we give a short review of scattering theory which is necessary to state the main result in Section 2. For a more detailed introduction we refer to [14, Section 1.3].

Definition 1.3 (Basic components of scattering theory)**.** *We denote by $\mathfrak{h}_0$ the set of smooth complex-valued functions on $\mathbb{R}^3$ with compact support contained in $\mathbb{R}^3 \setminus \{0\}$.*

We define the following objects:

(i) For $h \in \mathfrak{h}_0$ and $\Psi \in \mathcal{K} \otimes \mathcal{D}(H_f^{1/2})$, the asymptotic annihilation operators

$$a_\pm(h)\Psi := \lim_{t\to\pm\infty} a_t(h)\Psi, \quad a_t(h) := e^{itH} a(h_t) e^{-itH}, \quad h_t(k) := h(k)e^{-it\omega(k)}. \tag{1.17}$$

Moreover, we define the asymptotic creation operators $a_\pm^*(h)$ as the respective adjoints.

(ii) The asymptotic Hilbert spaces

$$\mathcal{H}^\pm := \mathcal{K}^\pm \otimes \mathcal{F}[\mathfrak{h}] \quad \text{where} \quad \mathcal{K}^\pm := \{\Psi \in \mathcal{H} : a_\pm(h)\Psi = 0 \ \ \forall h \in \mathfrak{h}_0\}. \tag{1.18}$$

(iii) The wave operators

$$\Omega_\pm : \mathcal{H}^\pm \to \mathcal{H} \tag{1.19}$$
$$\Omega_\pm \Psi \otimes a^*(h_1)...a^*(h_n)\Omega := a_\pm^*(h_1)...a_\pm^*(h_n)\Psi, \quad h_1, ..., h_n \in \mathfrak{h}_0, \quad \Psi \in \mathcal{K}^\pm.$$

(iv) The scattering operator $S := \Omega_+^* \Omega_-$.

The limit operators $a_\pm$ and $a_\pm^*$ are called asymptotic outgoing/ingoing annihilation and creation operators. The existence of the limits in (1.17) and their properties (for example that $\Psi_{\lambda_0} \in \mathcal{K}^\pm$) are well-known (see e.g. [23, 22, 16, 25, 24, 17, 18, 19, 20, 10]). For a detailed proof we refer to [14, Lemma 4.1]. We can thus define the following scattering matrix coefficients for one-boson processes:

$$S(h,l) = \|\Psi_{\lambda_0}\|^{-2} \left\langle a_+^*(h)\Psi_{\lambda_0}, a_-^*(l)\Psi_{\lambda_0} \right\rangle, \qquad \forall h,l \in \mathfrak{h}_0, \tag{1.20}$$

where the factor $\|\Psi_{\lambda_0}\|^{-2}$ appears due to the fact that, as already mentioned above, in our notation, the ground state Ψ_{λ_0} is not necessarily normalized. In addition, it will be convenient to work with the corresponding transition matrix coefficients for one-boson processes given by

$$T(h,l) = S(h,l) - \langle h,l \rangle_2 \qquad \forall h,l \in \mathfrak{h}_0. \tag{1.21}$$

Physically, these matrix coefficients may be interpreted as transition amplitudes of the scattering process in which an incoming boson with wave function l is scattered at the two-level atom into an outgoing boson with wave function h. Notice that the transition matrix coefficients of multi-boson processes can be defined likewise but in this work we focus on one-boson processes only.

2 Main results

We are now able to state our main result which provides the precise relation between the one-boson transition matrix elements and the resolvent of the complex dilated Hamiltonian. The corresponding proofs will be provided in Section 3.

Theorem 2.1 (Scattering Formula)**.** *For sufficiently small g, θ in a suitable subset $\mathcal{S} \subset \mathbb{C}$ (see* (A.3)*), and for all $h, l \in \mathfrak{h}_0$, the transition matrix coefficients for one-boson processes are given by*

$$T(h,l) = \int \mathrm{d}^3k \mathrm{d}^3k' \, \overline{h(k)} l(k') \delta(\omega(k) - \omega(k')) T(k,k') \tag{2.1}$$

where

$$\begin{aligned} T(k,k') = -2\pi i g^2 f(k) f(k') \|\Psi_{\lambda_0}\|^{-2} \Bigg(&\left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - \lambda_0 - |k'|\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle \\ &+ \left\langle \sigma_1 \Psi_{\lambda_0}^{\theta}, \left(H^{\overline{\theta}} - \lambda_0 + |k'|\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}} \right\rangle \Bigg). \end{aligned} \tag{2.2}$$

The integral with respect to the Dirac's delta distribution distribution δ in (2.1) is to be understood as

$$T(h,l) = \int_0^\infty \mathrm{d}|k| \int \mathrm{d}\Sigma \mathrm{d}\Sigma' \, \overline{h(|k|,\Sigma)} l(|k|,\Sigma') T(|k|,\Sigma,|k|,\Sigma'), \tag{2.3}$$

where we have introduced spherical coordinates $k = (|k|, \Sigma)$ with Σ being the solid angle and $T(k,k') \equiv T(|k|, \Sigma, |k|, \Sigma')$ is given by (2.2). Notice that (2.2) is not defined for $k = 0$ or $k' = 0$. However, since we take $h, l \in \mathfrak{h}_0$, the expression (2.1) is well-defined. Representing such matrix elements in terms of a distribution kernel is convenient (in our case, e.g., it makes the energy conservation apparent) and also frequently used in the literature. In particular, similar distribution kernels in a closely related model have been studied in [10, 14].

Remark 2.2. *In a similar vein as in [14], we can apply perturbation theory together with the spectral properties obtained in [13] in order to deduce a result as [14, Theorem 2.2] from Theorem 2.1 above. Then, one can again see the Lorentzian shape of the integral kernel which was explained in detail in [14].*

In the remainder of this work we denote by C any generic (indeterminate), positive constant that might change from line to line but does not depend on the coupling constant.

3 Proof of the main result

In the remainder of this work we provide the proof of Theorem 2.1. This section has three parts: In Section 3.1, we recall a preliminary formula for the scattering matrix coefficients; c.f. Theorem 3.1 below, which was proven in [14, Theorem 4.3]. This formula together with several technical ingredients provided in Section 3.2 and 3.3 pave the way for the proof of our main result given in Section 3.4.

3.1 Preliminary scattering formula

The following theorem has been proven in [14, Theorem 4.3].

Theorem 3.1 (Preliminary Scattering Formula)**.** *For $h, l \in \mathfrak{h}_0$, the transition matrix coefficient for one-boson processes $T(h,l)$ defined in* (1.21) *fulfills*

$$T(h,l) = \lim_{t\to-\infty} \int \mathrm{d}^3k \mathrm{d}^3k' \, \overline{h(k)} l(k') \delta(\omega(k) - \omega(k')) T_t(k,k') \tag{3.1}$$

for the integral kernel

$$T_t(k,k') = -2\pi i g f(k) \left\| \Psi_{\lambda_0} \right\|^{-2} \langle \sigma_1 \Psi_{\lambda_0}, a_t(k')^* \Psi_{\lambda_0} \rangle. \tag{3.2}$$

The integral in (3.1) is to be understood as

$$T(h,l) = -2\pi i g \left\| \Psi_{\lambda_0} \right\|^{-2} \left\langle \sigma_1 \Psi_{\lambda_0}, a_-(W)^* \Psi_{\lambda_0} \right\rangle \tag{3.3}$$

for $W \in \mathfrak{h}_0$ given by

$$\mathbb{R}^3 \ni k \mapsto W(k) := |k|^2 l(k) \int \mathrm{d}\Sigma \, \overline{h(|k|, \Sigma)} f(|k|, \Sigma) \tag{3.4}$$

using spherical coordinates $k = (|k|, \Sigma)$ with Σ being the solid angle.

3.2 General ingredients for the proof of the main theorem

Here, we state some general results which are applied in the proof of our main result, see Section 3.4. Most of the statements in this section are formulated without motivation. However, their importance becomes clear later in Section 3.4. At first, we recall a representation formula of the time-evolution operator similar to the Laplace transform representation (see, e.g., [2]). This formula is an important ingredient for the proof of the perturbative scattering formula in [14] and it plays a relevant role in the present work. For a detailed proof we refer to [14, Lemma 4.5].

Lemma 3.2. *For $\epsilon > 0$, $\nu = \operatorname{Im}\theta > 0$ and sufficiently large $R > 0$, we consider the concatenated contour $\Gamma(\epsilon, R) := \Gamma_-(\epsilon, R) \cup \Gamma_c(\epsilon) \cup \Gamma_d(R)$ (see Figure 1), where*

$$\begin{aligned}\Gamma_-(\epsilon, R) &:= [-R, \lambda_0 - \epsilon] \cup [\lambda_0 + \epsilon, R],\\ \Gamma_d(R) &:= \left\{-R - ue^{i\frac{\nu}{4}} : u \geq 0\right\} \cup \left\{R + ue^{-i\frac{\nu}{4}} : u \geq 0\right\},\\ \Gamma_c(\epsilon) &:= \left\{\lambda_0 - \epsilon e^{-it} : t \in [0, \pi]\right\}. \end{aligned} \tag{3.5}$$

The orientations of the contours in (3.5) are given by the arrows depicted in Figure 1. Then, for all analytic vectors $\phi, \psi \in \mathcal{H}$ (analytic in a – connected – domain containing 0) and $t > 0$, the following identity holds true:

$$\left\langle \phi, e^{-itH}\psi \right\rangle = \frac{1}{2\pi i} \int_{\Gamma(\epsilon,R)} \mathrm{d}z\, e^{-itz} \left\langle \psi^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \phi^\theta \right\rangle. \tag{3.6}$$

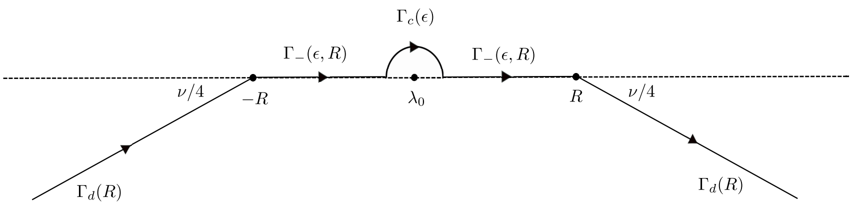

Figure 1: An illustration of the contour $\Gamma(\epsilon, R) := \Gamma_-(\epsilon, R) \cup \Gamma_c(\epsilon) \cup \Gamma_d(R)$.

In this paper we use a non-standard definition of the Fourier transform and its inverse:

$$\mathfrak{F}[u](x) := \int_{\mathbb{R}} \mathrm{d}s\, u(s)e^{-isx}, \qquad \mathfrak{F}^{-1}[u](x) := (2\pi)^{-1} \int_{\mathbb{R}} \mathrm{d}s\, u(s)e^{isx}, \tag{3.7}$$

where $u \in S(\mathbb{R}, \mathbb{C})$ (the Schwartz space). We utilize the same symbols (and names) for their dual transformation on $S'(\mathbb{R}, \mathbb{C})$ (the space of tempered distributions). We identify, as usual, functions $f \in L^p(\mathbb{R}, \mathbb{C})$ (for some $p \in [1, \infty]$) with their induced tempered distributions in $S'(\mathbb{R}, \mathbb{C})$ ($f(u) = \int uf$) and, similarly, we identify functions $f \in L^1_{\mathrm{loc}}(\mathbb{R}, \mathbb{C})$ with their induced distributions in $\left(C_0^\infty(\mathbb{R}, \mathbb{C})\right)'$. We denote by Θ the

Heaviside function (or distribution, or tempered distribution) and by δ the Dirac δ distribution (or tempered distribution):

$$\Theta(x) := \begin{cases} 1 & \text{for} \quad x \geq 0 \\ 0 & \text{for} \quad x < 0 \end{cases}, \qquad \Theta(u) = \int_0^\infty u(x)dx, \qquad \delta(u) = u(0), \tag{3.8}$$

for $u \in S'(\mathbb{R}, \mathbb{C})$.

Lemma 3.3. *We denote by* $(PV(1/\bullet)) \in S'(\mathbb{R}, \mathbb{C})$ *the principal value:*

$$(PV(1/\bullet))(\varphi) \equiv PV \int_{\mathbb{R}} \mathrm{d}s \, \frac{1}{s} \varphi(s) := \lim_{\eta \to 0^+} \int_{\mathbb{R} \setminus [-\eta, \eta]} \mathrm{d}s \, \frac{1}{s} \varphi(s) \qquad \forall \varphi \in S(\mathbb{R}, \mathbb{C}). \tag{3.9}$$

It follows that

$$\mathfrak{F}[\Theta] = \pi\delta - iPV(1/\bullet). \tag{3.10}$$

The above result can be shown using methods from standard distribution theory. However, for the sake of completeness, we present a proof in Appendix B.

3.3 Key estimates

In this section we establish two key estimates for the proof of the main theorem. We point out to the reader that they strongly rely on the results obtained in [13]. However, for simplicity and due to the fact that the important features have already been studied in [14, Section 4.3], we omit the details related to the multiscale analysis carried out in [13], and give precise references instead.

Definition 3.4. *(c.f. [14, Definition 4.6]) For every fixed numbers* $\rho_0 \in (0,1)$ *and* $\rho \in (0, \min(1, e_1/4))$ *satisfying* (A.13)*, we define the sequences*

$$\rho_n := \rho_0 \rho^n, \qquad \epsilon_n := 20\rho_n^{1+\mu/4}, \qquad \forall n \in \mathbb{N}. \tag{3.11}$$

Lemma 3.5. *Set* $G \in \mathcal{C}_c^\infty(\mathbb{R} \setminus \{0\}, \mathbb{C})$*,* $n \in \mathbb{N}$ *large enough and* $\eta > 0$ *small enough such that* $G(x) = 0$*, for* $|x| \leq 2(\epsilon_n + \eta)$*. We define*

$$T_{n,R}(\eta) := \int_{\Gamma_-(\epsilon_n, R)} \mathrm{d}z \, u(z) \int_{\mathbb{R}} \mathrm{d}r \, \frac{G(r)}{z - \lambda_0 - r} \left(1 - \mathbb{1}_{I_\eta(z)}(r)\right), \tag{3.12}$$

where $\mathbb{1}_{I_\eta(z)}$ *is the characteristic function of the set* $I_\eta(z) := [z - \lambda_0 - \eta, z - \lambda_0 + \eta]$*,* $\Gamma_-(\epsilon_n, R)$ *is defined in* (3.5) *and*

$$u : \overline{\mathbb{C}^+} \setminus \{\lambda_0\} \to \mathbb{C}, \qquad z \mapsto u(z) := \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle. \tag{3.13}$$

Then, for sufficiently large R *(independent of* n *and* $\theta \in \mathcal{S}$*), there is a constant* C *(that does not depend on* n*, but it does depend on* G*,* θ*,* e_1 *and* m *– see above* (A.9) *below) such that*

$$\left| T_{n,R}(\eta) - \pi i \int_{\mathbb{R}} \mathrm{d}r \, G(r) u(r + \lambda_0) \right| \leq C \left(\rho_n^{\mu/8} + \frac{1}{R} + \eta \right). \tag{3.14}$$

Proof. The integrand in (3.12) is absolutely integrable with respect to the variables z and r because the singularity is cut off by the characteristic function. We apply Fubini's theorem to get

$$T_{n,R}(\eta) = \int_{\mathbb{R}} \mathrm{d}r\, G(r) \int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\, u(z) \frac{1}{z-\lambda_0-r} \Big(1 - \mathbb{1}_{I_\eta(z)}(r)\Big) . \tag{3.15}$$

Next, we analyze the inner integral above for r in the support of G. Set $\Gamma_{(r)}$ the half circle in the upper half complex plane with center $r+\lambda_0$ and radius η. Moreover, set $\Gamma^{(R)}$ the half-circle in the upper half complex plane with center 0 and radius R. As

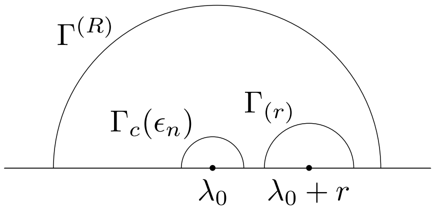

Figure 2: An illustration of the half circles $\Gamma_c(\epsilon_n)$ and $\Gamma_{(r)}$.

despicted in Figure 2, the two half circles $\Gamma_c(\epsilon_n)$ and $\Gamma_{(r)}$ do not intersect each other for all r in the support of G. This is a consequence of the assumption that the support of G does not intersect with the interval $(-2(\epsilon_n+\eta), 2(\epsilon_n+\eta))$. Moreover, we find that both half circles $\Gamma_c(\epsilon_n)$ and $\Gamma_{(r)}$ are contained in $\Gamma^{(R)}$ for large enough R (the value of R can be chosen uniformly with respect to n and $\theta \in \mathcal{S}$, but it depends on the support of G independent of n and $\theta \in \mathcal{S}$, but dependent on the support of G).

Note that there is a constant C (that depends on the support of G, but not on n, $\theta \in S$, ρ and ρ_0) such that (see (A.12))

$$\Big| u(z) \frac{1}{z-\lambda_0-r} \Big| \le \frac{C}{R^2}, \qquad \forall z \in \Gamma^{(R)}. \tag{3.16}$$

Moreover, there is a constant C (that depends on the support of G, but not on n, ρ and ρ_0) such that (see (A.15))

$$\Big| u(z) \frac{1}{z-\lambda_0-r} \Big| \le C\boldsymbol{C}^{n+1} \frac{1}{\rho_n}, \qquad \forall z \in \Gamma_c(\epsilon_n), \tag{3.17}$$

where $\rho_n = \rho_0\rho^n$ and $\rho_0 > 0$, $0 < \rho < 1$ and $\boldsymbol{C} > 0$ are specific numbers defined in [13, Definition 4.1 and 4.2] and fulfilling (A.13). We know from (A.10) and (A.11) that the only spectral point of H^θ in $\overline{\mathbb{C}^+}$ is λ_0. Hence, there is a constant C (that depends on the support of G, but not on n) such that

$$|u(z) - u(\lambda_0 + r)| \le C\eta, \qquad \forall z \in \Gamma_{(r)}. \tag{3.18}$$

A direct calculation shows that

$$\int_{\Gamma_{(r)}} dz\, u(\lambda_0 + r)\, \frac{1}{z - \lambda_0 - r} = -u(\lambda_0 + r) i\pi. \tag{3.19}$$

We choose the contour which follows the following set of points $\Big(\Gamma_-(\epsilon_n, R) \setminus (r + \lambda_0 - \eta, r + \lambda_0 + \eta)\Big) \cup \Gamma^{(R)} \cup \Gamma(r) \cup \Gamma_c(\epsilon_n)$ along the mathematical positive orientation. This is a closed contour where the function $z \mapsto \frac{u(z)}{z - \lambda_0 - r}$ is continuous, and an it is analytic on its interior. Then, it follows from Cauchy's integral formula that (notice that, for z in the real numbers, $\mathbb{1}_{I_\eta(z)}(r) = \mathbb{1}_{[r+\lambda_0-\eta, r+\lambda_0+\eta]}(z)$)

$$\begin{aligned}\int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\, \frac{u(z)}{z - \lambda_0 - r} \Big(1 - \mathbb{1}_{I_\eta(z)}(r)\Big) &= \int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\, \frac{u(z)}{z - \lambda_0 - r} \Big(1 - \mathbb{1}_{[r+\lambda_0-\eta, r+\lambda_0+\eta]}(z)\Big) \\ &= \int_{\Gamma_-(\epsilon_n,R) \setminus (r+\lambda_0-\eta, r+\lambda_0+\eta)} \mathrm{d}z\, \frac{u(z)}{z - \lambda_0 - r} \\ &= -\int_{\Gamma^{(R)} \cup \Gamma(r) \cup \Gamma_c(\epsilon_n)} dz\, \frac{u(z)}{z - \lambda_0 - r},\end{aligned} \tag{3.20}$$

which together with (3.15)-(3.19) imply the desired result, we additionally use Definition 3.4 and (A.13) to estimate the integral over $\Gamma_c(\epsilon_n)$. □

Lemma 3.6. *Let $n \geq 2$ and $R > 0$ be large enough. For $0 < q < 1 < Q < \infty$ and $\zeta \in S(\mathbb{R}, \mathbb{C})$, we define*

$$A(Q, n, R) := \int_q^Q \mathrm{d}s\, \zeta(s) \int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\, e^{-is(z-\lambda_0)} \Big\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \Big(H^\theta - z\Big)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \Big\rangle. \tag{3.21}$$

Then, the limits $A(Q, \infty, \infty) := \lim_{n,R\to\infty} A(Q, n, R)$ and $A(\infty, n, R) := \lim_{Q\to\infty} A(Q, n, R)$ exist and they are uniform with respect to Q and (n, R), respectively. Moreover, there is a constant C (independent of n, q, Q and R) such that

$$|A(Q, n, R) - A(\infty, n, R)| \leq C/Q. \tag{3.22}$$

Additionally, the limits

$$\lim_{Q\to\infty} \lim_{n,R\to\infty} A(Q, n, R), \qquad \lim_{n,R\to\infty} A(\infty, n, R) \tag{3.23}$$

exist and they are equal.

Proof. For $0 < q < Q < \infty$, $n \in \mathbb{N}$ and $R \in \mathbb{R}^+$ sufficiently large, we write

$$A(Q, n, R) = A^{(1)}(Q, n, R) + A^{(2)}(Q, n, R), \tag{3.24}$$

where

$$A^{(1)}(Q,n) := \int_q^Q \mathrm{d}s\,\zeta(s) \int_{I_n} \mathrm{d}z\, e^{-is(z-\lambda_0)} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle, \tag{3.25}$$

$$A^{(2)}(Q,R) := \int_q^Q \mathrm{d}s\,\zeta(s) \int_{I_1} \mathrm{d}z\, e^{-is(z-\lambda_0)} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle. \tag{3.26}$$

Here, we split the the domain of integration $\Gamma_-(\epsilon_n, R) = I_1 \cup I_n$, where $I_1 := [-R, R] \setminus (\lambda_0 - \epsilon_1, \lambda_0 + \epsilon_1)$ and $I_n := [\lambda_0 - \epsilon_1, \lambda_0 + \epsilon_1] \setminus (\lambda_0 - \epsilon_n, \lambda_0 + \epsilon_n)$. We analyze first (3.26). We obtain from the integration by parts formula (in the variable s) together with $e^{-is(z-\lambda_0)} = i(z-\lambda_0)^{-1}\partial_s e^{-is(z-\lambda_0)}$ that there is a constant C such that, for $\tilde{Q} > Q$,

$$\begin{aligned}
&A^{(2)}(\tilde{Q},R) - A^{(2)}(Q,R)\\
&= i\int_Q^{\tilde{Q}} \mathrm{d}s\,\zeta(s) \int_{I_1} \mathrm{d}z\,(z-\lambda_0)^{-1}\partial_s e^{-is(z-\lambda_0)} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle.\\
&= i\int_{I_1} \mathrm{d}z\, \left(\zeta(\tilde{Q})e^{-i\tilde{Q}(z-\lambda_0)} - \zeta(Q)e^{-iQ(z-\lambda_0)}\right)(z-\lambda_0)^{-1} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle\\
&- i\int_Q^{\tilde{Q}} \mathrm{d}s\, \left(\partial_s\zeta(s)\right) \int_{I_1} \mathrm{d}z\,(z-\lambda_0)^{-1} e^{-is(z-\lambda_0)} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle.
\end{aligned} \tag{3.27}$$

Since $\zeta \in S(\mathbb{R},\mathbb{C})$, there is a constant C such that, for all $s \in \mathbb{R}$, $|\zeta(s)|, |\partial_s\zeta(s)| \le C/(1+s^2)$, and hence, there is a constant C such that

$$\left|A^{(2)}(\tilde{Q},R) - A^{(2)}(Q,R)\right| \le CQ^{-1} \int_{I_1} \mathrm{d}z\, |z-\lambda_0|^{-1} \left| \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle \right|. \tag{3.28}$$

It follows from (A.12) and (A.15) that there is a constant C (independent of n, R, q and Q) such that

$$\left|A^{(2)}(\tilde{Q},R) - A^{(2)}(Q,R)\right| \le C/Q. \tag{3.29}$$

Similarly, using that $\zeta \in S(\mathbb{R},\mathbb{C})$, we find a constant C (independent of n, R, q and Q) such that

$$\begin{aligned}
\left|A^{(1)}(\tilde{Q},n) - A^{(1)}(Q,n)\right| &\le CQ^{-1} \int_{I_n} \mathrm{d}z\, \left| \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle \right|\\
&\le CQ^{-1} \sum_{j=1}^{n-1} \int_{I_{j,j+1}} \mathrm{d}z\, \left| \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle \right|,
\end{aligned} \tag{3.30}$$

where $I_{j,j+1} := [\lambda_0 - \epsilon_j, \lambda_0 + \epsilon_j] \setminus (\lambda_0 - \epsilon_{j+1}, \lambda_0 + \epsilon_{j+1})$. We observe from (A.15) together with Definition 3.4 that there is a constant C (independent of n, R, q and Q) such that

$$\left|A^{(1)}(\tilde{Q},n) - A^{(1)}(Q,n)\right| \le CQ^{-1} \sum_{j=1}^{\infty} \int_{I_{j,j+1}} \mathrm{d}z\, \frac{\boldsymbol{C}^{j+2}}{\rho_{j+1}} \le CQ^{-1} \sum_{j=1}^{\infty} \frac{\boldsymbol{C}^{j+2}\epsilon_j}{\rho_{j+1}}. \tag{3.31}$$

From Definition 3.4 and (A.13), we obtain that

$$\left|A^{(1)}(\tilde{Q},n) - A^{(1)}(Q,n)\right| \le C/Q. \tag{3.32}$$

This together with (3.29) implies that there is a constant C such that

$$\left|A(\tilde{Q},n,R) - A(Q,n,R)\right| \le C/Q. \tag{3.33}$$

Consequently, the limit $\lim_{\tilde{Q}\to\infty} A(\tilde{Q},n,R)$ exists and it converges uniformly with respect to n and R. We denote the limit by $A(\infty,n,R) = \lim_{Q\to\infty} A(Q,n,R)$. It follows that (3.22) holds true.

For fixed Q and $\tilde{n} > n$ and $\tilde{R} > R$, we have

$$\left|A(Q,\tilde{n},\tilde{R}) - A(Q,n,R)\right| \le \left|A(Q,\tilde{n},\tilde{R}) - A(Q,\tilde{n},R)\right| + \left|A(Q,\tilde{n},R) - A(Q,n,R)\right|. \tag{3.34}$$

For $\tilde{n}$ and $\tilde{R}$ large enough, employing a similar calculation as in (3.28), we get from (3.24), (3.25), (3.26) that there is a constant C (that does not depend on Q) such that

$$\begin{aligned}&\left|A(Q,\tilde{n},\tilde{R}) - A(Q,\tilde{n},R)\right| = \left|A^{(2)}(Q,\tilde{R}) - A^{(2)}(Q,R)\right| \\ &\le C' \int_{[-\tilde{R},-R]\cup[R,\tilde{R}]} \mathrm{d}z\ |z-\lambda_0|^{-1} \left|\left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta}\right\rangle\right| \le C/R,\end{aligned} \tag{3.35}$$

and furthermore, similarly as in (3.31), we obtain that there is a constant C such that

$$\left|A(Q,\tilde{n},R) - A(Q,n,R)\right| = \left|A^{(1)}(Q,\tilde{n}) - A^{(1)}(Q,n)\right| \le C \sum_{j=n}^{\tilde{n}-1} \frac{\boldsymbol{C}^{j+2}\epsilon_j}{\rho_{j+1}}, \tag{3.36}$$

and consequently, it follows from Definition 3.4 together with (A.13) that there is a constant C (that does not depend on Q) such that

$$\left|A(Q,\tilde{n},R) - A(Q,n,R)\right| \le C/n. \tag{3.37}$$

This together with (3.34) and (3.35) yields that there there is a constant C (that does not depend on Q) such that

$$\left|A(Q,\tilde{n},\tilde{R}) - A(Q,n,R)\right| \le C(R^{-1} + n^{-1}). \tag{3.38}$$

We conclude that the limit $A(Q,\infty,\infty) := \lim_{n,R\to\infty} A(Q,n,R)$ exists (uniformly with respect to Q). This completes the first part of the lemma.

Now we prove the second part of the lemma. At first, we show the existence of the limit $\lim_{n,R\to\infty} A(\infty,n,R)$. For $\tilde{n} > n$ and $\tilde{R} > R$, we estimate

$$\begin{aligned}&\left|A(\infty,\tilde{n},\tilde{R}) - A(\infty,n,R)\right| \\ &\le \left|A(\infty,\tilde{n},\tilde{R}) - A(Q,\tilde{n},\tilde{R})\right| + \left|A(Q,\tilde{n},\tilde{R}) - A(Q,n,R)\right| + \left|A(Q,n,R) - A(\infty,n,R)\right|.\end{aligned} \tag{3.39}$$

For $\epsilon > 0$, we take $Q_0 > 0$ such that for all $Q \geq Q_0$

$$\left| A(\infty, \tilde{n}, \tilde{R}) - A(Q, \tilde{n}, \tilde{R}) \right| \leq \epsilon/3 \quad \text{and} \quad |A(\infty, n, R) - A(Q, n, R)| \leq \epsilon/3. \tag{3.40}$$

We obtain from (3.38) that, for $\epsilon > 0$, there are constants $n_0, R_0 > 0$ such that, for all $n, \tilde{n} \geq n_0$ and $R, \tilde{R} \geq R_0$,

$$\left| A(Q, \tilde{n}, \tilde{R}) - A(Q, n, R) \right| \leq \epsilon/3. \tag{3.41}$$

This together with (3.40) and (3.39) yields that, for $\epsilon > 0$, there are $n_0 > 0$ and $R_0 > 0$ such that, for $n \geq n_0$ and $R \geq R_0$, we have

$$\left| A(\infty, \tilde{n}, \tilde{R}) - A(\infty, n, R) \right| \leq \epsilon. \tag{3.42}$$

This implies the existence of the limit $\lim_{n,R\to\infty} A(\infty, n, R) =: A(\infty, \infty, \infty)$. We fix $\epsilon > 0$. According to (3.42) we obtain that for large enough n, R, $|A(\infty, \infty, \infty) - A(\infty, n, R)| < \epsilon/3$. Since $\lim_{Q\to\infty} A(Q, n, R) = A(\infty, n, R)$ uniformly with respect to n, R, then for large enough Q (independently of n, R) $|A(\infty, n, R) - A(Q, n, R)| < \epsilon/3$. Moreover, because $A(Q, \infty, \infty) = \lim_{n,R\to\infty} A(Q, n, R)$ (uniformly with respect to Q), for large enough n, R (independently of Q) we have that $|A(Q, n, R) - A(Q, \infty, \infty)| < \epsilon/3$. We conclude that there are $\boldsymbol{n} \in \mathbb{N}$, $\boldsymbol{R} > 0$ and $\boldsymbol{Q} > 0$ such that, for $n \geq \boldsymbol{n}$, $Q \geq \boldsymbol{Q}$ and $R \geq \boldsymbol{R}$, we have

$$\begin{aligned} |A(\infty, \infty, \infty) - A(Q, \infty, \infty)| \leq & |A(\infty, \infty, \infty) - A(\infty, n, R)| + |A(\infty, n, R) - A(Q, n, R)| \\ & + |A(Q, n, R) - A(Q, \infty, \infty)| < \epsilon. \end{aligned} \tag{3.43}$$

This proves that $\lim_{Q\to\infty} A(Q, \infty, \infty) = A(\infty, \infty, \infty)$ and completes the proof of the second part of the lemma. □

Remark 3.7. *The absolute value of the integrand in the definition of $A(Q, n, R)$ in Lemma 3.6 is*

$$|\zeta(s)| \left| \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^{\theta} - z \right)^{-1} \sigma_1 \Psi_{\lambda_0}^{\theta} \right\rangle \right|, \tag{3.44}$$

and since the norm of the resolvent operator behaves as $\left| 1/z \right|$ for large $|z|$, it is expected that the integral of (3.44) *over $\Gamma_-(\epsilon_n, R)$ diverges as R tends to infinity. A uniform bound of the from* (3.22) *is possible because the oscillatory factor $e^{-is(z-\lambda_0)}$is being integrated: we treat $A(Q, n, R)$ as an oscillatory integral, and use the usual tools from this area (we use a clever division of the integration domain, apply integration by parts in different forms and interchange orders of integration). This is only possible if the variable s is integrated (otherwise we loose the power of the oscillatory factor and we cannot perform integration by parts in the way we do). This is the reason why do not differentiate with respect to Q and utilize the fundamental theorem of calculus (which is called Cook method in the context of scattering theory), since the derivative of $A(Q, n, R)$ with respect to Q does not contain an integration with respect to s.*

3.4 Proof of Theorem 2.1

Proof of Theorem 2.1. Let $h, l \in \mathfrak{h}_0$; see Definition 1.3. Recall the definition of W given in (3.4) and the form factor f in (1.3). Thanks to the fact that $f \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})$, we find that

$$hf, lf, W \in \mathfrak{h}_0. \tag{3.45}$$

Theorem 3.1, i.e., Equation (3.3) together with (A.2) yields

$$T(h,l) = -2\pi ig \left\|\Psi_{\lambda_0}\right\|^{-2} \langle a_-(W)\sigma_1\Psi_{\lambda_0}, \Psi_{\lambda_0}\rangle = -2\pi ig \left\|\Psi_{\lambda_0}\right\|^{-2} \langle [a_-(W), \sigma_1]\Psi_{\lambda_0}, \Psi_{\lambda_0}\rangle, \tag{3.46}$$

and furthermore, recalling that $\omega(k) = |k|$, and (A.1), we obtain that

$$\begin{aligned} T(h,l) &= -2\pi(ig)^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \int_{-\infty}^0 \mathrm{d}s\, \overline{\langle W_s, f\rangle_2} \left\langle \left[e^{isH}\sigma_1 e^{-isH}, \sigma_1\right] \Psi_{\lambda_0}, \Psi_{\lambda_0}\right\rangle \\ &= 2\pi g^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \int_0^\infty \mathrm{d}s\, \langle f, W_{-s}\rangle_2 \left\langle \left[e^{-isH}\sigma_1 e^{isH}, \sigma_1\right] \Psi_{\lambda_0}, \Psi_{\lambda_0}\right\rangle \\ &= ig^2 \left\|\Psi_{\lambda_0}\right\|^{-2} \left(T^{(1)} - T^{(2)}\right), \end{aligned} \tag{3.47}$$

where we use the abbreviations

$$T^{(j)} := \lim_{q\to 0^+} \lim_{Q\to\infty} T^{(j),q,Q} \tag{3.48}$$

for $j = 1, 2$ with

$$\begin{aligned} T^{(1),q,Q} : &= -2\pi i \int_q^Q \mathrm{d}s \int \mathrm{d}^3k\, W(k) f(k) e^{is(|k|+\lambda_0)} \left\langle \sigma_1\Psi_{\lambda_0}, e^{-isH}\sigma_1\Psi_{\lambda_0}\right\rangle \\ &= -2\pi i \int_q^Q \mathrm{d}s \int \mathrm{d}r\, G(r) e^{is(r+\lambda_0)} \left\langle \sigma_1\Psi_{\lambda_0}, e^{-isH}\sigma_1\Psi_{\lambda_0}\right\rangle \end{aligned} \tag{3.49}$$

and

$$T^{(2),q,Q} := -2\pi i \int_q^Q \mathrm{d}s \int \mathrm{d}r\, G(r) e^{is(r-\lambda_0)} \left\langle \sigma_1\Psi_{\lambda_0}, e^{isH}\sigma_1\Psi_{\lambda_0}\right\rangle. \tag{3.50}$$

Here, we use the notation

$$G : \mathbb{R} \to \mathbb{C}, \qquad r \mapsto G(r) := \begin{cases} \int \mathrm{d}\Sigma \mathrm{d}\Sigma'\, r^4 \overline{h(r,\Sigma)} l(r,\Sigma') f(r)^2 & \text{for} \quad r \geq 0 \\ 0 & \text{for} \quad r < 0, \end{cases} \tag{3.51}$$

where we write spherical coordinates $k = (r, \Sigma)$ and $k' = (r', \Sigma')$ in (3.1) and (3.4) recalling the definition of W and that $f(k) \equiv f(|k|)$ only depends on the radial coordinate $r = |k|$. Thanks to (3.45), we observe

$$G \in C_c^\infty(\mathbb{R} \setminus \{0\}, \mathbb{C}) \subset \mathcal{S}(\mathbb{R}, \mathbb{C}). \tag{3.52}$$

Term $T^{(1),q,Q}$: [13, Theorem 2.3] guarantees that Ψ_{λ_0}, and therefore, also $\sigma_1\Psi_{\lambda_0}$ is an analytic vector (see Definition 1.2). As pointed out earlier, for the ground state, we can take the set $\mathcal{S}$ to be a neighborhood of 0 which allows us to apply Lemma 3.2 and find

$$T^{(1),q,Q} = -\int_q^Q \mathrm{d}s \int \mathrm{d}r\, G(r) e^{is(r+\lambda_0)} \int_{\Gamma(\epsilon_n,R)} \mathrm{d}z\, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle. \tag{3.53}$$

Here, $\Gamma(\epsilon_n, R) = \Gamma_-(\epsilon_n, R) \cup \Gamma_c(\epsilon_n) \cup \Gamma_d(R)$ is the contour defined in Lemma 3.2, i.e., (3.5), for sufficiently large $R > 0$ and $n > 2$. We split the term

$$T^{(1),q,Q} = T_{\epsilon_n,R}^{(1),q,Q} + T_{\epsilon_n}^{(1),q,Q} + T_R^{(1),q,Q} \tag{3.54}$$

according to the different contours parts, see (3.5), in the dz-integrals:

$$T_{\epsilon_n,R}^{(1),q,Q} := -\int_q^Q \mathrm{d}s\, J(s) \int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle, \tag{3.55}$$

$$T_{\epsilon_n}^{(1),q,Q} := -\int_q^Q J(s) \int_{\Gamma_c(\epsilon_n)} \mathrm{d}z\, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle, \tag{3.56}$$

$$T_R^{(1),q,Q} := -\int_q^Q \mathrm{d}s\, J(s) \int_{\Gamma_d(R)} \mathrm{d}z\, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle, \tag{3.57}$$

and we use the definition

$$J : \mathbb{R} \to \mathbb{C}, \qquad s \mapsto J(s) = \int \mathrm{d}r\, G(r) e^{is(r+\lambda_0)}. \tag{3.58}$$

We observe that, thanks to (3.52), we have $J \in S(\mathbb{R}, \mathbb{C})$ which implies

$$|J(s)| \le C(1 + |s|^2)^{-1} \tag{3.59}$$

for some constant C. Moreover, we have (see (A.12))

$$\left| e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \right| \le C \|\Psi_{\lambda_0}\|^2 \frac{e^{s \operatorname{Im} z}}{|z - e_1|}, \qquad \forall z \in \Gamma_d(R). \tag{3.60}$$

Contribution $T_{\epsilon_n}^{(1),q,Q}$ in (3.56)**:** Using (3.59), we may start with the bound

$$|T_{\epsilon_n}^{(1),q,Q}| \le C \sup_{s \in [q,Q]} \left| \int_{\Gamma_c(\epsilon_n)} \mathrm{d}z\, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \right|. \tag{3.61}$$

It follows from (A.15) together with Definition 3.4 that there is a constant C such that, for $s \in [q, Q]$, we have

$$\left| \int_{\Gamma_c(\epsilon_n)} \mathrm{d}z\, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \right| \le C e^{\epsilon_n Q} \frac{\epsilon_n}{\rho_n} \boldsymbol{C}^{n+1} \le C e^{\epsilon_n Q} \rho_n^{\mu/8}, \tag{3.62}$$

where we use (A.13). In conclusion, we have that, for all $0 < q < Q < \infty$,

$$\lim_{n \to 0} T_{\epsilon_n}^{(1),q,Q} = 0. \tag{3.63}$$

Contribution $T_R^{(1),q,Q}$ in (3.57)**:** Using (3.59) again, we find

$$|T_R^{(1),q,Q}| \leq C \int_q^Q \mathrm{d}s \, \frac{1}{1+|s|^2} \left| \int_{\Gamma_d(R)} \mathrm{d}z \, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \right|. \tag{3.64}$$

For $s \in [q, Q]$, we observe that there is a constant C such that (see (A.12))

$$\left| \int_{\Gamma_d(R)} \mathrm{d}z \, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \right| \leq \frac{C}{R} \int_0^\infty \mathrm{d}u \, e^{-su \sin(\nu/4)}. \tag{3.65}$$

Thereby, as in (3.65), we obtain the estimate

$$\begin{aligned} &\lim_{R\to\infty} \int_q^Q \mathrm{d}s \, \frac{1}{1+|s|^2} \int_{\Gamma_d(R)} \mathrm{d}z \left| e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \right| \\ &\leq \lim_{R\to\infty} \frac{C}{R} \int_q^Q \mathrm{d}s \, \frac{1}{1+|s|^2} \frac{1}{|s|} = 0. \end{aligned} \tag{3.66}$$

Then, we conclude for all $0 < q < Q < \infty$

$$\lim_{R\to\infty} T_R^{(1),q,Q} = 0. \tag{3.67}$$

This together with (3.63) and (3.54) yields that for all $0 < q < Q < \infty$

$$T^{(1),q,Q} = \lim_{n,R\to\infty} T_{\epsilon_n,R}^{(1),q,Q}. \tag{3.68}$$

Note that $J \in S(\mathbb{R}, \mathbb{C})$. Therefore, we are in the position to apply Lemma 3.6 and find

$$T^{(1),q,\infty} := \lim_{Q\to\infty} T^{(1),q,Q} = \lim_{Q\to\infty} \lim_{n,R\to\infty} T_{\epsilon_n,R}^{(1),q,Q} = \lim_{n,R\to\infty} T_{\epsilon_n,R}^{(1),q,\infty}, \tag{3.69}$$

where

$$T_{\epsilon_n,R}^{(1),q,\infty} := \lim_{Q\to\infty} T_{\epsilon_n,R}^{(1),q,Q} = -\int_q^\infty \mathrm{d}s \, J(s) \int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z \, e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle. \tag{3.70}$$

For fixed n and R, the function $z \mapsto e^{-isz} \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle$ is bounded in $\Gamma_-(\epsilon_n, R)$. Then, thanks to (3.59), we may apply Fubini's theorem and find:

$$\begin{aligned} T_{\epsilon_n,R}^{(1),q,\infty} &= -\int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z \, \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \int_q^\infty \mathrm{d}s \int \mathrm{d}r \, G(r) e^{is(r+\lambda_0-z)} \\ &= -\int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z \, \left\langle \sigma_1 \Psi_{\lambda_0}^{\overline{\theta}}, \left(H^\theta - z\right)^{-1} \sigma_1 \Psi_{\lambda_0}^\theta \right\rangle \int \mathrm{d}s \, \Theta(s-q) \int \mathrm{d}r \, G^{(z)}(r) e^{-isr}. \end{aligned} \tag{3.71}$$

In the last step, we use the coordinate transformation $r \to z - \lambda_0 - r$ and the notation

$$G^{(z)} : \mathbb{R} \to \mathbb{C}, \qquad r \mapsto G^{(z)}(r) := G(z - \lambda_0 - r) \qquad z \in \mathbb{R}. \tag{3.72}$$

Then, it follows from (3.52) together with (3.7) that

$$\int \mathrm{d}s\,\Theta(s-q)\int \mathrm{d}r\,G^{(z)}(r)e^{-isr} = \int \mathrm{d}s\,\Theta(s)\int \mathrm{d}r\,G^{(z)}(r)e^{-iqr}e^{-isr} = \Theta(\mathfrak{F}[G^{(z),q}]) = \mathfrak{F}[\Theta](G^{(z),q}), \tag{3.73}$$

where, for $q > 0$, we define

$$G^{(z),q}(r) := G^{(z)}(r)e^{-iqr}. \tag{3.74}$$

Thanks to (3.52), we have for $z \in \mathbb{R}$ and $q \geq 0$

$$G^{(z),q} \in C_c^\infty(\mathbb{R}\setminus\{z-\lambda_0\},\mathbb{C}) \subset \mathcal{S}(\mathbb{R},\mathbb{C}). \tag{3.75}$$

It follows from Lemma 3.3 that for $z \in \mathbb{R}$

$$\int \mathrm{d}s\,\Theta(s-q)\int \mathrm{d}r\,G^{(z)}(r)e^{-isr} = \pi\delta(G^{(z),q}) - i\,(\mathrm{PV}\,(1/\bullet))\,(G^{(z),q}). \tag{3.76}$$

This together with (3.71) yields that

$$T^{(1),q,\infty}_{\epsilon_n,R} = T^{(1,1),q,\infty}_{\epsilon_n,R} + T^{(1,2),q,\infty}_{\epsilon_n,R}, \tag{3.77}$$

where

$$T^{(1,1),q,\infty}_{\epsilon_n,R} := -\pi\int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\,\left\langle \sigma_1\Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - z\right)^{-1}\sigma_1\Psi^\theta_{\lambda_0}\right\rangle G(z-\lambda_0) \tag{3.78}$$

$$T^{(1,2),q,\infty}_{\epsilon_n,R} := i\int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\,\left\langle \sigma_1\Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - z\right)^{-1}\sigma_1\Psi^\theta_{\lambda_0}\right\rangle \lim_{\eta\to 0^+}\int_{\mathbb{R}\setminus[-\eta,\eta]} \mathrm{d}r\,\frac{G(z-\lambda_0-r)e^{-iqr}}{r} \tag{3.79}$$

In the following, we shall compute both contributions explicitly.

Contribution $T^{(1,1)}_{\epsilon_n,R}(h,l)$: It follows from (3.52) that there are numbers $M > \kappa > 0$ such that $\operatorname{supp} G \subset [\kappa, M]$. Recall that everything so far holds for any choice of $n, R > 0$ large enough. For the rest of this proof we will restrict this choice to $R > M$ and $n > 0$ large enough such that $\epsilon_n < \kappa/4$. In this setting, we may turn the dz-integral in an indefinite one, exploiting, the compact support of G and the definition of the contour $\Gamma_-(\epsilon_n, R)$. We thus obtain

$$\begin{aligned} T^{(1,1),q,\infty}_{\epsilon_n,R} &= -\pi\int_{\Gamma_-(\epsilon_n,R)} \mathrm{d}z\,\left\langle \sigma_1\Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - z\right)^{-1}\sigma_1\Psi^\theta_{\lambda_0}\right\rangle G(z-\lambda_0) \\ &= -\pi\int_{\Gamma_-(\epsilon_n,R)-\lambda_0} \mathrm{d}z\,\left\langle \sigma_1\Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta -\lambda_0- z\right)^{-1}\sigma_1\Psi^\theta_{\lambda_0}\right\rangle G(z) \\ &= -\pi\int_0^\infty \mathrm{d}z\,\left\langle \sigma_1\Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta -\lambda_0- z\right)^{-1}\sigma_1\Psi^\theta_{\lambda_0}\right\rangle G(z) \end{aligned} \tag{3.80}$$

Contribution $T^{(1,2)}_{\epsilon_n,R}(h,l)$: In order to calculate $T^{(1,2)}_{\epsilon_n,R}(h,l)$ we can now fall back to Lemma 3.5. We recall Definition 3.4 and notice that $0<\epsilon_n<\kappa/4$ for sufficiently large n. Then, as a direct consequence of Lemma 3.5, we find (for sufficiently large R)

$$\begin{aligned}\lim_{n,R\to\infty} T^{(1,2),q,\infty}_{\epsilon_n,R} &= i \lim_{n,R\to\infty,\eta\to 0} T_{n,R}(\eta)\\ &= -\pi \int_{\mathbb{R}} \mathrm{d}r\, G(r) e^{-iqr} \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - \lambda_0 - r\right)^{-1} \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle\\ &= -\pi \int_0^\infty \mathrm{d}z \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - \lambda_0 - z\right)^{-1} \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle G(z) e^{-iqz}, \qquad (3.81)\end{aligned}$$

where $T_{n,R}(\eta)$ is defined in (3.12).

Collecting the contributions of (3.77), i.e, (3.80) and (3.81), we establish the identity

$$\begin{aligned} T^{(1)} &= \lim_{q\to 0^+} \lim_{n,R\to\infty} T^{(1),q,\infty}_{\epsilon_n,R} \qquad (3.82)\\ &= -\pi \lim_{q\to 0^+} \int_0^\infty \mathrm{d}z \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - \lambda_0 - z\right)^{-1} \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle G(z)(1+e^{-iqz})\\ &= -2\pi \int_0^\infty \mathrm{d}z \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - \lambda_0 - z\right)^{-1} \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle G(z)\\ &= -2\pi \int \mathrm{d}^3k \mathrm{d}^3k'\, \overline{h(k)} l(k') f(k) f(k') \delta(|k|-|k'|) \left\langle \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0}, \left(H^\theta - \lambda_0 - |k'|\right)^{-1} \sigma_1 \Psi^{\theta}_{\lambda_0} \right\rangle. \end{aligned}$$

In the third line we applied the dominated convergence theorem which is justified by (3.52). Moreover, we have inserted the definition of G using the symbolic notation of the Dirac-delta distribution in the last step.

Term $T^{(2)}$: The second term $T^{(2)}$ can be inferred by repeating the calculation with θ replaced by $\overline{\theta}$ and reflecting the path of integration $\Gamma(\epsilon_n,R)$ on the real axis when applying Lemma 3.2. In this case one has to consider the Hamiltonian $H^{\overline{\theta}}$ whose spectrum is given by mirroring the spectrum of H^θ at the real axis. Due to the similarity of the calculation, we omit a proof but only state the result

$$T^{(2)} = 2\pi \int \mathrm{d}^3k \mathrm{d}^3k'\, \overline{h(k)} l(k') f(k) f(k') \delta(|k|-|k'|) \left\langle \sigma_1 \Psi^{\theta}_{\lambda_0}, \left(H^{\overline{\theta}} - \lambda_0 + |k'|\right)^{-1} \sigma_1 \Psi^{\overline{\theta}}_{\lambda_0} \right\rangle. \qquad (3.83)$$

The relative sign in comparison with (3.82) is due to the the opposite mathematical orientation of the contour. Inserting (3.82) and (3.83) in (3.47) completes the proof. □

A Collection of previous results used in this work

In this section we collect the relevant results of [14] and [13] which are used in the proofs contained in this work.

A.1 Scattering Theory

Let $\Psi \in \mathcal{K} \otimes D(H_f^{1/2})$ and $h, l \in \mathfrak{h}_0$. Then, we recall from [14, Lemma 4.1] that

$$a_-(h)\Psi = a(h)\Psi + ig \int_{-\infty}^{0} \mathrm{d}s\, e^{isH} \langle h_s, f\rangle_2\, \sigma_1 e^{-isH}\Psi. \tag{A.1}$$

It can be shown by integration by parts that there is constant C such that $|\langle h_s, f\rangle_2| \leq C/(1+s^2)$ for $s \in \mathbb{R}$ (see [14, Eq. (C.7)]). Hence, the integral above is convergent. Moreover, it is proven in [14, Lemma 4.1 (iv)] that

$$a_\pm(h)\Psi_{\lambda_0} = 0. \tag{A.2}$$

A.2 Spectral Properties

We define

$$\mathcal{S} := \left\{\theta \in \mathbb{C} : -10^{-3} < \operatorname{Re}\theta < 10^{-3} \text{ and } \boldsymbol{\nu} < \operatorname{Im}\theta < \pi/16\right\}, \tag{A.3}$$

where $\boldsymbol{\nu} \in (0, \pi/16)$ is a fixed number (see [13, Definition 1.4]).

In order to specify some of the spectral properties of H^θ we define certain regions in the complex plane:

Definition A.1. *(c.f. [14, Definition 3.2]) For fixed $\theta \in \mathcal{S}$, we set $\delta = e_1 - e_0 = e_1$ and define the regions*

$$A := A_1 \cup A_2 \cup A_3, \tag{A.4}$$

where

$$A_1 := \{z \in \mathbb{C} : \operatorname{Re} z < e_0 - \delta/2\} \tag{A.5}$$

$$A_2 := \left\{z \in \mathbb{C} : \operatorname{Im} z > \frac{1}{8}\delta \sin(\nu)\right\} \tag{A.6}$$

$$A_3 := \{z \in \mathbb{C} : \operatorname{Re} z > e_1 + \delta/2, \operatorname{Im} z \geq -\sin(\nu/2)\,(\operatorname{Re}(z) - (e_1 + \delta/2))\}, \tag{A.7}$$

and for $i = 0, 1$, we define

$$B_i^{(1)} := \left\{z \in \mathbb{C} : |\operatorname{Re} z - e_i| \leq \frac{1}{2}\delta, -\frac{1}{2}\rho_1 \sin(\nu) \leq \operatorname{Im} z \leq \frac{1}{8}\delta \sin(\nu)\right\}. \tag{A.8}$$

These regions are depicted in Figure 3.

For a fixed $m \in \mathbb{N}$, $m \geq 4$, we define the cone

$$\mathcal{C}_m(z) := \left\{z + xe^{-i\alpha} : x \geq 0, |\alpha - \nu| \leq \nu/m\right\}. \tag{A.9}$$

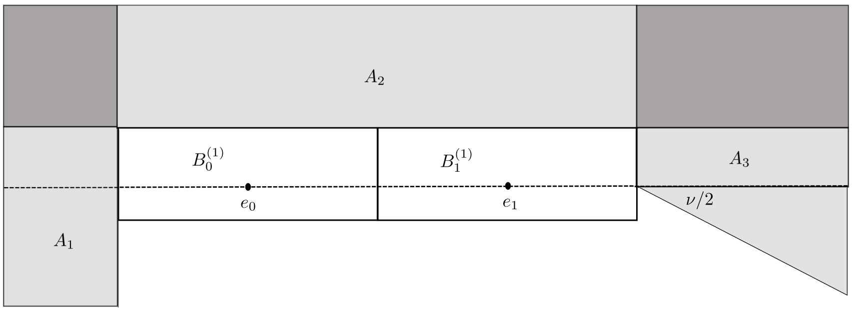

Figure 3: An illustration of the subsets of the complex plane introduced in Definition A.1.

It follows from the induction scheme in [13, Section 4] that $\lambda_i \in B_i^{(1)}$, and moreover, [13, Theorem 2.7] together with [13, Lemma 3.13] yields

$$\sigma(H^\theta) \subset \mathbb{C} \setminus \Big[A \cup (B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0)) \cup (B_1^{(1)} \setminus \mathcal{C}_m(\lambda_1))\Big]. \tag{A.10}$$

For g small enough, we recall from [14, Eq. (3.13)] that there is constant $\boldsymbol{c} > 0$ such that

$$\operatorname{Im} \lambda_1 < -g^2 \boldsymbol{c} < 0. \tag{A.11}$$

In the following we collect some important resolvent estimates. The region A is far away from the spectrum, and therefore, resolvent estimates in this region are easy. In [13, Lemma 3.2], we prove that there is a constant C (that does not depend on n, g, ρ_0 and ρ) such that

$$\Big\| \frac{1}{H^\theta - z} \Big\| \leq C \frac{1}{|z - e_1|}, \qquad \forall z \in A. \tag{A.12}$$

As in [14, Eq. (3.31)], we select the auxiliary numbers ρ

$$\boldsymbol{C}^8 \rho_0^\mu \leq 1, \qquad \boldsymbol{C}^8 \rho^\mu \leq 1/4, \qquad \text{(and hence} \qquad \boldsymbol{C} \rho^{\frac{1}{2}\iota(1+\mu/4)} \leq 1), \tag{A.13}$$

where

$$\iota = \frac{\mu/4}{(1+\mu/4)} \in (0,1). \tag{A.14}$$

In [14, Lemma 4.7] we show that for all $n \in \mathbb{N}$, a fixed (arbitrary) $m \geq 4$ and $\theta \in \mathcal{S}$, there is a constant C (that depends on m) such that

$$\Big\| \frac{1}{H^\theta - z} \sigma_1 \Psi_{\lambda_0}^\theta \Big\| \leq C \boldsymbol{C}^{n+1} \frac{1}{\rho_n}, \tag{A.15}$$

for every $z \in B_0^{(1)} \setminus \mathcal{C}_m(\lambda_0 - 2\rho_n^{1+\mu/4} e^{-i\nu})$, where the cone $\mathcal{C}_m$ is defined in (A.9). It can be seen from [14, Lemma 4.7] that C does not depend on n, ρ_0 and ρ. Here, we recall from [14, Eq. (4.51)] that

$$\mathcal{C}_m(\lambda_0 - 2\rho_n^{1+\mu/4} e^{-i\nu}) \cap \left(\overline{\mathbb{C}^+} + \lambda_0 - i2\sin(\nu)\rho_n^{1+\mu/4}\right) \subset D(\lambda_0, \epsilon_n) \subset D(\lambda_0, 2\epsilon_n) \subset B_0^{(1)}. \tag{A.16}$$

B Proof of Lemma 3.3

Proof of Lemma 3.3. For $\alpha > 0$, we define $g_\alpha \in S'(\mathbb{R}, \mathbb{C})$ by

$$g_\alpha : S(\mathbb{R}, \mathbb{C}) \to \mathbb{C}, \qquad \varphi \mapsto g_\alpha(\varphi) = \int_0^\infty \mathrm{d}x\, e^{-\alpha x} \varphi(x). \tag{B.1}$$

It follows from (3.7) that for $\varphi \in S(\mathbb{R}, \mathbb{C})$

$$\mathfrak{F}[g_\alpha](\varphi) = g_\alpha(\mathfrak{F}[\varphi]) = \int_0^\infty \mathrm{d}x\, e^{-\alpha x} \mathfrak{F}[\varphi](x) = \int_0^\infty \mathrm{d}x\, e^{-\alpha x} \int_{\mathbb{R}} \mathrm{d}s\, \varphi(s) e^{-isx}. \tag{B.2}$$

The integrand on the right-hand side of (B.2) is absolutely integrable because of $\varphi \in S(\mathbb{R}, \mathbb{C})$, and hence, the Fubini-Tonelli theorem yields that

$$\mathfrak{F}[g_\alpha](\varphi) = \int_{\mathbb{R}} \mathrm{d}s\, \varphi(s) \int_0^\infty \mathrm{d}x\, e^{-x(\alpha + is)}. \tag{B.3}$$

This together with

$$\int_0^\infty \mathrm{d}x\, e^{-x(\alpha+is)} = \frac{1}{\alpha + is} = \frac{\alpha}{(\alpha^2 + s^2)} - i \frac{s}{(\alpha^2 + s^2)} \tag{B.4}$$

implies that

$$\mathfrak{F}[g_\alpha](\varphi) = G_\alpha^{(1)}(\varphi) - i G_\alpha^{(2)}(\varphi), \tag{B.5}$$

where

$$G_\alpha^{(1)}(\varphi) = \int_{\mathbb{R}} \mathrm{d}s\, \frac{\alpha}{(\alpha^2 + s^2)} \varphi(s) \tag{B.6}$$

and

$$G_\alpha^{(2)}(\varphi) = \int_{\mathbb{R}} \mathrm{d}s\, \frac{s}{(\alpha^2 + s^2)} \varphi(s). \tag{B.7}$$

Using the coordinate transformation $s \to \alpha s$ we obtain that

$$\lim_{\alpha \to 0^+} G_\alpha^{(1)}(\varphi) = \lim_{\alpha \to 0^+} \int_{\mathbb{R}} \mathrm{d}s\, \frac{\varphi(\alpha s)}{1 + s^2} = \varphi(0) \int_{\mathbb{R}} \mathrm{d}s\, \frac{1}{1 + s^2} = \pi \varphi(0) = \pi \delta(\varphi), \tag{B.8}$$

where the second step follows from the dominated convergence theorem together with the continuity of φ. Moreover, we have

$$G_\alpha^{(2)}(\varphi) = G_\alpha^{(2,1)}(\varphi) + G_\alpha^{(2,2)}(\varphi), \tag{B.9}$$

where

$$G_\alpha^{(2,1)}(\varphi) := \int_{\mathbb{R}\setminus[-\alpha^8,\alpha^8]} \mathrm{d}s \, \frac{s}{(\alpha^2+s^2)}\varphi(s) \tag{B.10}$$

and

$$G_\alpha^{(2,2)}(\varphi) := \int_{-\alpha^8}^{\alpha^8} \mathrm{d}s \, \frac{s}{(\alpha^2+s^2)}\varphi(s). \tag{B.11}$$

We treat these two terms separately. At first, we obtain

$$\begin{aligned}\left|G_\alpha^{(2,2)}(\varphi)\right| &\leq \int_{-\alpha^8}^{\alpha^8} \mathrm{d}s \left|\frac{s}{(\alpha^2+s^2)}\left(\varphi(s)-\varphi(0)\right)\right| + |\varphi(0)| \left|\int_{-\alpha^8}^{\alpha^8} \mathrm{d}s \, \frac{s}{(\alpha^2+s^2)}\right| \\ &\leq 2\alpha^{14} \sup_{s\in[-\alpha^8,\alpha^8]} |\varphi(s)-\varphi(0)| + \frac{|\varphi(0)|}{2}\left|\int_{-\alpha^{16}}^{\alpha^{16}} \mathrm{d}s \, \frac{1}{\alpha^2+s}\right| \end{aligned} \tag{B.12}$$

where we have used the coordinate transformation $s' = s^2$ for the second term in the last line. Then, we obtain

$$\left|G_\alpha^{(2,2)}(\varphi)\right| \leq 2\alpha^{14} \sup_{s\in[-\alpha^8,\alpha^8]} |\varphi(s)-\varphi(0)| + \frac{\varphi(0)}{2}\left|\ln(1+\alpha^8) - \ln(1-\alpha^8)\right|. \tag{B.13}$$

Note that $\ln(\cdot)$ is continuous close to 1 and $\sup_{s\in[-\alpha^8,\alpha^8]} |\varphi(s)-\varphi(0)| < \infty$ since a continuous function has a maximum on a compact set. We conclude

$$\lim_{\alpha\to 0^+} G_\alpha^{(2,2)}(\varphi) = 0. \tag{B.14}$$

Finally, for some $R > 0$, we obtain

$$\begin{aligned} G_\alpha^{(2,1)}(\varphi) = &\int_{[-R,R]\setminus[-\alpha^8,\alpha^8]} \mathrm{d}s \, \frac{s}{(\alpha^2+s^2)}\left(\varphi(s)-\varphi(0)\right) + \int_{[-R,R]\setminus[-\alpha^8,\alpha^8]} \mathrm{d}s \, \frac{s}{(\alpha^2+s^2)}\varphi(0) \\ &+ \int_{\mathbb{R}\setminus[-R,R]} \mathrm{d}s \, \frac{s}{(\alpha^2+s^2)}\varphi(s). \end{aligned} \tag{B.15}$$

Due to symmetry, the second term vanishes independently of R, and moreover, the mean value theorem implies that

$$|\varphi(s)-\varphi(0)| \leq |s| \left\|\varphi'\right\|_\infty. \tag{B.16}$$

Altogether, this yields that

$$\left|\frac{s}{(\alpha^2+s^2)}\left(\varphi(s)-\varphi(0)\right)\chi_{[-R,R]\setminus[-\alpha^8,\alpha^8]}(s)\right| \leq \left\|\varphi'\right\|_\infty \chi_{[-R,R]}(s), \tag{B.17}$$

$$\left|\frac{s}{(\alpha^2+s^2)}\varphi(s)\chi_{\mathbb{R}\setminus[-R,R]}(s)\right| \leq \left|\frac{\phi(s)}{s}\chi_{\mathbb{R}\setminus[-R,R]}(s)\right|, \tag{B.18}$$

where χ_A is the characteristic (indicator) function of the set A. This allows us to apply the dominated convergence theorem in order to find

$$\lim_{\alpha\to 0^+} G_\alpha^{(2,1)}(\varphi) = \mathrm{PV}\int_{\mathbb{R}} \mathrm{d}s\, \frac{1}{s}\varphi(s) = (\mathrm{PV}\,(1/\bullet))\,(\varphi). \tag{B.19}$$

This together with (B.14), (B.9), (B.8) and (B.5) implies that

$$\lim_{\alpha\to 0^+} \mathfrak{F}[g_\alpha](\varphi) = \pi\delta(\varphi) - i\,(\mathrm{PV}\,(1/\bullet))\,(\varphi) \qquad \forall\varphi \in S(\mathbb{R},\mathbb{C}). \tag{B.20}$$

We conclude the proof by (3.7) which yields

$$\lim_{\alpha\to 0^+} \mathfrak{F}[g_\alpha](\varphi) = \lim_{\alpha\to 0^+} g_\alpha(\mathfrak{F}[\varphi]) = \Theta(\mathfrak{F}[\varphi]) = \mathfrak{F}[\Theta](\varphi) \qquad \forall\varphi \in S(\mathbb{R},\mathbb{C}). \tag{B.21}$$

□

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A Perspective on External Field QED

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Abstract

In light of the conference *Quantum Mathematical Physics* held in Regensburg in 2014, we give our perspective on the external field problem in quantum electrodynamics (QED), i.e., QED without photons in which the sole interaction stems from an external, time-dependent, four-vector potential. Among others, this model was considered by Dirac, Schwinger, Feynman, and Dyson as a model to describe the phenomenon of electron-positron pair creation in regimes in which the interaction between electrons can be neglected and a mean field description of the photon degrees of freedom is valid (e.g., static field of heavy nuclei or lasers fields). Although it may appear as second easiest model to study, it already bares a severe divergence in its equations of motion preventing any straight-forward construction of the corresponding evolution operator. In informal computations of the vacuum polarization current this divergence leads to the need of the so-called *charge renormalization*. In an attempt to provide a bridge between physics and mathematics, this work gives a review ranging from the heuristic picture to our rigorous results in a way that is hopefully also accessible to non-experts and students. We discuss how the evolution operator can be constructed, how this construction yields well-defined and unique transition probabilities, and how it provides a family of candidates for charge current operators without the need of removing ill-defined quantities. We conclude with an outlook of what needs to be done to identify the physical charge current among this family.

1 Heuristic introduction

We begin with a basic and informal introduction inspired by Dirac's original work [9] to provide a physical intuition for the external field QED model. Specialists among the readers are referred directly to Section 1.1. As it is well-known, the free one-particle Dirac equation, in units such that $\hbar = 1$ and $c = 1$,

$$(i\partial\!\!\!/ - m)\psi(x) = 0, \qquad \text{for } \psi \in \mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4), \tag{1}$$

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was originally suggested to describe free motion of single electrons. Curiously enough, it allows for wave functions in the negative part $(-\infty, -m]$ of the energy spectrum $\sigma(H^0) = (-\infty, -m] \cap [+m, \infty)$ of the corresponding Hamiltonian $H^0 = \gamma^0(-i\boldsymbol{\gamma} \cdot \nabla + m)$. As the spectrum is not bounded from below, physicists rightfully argue [17] that a Dirac electron coupled to the electromagnetic field may cascade to ever lower and lower energies by means of radiation; the reason for this unphysical instability is that the electromagnetic field is an open system, which may transport energy to spacial infinity. Other peculiarities stemming from the presence of a negative energy spectrum are the so-called *Zitterbewegung* first observed by Schrödinger [29] and *Klein's paradox* [20]. As Dirac demonstrated [9], those peculiarities can be reconciled in a coherent description when switching from the one-particle Dirac equation (1) to a many, in the mathematical idealization even infinitely many, particle description known as the *second-quantization* of the Dirac equation. Perhaps the most striking consequence of this description is the phenomenon of electron-positron pair creation, which only little later was observed experimentally by Anderson [1].

In order to get rid of peculiarities due to the negative energy states, Dirac proposed to introduce a "sea" of electrons occupying all negative energy states. The Pauli exclusion principle then acts to prevent any additional electron in the positive part of the spectrum to dive into the negative one. Let us introduce the orthogonal projectors P^+ and P^- onto the positive and negative energy subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$, respectively, i.e., $\mathcal{H}^+ = P^+\mathcal{H}$ and $\mathcal{H}^- = P^-\mathcal{H}$. Dirac's heuristic picture amounts to introducing an infinitely many-particle wave function of this sea of electrons, usually referred to as *Dirac sea*,

$$\Omega = \varphi_1 \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots, \qquad (\varphi_n)_{n\in\mathbb{N}} \text{ being an orthonormal basis of } \mathcal{H}^-, \tag{2}$$

where $\wedge$ denotes the antisymmetric tensor product w.r.t. Hilbert space $\mathcal{H}$. Given a one-particle evolution operator $U : \mathcal{H} \circlearrowleft$, such a Dirac sea may then be evolved with an operator $\mathcal{L}_U$ according to

$$\mathcal{L}_U \Omega = U\varphi_1 \wedge U\varphi_2 \wedge U\varphi_3 \wedge \ldots. \tag{3}$$

Such an ansatz may seem academic and ad-hoc. First, the Coulomb repulsion between the electrons is neglected (not to mention radiation), second, the choice of Ω is somewhat arbitrary. These assumptions clearly would have to be justified starting from a yet to be found full version of QED. For the time being we can only trust Dirac's intuition that the Dirac sea, when left alone, is so homogeneously distributed that effectively every electron in it feels the same net interaction from each solid angle, and in turn, moves freely so that it lies near to neglect the Coulomb repulsion; see also [3] for a more detailed discussion. Since then none of the particle effectively "sees" the others, physicists refer to such a state as the "vacuum". A less ad-hoc candidate for Ω would of course be the ground state of a fully interacting theory. Even though the net interaction may cancel out, electrons in the ground state will be highly entangled. The hope in using the product state (2) instead, i.e., the ground state of the free theory, to model the vacuum is that in certain regimes the particular entanglement and motion deep down in the sea might be irrelevant. The success of QED in arriving at predictions which are in astonishing agreement with experimental data substantiates this hope.

As a first step to introduce an interaction one allows for an external disturbance of the electrons in Ω modeled by a prescribed, time-dependent, four-vector potential A. This turns the one-particle Dirac equation into

$$(i\partial\!\!\!/ - m)\psi(x) = eA\!\!\!/(x)\psi(x). \tag{4}$$

The potential A may now allow for transitions of states between the subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$. Heuristically speaking, a state $\varphi_1 \in \mathcal{H}$ in the Dirac sea Ω may be bound by the potential and over time dragged to the positive energy subspace $\chi \in \mathcal{H}^+$. For an (as we shall see, oversimplified) example, let us assume that up to a phase the resulting state can be represented as

$$\Psi = \chi \wedge \varphi_2 \wedge \varphi_3 \wedge \dots \tag{5}$$

in which φ_1 is missing. Due to (4), states in $\mathcal{H}^+$ move rather differently as compared to the ones in $\mathcal{H}^-$. Thus, an electron described by $\chi \in \mathcal{H}^+$ will emerge from the "vacuum" and so does the "hole" described by the missing $\varphi_1 \in \mathcal{H}^-$ in the Dirac sea (5), which is left behind. Following Dirac, the *hole* itself can be interpreted as a particle, which is referred to as *positron*, and both names can be used as synonyms. If, as in this example, the electrons deeper down in the sea are not affected too much by this disturbance, it makes sense to switch to a more economic description. Instead of tracking all infinitely many particles, it then suffices to describe the motion of the electron χ, of the corresponding hole φ_1, and of the net evolution of Ω only. Since the number of electron-hole pairs may vary over time, a formalism for variable particle numbers is needed. This is provided by the Fock space formalism of quantum field theory, i.e., the so-called "second quantization". One introduces a so-called *creation* operator a^* that formally acts as

$$a^*(\chi)\varphi_1 \wedge \varphi_2 \wedge \dots = \chi \wedge \varphi_1 \wedge \varphi_2 \wedge \dots, \tag{6}$$

and also its corresponding adjoint a, which is called *annihilation* operator. The state Ψ from example in (5) can then be written as $\Psi = a^*(\chi)a(\varphi_1)\Omega$. With the help of a^*, one-particle operators like the evolution operator U^A generated by (4) can be lifted to an operator $\widetilde{U}$ on $\mathcal{F}$ in a canonical way by requiring that

$$\widetilde{U}^A a^*(f)(\widetilde{U}^A)^{-1} = a^*(U^A f). \tag{7}$$

This condition determines a lift up to a phase as can be seen from the left-hand side of (7). Since the operator $a^*(f)$ is linear in its argument $f \in \mathcal{H}$, it is commonly split into the sum

$$a^*(f) = b^*(f) + c^*(f) \qquad \text{with} \qquad b^*(f) := a^*(P^+ f), \quad c^*(f) := a^*(P^- f). \tag{8}$$

Hence, b^* and c^* and their adjoints are creation and annihilation operators of electrons having positive and negative energy, respectively. In order to be able to disregard the infinitely many-particle wave function Ω in the notation, one introduces the following change in language. First, the space generated by states of the form $b^*(f_1)b^*(f_2)\dots b^*(f_n)\Omega$ for $f_k \in \mathcal{H}^+$ is identified with the *electron Fock space*

$$\mathcal{F}_e = \bigoplus_{n\in\mathbb{N}_0} (\mathcal{H}^+)^{\wedge n}. \tag{9}$$

Second, the space generated by the states of the form $c(g_1)c(g_2)\dots c(g_n)\Omega$ for $g_k \in \mathcal{H}^-$ is identified with the *hole Fock space*

$$\mathcal{F}_h = \bigoplus_{n\in\mathbb{N}_0} (\mathcal{H}^-)^{\wedge n}. \tag{10}$$

Note that this time the *annihilation* operator of *negative* energy states is employed to generate the Fock space. To make this evident in the notation, one usually replaces $c(g)$ by a creation operator $d^*(g)$. However, unlike creation operators, $c(g)$ is *anti-linear* in its argument $g \in \mathcal{H}^-$. Thus, in a third step one replaces $\mathcal{H}^-$ by its complex conjugate $\overline{\mathcal{H}^-}$, i.e., the set $\mathcal{H}^-$ equipped with the usual $\mathbb{C}$-vector space structure except for the scalar multiplication $\cdot^\star : \mathbb{C} \times \overline{\mathcal{H}^-} \to \overline{\mathcal{H}^-}$ which is redefined by $\lambda \cdot^\star g = \lambda^* g$ for all $\lambda \in \mathbb{C}$ and $g \in \overline{\mathcal{H}^-}$. This turns $\mathcal{F}_h$ into

$$\overline{\mathcal{F}_h} = \bigoplus_{n\in\mathbb{N}_0} (\overline{\mathcal{H}^-})^{\wedge n}, \tag{11}$$

and the hole creation operator $d^*(g) = c(g)$ becomes *linear* in its argument $g \in \overline{\mathcal{H}^-}$. To treat electrons and holes more symmetrically, one also introduces the *anti-linear* charge conjugation operator $C : \mathcal{H} \to \mathcal{H}$, $C\psi = i\gamma^2\psi^*$. This operator exchanges $\mathcal{H}^+$ and $\mathcal{H}^-$, i.e., $C\mathcal{H}^\pm = \mathcal{H}^\mp$, and thus, gives rise to a *linear* map $C : \overline{\mathcal{H}^-} \to \mathcal{H}^+$. A hole wave function $g \in \overline{\mathcal{H}^-}$ living in the space negative states can then be represented by a wave function $Cg \in \mathcal{H}^+$ living in the positive energy space. Our discussion of the Dirac sea above may appear to break the charge symmetry as Ω is represented by a sea of electrons in $\mathcal{H}^-$. However, an equivalent description that makes the charge symmetry explicit is possible by representing the vacuum Ω through a pair of two seas, one in $\mathcal{H}^+$ and one in $\mathcal{H}^-$. Nevertheless, as the charge symmetry will not play a role in this overview we will continue using Dirac's picture with a sea of electrons in $\mathcal{H}^-$.

By definition (6) it can be seen that b, b^* and d, d^* fulfill the well-known anti-commutator relations:

$$\begin{aligned} \{b(g), b(h)\} = 0 = \{b^*(g), b^*(h)\}, \qquad \{b^*(g), b(h)\} = \langle g, P^+h\rangle \, \mathrm{id}_{\mathcal{F}_e}, \\ \{d(g), d(h)\} = 0 = \{d^*(g), d^*(h)\}, \qquad \{d^*(g), d(h)\} = \langle g, P^-h\rangle \, \mathrm{id}_{\overline{\mathcal{F}_h}}. \end{aligned} \tag{12}$$

The full Fock space for the electrons and positrons is then given by

$$\mathcal{F} = \mathcal{F}_e \otimes \overline{\mathcal{F}_h}. \tag{13}$$

In this space the vacuum wave function Ω in (2) is represented by $|0\rangle = 1 \otimes 1$ and the pair state Ψ in (5) by $a^*(\chi)d^*(\varphi_1)|0\rangle$. Thus, in this notation one only describes the excitations of the vacuum, i.e., those electrons that deviate from it. The infinitely many other electrons in the Dirac sea one preferably would like to forget about are successfully hidden in the symbol $|0\rangle$. Here, however, the story ends abruptly.

1.1 The problem and a program for a cure

For a prescribed external potential A, one would be inclined to compute transition probabilities for the creation of pairs, as for example for a transition from Ω to Ψ as in (2) and (5), right away. Given the one-particle Dirac evolution operator $U^A = U^A(t_1, t_0)$ generated by (4) and any orthonormal basis $(\chi_n)_n$ of $\mathcal{H}^+$, the first order of perturbation of the probability of a possible pair creation is given by

$$\sum_{nm} \left| \langle \chi_n, U^A \varphi_m \rangle \right|^2 = \| U^A_{+-} \|_{I_2}, \tag{14}$$

where $I_2(\mathcal{H})$ denotes the space of bounded operators with finite Hilbert-Schmidt norm $\|\cdot\|_{I_2}$, and we use the notation $U^A_{\pm\mp} = P^{\pm} U^A P^{\mp}$. For quite general potentials $A = (A^0, \mathbf{A})$, it turns out that:

Theorem 1.1 ([26])**.** *Term* (14) $< \infty$ *for all times* $t_0, t_1 \in \mathbb{R} \Leftrightarrow \mathbf{A} = 0$.

In view of (14), the transition probability is thus only defined for external potentials A that have zero spatial components $\mathbf{A}$. Even worse, the criterion for the well-definedness of a possible lift $\widetilde{U}$ of any unitary one-particle operator U according to (7) is given by:

Theorem 1.2 ([30])**.** *There is a unitary operator* $\widetilde{U} : \mathcal{F} \circlearrowleft$ *that fulfills* (7) $\Leftrightarrow U_{+-}, U_{-+} \in I_2(\mathcal{H})$.

Applying this result to the evolution operator U^A, (14) and Theorem 1.1 imply that the criterion in Theorem 1.2 is only fulfilled for external potentials A with zero spatial components $\mathbf{A}$. Even more peculiar, the given criterion is not gauge covariant (not to mention the Lorentz covariance). Although the free evolution operator $U^{A=0}$ has a lift, in the case that some spatial derivatives of a scalar field Γ are non-zero, the gauge transformed $U^{A=\partial\Gamma}$ does not. This indicates that an unphysical assumption must have been made.

What singles out the spatial components of A? Mathematically, they appear in the Hamiltonian, $H^A = \gamma^0(-i\boldsymbol{\gamma} \cdot \boldsymbol{\Delta} + m) + A_0 - \gamma^0 \boldsymbol{\gamma} \cdot \mathbf{A}$, preceded by the spinor matrix $\gamma^0\boldsymbol{\gamma}$ whereas A_0 is only a multiple of the identity. Heuristically, if $\mathbf{A}$ is non-zero then the $\gamma^0\boldsymbol{\gamma}$ matrix transforms the negative energy states φ_n in spinor space to develop components in $\mathcal{H}^+$. There is no mechanism that would limit this development, not even smallness of $|\mathbf{A}|$, so there is no reason why the infinite sum (14) should be finite – and in general this is also not the case as Theorem 1.1 shows. In other words, for $\mathbf{A} \neq 0$, instantly infinitely many electron-positron pairs are created from the vacuum state Ω. Therefore, the picture is not nearly as peaceful as suggested by example state (5). However, if A is switched off at some later time one can expect that almost all of these pairs disappear again, and only a few excitations of the vacuum as in (5) will remain (hence, the name *virtual pairs* that is used by physicists). Assuming that at initial and final times $A = 0$, it can indeed be shown that the scattering matrix S^A fulfills the conditions of Theorem 1.2. The physical reason why the spatial components are singled out is due to the use of equal-time hyperplanes and will be discussed more geometrically in Section 2; see Theorem 2.8 below.

In conclusion, the problem lies in the fact that even the “vacuum” Ω consists of infinitely many particles. In the formalism of the free theory this fact is usually hidden by the use of normal ordering. Without it the ground state energy of Ω would be the infinite sum of all negative energies, or the charge current operator expectation value $\langle \Omega, \overline{a}\gamma^\mu a \Omega \rangle$ of the vacuum would simply be the infinite sum of all one-particle currents $\overline{\varphi}_n \gamma^\mu \varphi_n$ – both quantities that diverge. The rational behind the ad-hoc introduction of normal ordering of, e.g., the charge current operator is again the assumption that in the vacuum state these currents are effectively not observable since the net interaction between the particles vanishes.

The incompatibility of Theorem 1.2 with the gauge freedom however shows that, although the choice of Ω may be distinguished for $A = 0$ by the ground state property, it is somehow arbitrary when $A \neq 0$, and so is the choice in the splitting of $\mathcal{H}$ into $\mathcal{H}^+$ and $\mathcal{H}^-$, which is usually referred to as *polarization*. As a program for a cure of these divergences, one may therefore attempt to carefully adapt the choice of the polarization depending on the evolution of A instead of keeping it fixed. Several attempts have been made to give a definition of a more physical polarization, one of them being the *Furry picture*. It defines the polarization according to the positive and negative parts of the spectrum of H^A given a fixed A. Unfortunately, none of the proposed choices are Lorentz invariant as it is shown in [10] since the vacuum state w.r.t. one of such choices in one frame of reference may appear as a many-particle state in another. This is due to the fact that the energy spectrum is obviously not invariant under Lorentz boosts.

Although a fully developed QED may be able to distinguish a class of states that can be regarded as physical vacuum states, simply by verifying the assumption above that the net interaction between the particles vanishes, the external field QED model has no mathematical structure to do so. Nevertheless, whenever a distinction between electrons and positrons by means of a polarization is not necessary, e.g., in the case of vacuum polarization in which the exact number of pairs is irrelevant, it should still be possible to track the time evolution $\widetilde{U}^A\Omega$ and study the generated dynamics – not only asymptotically in scattering theory but also at intermediate times. The choice in admissible polarizations can then be seen to be analogous to the choice of a convenient coordinate system to represent the Dirac seas. Since the employed Fock space $\mathcal{F}$ depends directly on the polarization of $\mathcal{H}$ into $\mathcal{H}^+$ and $\mathcal{H}^-$, see (9)-(10) and (13), the standard formalism has to be adapted to allow the Fock space to also vary according to A, and the evolution operator $\widetilde{U}^A$ must be implemented mapping one Fock space into another. While the idea of varying Fock space may be unfamiliar from the non-relativistic setting, it is natural when considering a relativistic formalism. A Lorentz boost, for example, tilts an equal-time hyperplane to a Cauchy surface Σ which requires a change from the standard Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ to one that is attached to Σ, and likewise, for the corresponding Fock spaces. Hence, a Lorentz transform will naturally be described by a map from one Fock space into another [5]. In the special case of equal-time hyperplanes, parts of this program have been carried out in [21, 22] and [4]. In the former two works the time evolution operator is nevertheless implemented on standard Fock space $\mathcal{F}$ by conjugation of the evolution operator with a convenient (non-unique) unitary "renormalization" transformation. In the latter work it is implemented between time-varying Fock spaces, so-called infinite wedge spaces, and furthermore, the degrees of freedom in the construction have been identified. These latter results have been extended recently to allow for general Cauchy surfaces in [5, 6] and are presented in Section 2. All these results ensure the existence of an evolution operator by a quite abstract argument. Therefore, we review a construction of it in Section 3 based on [4]. It utilizes a notation that is very close to Dirac's original view of a sea of electrons as in (2). Though it is canonically equivalent to the Fock space formalism, it provided us a more intuitive view of the problem and helped in identifying the degrees of freedom involved in the construction. In Section 4 we conclude with a discussion of the unidentified phase of the evolution operator and its meaning for the charge current in. Beside the publications cited so far, there are several recent contributions which also take up on Dirac's original idea. As a more fundamental approach we want to mention the one of the so-called "Theory of Causal Fermion Systems" [11, 12, 13], which is based on a reformulation of quantum electrodynamics from first principles. The phenomenon of adiabatic pair creation was treated rigorously in [24]. Furthermore, there is a series of works treating the Dirac sea in the Hartree-Fock approximation. The most general is [16] in which the effect of vacuum polarization was treated self-consistently for static external sources.

2 Varying Fock spaces

In order to better understand why the spatial components of A had been singled out in the discussion above, it is helpful to consider the Dirac evolution not only on equal-time hyperplanes but on more general Cauchy surfaces.

Definition 2.1. *A Cauchy surface Σ in $\mathbb{R}^4$ is a smooth, 3-dimensional submanifold of $\mathbb{R}^4$ that fulfills the following two conditions:*

(a) Every inextensible, two-sided, time- or light-like, continuous path in $\mathbb{R}^4$ intersects Σ in a unique point.

(b) For every $x \in \Sigma$, the tangent space $T_x\Sigma$ of Σ at x is space-like.

To each Cauchy surface Σ we associated a Hilbert space $\mathcal{H}_\Sigma$.

Definition 2.2. *Let $\mathcal{H}_\Sigma = L^2(\Sigma, \mathbb{C}^4)$ denote the vector space of all 4-spinor valued measurable functions $\phi : \Sigma \to \mathbb{C}^4$ (modulo changes on null sets) having a finite norm $\|\phi\| = \sqrt{\langle \phi, \phi \rangle} < \infty$ w.r.t. the scalar product*

$$\langle \phi, \psi \rangle = \int_\Sigma \overline{\phi(x)} i_\gamma(d^4x)\psi(x). \tag{15}$$

Here, $i_\gamma(d^4x)$ denotes the contraction of the volume form $d^4x = dx^0 \wedge dx^1 \wedge dx^2 \wedge dx^3$ with the spinor-matrix valued vector γ^μ, $\mu = 0, 1, 2, 3$. The corresponding dense subset of smooth and compactly supported functions will be denoted by $\mathcal{C}_\Sigma$.

The well-posedness of the initial value problem related to (4) for initial data on Cauchy surfaces has been studied in the literature; e.g., see [18, 31] for general hyperbolic systems and more specifically for wave equations on Lorentzian manifolds [8], [2], [25], [14], and [7]. For the purpose of our study we furthermore introduced generalized Fourier transforms for the Dirac equation in [5] and extended the standard Sobolev and Paley-Wiener methods in $\mathbb{R}^n$ to the geometry given by the Cauchy surfaces and the mass shell of the Dirac equation. These methods were required for the analysis of solutions. They play along nicely with Lorentz and gauge transforms and allow for the introduction of an interaction picture. As a byproduct, these methods also ensure existence, uniqueness, and causal structure of strong solutions. Since we avoid technicalities in this paper, we assume A is a smooth and compactly supported (although sufficient strong decay would be sufficient), and the following theorem will suffice to discuss the one-particle Dirac evolution.

Theorem 2.3 (Theorem 2.23 in [5])**.** *Let Σ, Σ' be two Cauchy surfaces and $\psi_\Sigma \in \mathcal{C}_\Sigma$ the initial data. There is a unique strong solution $\psi \in \mathcal{C}^\infty(\mathbb{R}^4, \mathbb{C}^4)$ to (4) being supported in the forward and backward light cone of $\operatorname{supp}\psi_\Sigma$ such that $\psi|_\Sigma = \psi_\Sigma$ holds. Furthermore, there is an isometric isomorphism $U^A_{\Sigma'\Sigma} : \mathcal{C}_\Sigma \to \mathcal{C}_{\Sigma'}$ fulfilling $\psi|_{\Sigma'} = U^A_{\Sigma'\Sigma}\psi_\Sigma$. Its unique extension to a unitary map $U^A_{\Sigma'\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$ is denoted by the same symbol.*

Similarly to the standard Fock space (13) we define the Fock space for a Cauchy surface on the basis of a polarization.

Definition 2.4. *Let $\texttt{Pol}(\mathcal{H}_\Sigma)$ denote the set of all closed, linear subspaces $V \subset \mathcal{H}_\Sigma$ such that V and $V^\perp$ are both infinite dimensional. Any $V \in \texttt{Pol}(\mathcal{H}_\Sigma)$ is called a* polarization *of $\mathcal{H}_\Sigma$. For $V \in \texttt{Pol}(\mathcal{H}_\Sigma)$, let $P^V_\Sigma : \mathcal{H}_\Sigma \to V$ denote the orthogonal projection of $\mathcal{H}_\Sigma$ onto V.*

The Fock space attached to Cauchy surface Σ and corresponding to polarization $V \in \texttt{Pol}(\mathcal{H}_\Sigma)$ is defined by

$$\mathcal{F}(V,\Sigma) := \bigoplus_{c\in\mathbb{Z}} \mathcal{F}_c(V,\mathcal{H}_\Sigma), \qquad \mathcal{F}_c(V,\Sigma) := \bigoplus_{\substack{n,m\in\mathbb{N}_0\\ c=m-n}} (V^\perp)^{\wedge n} \otimes \overline{V}^{\wedge m}. \tag{16}$$

Note that the standard Fock space is included in this definition by choosing $\Sigma = \{0\} \times \mathbb{R}^3$ and $V = \mathcal{H}^-$.

Given two Cauchy surfaces Σ and Σ', polarizations $V \in \texttt{Pol}(\mathcal{H}_\Sigma)$ and $V' \in \texttt{Pol}(\mathcal{H}_{\Sigma'})$, and the one-particle evolution operator $U^A_{\Sigma'\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$, we need a condition analogous to (7) that allows us to find an evolution operator $\widetilde{U}^A_{V',\Sigma';V,\Sigma} : \mathcal{F}(V,\Sigma) \to \mathcal{F}(V',\Sigma')$. For the discussion, let a^*_Σ and a_Σ denote the corresponding creation and annihilation operators on any $\mathcal{F}(W,\Sigma)$ for $W \in \texttt{Pol}(\mathcal{H}_\Sigma)$; note that the defining expression of a^* in (6) does not depend on the choice of a polarization W. In this notation, the lift requirement reads

$$\widetilde{U}^A_{V',\Sigma';V,\Sigma}\, a^*_\Sigma(f) \left(\widetilde{U}^A_{V',\Sigma';V,\Sigma}\right)^{-1} = a^*_{\Sigma'}(U^A_{\Sigma'\Sigma} f), \qquad \forall f \in \mathcal{H}_\Sigma. \tag{17}$$

The condition under which such a lift of the one-particle evolution operator $U^A_{\Sigma'\Sigma}$ exists can be inferred from a slightly rewritten version of the Shale-Stinespring Theorem 1.2:

Corollary 2.5. *Let Σ, Σ' be Cauchy surfaces, $V \in \texttt{Pol}(\mathcal{H}_\Sigma)$, and $V' \in \texttt{Pol}(\mathcal{H}_{\Sigma'})$. Then the following statements are equivalent:*

(a) There is a unitary operator $\widetilde{U}^A_{V'\Sigma';V,\Sigma} : \mathcal{F}(V,\Sigma) \to \mathcal{F}(V',\Sigma')$ which fulfills (17).

(b) The off-diagonals $P^{V'^\perp}_{\Sigma'} U^A_{\Sigma'\Sigma} P^V_\Sigma$ and $P^{V'}_{\Sigma'} U^A_{\Sigma'\Sigma} P^{V^\perp}_\Sigma$ are Hilbert-Schmidt operators.

Note again that if such a lift exists, its phase is not fixed by (17) and the corollary above does not provide any information about it. Therefore, we will discuss a direct construction of the lifted operator $\widetilde{U}^A_{V'\Sigma';V,\Sigma}$ in Section 3, which makes the involved degrees of freedom apparent.

Coming back to the question which polarizations $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ and $V' \in \mathtt{Pol}(\mathcal{H}_{\Sigma'})$ guarantee the existence of a lifted evolution operator $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V,\Sigma) \to \mathcal{F}(V',\Sigma')$, one readily finds a trivial choice. Let us pick a Cauchy surface Σ_{in} in the remote past fulfilling:

$$\Sigma_{\text{in}} \text{ is a Cauchy surface such that } \operatorname{supp} A \cap \Sigma_{\text{in}} = \emptyset. \tag{18}$$

When transporting the standard polarization along with the Dirac evolution we get

$$V = U^A_{\Sigma\Sigma_{\text{in}}} P^-_{\Sigma_{\text{in}}} \mathcal{H}_{\Sigma_{\text{in}}} \in \mathtt{Pol}(\mathcal{H}_\Sigma), \qquad V' = U^A_{\Sigma'\Sigma_{\text{in}}} P^-_{\Sigma_{\text{in}}} \mathcal{H}_{\Sigma_{\text{in}}} \in \mathtt{Pol}(\mathcal{H}_{\Sigma'}), \tag{19}$$

which automatically fulfills condition (b) of Theorem 2.5 as then the off-diagonals $(U^A_{\Sigma\Sigma_{\text{in}}})_{\pm\mp}$ become zero. This choice is usually called the *interpolation picture*. Its drawback is that the polarizations V and V' depend on the whole history of A between Σ_{in} and Σ and Σ'. Moreover, such V and V' are rather implicit. Luckily, there are other choices. Statement (b) in Theorem 2.5 allows to differ from the projectors P^V_Σ and $P^{V'}_{\Sigma'}$ by a Hilbert-Schmidt operator. Hence, all admissible polarizations can be collected and characterized by means of the following classes:

Definition 2.6. *For a Cauchy surface Σ we define the class*

$$\mathtt{C}_\Sigma(A) := \left\{ W \in \mathtt{Pol}(\mathcal{H}_\Sigma) \,\middle|\, W \approx U^A_{\Sigma\Sigma_{\text{in}}} \mathcal{H}^-_{\Sigma_{\text{in}}} \right\} \tag{20}$$

where for $V, W \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, $V \approx W$ means that the difference of the corresponding orthogonal projectors $P^V_\Sigma - P^W_\Sigma$ is a Hilbert-Schmidt operator.

As simple implication of Corollary 2.5 one gets:

Corollary 2.7. *Let Σ, Σ' be Cauchy surfaces and polarizations $V \in C_\Sigma(A)$ and $W \in C_{\Sigma'}(A)$. Then up to a phase there is a unitary operator $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V,\mathcal{H}_\Sigma) \to \mathcal{F}(W,\mathcal{H}_{\Sigma'})$ obeying (17).*

We emphasize again that any other possible polarization than the choice in (19) is comprised in the respective class $C_\Sigma(A)$ as Corollary 2.5 only allows for the freedom encoded in the equivalence relation $\approx$. Although the polarization (19) depends on the history of the evolution it turns out that the classes $C_\Sigma(A)$ are independent thereof. The sole dependence of the classes $C_\Sigma(A)$ is on the tangential components of A, which can be stated as follows.

Theorem 2.8 (Theorem 1.5 in [6])**.** *Let Σ be a Cauchy surface and let A and $\widetilde{A}$ be two smooth and compactly supported external fields. Then*

$$C_\Sigma(A) = C_\Sigma(\widetilde{A}) \qquad \Leftrightarrow \qquad A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}, \tag{21}$$

where $A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}$ means that for all x in Σ and all vectors y in the tangent space $T_x\Sigma$ of Σ at x, the relation $A_\mu(x)y^\mu = \widetilde{A}_\mu(x)y^\mu$ holds.

This theorem is a generalization of Ruijsenaar's result [27] and helps to understand why on equal-time hyperplanes the spatial components of A appeared to play such a special role. The spatial components $\mathbf{A}$ are the tangential ones w.r.t. such Cauchy surfaces. Furthermore, the classes $C_\Sigma(A)$ transform nicely under Lorentz and gauge transformations:

Theorem 2.9 (Theorem 1.6 in [6]).

(i) Consider a Lorentz transformation given by $L_\Sigma^{(S,\Lambda)} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Lambda\Sigma}$ *for a spinor transformation matrix* $S \in \mathbb{C}^{4\times 4}$ *and an associated proper orthochronous Lorentz transformation matrix* $\Lambda \in \mathrm{SO}^\uparrow(1,3)$*, see for example [5, Section 2.3]. Then:*

$$V \in \mathtt{C}_\Sigma(A) \qquad \Leftrightarrow \qquad L_\Sigma^{(S,\Lambda)} V \in \mathtt{C}_{\Lambda\Sigma}(\Lambda A(\Lambda^{-1}\cdot)). \tag{22}$$

(ii) Consider a gauge transformation $A' = A + \partial\Gamma$ *for some* $\Gamma \in \mathcal{C}_c^\infty(\mathbb{R}^4, \mathbb{R})$ *given by the multiplication operator* $e^{-i\Gamma} : \mathcal{H}_\Sigma \to \mathcal{H}_\Sigma$*,* $\psi \mapsto \psi' = e^{-i\Gamma}\psi$*. Then:*

$$V \in \mathtt{C}_\Sigma(A) \qquad \Leftrightarrow \qquad e^{-i\Gamma} V \in \mathtt{C}_\Sigma(A + \partial\Gamma). \tag{23}$$

As an analogy from geometry one could think of the particular polarization as a particular choice of coordinates to represent the Dirac sea. Corollary 2.5 and Theorem 2.9 explain why gauge transformations that introduce spatial components in the external fields do not comply with the condition to the Shale-Stinespring Theorem 1.2 in which the “coordinates” $\mathcal{H}^+$ and $\mathcal{H}^-$ were fixed.

The key idea in the proofs of Theorem 2.8 and 2.9 is to guess a simple enough operator $P_\Sigma^A : \mathcal{H}_\Sigma \circlearrowleft$ depending only on the restriction $A|_\Sigma$ so that

$$U_{\Sigma\Sigma_{\mathrm{in}}}^A P_{\Sigma_{\mathrm{in}}}^- U_{\Sigma_{\mathrm{in}}\Sigma}^A - P_\Sigma^A \in I_2(\mathcal{H}_\Sigma), \qquad \text{and} \qquad (P_\Sigma^A)^2 - P_\Sigma^A \in I_2(\mathcal{H}_\Sigma). \tag{24}$$

The claims about the properties of the polarization classes $C_\Sigma(A)$ can then be inferred directly from the properties of P_Σ^A. This is due to the fact that (24) is compatible with the Hilbert-Schmidt operator freedom encoded in the $\approx$ equivalence relation. The intuition behind the guess of P_Σ^A used in the proofs presented in [6] comes from the gauge transform. Imagine the special situation in which an external potential A could be gauged to zero, i.e., $A = \partial\Gamma$ for a given scalar field Γ. In this case $e^{-i\Gamma} P_\Sigma^- e^{i\Gamma}$ is a good candidate for P_Σ^A. Now in the case of general external potentials A that cannot be attained by a gauge transformation of the zero potential, the idea is to implement gauge transforms locally at each space-time point. For example, if $p_-(x,y)$ denotes the informal integral kernel of the operator P_Σ^-, one could try to define P_Σ^A as the operator corresponding to the informal kernel $p^A(x,y) = e^{-i\lambda_A(x,y)} p_-(x,y)$ for the choice $\lambda_A(x) = A(x)_\mu (y-x)^\mu$. The effect of $\lambda_A(x,y)$ on the projector can be interpreted as a local gauge transform of $p_-(x,y)$ from the zero potential to the potential $A_\mu(x)$ at space-time point x. A careful analysis of P_Σ^A, which was conducted in Section 2 of [6], shows that P_Σ^A fulfills (24).

Finally, given Cauchy surface Σ, there is also an explicit representative of the polarization class $C_\Sigma(A)$ which can be given in terms of the bounded operator $Q_\Sigma^A : \mathcal{H}_\Sigma \circlearrowleft$ defined by

$$Q_\Sigma^A := P_\Sigma^+ (P_\Sigma^A - P_\Sigma^-) P_\Sigma^- - P_\Sigma^- (P_\Sigma^A - P_\Sigma^-) P_\Sigma^+. \tag{25}$$

With it, the polarization class can be identified as follows:

Theorem 2.10 (Theorem 1.7 in [6]). *Given Cauchy surface* Σ*,* $\mathtt{C}_\Sigma(A) = \left[e^{Q_\Sigma(A)} \mathcal{H}_\Sigma^- \right]_\approx$*.*

The implications of these results on the physical picture can be seen as follows. The Dirac sea on Cauchy surface Σ can be described in any Fock space $\mathcal{F}(V, \mathcal{H}_\Sigma)$ for any choice of polarization $V \in C_\Sigma(A)$. The polarization class $C_\Sigma(A)$ is uniquely determined by the tangential components of the external potential A on Σ. When regarding the Dirac evolution from one Cauchy surface Σ to Σ', another choice of "coordinates" $V' \in C_{\Sigma'}(A)$ has to be made. Then one yields an evolution operator $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(V', \mathcal{H}_{\Sigma'})$ which is unique up to an arbitrary phase. Transition probabilities $|\langle \Psi, \widetilde{U}^A_{\Sigma'\Sigma}\Phi\rangle|^2$ for $\Psi \in \mathcal{F}(V', \mathcal{H}_{\Sigma'})$ and $\Phi \in \mathcal{F}(V, \mathcal{H}_\Sigma)$ are well-defined and unique without the need of a renormalization method. Finally, for a family of Cauchy surfaces $(\Sigma_t)_{t\in\mathbb{R}}$ that interpolates smoothly between Σ and Σ' one can also infer an infinitesimal version of how the external potential A changes the polarization in terms of the flow parameter t; see Theorem 2.6 in [6].

We remark that the kernel of the orthogonal projector corresponding to a polarization in $\mathtt{C}_\Sigma(A)$, which can be interpreted as a distribution, is frequently called *two-point function*. Two kernels belonging to two polarizations in the same class $\mathtt{C}_\Sigma(A)$ may differ by a square-integrable kernel. This stands in contrast to the so-called Hadamard property (see, e.g., [19]) which allows changes with $\mathcal{C}^\infty$ kernels as freedom in two-point functions.

3 An explicit construction of the evolution operator

The argument in Section 2 that ensures the existence of dynamics on varying Fock spaces is quite abstract. In this section we present a more direct approach that is also closer to Dirac's original picture in describing infinite particle wave functions like in (2). As discussed, the infinitely many particles are also present in the usual Fock space formalism but commonly hidden by use of normal ordering. But since the very obstacle in a straight-forward construction of the evolution operator is due to their presence, it seems to make sense to work with a formalism that makes them apparent. One such formalism, introduced in Section 2 of [4], employs so-called infinite wedge spaces and will be used in the following.

To leave our discussion general, let $\mathcal{H}$ be a one-particle Hilbert space (e.g., $\mathcal{H} = \mathcal{H}_\Sigma$ as in Section 2) and let $V \in \mathtt{Pol}(\mathcal{H})$ be a polarization thereof. The Dirac sea corresponding to that choice of polarization can be represented, using any orthonormal basis $(\varphi_n)_{n\in\mathbb{N}}$ that spans V, by the infinite wedge product

$$\Lambda\Phi = \varphi_1 \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots, \tag{26}$$

i.e., the anti-symmetric product of all wave functions φ_n, $n \in \mathbb{N}$. Slightly more general, it suffices if $(\varphi_n)_{n\in\mathbb{N}}$ is only *asymptotically* orthonormal in the sense that the infinite matrix $(\langle\varphi_n, \varphi_m\rangle)_{n,m\in\mathbb{N}}$ has a (Fredholm) determinant, i.e., that it differs from the identity only by a matrix that has a trace. The reason for this property will become clear when introducing the scalar product of two infinite wedge products.

In order to keep the formalism short, we encode the basis $(\varphi_n)_{n\in\mathbb{N}}$ by a bounded linear operator

$$\Phi : \ell \to \mathcal{H}, \qquad \Phi\, e_n = \varphi_n \tag{27}$$

on a Hilbert space ℓ. The role of ℓ is only that of an index space, and one example we have in mind is $\ell = \ell^2(\mathbb{N})$, i.e., the space of square summable sequences where the vectors e_n, $n \in \mathbb{N}$, denote the canonical basis. In this language, the asymptotic orthonormality requirement from above can be rewritten as $\Phi^*\Phi \in \mathrm{id}_\ell + I_1(\ell)$, where $I_1(\ell)$ is the space of bounded linear maps $\ell \to \ell$ which have a trace, the so-called *trace class*. We will also write $\Lambda\Phi = \varphi_1 \wedge \varphi_2 \wedge \dots$ which denotes the infinite wedge product (26) and refer to all such Φ as *Dirac seas*.

Given another Dirac sea Ψ with $\psi_n = \Psi e_n$, $n \in \mathbb{N}$, the pairing that will later become a scalar product

$$\langle \Lambda\Psi, \Lambda\Phi \rangle = \langle \psi_1 \wedge \psi_2 \wedge \dots, \varphi_1 \wedge \varphi_2 \wedge \dots \rangle = \det(\langle \psi_n, \varphi_m \rangle)_{nm} = \det \Psi^*\Phi \tag{28}$$

is well-defined if $\Psi^*\Phi$ has a determinant, which is the case if $\Psi^*\Phi \in \mathrm{id}_\ell + I_1(\ell)$. Thus, it makes sense to build a Fock space, referred to as "infinite wedge space $\mathcal{F}_{\Lambda\Phi}$", based on a basis encoded by Φ. It is defined by the completion w.r.t. the pairing (28) of the space of *formal* linear combinations of all such Ψ; see Section 2.1 in [4] for a rigorous construction. This space consists of the sea wave function $\Lambda\Phi$, its excitations $\Lambda\Psi$ that form a generating set, and superpositions thereof. An example excitation analogous to (5) representing an electron-positron pair with electron wave function $\chi \in V^\perp$ and positron wave function $\varphi_1 \in V$ is given by

$$\Lambda\Psi = \chi \wedge \varphi_2 \wedge \varphi_3 \wedge \varphi_4 \wedge \dots. \tag{29}$$

Note, however, that mathematically Φ is not distinguished as "the one vacuum" state as it turns out that $\mathcal{F}_{\Lambda\Phi} = \mathcal{F}_{\Lambda\Psi}$ if and only if $\Psi^*\Phi$ has a determinant, i.e., if the scalar product $\langle \Lambda\Psi, \Lambda\Phi \rangle$ in (28) is well-defined. This is due to the that fact $\Psi \sim \Phi :\Leftrightarrow \Psi^*\Phi \in \mathrm{id}_\ell + I_1(\ell)$ is an equivalence relation on the set of all Dirac seas; see Corollary 2.9 in [4].

Next, let us consider another one-particle Hilbert space $\mathcal{H}'$ and a one-particle unitary operator $U : \mathcal{H} \to \mathcal{H}'$ such as the one-particle Dirac evolution operator $U^A_{\Sigma'\Sigma}$. To infer from this a corresponding evolution of the Dirac seas, we define a canonical operation from the left as follows

$$\mathcal{L}_U : \mathcal{F}_{\Lambda\Phi} \to \mathcal{F}_{\Lambda U\Phi}, \qquad \mathcal{L}_U \, \Lambda\Psi := \Lambda U\Psi = (U\psi_1) \wedge (U\psi_2) \wedge \dots. \tag{30}$$

Here, Ψ is taken from the generating set of Dirac seas fulfilling $\Psi^*\Phi \in 1 + I_1(\ell)$; see Section 2.2 in [4]. That the range of $\mathcal{L}_U$ is $\mathcal{F}_{\Lambda U\Phi}$ is due to the fact that $\Psi^*\Phi$ has a determinant if and only if $(U\Psi)^*(U\Phi)$ does. Such a map $\mathcal{L}_U$ represents an evolution operator from one infinite wedge space into another that in the sense of (6) also complies with the previously discussed lift condition (7).

Nevertheless, the construction of the evolution operator for the Dirac seas does not end here because the target space $\mathcal{F}_{\Lambda U\Phi}$ in (30) is completely implicit, and hence, $\mathcal{L}_U$ alone is not very helpful. On the contrary, relying on the observations made in Section 2, physics should allow us to decide beforehand between which infinite wedge spaces the evolution operator should be implemented. Consider the example situation of

$$\begin{gathered}\text{an evolution operator } U = U^A_{\Sigma'\Sigma} \text{ from Theorem 2.3,} \\ \mathcal{H} = \mathcal{H}_\Sigma, \quad V \in \mathtt{Pol}(\mathcal{H}_\Sigma), \quad \Phi : \ell \to \mathcal{H}_\Sigma \text{ such that } \operatorname{range}\Phi = V, \\ \mathcal{H}' = \mathcal{H}_{\Sigma'}, \quad V' \in \mathtt{Pol}(\mathcal{H}_{\Sigma'}), \quad \Phi' : \ell' \to \mathcal{H}_{\Sigma'} \text{ such that } \operatorname{range}\Phi' = V'.\end{gathered} \tag{31}$$

In this situation one would wish for an evolution operator of the form $\widetilde{U} : \mathcal{F}_{\wedge\phi} \to \mathcal{F}_{\wedge\Phi'}$ instead of $\widetilde{U} : \mathcal{F}_{\wedge\phi} \to \mathcal{F}_{\wedge U\Phi}$. If we are not in the lucky case $\mathcal{F}_{\Phi'} = \mathcal{F}_{\wedge U\Phi}$, there are two ways in which the equality may fail. First, Corollary 2.5 suggests that polarization V and V' must be elements of the appropriate polarization classes, more precisely, $V \in C_{\Sigma}(A)$ and $V' \in C_{\Sigma'}(A)$. However, there is a more subtle obstacle as for $\mathcal{F}_{\Phi'} = \mathcal{F}_{\wedge U\Phi}$ to hold we need to ensure that $\langle \Phi', U\Phi \rangle$ is well-defined, which even for $\ell = \ell'$ and admissible V and V' does need not to be the case. Thus, in general $U\Phi$ and Φ' belong to entirely different infinite wedge spaces as the choice of orthonormal bases encoded in Φ and Φ' was somehow arbitrary. However, let $\Psi : \ell \to \mathcal{H}'$ be another Dirac sea with range $\Psi = V'$, then there is a unitary $R : \ell' \to \ell$ such that $\Phi' = \Psi R$. The action of R gives rise to a unitary operation from the right $\mathcal{R}_R$ characterized by

$$\mathcal{R}_R : \mathcal{F}_{\wedge\Psi} \to \mathcal{F}_{\wedge\Psi R}, \qquad \mathcal{R}_R \wedge\tilde{\Psi} = \wedge(\tilde{\Psi} R) \tag{32}$$

for all $\tilde{\Psi} : \ell \to \mathcal{H}'$ in the generating system of $\mathcal{F}_{\wedge\Psi}$, which connects the infinite wedge spaces $\mathcal{F}_{\wedge\Psi}$ and $\mathcal{F}_{\wedge\Phi'}$. The spaces $\mathcal{F}_{\wedge\Psi}$ and $\mathcal{F}_{\wedge\Phi'}$ coincide if and only if $\ell = \ell'$ and R has a determinant. Slightly more generally, it suffices if R is only *asymptotically* unitary in the sense that R^*R has a non-zero determinant. Then the operation from the right $\det(R^*R)^{-1/2}\mathcal{R}_R$ is unitary. Whether there is a unitary $R : \ell' \to \ell$ in the situation of example (31) above such that $\mathcal{F}_{\wedge U\Phi R} = \mathcal{F}_{\wedge\Phi'}$ is answered by the next theorem. It can be seen as yet another version of the Shale and Stinespring's Theorem:

Theorem 3.1 (Theorem 2.26 of [4]). *Let $\mathcal{H}, \ell, \mathcal{H}', \ell'$ be Hilbert spaces, $V \in \mathtt{Pol}(\mathcal{H})$ and $V' \in \mathtt{Pol}(\mathcal{H}')$ polarizations, $\Phi : \ell \to \mathcal{H}$ and $\Phi' : \ell' \to \mathcal{H}'$ Dirac seas such that* range $\Phi = V$ *and* range $\Phi' = V'$. *Then the following statements are equivalent:*

(a) The off-diagonals $P^{V'^\perp} U P^V$ and $P^{V'} U P^{V^\perp}$ are Hilbert-Schmidt operators.

(b) There is a unitary $R : \ell' \to \ell$ such that $\mathcal{F}_{\wedge\Phi'} = \mathcal{F}_{\wedge U\Phi R}$.

Coming back to the example (31) from above, in the case $V \in C_{\Sigma}(A)$ and $V' \in C_{\Sigma'}(A)$, i.e., that the chosen polarization belong to the admissible classes of polarizations, condition (a) of Theorem 3.1 is fulfilled, which implies the existence of a unitary map $R : V' \to V$ such that the evolution operator

$$\widetilde{U}^A_{V,\Sigma;V'\Sigma'} : \mathcal{F}_{\wedge\Phi} \to \mathcal{F}_{\wedge\Phi'}, \qquad \widetilde{U}^A_{V,\Sigma;V'\Sigma'} = \mathcal{R}_R \circ \mathcal{L}_{U^A_{\Sigma'\Sigma}} \tag{33}$$

is well-defined and unitary. An immediate question is of course how many such maps exist, and it turns out that any other operation from the right $\mathcal{R}_{R'}$ for which $\mathcal{R}_{R'} \circ \mathcal{L}_U : \mathcal{F}_{\wedge\Phi} \to \mathcal{F}_{\wedge\Phi'}$ is well-defined and unitary fulfills $\widetilde{U}^A_{V,\Sigma;V'\Sigma'} = e^{i\theta}\mathcal{R}_{R'} \circ \mathcal{L}_U$ for some $\theta \in \mathbb{R}$; see [4, Corollary 2.28]. Now Φ and Φ' are Dirac seas in which all states in V and V' are occupied, respectively. A canonical choice for their representation is to choose $\ell = V$, $\ell' = V'$, and to define the inclusion maps $\Phi : V \hookrightarrow \mathcal{H}_{\Sigma}$, $\Phi v = v$ for all $v \in V$, and $\Phi' : V' \hookrightarrow \mathcal{H}_{\Sigma'}$, $\Phi' v' = v'$ for all $v' \in V'$. In this case there is a canonical isomorphism between the spaces $\mathcal{F}_{\wedge\Phi}$ and $\mathcal{F}_{V,\Sigma}$ as well as between $\mathcal{F}_{\wedge\Phi'}$ and $\mathcal{F}_{V',\Sigma'}$. Hence, we are again in the situation of Corollary 2.5. We can identify the evolution of the Dirac seas only up to a phase $\theta \in \mathbb{R}$. However, now we have a more direct construction at hand which identifies the involved degrees of freedom:

(a) The choice of particular polarizations $V \in C_\Sigma(A)$ and $V' \in C_{\Sigma'}(A)$.

(b) The choice of particular bases encoded in Φ and Φ'.

The restriction of the polarizations to polarization classes in (a) has been discussed in Section 2. Moreover, choice (b) can be given a quite intuitive picture coming from Dirac's original idea that the motion deep down in the sea should be irrelevant when studying the excitations on its "surface". Clearly, when a sea wave function $\Lambda\Psi \in \mathcal{F}_{\Lambda\Phi}$, which could represent an excitation w.r.t. $\Lambda\Phi$, is evolved from Σ to $\Lambda\Psi'$ on Σ', clearly also the particles deep down in the sea will "move". Since there are infinitely many it will be impossible to directly compare Ψ' with Ψ in general. Writing $U = U^A_{\Sigma'\Sigma}$ in matrix notation

$$U = \begin{pmatrix} U_{++} & U_{+-} \\ U_{-+} & U_{--} \end{pmatrix} = \begin{pmatrix} P^{V'^\perp}_{\Sigma'} U P^{V^\perp}_{\Sigma} & P^{V'^\perp}_{\Sigma'} U P^{V}_{\Sigma} \\ P^{V'}_{\Sigma'} U P^{V^\perp}_{\Sigma} & P^{V'}_{\Sigma'} U P^{V}_{\Sigma} \end{pmatrix}, \tag{34}$$

the motion deep down in the sea is governed by U_{--}. Now, if according to Dirac's original idea the motion deep down in the sea can be considered irrelevant for the behavior of the excitations on its surface one should still be able to compare $\Lambda\Psi'$ to $\Lambda\Psi$ when reversing the motion deep down in the sea with $(U_{--})^{-1}$. If U is for example sufficiently close to the identity this can be done explicitly since then U_{--} has an inverse $R = (U_{--})^{-1}$. As we shall see now, the inversion of the motion deep down in the sea can be implemented by means of an operation from the right $\mathcal{R}_R$. For R to induce an operation from the right it has to be asymptotically orthonormal, i.e., R^*R must have a determinant. Recall that condition (a) in Theorem 3.1 states that the off-diagonals U_{+-} and U_{-+} are Hilbert-Schmidt operators. Thanks to $U^*U = \mathrm{id}_\mathcal{H}$ the identity

$$U^*_{--}U_{--} = \mathrm{id}_V - (U^*)_{-+}U_{+-} \tag{35}$$

holds, and since the product of two Hilbert-Schmidt operators has a trace, one finds $U^*_{--}U_{--} \in \mathrm{id}_V + I_1(V)$. Thus, $U^*_{--}U_{--}$ and then also R^*R have determinants. Note that in general $\det(R^*R) \neq 1$, which implies that $\mathcal{R}_R$ may fail to be unitary up to the factor $\det|R|$. By definition one finds

$$\mathcal{R}_R \circ \mathcal{L}_U \mathcal{F}_{\Lambda\Phi} = \mathcal{F}_{\Lambda U\Phi R} = \mathcal{F}_{\Lambda\Phi'} \tag{36}$$

because $\Phi'^* U\Phi R = P^{V'}(U_{+-} + U_{--})R = \mathrm{id}_{V'}$, and therefore, has a determinant. In consequence, we yield the unitary Dirac evolution

$$\widetilde{U}^A_{V,\Sigma;V'\Sigma'} : \mathcal{F}_{\Lambda\Phi} \to \mathcal{F}_{\Lambda\Phi'}, \quad \widetilde{U}^A_{V,\Sigma;V'\Sigma'} = \det|(U^A_{\Sigma'\Sigma})_{--}|\, \mathcal{R}_{[(U^A_{\Sigma'\Sigma})_{--}]^{-1}} \circ \mathcal{L}_{U^A_{\Sigma'\Sigma}}, \tag{37}$$

which implements both the forward evolution of the whole Dirac sea and the backward evolution of the states deep down in the sea.

4 The charge current and the phase of the evolution operator

Although the construction of the second-quantized evolution operator according to the above program is successful, it fails to identify the phase. This short-coming has no effect on the uniqueness of transition probabilities but it turns out that the charge current depends directly on this phase. One way to see that is from Bogolyubov's formula of the current

$$J^\mu(x) = i\,\widetilde{U}^A_{V_\text{in},\Sigma_\text{in};V_\text{out}\Sigma_\text{out}}\,\frac{\delta}{\delta A_\mu(x)}\,\widetilde{U}^A_{V_\text{out},\Sigma_\text{out};V_\text{in},\Sigma_\text{in}}, \tag{38}$$

where Σ_out is a Cauchy surface in the remote future of the support of A such that $\Sigma_\text{out} \cap \operatorname{supp} A = \emptyset$. Changing the evolution operator by an A-dependent phase generates another summand on the right hand side of (38) by the chain rule. Until some phase is distinguished, (38) has no particular physical meaning as charge current. Nevertheless, all possible currents can be derived from (38) given an evolution operator and a particular phase. Therefore, the situation is better than in standard QED. There, the charge current is a quantity whose formal perturbation series leads to several divergent integrals which have to be taken out by hand until only a logarithmic divergent is left, which in turn is remedied by means of charge renormalization. On the contrary, here, the currents are well-defined and in a sense the correct one only needs to be identified by determining the phase of the evolution operator. As already envisioned in [28] and discussed by [22, 15], this may be done by imposing extra conditions on the evolution operator. One of them is clearly the following property. For any choice of a future oriented foliation of space-time into a family of Cauchy surfaces $(\Sigma_t)_{t\in\mathbb{R}}$ and polarization $V_t \in C_{\Sigma_t}(A)$, $t \in \mathbb{R}$, the assigned phase of the evolution operator $\widetilde{U}^A(t_1,t_0) = \widetilde{U}^A_{\Sigma_{t_1},V_{t_1};\Sigma_{t_0},V_{t_0}}$ constructed in Section 3 should be required to fulfill $\widetilde{U}(t_1,t_0) = \widetilde{U}(t_1,t)\widetilde{U}(t,t_0)$. Other constraints come from the fact that $J^\mu(x)$ must be Lorentz and gauge covariant, and its vacuum expectation value for $A = 0$ should be zero. The hope is that the collection of all such physical constraints restrict the possible currents (38) to a class which can be parametrized by a real number only, the electric charge of the electron. In the case of equal-time hyperplanes one possible choice of the phase was given by Mickelsson via a parallel transport argument [23]. On top of the nice geometric construction and despite the fact that there are still degrees of freedom left, Mickelsson's current agrees with conventional perturbation theory up to second order. The aim of this program is to settle the question which conditions are required to identify the charge current upon changes of the value of the electric charge.

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External Field QED on Cauchy Surfaces for varying Electromagnetic Fields

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Abstract

The Shale-Stinespring Theorem (1965) together with Ruijsenaar's criterion (1977) provide a necessary and sufficient condition for the implementability of the evolution of external field quantum electrodynamics between constant-time hyperplanes on standard Fock space. The assertion states that an implementation is possible if and only if the spatial components of the external electromagnetic four-vector potential A_μ are zero. We generalize this result to smooth, space-like Cauchy surfaces and, for general A_μ, show how the second-quantized Dirac evolution can always be implemented as a map between varying Fock spaces. Furthermore, we give equivalence classes of polarizations, including an explicit representative, that give rise to those admissible Fock spaces. We prove that the polarization classes only depend on the tangential components of A_μ w.r.t. the particular Cauchy surface, and show that they behave naturally under Lorentz and gauge transformations.

1 Introduction and Setup

We consider the external field model of quantum electrodynamics (QED) or no-photon QED which describes a Dirac sea of electrons evolving subject to a prescribed external electromagnetic four-vector potential A_μ. To infer the evolution operator of this model one attempts to implement the one-particle Dirac evolution

$$(i\partial\!\!\!/ - A\!\!\!/)\psi = m\psi \tag{1}$$

in second-quantized form. Here, $m > 0$ denotes the mass of the electron; the elementary charge of the electron e (having a negative sign in the case of an electron) is already absorbed in A; units are chosen such that $\hbar = 1$ and $c = 1$. The employed relativistic notation is introduced with all other notations in Section 1.3. For sake of simplicity we will restrict us to smooth and compactly supported A_μ, i.e.,

$$A = (A_\mu)_{\mu=0,1,2,3} = (A_0, \mathbf{A}) \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4), \tag{2}$$

although this condition is unnecessarily strong.

It is well-known [21, 18] that, on standard Fock space and for equal-time hyperplanes, a second quantization of the one particle Dirac evolution (1) is possible if and only if $\mathbf{A} = 0$, i.e., the spatial components of the external field vanish – a condition that appears strange in view of gauge invariance. In physics the ill-definedness of the evolution operator and its generator for general vector potentials A is usually ignored at first which later manifests itself in the appearance of infinities in informal perturbation series. Those infinities have to be taken out by hand or, as for example in the case of the vacuum expectation value of the charge current, absorbed in the coefficient of the electron charge. Nevertheless, since the sole interaction arises only from a prescribed four-vector field one may rather expect that it should be possible to control the time evolution non-perturbatively. One way to construct a well-defined second-quantized time evolution operator, as sketched in [6], is to implement it between time-varying Fock spaces. Such constructions have been carried out, e.g., in [14, 15, 2]. While the idea of changing Fock spaces might be unfamiliar as seen from the non-relativistic setting, in a relativistic formulation it is to be expected. A Lorentz boost for instance may tilt an equal-time hyperplane to a space-like space-like hyperplane Σ, which requires a change from standard Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^4)$ to one attached to Σ, and likewise, for the corresponding Fock spaces.

In this work we extend the existing constructions in [14, 15, 2], which deal exclusively with equal-time hyperplanes, by implementing the second-quantized Dirac evolution from one Cauchy surface to another. The resulting formulation of external field QED has several advantages: 1) Its Lorentz and gauge covariance can be made explicit; 2) as it treats the initial value problem for general Cauchy surfaces it allows to study the evolution in the form of local deformations of Cauchy surfaces in the spirit of Tomonaga and Schwinger, e.g., [22, 20]; 3) it gives a geometric and more general version of the implementability condition $\mathbf{A} = 0$ that was found in the special case of equal-time hyperplanes.

Before presenting our main results in Section 1.1 we outline the construction of the evolution operator for general space-like Cauchy surfaces. Given a Cauchy surface Σ in Minkowski space-time (see Definition 1.9 below), the states of the Dirac sea on Σ are represented by vectors in a conveniently chosen Fock space, here, denoted by the symbol $\mathcal{F}(V, \mathcal{H}_\Sigma)$. In this notation $\mathcal{H}_\Sigma$ is the Hilbert space of $\mathbb{C}^4$-valued, square integrable functions on Σ (see Definition 1.10 below) and $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ is one of its polarizations:

Definition 1.1. *Let $\mathtt{Pol}(\mathcal{H}_\Sigma)$ denote the set of all closed, linear subspaces $V \subset \mathcal{H}_\Sigma$ such that V and $V^\perp$ are both infinite dimensional. Any $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ is called a* polarization *of $\mathcal{H}_\Sigma$. For $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, let $P^V_\Sigma : \mathcal{H}_\Sigma \to V$ denote the orthogonal projection of $\mathcal{H}_\Sigma$ onto V.*

The Fock space corresponding to polarization V on Cauchy surface Σ is then defined by

$$\mathcal{F}(V, \mathcal{H}_\Sigma) := \bigoplus_{c \in \mathbb{Z}} \mathcal{F}_c(V, \mathcal{H}_\Sigma), \qquad \mathcal{F}_c(V, \mathcal{H}_\Sigma) := \bigoplus_{\substack{n,m \in \mathbb{N}_0 \\ c = m-n}} (V^\perp)^{\wedge n} \otimes \overline{V}^{\wedge m}, \tag{3}$$

where $\bigoplus$ denotes the Hilbert space direct sum, $\wedge$ the antisymmetric tensor product of Hilbert spaces, and $\overline{V}$ denotes the conjugate complex vector space of V, which coincides with V as a set and has the same vector space operations as V with the exception of the scalar multiplication, which is redefined by $(z, \psi) \mapsto z^* \psi$ for $z \in \mathbb{C}$, $\psi \in V$.

Each polarization V splits the Hilbert space $\mathcal{H}_\Sigma$ into a direct sum, i.e., $\mathcal{H}_\Sigma = V^\perp \oplus V$. The so-called standard polarizations $\mathcal{H}_\Sigma^+$ and $\mathcal{H}_\Sigma^-$ are determined by the orthogonal projectors P_Σ^+ and P_Σ^- onto the free positive and negative energy Dirac solutions, respectively, restricted to Σ:

$$\mathcal{H}_\Sigma^+ := P_\Sigma^+ \mathcal{H}_\Sigma = (1 - P_\Sigma^-)\mathcal{H}_\Sigma, \qquad \mathcal{H}_\Sigma^- := P_\Sigma^- \mathcal{H}_\Sigma. \tag{4}$$

Loosely speaking, in terms of Dirac's hole theory, the polarization $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ indicates the "sea level" of the Dirac sea, and electron wave functions in $V^\perp$ and V are considered to be "above" and "below" sea level, respectively. However, it has to be stressed that the mathematical structure of the external field problem in QED does not seem to discriminate between particular choices of polarizations V. Hence, unless an additional physical condition is delivered, the V-dependent labels "electron" and "positron" are somewhat arbitrary, and V should rather be regarded as a choice of coordinate system w.r.t. which the states of the Dirac sea are represented. To describe pair-creation on the other hand it is necessary to have a distinguished V, and the common (and seemingly most natural) ad hoc choice in situations when the external field vanishes is $V = \mathcal{H}_\Sigma^-$. Nevertheless, it is conceivable that only a yet to be found full version of QED, including the interaction with the photon field, may distinguish particular polarizations V in general situations.

Given two Cauchy surfaces Σ, Σ' and two polarizations $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ and $W \in \mathtt{Pol}(\mathcal{H}_{\Sigma'})$ a sensible lift of the one-particle Dirac evolution $U^A_{\Sigma'\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$ (see Definition 1.13) should be given by a unitary operator $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ that fulfills

$$\widetilde{U}^A_{\Sigma'\Sigma}\, \psi_{V,\Sigma}(f)\, (\widetilde{U}^A_{\Sigma'\Sigma})^{-1} = \psi_{W,\Sigma'}(U^A_{\Sigma'\Sigma} f), \qquad \forall\, f \in \mathcal{H}_\Sigma. \tag{5}$$

Here, $\psi_{V,\Sigma}$ denotes the Dirac field operator corresponding to Fock space $\mathcal{F}(V, \Sigma)$, i.e.,

$$\psi_{V,\Sigma}(f) := b_\Sigma(P_\Sigma^{V^\perp} f) + d_\Sigma^*(P_\Sigma^V f), \qquad \forall\, f \in \mathcal{H}_\Sigma. \tag{6}$$

Here, b_Σ, d^*_Σ denote the annihilation and creation operators on the $V^\perp$ and $\overline{V}$ sectors of $\mathcal{F}_c(V, \mathcal{H}_\Sigma)$, respectively. Note that $P_\Sigma^V : \mathcal{H} \to \overline{V}$ is *anti-linear*; thus, $\psi_{V,\Sigma}(f)$ is anti-linear in its argument f. The condition under which such a lift $\widetilde{U}^A_{\Sigma'\Sigma}$ exists can be inferred from a straight-forward application of Shale and Stinespring's well-known theorem [21]:

Theorem 1.2 (Shale-Stinespring)**.** *The following statements are equivalent:*

(a) There is a unitary operator $\widetilde{U}^A_{\Sigma\Sigma'} : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ *which fulfills* (5).

(b) The off-diagonals $P_{\Sigma'}^{W^\perp} U^A_{\Sigma'\Sigma} P_\Sigma^V$ *and* $P_{\Sigma'}^{W} U^A_{\Sigma'\Sigma} P_\Sigma^{V^\perp}$ *are Hilbert-Schmidt operators.*

Note that the phase of the lift is not fixed by condition (5). Even worse, as indicated earlier, depending on the external field A this condition is not always satisfied; see [18]. On the other hand, the choices made for the polarizations V and W were completely arbitrary. We shall see next that adapting these choices carefully will however yield an evolution of the Dirac sea in the corresponding Fock space representations.

There is a trivial but not so useful choice. Pick a Σ_{in} in the remote past of the support of A fulfilling

$$\Sigma_{\text{in}} \text{ is a Cauchy surface such that } \operatorname{supp} A \cap \Sigma_{\text{in}} = \emptyset. \tag{7}$$

Then the choices $V = U^A_{\Sigma\Sigma_{\text{in}}}\mathcal{H}^-_{\Sigma_{\text{in}}}$ and $W = U^A_{\Sigma'\Sigma_{\text{in}}}\mathcal{H}^-_{\Sigma_{\text{in}}}$ fulfill (b) of Theorem 1.2 as the off-diagonals are zero. The drawback of these choices is that the resulting lift depends on the whole history of A between Σ_{in} and Σ, Σ'. Moreover, such V and W are rather implicit. But statement (b) in Theorem 1.2 also allows to differ from the projectors P^V_Σ and $P^W_{\Sigma'}$ by a Hilbert-Schmidt operator. Hence, it lies near to characterize polarizations according to the following classes:

Definition 1.3 (Physical Polarization Classes)**.** *For a Cauchy surface Σ we define*

$$\mathcal{C}_\Sigma(A) := \left[U^A_{\Sigma\Sigma_{\text{in}}}\mathcal{H}^-_{\Sigma_{\text{in}}}\right]_\approx, \tag{8}$$

where for $V, V' \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, $V \approx V'$ means that $P^V_\Sigma - P^{V'}_\Sigma \in I_2(\mathcal{H}_\Sigma)$, i.e., is a Hilbert-Schmidt operator $\mathcal{H}_\Sigma \circlearrowleft$.

The equivalence relation $\approx$ can be refined to give another equivalence relation $\approx_0$ describing polarization classes of equal charge; c.f. [2] and Remark 1.8. As a simple corollary of Theorem 1.2 one gets:

Corollary 1.4 (Dirac Sea Evolution)**.** *Let Σ, Σ' be Cauchy surfaces. Then any choice $V \in \mathcal{C}_\Sigma(A)$ and $W \in \mathcal{C}_{\Sigma'}(A)$ implies condition (b) of Theorem 1.2 and therefore the existence of a lift $\widetilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ obeying (5).*

Consequently, any choice $V \in \mathcal{C}_\Sigma(A)$ and $W \in \mathcal{C}_{\Sigma'}(A)$ gives rise to a lift of the one-particle Dirac evolution between the corresponding $\mathcal{F}(V, \mathcal{H}_\Sigma)$ and $\mathcal{F}(W, \mathcal{H}_{\Sigma'})$ that is unique up to a phase. The crucial questions are: 1) On which properties of A and Σ do these polarization classes depend? 2) How do they behave under Lorentz and gauge transforms? 3) Is there an explicit representative for each class? These question will be answered by our main results given in the next section. The next important question is about the unidentified phase. Although transition probabilities are independent of this phase, dynamic quantities like the charge current will depend directly on it. We briefly discuss this in Section 1.2 and give an outlook of what needs to be done to derive the vacuum expectation of the polarization current.

1.1 Main Results

The definition (8) of the physical polarization classes involves the one-particle Dirac evolution operator and is therefore not very useful in finding an explicit description of admissible Fock spaces for the implementation of the second-quantized Dirac evolution. In our main results Theorems 1.5-1.7 we give a more direct identification of the polarization classes classes $\mathcal{C}_\Sigma(A)$ and state some of their fundamental geometric properties.

The first one ensures that the classes $\mathcal{C}_\Sigma(A)$ are independent of the history of A, instead they depend on the tangential components of A on Σ only.

Theorem 1.5 (Identification of Polarization Classes)**.** *Let Σ be a Cauchy surface and let A and $\widetilde{A}$ be two smooth and compactly supported external fields. Then*

$$\mathcal{C}_\Sigma(A) = \mathcal{C}_\Sigma(\widetilde{A}) \qquad \Leftrightarrow \qquad A|_{T\Sigma} = \widetilde{A}|_{T\Sigma} \tag{9}$$

where $A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}$ means that for all $x \in \Sigma$ and $y \in T_x\Sigma$ we have $A_\mu(x)y^\mu = \widetilde{A}_\mu(x)y^\mu$.

Ruijsenaar's result, see [18], may be viewed as the special case of this theorem pertaining to $\widetilde{A} = 0$ and, for t fixed, $\Sigma = \Sigma_t = \{x \in \mathbb{R}^4 | \, x^0 = t\}$ being an equal-time hyperplane.

Furthermore, the polarization classes transform naturally under Lorentz and gauge transformations:

Theorem 1.6 (Lorentz and Gauge Transforms)**.** *Let $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ be a polarization.*

(i) Consider a Lorentz transformation *given by $L_\Sigma^{(S,\Lambda)} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Lambda\Sigma}$ for a spinor transformation matrix $S \in \mathbb{C}^{4\times 4}$ and an associated proper orthochronous Lorentz transformation matrix $\Lambda \in \mathrm{SO}^\uparrow(1,3)$, cf. [3, Section 2.3]. Then:*

$$V \in \mathcal{C}_\Sigma(A) \qquad \Leftrightarrow \qquad L_\Sigma^{(S,\Lambda)} V \in \mathcal{C}_{\Lambda\Sigma}(\Lambda A(\Lambda^{-1}\cdot)). \tag{10}$$

(ii) Consider a gauge transformation *$A \mapsto A + \partial\Omega$ for some $\Omega \in C_c^\infty(\mathbb{R}^4, \mathbb{R})$ given by the multiplication operator $e^{-i\Omega} : \mathcal{H}_\Sigma \to \mathcal{H}_\Sigma$, $\psi \mapsto \psi' = e^{-i\Omega}\psi$. Then:*

$$V \in \mathcal{C}_\Sigma(A) \qquad \Leftrightarrow \qquad e^{-i\Omega} V \in \mathcal{C}_\Sigma(A + \partial\Omega). \tag{11}$$

As we are mainly interested in a *local* study of the second-quantized Dirac evolution, we only allow compactly supported vector potentials A, and therefore, have to restrict the gauge transformations $e^{-i\Omega}$ to compactly supported Ω as well. Treating more general vector potentials A and gauge transforms $e^{-i\Omega}$ would require an analysis of decay properties at infinity which is not our focus here.

Finally, given Cauchy surface Σ, there is an explicit representative of the equivalence class of polarizations $\mathcal{C}_\Sigma(A)$ which can be given in terms of a compact, skew-adjoint linear operator $Q_\Sigma^A : \mathcal{H}_\Sigma \circlearrowleft$, as defined in (56) below. With it the polarization class can be identified as follows:

Theorem 1.7. *Given Cauchy surface Σ, we have $\mathcal{C}_\Sigma(A) = \left[e^{Q_\Sigma^A} \mathcal{H}_\Sigma^- \right]_\approx$.*

Other representatives for polarization classes $\mathcal{C}_\Sigma(A)$ beyond the "interpolating representation" $U_{\Sigma\Sigma_{\mathrm{in}}}^A \mathcal{H}_{\Sigma_{\mathrm{in}}}^-$, as used in Definition 1.3, can be inferred from the so-called Furry picture, as worked out for equal-time hyperplanes in [6], and from the global constructions of the fermionic projector given in [11, 10]. In contrast to global constructions, the representation given in Theorem 1.7 uses only *local* geometric information of the vector potential A at Σ; cf. (56), (39), and Lemma 2.3 below.

The implications on the physical picture can be seen as follows. The Dirac sea on Cauchy surface Σ can be described in any Fock space $\mathcal{F}(V, \mathcal{H}_\Sigma)$ for any choice of polarization $V \in \mathcal{C}_\Sigma(A)$. The polarization class $\mathcal{C}_\Sigma(A)$ is uniquely determined by the tangential components of the external potential A on Σ. This is an object that transforms covariantly under Lorentz and gauge transformations. The choice of the particular polarization can then be seen as a "choice of coordinates" in which the Dirac sea is described. When regarding the Dirac evolution from one Cauchy surface Σ to Σ' another "choice of coordinates" $W \in \mathcal{C}_{\Sigma'}(A)$ has to be made. Then one yields an evolution operator $\widetilde{U}_{\Sigma'\Sigma}^A : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ which is unique up to an arbitrary phase Corollary 1.4. Transition probabilities of the kind $|\langle \Psi, \widetilde{U}_{\Sigma'\Sigma}^A \Phi \rangle|^2$ for $\Psi \in \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ and $\Phi \in \mathcal{F}(V, \mathcal{H}_\Sigma)$ are well-defined and unique without the need of a renormalization method. Finally, for a family of Cauchy surfaces $(\Sigma_t)_{t\in\mathbb{R}}$ that interpolates smoothly between Σ and Σ' we also give an infinitesimal version of how the external potential A changes the polarization in terms of the flow parameter t; see Theorem 2.8 below.

Remark 1.8 (Charge Sectors)**.** *Given two polarizations $V, W \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ such that $P_\Sigma^V - P_\Sigma^W$ is a compact operator, e.g., as in the case $V \approx W$ as defined in (8), one can define their relative charge, denoted by* $\mathrm{charge}(V,W)$*, to be the Fredholm index of $P_\Sigma^W|_{V\to W}$; cf. [2]. The equivalence relation $\approx$ in the claim of Theorem 1.7 can then be replaced by the finer equivalence relation $\approx_0$, which is defined as follows: $V \approx_0 W$ if and only if $V \approx W$ and* $\mathrm{charge}(V,W) = 0$*. This is shown as an addendum to the proof of Theorem 1.7.*

1.2 Outlook

As indicated at the end of the introduction the current operator depends directly on the unspecified phase of $\widetilde{U}^A_{\Sigma'\Sigma}$. This can be seen from Bogolyubov's formula

$$j^\mu(x) = i\widetilde{U}^A_{\Sigma_{\rm in}\Sigma_{\rm out}} \frac{\delta \widetilde{U}^A_{\Sigma_{\rm out}\Sigma_{\rm in}}}{\delta A_\mu(x)} \tag{12}$$

where $\Sigma_{\rm out}$ is a Cauchy surfaces in the remote future of the support of A such that $\Sigma_{\rm out} \cap \operatorname{supp} A = \emptyset$. Hence, without identification of the derivative of the phase of $\widetilde{U}^A_{\Sigma'\Sigma}$ the physical current is not fully specified. Nevertheless, now the situation is slightly better than in the standard perturbative approach. As for each choice of admissible polarizations in $\mathcal{C}_{\Sigma'}(A)$ and $\mathcal{C}_\Sigma(A)$, identified above, there is a well-defined lift $\widetilde{U}^A_{\Sigma'\Sigma}$ of the Dirac evolution operator $U^A_{\Sigma'\Sigma}$ and therefore also a well-defined current (12). Now it is only the task to select the physical relevant one. One way of doing so is to impose extra conditions on the (12), and hence, the phase, so that the set of admissible phases shrinks to one that produces the same currents up to the known freedom of charge renormalization; see [5, 19, 15, 12]. In the case of equal-time hyperplanes a choice of the unidentified phase was given by parallel transport in [16]. On top of the geometric construction and despite the fact that there are still degrees of freedom left, Mickelsson's current is particularly interesting because it agrees with conventional perturbation theory up to second order. Yet the open question remains which additional physical requirements may constraint these degree of freedoms up to the one of the numerical value of the elementary charge e fixed by the experiment.

The issue of the unidentified phase particularly concerns the so-called phenomenon of "vacuum polarization" as well as the dynamical description of pair creation processes for which only a few rigorous treatments are available; e.g., see [13] for vacuum polarization in the Hartree-Fock approximation for static external sources, [17] for adiabatic pair creation, and for a more fundamental approach the so-called "Theory of Causal Fermion Systems" [7, 8, 9], which is based on a reformulation of quantum electrodynamics by means of an action principle.

1.3 Definitions, Constants, Notation, and previous Results

In this section we briefly review the notation and results about the one-particle Dirac evolution on Cauchy surfaces provided in a previous work [3]. The present article, dealing with the second-quantization Dirac evolution, is based on this work.

Space-time $\mathbb{R}^4$ is endowed with metric tensor $g = (g_{\mu\nu})_{\mu,\nu=0,1,2,3} = \text{diag}(1,-1,-1,-1)$, and its elements are denoted by four-vectors $x = (x^0, x^1, x^2, x^3) = (x^0, \mathbf{x}) = x^\mu e_\mu$, for e_μ being the canonical basis vectors. Raising and lowering of indices is done w.r.t. g. Moreover, we use Einstein's summation convention, the standard representation of the Dirac matrices $\gamma^\mu \in \mathbb{C}^{4\times 4}$ that fulfill $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$, and Feynman's slash-notation $\partial\!\!\!/ = \gamma^\mu \partial_\mu$, $A\!\!\!/ = \gamma^\mu A_\mu$. When considering subsets of space-time $\mathbb{R}^4$ we shall use the following notations: Causal := $\{x \in \mathbb{R}^4 |\ x_\mu x^\mu \geqslant 0\}$ and Past := $\{x \in \mathbb{R}^4 |\ x_\mu x^\mu > 0, x^0 < 0\}$.

The central geometric objects for posing the initial value problem for (1) are Cauchy surfaces defined as follows:

Definition 1.9 (Cauchy Surfaces)**.** *We define a Cauchy surface Σ in $\mathbb{R}^4$ to be a smooth, 3-dimensional submanifold of $\mathbb{R}^4$ that fulfills the following three conditions:*

(a) Every inextensible, two-sided, time- or light-like, continuous path in $\mathbb{R}^4$ intersects Σ in a unique point.

(b) For every $x \in \Sigma$, the tangential space $T_x\Sigma$ is space-like.

(c) The tangential spaces to Σ are bounded away from light-like directions in the following sense: The only light-like accumulation point of $\bigcup_{x\in\Sigma} T_x\Sigma$ is zero.

In coordinates, every Cauchy surface Σ can be parametrized as

$$\Sigma = \{\pi_\Sigma(\mathbf{x}) := (t_\Sigma(\mathbf{x}), \mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^3\} \tag{13}$$

with a smooth function $t_\Sigma : \mathbb{R}^3 \to \mathbb{R}$. For convenience and without restricting generality of our results we keep a global constant

$$0 < V_{\max} < 1 \tag{14}$$

fixed and work only with Cauchy surfaces Σ such that

$$\sup_{\mathbf{x}\in\mathbb{R}^3} |\nabla t_\Sigma(\mathbf{x})| \leqslant V_{\max}. \tag{15}$$

The assumption (c) in Definition 1.9 and (15) can be relaxed to $|\nabla t_\Sigma(\mathbf{x})| < 1$ for all $\mathbf{x} \in \mathbb{R}^3$ due to the causal structure of the solutions to the Dirac equation, although this is not worked out in this paper.

The standard volume form over $\mathbb{R}^4$ is denoted by $d^4x = dx^0\, dx^1\, dx^2\, dx^3$; the product of forms is understood as wedge product. The symbols d^3x and $d^3\mathbf{x}$ mean the 3-form $d^3x = dx^1\, dx^2\, dx^3$ on $\mathbb{R}^4$ and on $\mathbb{R}^3$, respectively. Contraction of a form ω with a vector v is denoted by $i_v(\omega)$. The notation $i_v(\omega)$ is also used for the spinor matrix valued vector $\gamma = (\gamma^0, \gamma^1, \gamma^2, \gamma^3) = \gamma^\mu e_\mu$:

$$i_\gamma(d^4x) = \gamma^\mu i_{e_\mu}(d^4x). \tag{16}$$

Furthermore, for a 4-spinor $\psi \in \mathbb{C}^4$ (viewed as column vector), $\overline{\psi}$ stands for the row vector $\psi^*\gamma^0$, where * denotes hermitian conjugation.

Smooth families $(\Sigma_t)_{t\in T}$ of Cauchy surfaces, indexed by an interval $T \subseteq \mathbb{R}$ and fulfilling (15), are denoted by

$$\mathbf{\Sigma} := \{(x,t) |\ t \in T,\ x \in \Sigma_t\}. \tag{17}$$

Given the external electromagnetic vector potential $A \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4)$ of interest, we assume that the set $\{(x,t) \in \mathbf{\Sigma} |\ x \in \operatorname{supp}(A)\}$ is compact. This condition is trivially fulfilled in the important case of a compact interval $T = [t_0, t_1]$ with $\mathbf{\Sigma}$ interpolating between two Cauchy surfaces Σ_{t_0} and Σ_{t_1}. The compactness condition is also automatically fulfilled in the case that $T = \mathbb{R}$ with $\mathbf{\Sigma}$ being a smooth foliation of the Minkowski space-time $\mathbb{R}^4$.

We assume furthermore that the family $(\Sigma_t)_{t\in T}$ is driven driven by a (Minkowski) normal vector field $vn : \mathbf{\Sigma} \to \mathbb{R}^4$, where $n : \mathbf{\Sigma} \to \mathbb{R}^4$, $(x,t) \mapsto n_t(x)$, denotes the future-directed (Minkowski) normal unit vector field to the Cauchy surfaces and $v : \mathbf{\Sigma} \to \mathbb{R}$, $(x,t) \mapsto v_t(x)$, denotes the speed at which the Cauchy surfaces move forward in normal direction. For technical reasons, in particular when using the chain rule, it is convenient to extend the "speed" v and the unit vector field n in a smooth way to the domain $\mathbb{R}^4 \times T$. In the case that $\mathbf{\Sigma}$ is a foliation of space-time, we may even drop the t–dependence of v and n. In this important case, some of the arguments below become slightly simpler.

Definition 1.10 (Spaces of Initial Data)**.** *For any Cauchy surface Σ we define the vector space $\mathcal{C}_\Sigma := C_c^\infty(\Sigma, \mathbb{C}^4)$. For a given Cauchy surface Σ, let $\mathcal{H}_\Sigma = L^2(\Sigma, \mathbb{C}^4)$ denote the vector space of all 4-spinor valued measurable functions $\phi : \Sigma \to \mathbb{C}^4$ (modulo changes on null sets) having a finite norm $\|\phi\| = \sqrt{\langle\phi,\phi\rangle} < \infty$ w.r.t. the scalar product*

$$\langle\phi,\psi\rangle = \int_\Sigma \overline{\phi(x)} i_\gamma(d^4x)\psi(x). \tag{18}$$

For $x \in \Sigma$, the restriction of the spinor matrix valued 3-form $i_\gamma(d^4x)$ to the tangential space $T_x\Sigma$ is given by

$$i_\gamma(d^4x) = \not{n}(x) i_n(d^4x) = \left(\gamma^0 - \sum_{\mu=1}^{3} \gamma^\mu \frac{\partial t_\Sigma(\mathbf{x})}{\partial x^\mu}\right) d^3x =: \Gamma(\mathbf{x}) d^3x \text{ on } (T_x\Sigma)^3. \tag{19}$$

As a consequence of the (15), there is a positive constant $\Gamma_{\max} = \Gamma_{\max}(V_{\max})$ such that

$$\|\Gamma(\mathbf{x})\| \leqslant \Gamma_{\max}, \qquad \forall\, \mathbf{x} \in \mathbb{R}^3. \tag{20}$$

The class of solutions to the Dirac equation (1) considered in this work is defined by:

Definition 1.11 (Solution Spaces)**.**

(i) Let $\mathcal{C}_A$ denote the space of all smooth solutions $\psi \in C^\infty(\mathbb{R}^4, \mathbb{C}^4)$ of the Dirac equation (1) which have a spatially compact causal support in the following sense: There is a compact set $K \subset \mathbb{R}^4$ such that $\operatorname{supp}\psi \subseteq K + \text{Causal}$.

(ii) We endow $\mathcal{C}_A$ with the scalar product given in (18); note that due to conservation of the 4-vector current $\overline{\phi}\gamma^\mu\psi$, the scalar product $\langle\cdot,\cdot\rangle : \mathcal{C}_A \times \mathcal{C}_A \to \mathbb{C}$ is independent of the particular choice of Σ.

(iii) Let $\mathcal{H}_A$ be the Hilbert space given by the (abstract) completion of $\mathcal{C}_A$.

Theorem 2.21 in [3] ensures:

Theorem 1.12 (Initial Value Problem and Support)**.** *Let Σ be a Cauchy surface and $\chi_\Sigma \in \mathcal{C}_c^\infty(\Sigma, \mathbb{C}^4)$ be given initial data. Then, there is a $\psi \in \mathcal{C}_A$ such that $\psi|_\Sigma = \chi_\Sigma$ and $\operatorname{supp}\psi \subseteq \operatorname{supp}\chi_\Sigma + \text{Causal}$. Moreover, suppose $\widetilde{\psi} \in C^\infty(\mathbb{R}^4, \mathbb{C}^4)$ solves the Dirac equation (1) for initial data $\widetilde{\psi}|_\Sigma = \chi_\Sigma$, then $\widetilde{\psi} = \psi$.*

This theorem gives rise to the following definition in which we use the notation $\psi|_\Sigma \in \mathcal{C}_\Sigma$ to denote the restriction of a $\psi \in \mathcal{C}_A$ to a Cauchy surface Σ.

Definition 1.13 (Evolution Operators)**.** *Let Σ, Σ' be Cauchy surfaces. In view of Theorem 1.12 we define the isomorphic isometries*

$$\begin{aligned} &U_{\Sigma A} : \mathcal{C}_A \to \mathcal{C}_\Sigma, && U_{\Sigma A}\,\phi := \phi|_\Sigma, \\ &U_{A\Sigma} : \mathcal{C}_\Sigma \to \mathcal{C}_A, && U_{\Sigma A}\,\chi_\Sigma := \psi, \\ &U^A_{\Sigma'\Sigma} : \mathcal{C}_\Sigma \to \mathcal{C}_{\Sigma'}, && U^A_{\Sigma'\Sigma} := U_{\Sigma' A} U_{A\Sigma}, \end{aligned} \tag{21}$$

where $\chi_\Sigma \in \mathcal{C}_\Sigma$, $\phi \in \mathcal{C}_A$, and ψ is the solution corresponding to initial value χ_Σ as in Theorem 1.12. These maps extend uniquely to unitary maps $U_{A\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_A$, $U_{\Sigma A} : \mathcal{H}_A \to \mathcal{H}_\Sigma$ and $U^A_{\Sigma'\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$.

Here we differ from the notation used in Theorem 2.23 in [3] where $U^A_{\Sigma'\Sigma}$ was denoted by $\mathcal{F}^A_{\Sigma'\Sigma}$. Furthermore, it will be useful to express the orthogonal projector P^-_Σ in an momentum integral representation over the mass shell

$$\mathcal{M} = \{p \in \mathbb{R}^4 |\ p_\mu p^\mu = m^2\} = \mathcal{M}_+ \cup \mathcal{M}_-, \qquad \mathcal{M}_\pm = \{p \in \mathcal{M} |\ \pm p^0 > 0\}; \tag{22}$$

cf. Lemma 2.1 and the definition of $\mathcal{F}_{\mathcal{M}\Sigma}$ in [3]. We endow $\mathcal{M}$ with the orientation that makes the projection $\mathcal{M} \to \mathbb{R}^3$, $(p^0, \mathbf{p}) \mapsto \mathbf{p}$ positively oriented. One finds that

$$i_p(d^4p) = \frac{m^2}{p^0} dp^1\, dp^2\, dp^3 = \frac{m^2}{p^0} d^3p \text{ on } (T_p\mathcal{M})^3. \tag{23}$$

General Notation. Positive constants and remainder terms are denoted by $C_1, C_2, C_3, \ldots$ and $r_1, r_2, r_3, \ldots$, respectively. They keep their meaning throughout the whole article. Any fixed quantity a constant depends on (except numerical constants like electron mass m and charge e) is displayed at least once when the constant is introduced. Furthermore, we classify the behavior of functions using the following variant of the Landau symbol notation.

Definition 1.14. *For lists of variables x, y, z we use the notation*

$$f(x, y, z) = O_y\left(g(x)\right), \qquad \textit{for all } (x, y, z) \in \text{domain} \tag{24}$$

to mean the following: There exists a constant $C(y)$ depending only on the parameters y, but neither on x nor on z, such that

$$|f(x, y, z)| \leqslant C(y)|g(x)|, \qquad \textit{for all } (x, y, z) \in \text{domain}, \tag{25}$$

where $|\cdot|$ stands for the appropriate norm applicable to f. Note that the notation (24) does not mean that $f(x, y, z) = f(x, y)$, i.e., that the value of f is independent of z. Rather, it just means that the bound is uniform in z.

2 Proofs

The key idea in the proofs of our main results Theorem 1.5, 1.6, and 1.7 is to guess a simple enough operator $P^A_\Sigma : \mathcal{H}_\Sigma \circlearrowleft$ so that

$$U^A_{\Sigma\Sigma_{\text{in}}} P^-_{\Sigma_{\text{in}}} U^A_{\Sigma_{\text{in}}\Sigma} - P^A_\Sigma \in I_2(\mathcal{H}_\Sigma). \tag{26}$$

It turns out that all claims about the properties of the polarization classes $\mathcal{C}_\Sigma(A)$ above can then be inferred from the properties of P^A_Σ. This is due to the fact that (26) is compatible with the Hilbert-Schmidt operator freedom encoded in the $\approx$ equivalence relation that was used to define the polarization classes $\mathcal{C}_\Sigma(A)$; see Definition 1.3.

The intuition behind our guess of P^A_Σ comes from gauge transforms. Imagine the special situation in which an external potential A could be gauged to zero, i.e., $A = \partial\Omega$ for a given scalar field Ω. In this case $e^{-i\Omega}P^-_\Sigma e^{i\Omega}$ is a good candidate for P^A_Σ. Now in the case of general external potentials A that cannot be attained by a gauge transformation of the zero potential, the idea is to implement different gauge transforms locally near to each space-time point. For example, if $p^-(y-x)$ denotes the informal integral kernel of the operator P^-_Σ, one could try to define P^A_Σ as the operator corresponding to the informal kernel $p^A(x,y) = e^{-i\lambda^A(x,y)}p^-(y-x)$ for the choice $\lambda^A(x) = \frac{1}{2}(A(x) + A(y))_\mu(y-x)^\mu$. Due to this choice, the action of $\lambda^A(x,y)$ can be interpreted as a local gauge transform of $p^-(y-x)$ from the zero potential to the potential $A_\mu(x)$ at space-time point x. It turns out that these local gauge transforms give rise to an operator P^A_Σ that fulfills (26).

Section Overview In Section 2.1 we define the operators P^-_Σ and P^A_Σ and state their main properties. Assuming these properties we prove our main results in Section 2.2. The proofs of those employed properties are delivered afterwards in Sections 2.3 and 2.4.

2.1 The Operators P^-_Σ and P^A_Σ

As described in the previous section, the central objects of our study are the operators P^-_Σ and operators which are derived from them like the discussed P^A_Σ. Lemma 2.1 describes the integral representation of the orthogonal projector P^-_Σ. For this we introduce the notation

$$r(w) := \sqrt{-w_\mu w^\mu} \quad \text{for} \quad w \in \text{domain}(r) := \{w \in \mathbb{C}^4 | \; -w_\mu w^\mu \in \mathbb{C}\backslash\mathbb{R}^-_0\}. \tag{27}$$

The square root is interpreted as its principal value $\sqrt{r^2 e^{2i\varphi}} = re^{i\varphi}$ for $r > 0$, $-\frac{\pi}{2} < \varphi < \frac{\pi}{2}$. We note that for a Cauchy surface Σ fulfilling (15) and $0 \neq z = y - x$ with $x, y \in \Sigma$ one has

$$\sqrt{1 - {V_{\max}}^2}|\mathbf{z}| \leqslant r(z) \leqslant |\mathbf{z}| \leqslant |z| \leqslant \sqrt{1 + {V_{\max}}^2}|\mathbf{z}|. \tag{28}$$

To deal with the singularity of the informal integral kernel $p^-(y-x)$ of the projection operator P^-_Σ at the diagonal $x = y$, we use a regularization shifting the argument $y - x$ a little in direction of the imaginary past.

Lemma 2.1. *For $\phi, \psi \in \mathcal{C}_\Sigma$ and any past-directed time-like vector $u \in$ Past one has*

$$\left\langle \phi, P^-_\Sigma \psi \right\rangle = \lim_{\epsilon \downarrow 0} \int_{x\in\Sigma} \overline{\phi}(x)\, i_\gamma(d^4x) \int_{y\in\Sigma} p^-(y - x + i\epsilon u)\, i_\gamma(d^4y)\, \psi(y), \tag{29}$$

where

$$p^- : \mathbb{R}^4 + i\,\mathrm{Past} \to \mathbb{C}^{4x4}, \quad p^-(w) = \frac{1}{(2\pi)^3 m}\int_{\mathcal{M}_-} \frac{\not{p}+m}{2m} e^{ipw}\, i_p(d^4p) = \frac{-i\not{\partial}+m}{2m} D(w), \quad (30)$$

$$D : \mathbb{R}^4 + i\,\mathrm{Past} \to \mathbb{C}, \quad D(w) = \frac{1}{(2\pi)^3 m}\int_{\mathcal{M}_-} e^{ipw}\, i_p(d^4p) = -\frac{m^3}{2\pi^2}\frac{K_1(mr(w))}{mr(w)}, \quad (31)$$

$$K_1 : \mathbb{R}^+ + i\mathbb{R} \to \mathbb{C}, \qquad K_1(\xi) = \xi \int_1^\infty e^{-\xi s}\sqrt{s^2-1}\, ds. \quad (32)$$

K_1 is the modified Bessel function of second kind of order one. The functions D and p^- have analytic continuations defined on domain(r)*. The corresponding continuations are denoted by the same symbols.*

The proof is given in Section 2.3. It is based on the momentum integral representation given in Theorem 2.15 in [3]. In the following we define several candidates for P^A_Σ fulfilling the key property (26) as discussed in the beginning of Section 2. We will denote these operators by $P^\lambda_\Sigma : \mathcal{H}_\Sigma \circlearrowleft$ where the superscript λ denotes an element out of the following class of "local" gauge functions:

Definition 2.2. *For $A \in C^\infty_c(\mathbb{R}^4, \mathbb{R}^4)$ let $\mathcal{G}(A)$ denote the set of all functions $\lambda : \mathbb{R}^4 \times \mathbb{R}^4 \to \mathbb{R}$ with the following properties:*

(i) $\lambda \in C^\infty(\mathbb{R}^4 \times \mathbb{R}^4, \mathbb{R})$.

(ii) There is a compact set $K \subset \mathbb{R}^4$ such that $\operatorname{supp}\lambda \subseteq K \times \mathbb{R}^4 \cup \mathbb{R}^4 \times K$.

(iii) λ vanishes on the diagonal, i.e., $\lambda(x,x) = 0$ for $x \in \mathbb{R}^4$.

(iv) On the diagonal the first derivatives fulfill

$$\partial^x \lambda(x,y) = -\partial^y \lambda(x,y) = A(x) \qquad \text{for } x = y \in \mathbb{R}^4. \quad (33)$$

Given a "local" gauge transform $\lambda \in \mathcal{G}(A)$ we define the corresponding operator P^λ_Σ using the heuristic idea behind P^A_Σ we discussed in the beginning of Section 2.

Lemma 2.3. *Given $A \in C^\infty_c(\mathbb{R}^4, \mathbb{R}^4)$ and $\lambda \in \mathcal{G}(A)$ there is a unique bounded operator $P^\lambda_\Sigma : \mathcal{H}_\Sigma \circlearrowleft$ with matrix elements*

$$\left\langle \phi, P^\lambda_\Sigma \psi \right\rangle = \lim_{\epsilon \downarrow 0} \left\langle \phi, P^{\lambda,\epsilon u}_\Sigma \psi \right\rangle \ \text{ with} \quad (34)$$

$$\left\langle \phi, P^{\lambda,\epsilon u}_\Sigma \psi \right\rangle := \int_{x\in\Sigma} \overline{\phi}(x)\, i_\gamma(d^4x) \int_{y\in\Sigma} e^{-i\lambda(x,y)} p^-(y - x + i\epsilon u)\, i_\gamma(d^4y)\, \psi(y). \quad (35)$$

for any given $\phi, \psi \in \mathcal{C}_\Sigma$ and any past-directed time-like vector $u \in$ Past. In particular, the limit in (34) does not depend on the choice of $u \in$ Past. For $\Delta P^\lambda_\Sigma := P^\lambda_\Sigma - P^-_\Sigma$, $\psi \in \mathcal{H}_\Sigma$, and almost all $x \in \Sigma$ it holds

$$\left(\Delta P^\lambda_\Sigma \psi\right)(x) = \int_{y\in\Sigma} (e^{-i\lambda(x,y)} - 1) p^-(y-x)\, i_\gamma(d^4y)\, \psi(y), \quad (36)$$

and furthermore:

(i) The operator norm of P_Σ^λ is bounded by a constant $C_1(V_{\max}, \lambda)$; cf. (15)*;*

(ii) ΔP_Σ^λ is a compact operator;

(iii) $|\Delta P_\Sigma^\lambda|^2$ is a Hilbert-Schmidt operator.

(iv) If $\lambda(x,y) = -\lambda(y,x)$ for all $x, y \in \Sigma$, then P_Σ^λ is self-adjoint.

This lemma is proven in Section 2.3. Two important examples of elements in $\mathcal{G}(A)$ are:

- The choice $\lambda(x,y) = \Omega(x) - \Omega(y)$ for $\Omega \in \mathcal{C}_c^\infty(\mathbb{R}^4, \mathbb{R})$ fulfills $\lambda \in \mathcal{G}(\partial\Omega)$. Such a λ delivers a good candidate for the operator P_Σ^A fulfilling (26) if the external field A can be attained from the zero field via a gauge transform $A = 0 \mapsto A = \partial\Omega$. We observe for any path $C_{y,x}$ from y to x

$$\lambda(x,y) = \int_{C_{y,x}} A_\mu(u)\, du^\mu = \frac{1}{2}(A_\mu(x) + A_\mu(y))(x^\mu - y^\mu) + O_A(|x-y|^3). \tag{37}$$

- For an arbitrary vector potential $A \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4)$ also

$$\lambda^A(x,y) := \frac{1}{2}(A_\mu(x) + A_\mu(y))(x^\mu - y^\mu) \tag{38}$$

  fulfills $\lambda^A \in \mathcal{G}(A)$. This choice is motivated by the special case (37). It will be particularly convenient for our work. Note that it has the symmetry $\lambda^A(x,y) = -\lambda^A(y,x)$; cf. part (iv) in Lemma 2.3. In particular, the operator P_Σ^A from the discussion will be given by

$$P_\Sigma^A := P_\Sigma^{\lambda^A}. \tag{39}$$

We shall show that for $\lambda \in \mathcal{G}(A)$ the operators P_Σ^λ obey the key property (26). Our first result about P_Σ^λ for a $\lambda \in \mathcal{G}(A)$ is that, up to a Hilbert-Schmidt operator, it depends only on the restriction of the 1-form A to the tangent bundle $T\Sigma$ of the Cauchy surface Σ.

Theorem 2.4. *Given $A, \widetilde{A} \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4)$ and $\lambda \in \mathcal{G}(A)$, $\widetilde{\lambda} \in \mathcal{G}(\widetilde{A})$, the following is true:*

$$P_\Sigma^\lambda - P_\Sigma^{\widetilde{\lambda}} \in I_2(\mathcal{H}_\Sigma) \quad \Leftrightarrow \quad A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}. \tag{40}$$

This theorem is also proven in Section 2.3. From our next result we can infer that the operators P_Σ^λ obey the key property (26).

Theorem 2.5. *Given $A \in C_c^\infty(\mathbb{R}^4, \mathbb{R}^4)$, $\lambda \in \mathcal{G}(A)$, and two Cauchy surfaces Σ, Σ', one has*

$$U_{A\Sigma'} P_{\Sigma'}^\lambda U_{\Sigma' A} - U_{A\Sigma} P_\Sigma^\lambda U_{\Sigma A} \in I_2(\mathcal{H}_A), \tag{41}$$

where $U_{A\Sigma}$ and $U_{\Sigma A}$ are the Dirac evolution operators given in Definition 1.13.

Instead of proving this theorem directly we prove it at the end of Section 2.4 as consequence of Theorem 2.8 below. The latter can be understood as an infinitesimal version of Theorem 2.5. To state Theorem 2.8 we consider a family $(\Sigma_t)_{t\in T}$ of Cauchy surfaces encoded by $\boldsymbol{\Sigma}$, see (17), such that $\Sigma = \Sigma_{t_0}$ and $\Sigma' = \Sigma_{t_1}$. In addition we need the following helper object s^A_Σ defined in Definition 2.6 below as well as the following notation. Given an electromagnetic potential $A \in C^\infty_c(\mathbb{R}^4, \mathbb{R}^4)$ and a Cauchy surface Σ with future-directed unit normal vector field n, we define the electromagnetic field tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and

$$E_\mu := F_{\mu\nu} n^\nu \tag{42}$$

referred to as the "electric field" with respect to the local Cauchy surface Σ. In the special case $n = e_0 = (1, 0, 0, 0)$, this encodes just the electric part of the electromagnetic field tensor.

Recall from the paragraph preceding Definition 1.10 that we extended the unit normal field n on the Cauchy surface to a smooth unit normal field $n : \mathbb{R}^4 \times T \to \mathbb{R}^4$ and velocity field $v : \mathbb{R}^4 \times T \to \mathbb{R}$, which induces the "electric field" E to be defined on $\mathbb{R}^4 \times T$ as well. In particular, after this extension, the partial derivative $\partial E_\mu(x, t)/\partial t = F_{\mu\nu}(x)\, \partial n_t{}^\nu(x)/\partial t$ then makes sense.

Definition 2.6. *Recall the definitions of $r(w)$ and $D(w)$ given in (27) and (31), respectively. For $\epsilon > 0$, $u \in \mathrm{Past}$, and $x, y \in \mathbb{R}^4$, we define the integral kernel*

$$s^{A,\epsilon u}_\Sigma(x, y) := \frac{1}{8m} \not{n}(x) \not{E}(x) r(w)^2 \not{\partial} D(w), \qquad \text{where } w = y - x + i\epsilon u. \tag{43}$$

Furthermore, for $x - y$ being space-like (in particular $x \neq y$), we also define the integral kernel

$$s^A_\Sigma(x, y) = s^{A,0}_\Sigma(x, y) := \lim_{\epsilon \downarrow 0} s^{A,\epsilon u}_\Sigma(x, y) = \frac{1}{8m} \not{n}(x) \not{E}(x) r(y - x)^2 \not{\partial} D(y - x). \tag{44}$$

We remark that restricted to x and y within a single Cauchy surface Σ, the value of the kernel $s^{A,\epsilon u}_\Sigma(x, y)$ depends only on Σ through its normal field $n : \Sigma \to \mathbb{R}^4$. In this case the definition makes sense without specifying neither the velocity field v nor the extension of n and v to $\mathbb{R}^4 \times T$. In particular, $s^{A,\epsilon u}_\Sigma(x, y)$ depends only on the Cauchy surface Σ but not on the choice of a family $(\Sigma_t)_{t\in T}$. This stands in contrast to the derivative $\partial s^{A,\epsilon u}_{\Sigma_t}/\partial t$, which makes sense everywhere only given a family $(\Sigma_t)_{t\in T}$ and the extended version of n.

Exploiting the properties of $D(w)$ given in Lemma 2.1 and in Corollary A.1 in the appendix we shall find:

Lemma 2.7. *Let $u \in \mathrm{Past}$.*

(i) The integral kernels $s^{A,\epsilon u}_\Sigma$, $\epsilon \geqslant 0$, give rise to Hilbert-Schmidt operators

$$S^{A,\epsilon u}_\Sigma : \mathcal{H}_\Sigma \circlearrowleft, \qquad S^{A,\epsilon u}_\Sigma \psi(x) := \int_\Sigma s^{A,\epsilon u}_\Sigma(x, y)\, i_\gamma(d^4 y)\, \psi(y) \quad \text{for almost all } x \in \Sigma, \tag{45}$$

$S^A_\Sigma := S^{A,0}_\Sigma$, with the property that $\|S^A_\Sigma - S^{A,\epsilon u}_\Sigma\|_{I_2(\mathcal{H}_\Sigma)} \xrightarrow{\epsilon \downarrow 0} 0$.

(ii) *Similarly, for $t \in T$, the integral kernels $\partial s^{A,\epsilon u}_{\Sigma_t}/\partial t$, $\epsilon \geqslant 0$, give rise to Hilbert-Schmidt operators*

$$\dot{S}^{A,\epsilon u}_{\Sigma_t} : \mathcal{H}_\Sigma \circlearrowleft, \qquad \dot{S}^{A,\epsilon u}_{\Sigma_t}\psi(x) := \int_{\Sigma_t} \frac{\partial s^{A,\epsilon u}_{\Sigma_t}}{\partial t}(x,y)\, i_\gamma(d^4y)\,\psi(y) \quad \text{for almost all } x \in \Sigma_t, \tag{46}$$

$\dot{S}^{A}_{\Sigma_t} := \dot{S}^{A,0}_{\Sigma_t}$, *with the property that* $\sup_{t\in T} \|\dot{S}^{A}_{\Sigma_t}\|_{I_2(\mathcal{H}_{\Sigma_t})} < \infty$ *and* $\|\dot{S}^{A}_{\Sigma_t} - \dot{S}^{A,\epsilon u}_{\Sigma_t}\|_{I_2(\mathcal{H}_{\Sigma_t})} \xrightarrow{\epsilon\downarrow 0} 0$ *for all* t.

With this ingredient our infinitesimal version of Theorem 2.5 can be formulated as follows; for technical convenience, we phrase it only for the special choice $\lambda^A \in \mathcal{G}(A)$ defined in (38).

Theorem 2.8. *Given $A \in C^\infty_c(\mathbb{R}^4, \mathbb{R}^4)$, any smooth family of Cauchy surfaces $\mathbf{\Sigma}$, cf. (17), and $t_0, t_1 \in T$, and one has*

$$U_{A\Sigma_{t_1}}\left(P^A_{\Sigma_{t_1}} + S^A_{\Sigma_{t_1}}\right)U_{\Sigma_{t_1}A} - U_{A\Sigma_{t_0}}\left(P^A_{\Sigma_{t_0}} + S^A_{\Sigma_{t_0}}\right)U_{\Sigma_{t_0}A} = \int_{t_0}^{t_1} U_{A\Sigma_t}R(t)U_{\Sigma_t A}\,dt \tag{47}$$

for a family of Hilbert-Schmidt operators $R(t)$, $t \in T$, with $\sup_{t\in T}\|R(t)\|_{I_2(\mathcal{H}_{\Sigma_t})} < \infty$. The integral in (47) is understood in the weak sense.

Note that for the choice $\lambda \in \mathcal{G}(A)$, $\Sigma_{t_1} = \Sigma$, $\Sigma_{t_0} = \Sigma_{\text{in}}$ one has $P^\lambda_{\Sigma_{\text{in}}} = P^-_{\Sigma_{\text{in}}}$, and the restriction of (41) to Cauchy surface Σ yields property $U^A_{\Sigma\Sigma_{\text{in}}}P^-_{\Sigma_{\text{in}}}U^A_{\Sigma_{\text{in}}\Sigma} - P^\lambda_\Sigma \in I_2(\mathcal{H}_\Sigma)$, i.e., the key property (26). The proof of Theorem 2.8 given in Section 2.4 is the heart of this work.

2.2 Proofs of Main Results

In this section, we prove the main results under the assumption that the claims in Section 2.1 are true. The proofs of these assumed claims are then provided in Sections 2.3-2.4. The connection of how to infer the properties of $\mathcal{C}_\Sigma(A)$ from the properties of the operators P^λ_Σ is given by the following lemma.

Lemma 2.9. *Let $A \in C^\infty_c(\mathbb{R}^4, \mathbb{R}^4)$, Σ be a Cauchy surface, and $\lambda \in \mathcal{G}(A)$. Then for every polarization V in $\mathcal{H}_\Sigma$, we have*

$$V \in \mathcal{C}_\Sigma(A) \quad \Leftrightarrow \quad P^V_\Sigma - P^\lambda_\Sigma \in I_2(\mathcal{H}_\Sigma). \tag{48}$$

Proof. By Definition 1.3, $V \in \mathcal{C}_\Sigma(A)$ is equivalent to

$$P^V_\Sigma - U^A_{\Sigma\Sigma_{\text{in}}}P^-_{\Sigma_{\text{in}}}U^A_{\Sigma_{\text{in}}\Sigma} \in I_2(\mathcal{H}_\Sigma). \tag{49}$$

On the other hand, Theorem 2.5 implies

$$P^\lambda_\Sigma - U^A_{\Sigma\Sigma_{\text{in}}}P^-_\Sigma U^A_{\Sigma_{\text{in}}\Sigma} \in I_2(\mathcal{H}_\Sigma). \tag{50}$$

Thus, statement (49) is equivalent to $P^V_\Sigma - P^\lambda_\Sigma \in I_2(\mathcal{H}_\Sigma)$. □

Proof of Theorem 1.5. $\mathcal{C}_\Sigma(A) = \mathcal{C}_\Sigma(\widetilde{A})$ holds true if and only if there are $V \in \mathcal{C}_\Sigma(A)$ and $W \in \mathcal{C}_\Sigma(\widetilde{A})$ such that

$$P_\Sigma^V - P_\Sigma^W \in I_2(\mathcal{H}_\Sigma). \tag{51}$$

Let $\lambda \in \mathcal{G}(A)$ and $\widetilde{\lambda} \in \mathcal{G}(\widetilde{A})$. In view of Lemma 2.9, statement (51) is equivalent to $P_\Sigma^\lambda - P_\Sigma^{\widetilde{\lambda}} \in I_2(\mathcal{H}_\Sigma)$. Due to Theorem 2.4 the latter is equivalent to $A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}$, which proves the claim. □

Proof of Thorem 1.6. Claim (i): Is is sufficient to prove that there exist $V \in \mathcal{C}_\Sigma(A)$ and $W \in \mathcal{C}_{\Lambda\Sigma}(\Lambda A(\Lambda^{-1}\cdot))$ such that $L^{(S,\Lambda)} P_\Sigma^V (L^{(S,\Lambda)})^{-1} - P_{\Lambda\Sigma}^W \in I_2(\mathcal{H}_{\Lambda\Sigma})$. We remark that for the *linear form* A, ΛA stands for the linear form with coordinates $\Lambda_\mu{}^\nu A_\nu$, while for a *vector* x, the term Λx stands for the vector with coordinates $\Lambda^\mu{}_\nu x^\nu$. We take $\lambda \in \mathcal{G}(A)$, e.g., $\lambda = \lambda^A$ from (38). Thanks to Lemma 2.9, for all $V \in \mathcal{C}_\Sigma(A)$ we have $P_\Sigma^V - P_\Sigma^\lambda \in I_2(\mathcal{H}_\Sigma)$. First, let us discuss how such a P_Σ^λ behaves under the Lorentz transforms $L^{(S,\Lambda)}$. For $\epsilon > 0$ and $u \in \text{Past}$, the integral kernel $p_\Sigma^{\lambda,\epsilon u}(x,y) = e^{-i\lambda(x,y)} p_-(y-x+i\epsilon u)$ of $P_\Sigma^{\lambda,\epsilon u}$, cf. (35), transforms as follows: The integral kernel of $L_\Sigma^{(S,\Lambda)} P_\Sigma^{\lambda,\epsilon u} (L_\Sigma^{(S,\Lambda)})^{-1}$ is given by

$$\begin{aligned} S p_\Sigma^{\lambda,\epsilon u}(\Lambda^{-1}x, \Lambda^{-1}y) S^* &= e^{-i\lambda(\Lambda^{-1}x,\Lambda^{-1}y)}\, S\, p^-(\Lambda^{-1}(y-x) + i\epsilon u))\, S^* \\ &= e^{-i\lambda(\Lambda^{-1}x,\Lambda^{-1}y)} p^-(y-x+i\epsilon\Lambda u) = p_{\Lambda\Sigma}^{\overline{\lambda},\epsilon\Lambda u}(x,y), \end{aligned} \tag{52}$$

where $\overline{\lambda}(x,y) = \lambda(\Lambda^{-1}x, \Lambda^{-1}y)$. We claim $\overline{\lambda} \in \mathcal{G}(\Lambda A(\Lambda^{-1}\cdot))$. Indeed, $\overline{\lambda}$ clearly fulfills conditions (i)-(iii) of the Definition 2.2 of $\mathcal{G}(\Lambda A(\Lambda^{-1}\cdot))$. It also fulfills condition (iv) since

$$\begin{aligned} \frac{\partial}{\partial x^\mu}\overline{\lambda}(x,y)\Big|_{y=x} &= \frac{\partial}{\partial x^\mu}\lambda(\Lambda^{-1}x, \Lambda^{-1}y)\Big|_{y=x} = (\Lambda^{-1})^\nu{}_\mu \frac{\partial}{\partial z^\nu}\lambda(z, \Lambda^{-1}y)\Big|_{z=\Lambda^{-1}x, y=x} \\ &= \Lambda_\mu{}^\nu A_\nu(\Lambda^{-1}x) \end{aligned} \tag{53}$$

and similarly $\partial_\mu^y \overline{\lambda}(x,y)\big|_{x=y} = -\Lambda_\mu{}^\nu A_\nu(\Lambda^{-1}x)$, where we have used $(\Lambda^{-1})^\nu{}_\mu = \Lambda_\mu{}^\nu$. This shows $L_\Sigma^{(S,\Lambda)} P_\Sigma^{\lambda,\epsilon u} (L_\Sigma^{(S,\Lambda)})^{-1} = P_\Sigma^{\overline{\lambda},\epsilon\Lambda u}$, which implies $L_\Sigma^{(S,\Lambda)} P_\Sigma^\lambda (L_\Sigma^{(S,\Lambda)})^{-1} = P_\Sigma^{\overline{\lambda}}$ in the limit as $\epsilon \downarrow 0$; recall from Lemma 2.3 that the limit does not depend on the choice of $u, \Lambda u \in \text{Past}$.

Again by Lemma 2.9, there is a $W \in \mathcal{C}_{\Lambda\Sigma}(\Lambda A(\Lambda^{-1}\cdot))$ such that $P_{\Lambda\Sigma}^W - P_{\Lambda\Sigma}^{\overline{\lambda}} \in I_2(\mathcal{H}_{\Lambda\Sigma})$. We conclude

$$L_\Sigma^{(S,\Lambda)} P_\Sigma^V \left(L_\Sigma^{(S,\Lambda)}\right)^{-1} - P_{\Lambda\Sigma}^W = L_\Sigma^{(S,\Lambda)} \left(P_\Sigma^V - P_\Sigma^\lambda\right) \left(L_\Sigma^{(S,\Lambda)}\right)^{-1} - \left(P_{\Lambda\Sigma}^W - P_{\Lambda\Sigma}^{\overline{\lambda}}\right) \in I_2(\mathcal{H}_{\Lambda\Sigma}). \tag{54}$$

Claim (ii): The integral kernel of $e^{-i\Omega} P_\Sigma^{\lambda,\epsilon u} e^{i\Omega}$ for $\lambda \in \mathcal{G}(A)$, $\epsilon > 0$ and $u \in \text{Past}$ equals

$$e^{-i\Omega(x)} p_\Sigma^{\lambda,\epsilon u}(x,y) e^{i\Omega(y)} = e^{-i\Omega(x)} e^{-i\lambda(x,y)} p^-(y-x+i\epsilon u) e^{i\Omega(y)} = p_\Sigma^{\overline{\lambda},\epsilon u}(x,y), \tag{55}$$

where $\overline{\lambda}(x,y) = \Omega(x) + \lambda(x,y) - \Omega(y)$, which clearly fulfills $\overline{\lambda} \in \mathcal{G}(A + \partial\Omega)$; cf. Definition 2.2. Taking the limit as $\epsilon \downarrow 0$, the claim follows from the same kind of reasoning as in part (i). □

Finally, one can also use the self-adjoint operator P_Σ^A from (39) to construct a unitary operator $e^{Q_\Sigma^A} : \mathcal{H}_\Sigma \circlearrowleft$ which adapts the standard polarization $\mathcal{H}_\Sigma^-$ to one corresponding to $A|_{T\Sigma}$, more precisely, $e^{Q_\Sigma^A}\mathcal{H}_\Sigma^- \in \mathcal{C}_\Sigma(A)$. It is defined as follows:

Definition 2.10. *We set*

$$Q_\Sigma^A := [P_\Sigma^A, P_\Sigma^-] = P_\Sigma^+(P_\Sigma^A - P_\Sigma^-)P_\Sigma^- - P_\Sigma^-(P_\Sigma^A - P_\Sigma^-)P_\Sigma^+. \tag{56}$$

Proof of Theorem 1.7. In this proof, we use a 2×2-matrix notation for linear operators of the type $\mathcal{H}_\Sigma \circlearrowleft$. This matrix notation always refers to the splitting $\mathcal{H}_\Sigma = \mathcal{H}_\Sigma^+ \oplus \mathcal{H}_\Sigma^-$. In particular, we set

$$\begin{pmatrix} \Delta_{++} & \Delta_{+-} \\ \Delta_{-+} & \Delta_{--} \end{pmatrix} = \Delta P_\Sigma^{\lambda^A} = P_\Sigma^A - P_\Sigma^-, \tag{57}$$

cf. (36) for $\lambda = \lambda^A$. Using this matrix notation, we write

$$Q_\Sigma^A = \begin{pmatrix} 0 & \Delta_{+-} \\ -\Delta_{-+} & 0 \end{pmatrix}. \tag{58}$$

In the following we use the notation $X = Y \mod I_2(\mathcal{H}_\Sigma)$ to mean $X - Y \in I_2(\mathcal{H}_\Sigma)$. By (iii) of Lemma 2.3 we know that $(\Delta P_\Sigma^{\lambda^A})^2 \in I_2(\mathcal{H}_\Sigma)$, and therefore

$$(P_\Sigma^A)^2 = (P_\Sigma^- + \Delta P_\Sigma^{\lambda^A})^2 = P_\Sigma^A + \begin{pmatrix} -\Delta_{++} & 0 \\ 0 & \Delta_{--} \end{pmatrix} \mod I_2(\mathcal{H}_\Sigma). \tag{59}$$

Furthermore, Lemma 2.9 implies for all $V \in \mathcal{C}_\Sigma(A)$ that the corresponding orthogonal projector P_Σ^V fulfills $P_\Sigma^A - P_\Sigma^V \in I_2(\mathcal{H}_\Sigma)$. However, this means also that $(P_\Sigma^A)^2 - P_\Sigma^A \in I_2(\mathcal{H}_\Sigma)$, and therefore, $\Delta_{++}, \Delta_{--} \in I_2(\mathcal{H}_\Sigma)$; see (59). In conclusion, we obtain

$$P_\Sigma^A = P_\Sigma^- + \Delta P_\Sigma^{\lambda^A} = \begin{pmatrix} 0 & \Delta_{+-} \\ \Delta_{-+} & \mathrm{id}_{\mathcal{H}_\Sigma^-} \end{pmatrix} \mod I_2(\mathcal{H}_\Sigma). \tag{60}$$

Since $(\Delta P_\Sigma^{\lambda^A})^2 \in I_2(\mathcal{H}_\Sigma)$ we have $\Delta_{-+}\Delta_{+-}, \Delta_{-+}\Delta_{+-} \in I_2(\mathcal{H}_\Sigma)$ and hence $(Q_\Sigma^A)^2 \in I_2(\mathcal{H}_\Sigma)$; cf. (58). Defining

$$\Pi_\Sigma^A := e^{Q_\Sigma^A} P_\Sigma^- e^{-Q_\Sigma^A}, \tag{61}$$

we conclude

$$\Pi_\Sigma^A = (\mathrm{id}_{\mathcal{H}_\Sigma} + Q_\Sigma^A) P_\Sigma^- (\mathrm{id}_{\mathcal{H}_\Sigma} - Q_\Sigma^A) = \begin{pmatrix} 0 & \Delta_{+-} \\ \Delta_{-+} & \mathrm{id}_{\mathcal{H}_\Sigma^-} \end{pmatrix} = P_\Sigma^A = P_\Sigma^V \mod I_2(\mathcal{H}_\Sigma). \tag{62}$$

Furthermore, we observe that $e^{Q_\Sigma^A}$ is unitary because Q_Σ^A is skew-adjoint, so that Π_Σ^A is an orthogonal projector. Summarizing, we have shown $e^{Q_\Sigma^A}\mathcal{H}_\Sigma^- = \Pi_\Sigma^A \mathcal{H}_\Sigma \in \mathcal{C}_\Sigma(A)$, which proves the claim of Theorem 1.7.

As an addendum we prove the refinement of Theorem 1.7 described in Remark 1.8. For this it is left to show that $\mathrm{charge}(U_{\Sigma\Sigma_{\mathrm{in}}}^A \mathcal{H}_{\Sigma_{\mathrm{in}}}^-, \Pi_\Sigma^A \mathcal{H}_\Sigma) = 0$. We choose a future oriented foliation $(\Sigma_t)_{t\in\mathbb{R}}$ of space-time such that $\Sigma_0 = \Sigma_{\mathrm{in}}$ and $\Sigma_1 = \Sigma$. Recall the choice of Σ_{in} described in (7). The operators $Q_{\Sigma_t}^A$ are compact because they are skew-adjoint and $(Q_{\Sigma_t}^A)^2 \in$

$I_2(\mathcal{H}_{\Sigma_t})$. Hence, the operators $e^{-Q^A_{\Sigma_t}}$ are compact perturbations of the identity operators $\mathrm{id}_{\mathcal{H}_{\Sigma_t}}$. Translating this fact to an interaction picture, the operators

$$Q_t := U^0_{\Sigma_{\mathrm{in}}\Sigma_t} e^{-Q^A_{\Sigma_t}} U^0_{\Sigma_t\Sigma_{\mathrm{in}}} \tag{63}$$

are as well compact perturbations of the identity operator $\mathrm{id}_{\mathcal{H}_{\Sigma_{\mathrm{in}}}}$. We define the evolution operators in the interaction picture

$$U_t := U^0_{\Sigma_{\mathrm{in}}\Sigma_t} U^A_{\Sigma_t\Sigma_{\mathrm{in}}}, \tag{64}$$

which are continuous in $t \in \mathbb{R}$ w.r.t. the operator norm; this follows from Lemma 3.9 in [3]. Moreover, using $V \approx W \Leftrightarrow P^V_\Sigma P^{W^\perp}_\Sigma, P^{V^\perp}_\Sigma P^W_\Sigma \in I_2(\mathcal{H}_\Sigma)$, the just proven Theorem 1.7 implies

$$e^{Q^A_\Sigma}\mathcal{H}^-_\Sigma \approx U^A_{\Sigma\Sigma_{\mathrm{in}}}\mathcal{H}^-_{\Sigma_{\mathrm{in}}} \Rightarrow P^\pm_\Sigma e^{-Q^A_\Sigma} U^A_{\Sigma\Sigma_{\mathrm{in}}} P^\mp_{\Sigma_{\mathrm{in}}} \in I_2(\mathcal{H}_\Sigma) \tag{65}$$

$$\Rightarrow U^0_{\Sigma_{\mathrm{in}}\Sigma} P^\pm_\Sigma e^{-Q^A_\Sigma} U^A_{\Sigma\Sigma_{\mathrm{in}}} P^\mp_{\Sigma_{\mathrm{in}}} \in I_2(\mathcal{H}_\Sigma) \tag{66}$$

$$\Rightarrow P^\pm_{\Sigma_{\mathrm{in}}} Q_t U_t P^\mp_{\Sigma_{\mathrm{in}}} = P^\pm_\Sigma U^0_{\Sigma_{\mathrm{in}}\Sigma} e^{-Q^A_\Sigma} U^A_{\Sigma\Sigma_{\mathrm{in}}} P^\mp_{\Sigma_{\mathrm{in}}} \in I_2(\mathcal{H}_{\Sigma_{\mathrm{in}}}). \tag{67}$$

Since $Q_t - \mathrm{id}_{\mathcal{H}_{\Sigma_{\mathrm{in}}}}$ is compact, the operator $P^\pm_{\Sigma_{\mathrm{in}}}(Q_t - \mathrm{id}_{\mathcal{H}_{\Sigma_{\mathrm{in}}}})U_t P^\mp_{\Sigma_{\mathrm{in}}}$ is compact as well. Taking the difference with the compact operator in (67) yields that $P^\pm_{\Sigma_{\mathrm{in}}} U_t P^\mp_{\Sigma_{\mathrm{in}}}$ is compact so that

$$\begin{pmatrix} P^+_{\Sigma_{\mathrm{in}}} U_t P^+_{\Sigma_{\mathrm{in}}} & 0 \\ 0 & P^-_{\Sigma_{\mathrm{in}}} U_t P^-_{\Sigma_{\mathrm{in}}} \end{pmatrix} = U_t - \begin{pmatrix} 0 & P^+_{\Sigma_{\mathrm{in}}} U_t P^-_{\Sigma_{\mathrm{in}}} \\ P^-_{\Sigma_{\mathrm{in}}} U_t P^+_{\Sigma_{\mathrm{in}}} & 0 \end{pmatrix} \tag{68}$$

deviates from the unitary operator U_t by a compact perturbation, and hence, is a Fredholm operator. This implies that $P^-_{\Sigma_{\mathrm{in}}} U_t P^-_{\Sigma_{\mathrm{in}}}|_{\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\circlearrowleft}$ is a Fredholm operator. We note that the Fredholm index of $P^-_{\Sigma_{\mathrm{in}}} U_{t=0} P^-_{\Sigma_{\mathrm{in}}}|_{\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\circlearrowleft} = \mathrm{id}_{\mathcal{H}^-_{\Sigma_{\mathrm{in}}}}$ equals zero. The map $t \mapsto P^-_{\Sigma_{\mathrm{in}}} U_t P^-_{\Sigma_{\mathrm{in}}}$ is continuous in the operator norm which implies that the Fredholm index is constant, and hence,

$$\begin{aligned} 0 &= \mathrm{index}\, P^-_{\Sigma_{\mathrm{in}}} U_{t=1}|_{\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\circlearrowleft} = \mathrm{index}\, P^-_{\Sigma_{\mathrm{in}}} U^0_{\Sigma_{\mathrm{in}}\Sigma} U^A_{\Sigma\Sigma_{\mathrm{in}}}|_{\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\circlearrowleft} \\ &= \mathrm{index}\, P^-_\Sigma U^A_{\Sigma\Sigma_{\mathrm{in}}}|_{\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\to\mathcal{H}^-_\Sigma} = \mathrm{index}\, P^-_\Sigma|_{U^A_{\Sigma\Sigma_{\mathrm{in}}}\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\to\mathcal{H}^-_\Sigma} = \mathrm{index}\, P^-_\Sigma e^{-Q^A_\Sigma}|_{U^A_{\Sigma\Sigma_{\mathrm{in}}}\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\to\mathcal{H}^-_\Sigma} \\ &= \mathrm{index}\, e^{Q^A_\Sigma} P^-_\Sigma e^{-Q^A_\Sigma}|_{U^A_{\Sigma\Sigma_{\mathrm{in}}}\mathcal{H}^-_{\Sigma_{\mathrm{in}}}\to\Pi^A_\Sigma\mathcal{H}_\Sigma} = \mathrm{charge}(U^A_{\Sigma\Sigma_{\mathrm{in}}}\mathcal{H}^-_{\Sigma_{\mathrm{in}}}, \Pi^A_\Sigma\mathcal{H}_\Sigma), \end{aligned} \tag{69}$$

where in the fifth equality we have used that $e^{-Q^A_\Sigma}$ is a compact perturbation of the identity. □

This concludes the proofs of the main results under the condition that the claims in Section 2.1 are true. The proofs of these claims will be provided in the next two sections.

2.3 Proof of Lemma 2.1, Lemma 2.3, and Theorem 2.4

Proof of Lemma 2.1. Given $\phi, \psi \in \mathcal{C}_\Sigma$, we set $\widehat{\phi} = \mathcal{F}_{\mathcal{M}\Sigma}\phi$ and $\widehat{\psi} = \mathcal{F}_{\mathcal{M}\Sigma}\psi$ where $\mathcal{F}_{\mathcal{M}\Sigma}$ is the generalized Fourier transform

$$(\mathcal{F}_{\mathcal{M}\Sigma}\psi)(p) = \frac{\not{p} + m}{2m}(2\pi)^{-3/2} \int_\Sigma e^{ipx}\, i_\gamma(d^4x)\, \psi(x) \qquad \text{for } \psi \in \mathcal{C}_\Sigma, p \in \mathcal{M}, \tag{70}$$

introduced in Theorem 2.15 of [3]. This theorem ensures that $\overline{\widehat{\phi}(p)}\widehat{\psi}(p)\, i_p(d^4p)$ is integrable on $\mathcal{M}_-$. Let $u \in$ Past. With justifications given below, we compute the following.

$$\langle \phi, P_\Sigma^- \psi \rangle = \lim_{\epsilon \downarrow 0} \int\limits_{p\in\mathcal{M}_-} e^{-\epsilon pu} \overline{\widehat{\phi}(p)}\widehat{\psi}(p) \frac{i_p(d^4p)}{m} \tag{71}$$

$$= \frac{1}{(2\pi)^3 m} \lim_{\epsilon\downarrow 0} \int\limits_{p\in\mathcal{M}_-} e^{-\epsilon pu} \int\limits_{x\in\Sigma} \overline{\phi(x)}\, i_\gamma(d^4x)\, e^{-ipx} \left(\frac{\not p + m}{2m}\right)^2 \int\limits_{y\in\Sigma} e^{ipy}\, i_\gamma(d^4y)\, \psi(y)\, i_p(d^4p) \tag{72}$$

$$= \frac{1}{(2\pi)^3 m} \lim_{\epsilon\downarrow 0} \int\limits_{p\in\mathcal{M}_-} \int\limits_{x\in\Sigma} \overline{\phi(x)}\, i_\gamma(d^4x) \frac{\not p + m}{2m} \int\limits_{y\in\Sigma} e^{ip(y-x+i\epsilon u)}\, i_\gamma(d^4y)\, \psi(y)\, i_p(d^4p) \tag{73}$$

$$= \frac{1}{(2\pi)^3 m} \lim_{\epsilon\downarrow 0} \int\limits_{x\in\Sigma} \overline{\phi(x)}\, i_\gamma(d^4x) \int\limits_{y\in\Sigma} \int\limits_{p\in\mathcal{M}_-} \frac{\not p + m}{2m} e^{ip(y-x+i\epsilon u)}\, i_p(d^4p)\, i_\gamma(d^4y)\, \psi(y) \tag{74}$$

$$= \lim_{\epsilon\downarrow 0} \int\limits_{x\in\Sigma} \overline{\phi}(x)\, i_\gamma(d^4x) \int\limits_{y\in\Sigma} p^-(y - x + i\epsilon u)\, i_\gamma(d^4y)\, \psi(y). \tag{75}$$

The interchange of the p-integral and the limit $\epsilon \downarrow 0$ in (71) is justified by dominated convergence since $\overline{\widehat{\phi}(p)}\widehat{\psi}(p) i_p(d^4p)$ is integrable on $\mathcal{M}_-$ and by $|e^{-\epsilon pu}| \leqslant 1$ for $\epsilon > 0$, $p \in \mathcal{M}_-$. In the step from (71) to (72) we have used (70) and that $\gamma^0(\gamma^\mu)^*\gamma^0 = \gamma^\mu$, from (72) to (73) that $\not p^2 = p^2$ and that $p^2 = m^2$ for $p \in \mathcal{M}_-$. In the step from (73) to (74) we have used Fubini's theorem to interchange the integrals. This is justified because ϕ and ψ are bounded and compactly supported, and because for any given $\epsilon > 0$, $|e^{ip(y-x+i\epsilon u)}| = e^{-\epsilon pu}$ tends exponentially fast to 0 as $|p| \to \infty$, $p \in \mathcal{M}_-$. This proves the claim (29).

Now we prove the claimed properties of D and p^-. For any $w \in \mathbb{R}^4 + i\,\mathrm{Past}$, the modulus $|e^{ipw}| = e^{-p\,\mathrm{Im}\, w}$ tends exponentially fast to 0 as $|p| \to \infty$, $p \in \mathcal{M}_-$. Consequently, exchanging differentiation and integration in the following calculation is justified:

$$\begin{aligned} p^-(w) &= \frac{1}{(2\pi)^3 m} \int_{\mathcal{M}_-} \frac{-i\not\partial^w + m}{2m} e^{ipw}\, i_p(d^4p) \\ &= \frac{1}{(2\pi)^3 m} \frac{-i\not\partial^w + m}{2m} \int_{\mathcal{M}_-} e^{ipw}\, i_p(d^4p) = \frac{-i\not\partial + m}{2m} D(w). \end{aligned} \tag{76}$$

To show the second equality in (31), we proceed as follows: First, we show that $w \in \mathbb{R}^4 + i\,\mathrm{Past}$ implies $-w_\mu w^\mu \in \mathbb{C}\backslash\mathbb{R}_0^- = \mathrm{domain}(\sqrt{\cdot})$. We take $w = z + iu$ with $z \in \mathbb{R}^4$ and $u \in$ Past, and assume $-w_\mu w^\mu \in \mathbb{R}$. Then $0 = \mathrm{Im}(w_\mu w^\mu) = 2z_\mu u^\mu$, i.e., z is orthogonal to u in the Minkowski sense. Because u is time-like, we conclude that z is space-like or zero. We obtain $w_\mu w^\mu = \mathrm{Re}(w_\mu w^\mu) = z_\mu z^\mu - u_\mu u^\mu < 0$, i.e., $-w_\mu w^\mu \in \mathrm{domain}(\sqrt{\cdot})$. It follows that $\sqrt{-w_\mu w^\mu} \in \mathbb{R}^+ + i\mathbb{R} = \mathrm{domain}(K_1)$. In particular,

$$\widetilde{D} : \mathbb{R}^4 + i\,\mathrm{Past} \ni w \mapsto -\frac{m^3}{2\pi^2} \frac{K_1(m\sqrt{-w_\mu w^\mu})}{m\sqrt{-w_\mu w^\mu}} \tag{77}$$

is a well-defined holomorphic function. Because $|e^{ipw}|$ decays fast as $|p| \to \infty$, $p \in \mathcal{M}_-$, uniformly for w in any compact subset of $\mathbb{R}^4 + i\,\text{Past}$,

$$D : \mathbb{R}^4 + i\,\text{Past} \ni w \mapsto \frac{1}{(2\pi)^3 m} \int_{\mathcal{M}_-} e^{ipw}\, i_p(d^4p) \tag{78}$$

is also a holomorphic function. We need to show $D = \widetilde{D}$. By the identity theorem for holomorphic functions, it suffices to show that the restrictions of D and $\widetilde{D}$ to $i\,\text{Past}$ coincide. Given $w = iu \in i\,\text{Past}$, we choose a proper, orthochronous Lorentz transform $\Lambda \in \text{SO}^{\uparrow}(1,3) \subseteq \mathbb{R}^{4\times 4}$ that maps u to the negative time axis:

$$\Lambda u = -te_0 = (-t, 0, 0, 0) \text{ with } t = \sqrt{u_\mu u^\mu} = \sqrt{-w_\mu w^\mu} > 0. \tag{79}$$

By Lorentz invariance of the volume-form $i_p(d^4p)$ on $\mathcal{M}_-$, we know

$$\int_{\mathcal{M}_-} e^{ipw}\, i_p(d^4p) = \int_{\mathcal{M}_-} e^{ip\Lambda w}\, i_p(d^4p) \tag{80}$$

and $\sqrt{-w_\mu w^\mu} = \sqrt{-(\Lambda w)_\mu (\Lambda w)^\mu}$. Summarizing, we have reduced the claim $D = \widetilde{D}$ to its special case $D(w) = \widetilde{D}(w)$ for $w = -ite_0$, $t = \sqrt{-w_\mu w^\mu} > 0$. This special case is proven as follows. Using

$$i_p(d^4p) = \frac{m^2}{p^0} d^3p \text{ on } (T_p\mathcal{M})^3, \tag{81}$$

rotational symmetry, and the substitution

$$s = \frac{\sqrt{k^2+m^2}}{m}, \quad k = m\sqrt{s^2-1}, \quad m^2 s\, ds = k\, dk, \tag{82}$$

we obtain with the abbreviation $E(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2}$:

$$\begin{aligned} \int_{\mathcal{M}_-} e^{ipw}\, i_p(d^4p) &= -m^2 \int_{\mathbb{R}^3} e^{-E(\mathbf{p})t} \frac{d^3\mathbf{p}}{E(\mathbf{p})} \\ &= -4\pi m^2 \int_0^\infty \exp\left(-t\sqrt{k^2+m^2}\right) \frac{k^2\, dk}{\sqrt{k^2+m^2}} \\ &= -4\pi m^4 \int_1^\infty e^{-mts}\sqrt{s^2-1}\, ds = -4\pi m^4 \frac{K_1(mt)}{mt}, \end{aligned} \tag{83}$$

using the definition of K_1 in (32), and hence, the claim $D(-ite_0) = \widetilde{D}(-ite_0)$.

The representation (77) of D shows also that D can be analytically extended to all arguments $w \in \mathbb{C}^4$ with $-w_\mu w^\mu \in \text{domain}(\sqrt{\cdot}) = \mathbb{C}\backslash\mathbb{R}_0^-$. The same holds true for $p^- = (2m)^{-1}(-i\partial\!\!\!/ + m)D$. To sum up, p^- has an analytic continuation $p^- : \text{domain}(r) \to \mathbb{C}^{4\times 4}$, which also concludes the proof of Lemma 2.1. □

Proof of Lemma 2.3. We remark that most of the arguments in this proof are valid without regularization, i.e., also in the case $\epsilon = 0$. This is in contrast to Section 2.4 below, where the regularization with $\epsilon > 0$ turns out to be very useful.

Let $A \in \mathcal{C}_c^\infty(\mathbb{R}^4, \mathbb{R}^4)$, $\lambda \in \mathcal{G}(A)$, and Σ be a Cauchy surface. Before proving the claim (34)-(35) it will be convenient to introduce the operators $\Delta P_\Sigma^{\lambda,\epsilon u}$, $\epsilon \geqslant 0$, which shall act on any $\psi \in \mathcal{H}_\Sigma$ as

$$\left(\Delta P_\Sigma^{\lambda,\epsilon u}\psi\right)(x) = \int_{y\in\Sigma} (e^{-i\lambda(x,y)} - 1)p^-(y - x + i\epsilon u)\, i_\gamma(d^4y)\,\psi(y), \tag{84}$$

where the fixed vector $u \in \mathbb{R}^4$ is past-directed time-like. We remark that the special case $\epsilon = 0$ is included in the form $\Delta P_\Sigma^{\lambda,0} = \Delta P_\Sigma^\lambda$; cf. (36).

We show now that $\Delta P_\Sigma^{\lambda,\epsilon u} : \mathcal{H}_\Sigma \circlearrowleft$ is well-defined. Recall the parametrization $\pi_\Sigma(\mathbf{x})$ of Σ as stated in (13) and the identity $i_\gamma(d^4x) = \Gamma(\mathbf{x})\, d^3x$ on $(T_x\Sigma)^3$ given in (19). We use the abbreviation $x = \pi_\Sigma(\mathbf{x})$, $y = \pi_\Sigma(\mathbf{y})$ in the following. Line (84) can be recast into

$$\left(\Delta P_\Sigma^{\lambda,\epsilon u}\psi\right)(x) = \int_{\mathbb{R}^3} \Delta p_\Sigma^{\lambda,\epsilon u}(\mathbf{x},\mathbf{y})\,\Gamma(\mathbf{y})\,\psi(y)\,d^3\mathbf{y} \quad \text{for} \tag{85}$$

$$\Delta p_\Sigma^{\lambda,\epsilon u}(\mathbf{x},\mathbf{y}) := \left(e^{-i\lambda(x,y)} - 1\right) p^-(y - x + i\epsilon u). \tag{86}$$

To show at the same time that the right-hand side of (85), i.e., (84), is well-defined for $\psi \in \mathcal{H}_\Sigma$ and almost every $x \in \Sigma$, and that $\Delta P_\Sigma^{\lambda,\epsilon}\psi \in \mathcal{H}_\Sigma$, it suffices to prove that for every $\phi \in \mathcal{H}_\Sigma$, we have

$$\int_{\mathbf{x}\in\mathbb{R}^3}\int_{\mathbf{y}\in\mathbb{R}^3} \left|\overline{\phi(x)}\Gamma(\mathbf{x})\Delta p_\Sigma^{\lambda,\epsilon u}(\mathbf{x},\mathbf{y})\Gamma(\mathbf{y})\psi(y)\right| d^3\mathbf{y} \leqslant C_2\|\phi\|\|\psi\| \tag{87}$$

with some constant $C_2(u, V_{\max})$. We collect the necessary ingredients:

- As λ is smooth and vanishes on the diagonal, there is a positive constant $C_3(\lambda)$ such that

$$|e^{-i\lambda(x,y)} - 1| \leqslant C_3|x - y|[1_K(x) \vee 1_K(y)] \text{ for } x, y \in \mathbb{R}^4. \tag{88}$$

  Note that this bound holds globally, not only locally close to the diagonal, because $e^{-i\lambda} - 1$ is bounded and vanishes outside $K \times \mathbb{R}^4 \cup \mathbb{R}^4 \times K$ for some compact set K.

- The bounds (28) from the appendix, cf. (15), show that for all $x, y \in \Sigma$ and $(z^0, \mathbf{z}) = z = y - x$ we find $|\mathbf{z}| \leqslant |z| \leqslant \sqrt{1 + V_{\max}{}^2}|\mathbf{z}|$.

- Formula (238) in Corollary A.1 of the Appendix ensures for all $\epsilon \geqslant 0$ that for all $z = (z^0, \mathbf{z})$ such that $z = y - x$ for $x, y \in \Sigma$ and $\mathbf{z} \neq 0$ that

$$\|p^-(z + i\epsilon u)\| \leqslant O_{u,V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^3}\right). \tag{89}$$

Thanks to these ingredients we find the estimate

$$\|\Delta p_\Sigma^{\lambda,\epsilon u}(\mathbf{x},\mathbf{y})\| \leqslant C_4 \frac{e^{-C_D|\mathbf{y}-\mathbf{x}|}}{|\mathbf{y}-\mathbf{x}|^2}[1_K(x) \vee 1_K(y)] \tag{90}$$

for all $x, y \in \Sigma$ such that $\mathbf{y}-\mathbf{x} \neq 0$ and $\epsilon \geqslant 0$ with some constant $C_4(u, V_{\max}, \lambda)$. Consequently, using the bound for Γ from (20), we have the dominating function

$$\sup_{\epsilon \geqslant 0} \left| \overline{\phi(x)} \Gamma(\mathbf{x}) \Delta p_\Sigma^{\lambda,\epsilon u}(\mathbf{x},\mathbf{y}) \Gamma(\mathbf{y}) \psi(y) \right| \leqslant C_4 {\Gamma_{\max}}^2 |\phi(x)| \frac{e^{-C_D|\mathbf{y}-\mathbf{x}|}}{|\mathbf{y}-\mathbf{x}|^2} |\psi(y)|, \tag{91}$$

which is integrable, as the following calculation shows:

$$C_4 {\Gamma_{\max}}^2 \int_{\mathbf{x}\in\mathbb{R}^3} \int_{\mathbf{y}\in\mathbb{R}^3} |\phi(x)| \frac{e^{-C_D|\mathbf{y}-\mathbf{x}|}}{|\mathbf{y}-\mathbf{x}|^2} |\psi(y)| \, d^3\mathbf{y} \, d^3\mathbf{x} \tag{92}$$

$$= C_4 {\Gamma_{\max}}^2 \int_{\mathbf{z}\in\mathbb{R}^3} \frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^2} \int_{\mathbf{x}\in\mathbb{R}^3} |\phi(\pi_\Sigma(\mathbf{x}))||\psi(\pi_\Sigma(\mathbf{x}+\mathbf{z}))| \, d^3\mathbf{x} \, d^3\mathbf{z} \tag{93}$$

$$\leqslant 4\pi C_4 {\Gamma_{\max}}^2 \int_0^\infty e^{-C_D s} \, ds \, \|\phi \circ \pi_\Sigma\|_2 \|\psi \circ \pi_\Sigma\|_2 \tag{94}$$

$$\leqslant C_2 \|\phi\| \, \|\psi\|, \tag{95}$$

for a constant $C_2(u, V_{\max}, \lambda)$. In the step from (93) to (94) we use the Cauchy-Schwarz inequality, and in the step from (94) to (95), we use that the norms $\|\cdot \circ \pi_\Sigma\|_2$ and $\|\cdot\|$ are equivalent. On the one hand, this proves claim (87), which implies that the operators $\Delta P_\Sigma^{\lambda,\epsilon u} : \mathcal{H}_\Sigma \circlearrowleft$ described in (85) and (86) are well-defined for all $\epsilon \geqslant 0$ and bounded by

$$\sup_{\epsilon \geqslant 0} \|\Delta P_\Sigma^{\lambda,\epsilon u}\|_{\mathcal{H}_\Sigma \circlearrowleft} \leqslant C_2. \tag{96}$$

On the other hand, we use again the integrable domination from (91) together with the point-wise convergence

$$\lim_{\epsilon \downarrow 0} p^-(y - x + i\epsilon u) = p^-(y - x) \tag{97}$$

for $x, y \in \Sigma$ with $x \neq y$; cf. the analytic continuation of p^- described in Lemma 2.1. Using these ingredients, the dominated convergence theorem yields the following convergence in the weak operator topology:

$$\left\langle \phi, \Delta P_\Sigma^{\lambda,\epsilon u} \psi \right\rangle \xrightarrow{\epsilon \downarrow 0} \left\langle \phi, \Delta P_\Sigma^{\lambda} \psi \right\rangle \text{ for } \phi, \psi \in \mathcal{H}_\Sigma. \tag{98}$$

The next argument needs this fact only restricted to $\phi, \psi \in \mathcal{C}_\Sigma$. Using the notation (35) and Lemma 2.1, we get for $\phi, \psi \in \mathcal{C}_\Sigma$

$$\left\langle \phi, P_\Sigma^{\lambda,\epsilon u} \psi \right\rangle = \left\langle \phi, P_\Sigma^{0,\epsilon u} \psi \right\rangle + \left\langle \phi, \Delta P_\Sigma^{\lambda,\epsilon u} \psi \right\rangle \xrightarrow{\epsilon \downarrow 0} \left\langle \phi, P_\Sigma^{-} \psi \right\rangle + \left\langle \phi, \Delta P_\Sigma^{\lambda} \psi \right\rangle. \tag{99}$$

Because $P_\Sigma^-, \Delta P_\Sigma^\lambda : \mathcal{H}_\Sigma \circlearrowleft$ are bounded operators and $\mathcal{C}_\Sigma$ is dense in $\mathcal{H}_\Sigma$, this implies that

$$P_\Sigma^\lambda := P_\Sigma^- + \Delta P_\Sigma^\lambda : \mathcal{H}_\Sigma \circlearrowleft \tag{100}$$

is the unique bounded operator that satisfies (34), together with the bound

$$\|P^\lambda_\Sigma\|_{\mathcal{H}_\Sigma\circlearrowleft} \leqslant \|P^-_\Sigma\|_{\mathcal{H}_\Sigma\circlearrowleft} + \|\Delta P^\lambda_\Sigma\|_{\mathcal{H}_\Sigma\circlearrowleft} \leqslant 1 + C_2(u, V_{\max}, \lambda) \tag{101}$$

coming from (96). Note that we may take any fixed $u \in$ Past, e.g., $u = (-1, 0, 0, 0)$, in this bound and in the bounds below.

Next, we show that $K^\lambda := |\Delta P^\lambda_\Sigma|^2$ is a Hilbert-Schmidt operator. It is the integral operator (here written in 3-vector notation)

$$K^\lambda \psi(x) = \int_{\mathbb{R}^3} k^\lambda(\mathbf{x}, \mathbf{y})\Gamma(\mathbf{y})\psi(y) d^3\mathbf{y} \tag{102}$$

for $\psi \in \mathcal{H}_\Sigma$ and almost all $x \in \Sigma$ with the integral kernel

$$k^\lambda(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^3} \gamma^0 \Delta p^{\lambda,0}_\Sigma(\mathbf{x}, \mathbf{z})^* \gamma^0 \Gamma(\mathbf{z}) \Delta p^{\lambda,0}_\Sigma(\mathbf{z}, \mathbf{y})\, d^3\mathbf{z}. \tag{103}$$

We remark that under the symmetry assumption $\lambda(x, y) = -\lambda(y, x)$, we have

$$\gamma^0 \Delta p^{\lambda,0}_\Sigma(\mathbf{x}, \mathbf{z})^* \gamma^0 = \Delta p^{\lambda,0}_\Sigma(\mathbf{z}, \mathbf{x}); \tag{104}$$

cf. formula (110) below. Thanks to the estimate (90) we find

$$\left\|k^\lambda(\mathbf{x}, \mathbf{y})\right\| \leqslant \Gamma_{\max} {C_4}^2 \int_{\mathbb{R}^3} \frac{e^{-C_D|\mathbf{x}-\mathbf{z}|}}{|\mathbf{x}-\mathbf{z}|^2} \frac{e^{-C_D|\mathbf{z}-\mathbf{y}|}}{|\mathbf{z}-\mathbf{y}|^2} (1_K(x) \vee 1_K(z))(1_K(z) \vee 1_K(y))\, d^3\mathbf{z}. \tag{105}$$

Next, we use the bound

$$e^{-C_D|\mathbf{x}-\mathbf{z}|} e^{-C_D|\mathbf{z}-\mathbf{y}|} (1_K(x) \vee 1_K(z))(1_K(z) \vee 1_K(y)) \leqslant C_5 e^{-C_D(|\mathbf{y}-\mathbf{x}|+|\mathbf{x}|)/2} \tag{106}$$

with the constant $C_5(\lambda, V_{\max}) = \sup_{z \in K} e^{C_D|\mathbf{z}|/2}$. Substituting this bound in (105) and carrying out the integration yields

$$\|k^\lambda(\mathbf{x}, \mathbf{y})\| \leqslant \Gamma_{\max} {C_4}^2 C_5 e^{-C_D(|\mathbf{y}-\mathbf{x}|+|\mathbf{x}|)/2} \int_{\mathbb{R}^3} \frac{d^3\mathbf{z}}{|\mathbf{x}-\mathbf{z}|^2|\mathbf{z}-\mathbf{y}|^2} = C_6 \frac{e^{-C_D(|\mathbf{y}-\mathbf{x}|+|\mathbf{x}|)/2}}{|\mathbf{y}-\mathbf{x}|} \tag{107}$$

for a finite constant $C_6(\lambda, V_{\max})$. We can therefore bound the Hilbert-Schmidt norm of K^λ as follows:

$$\begin{aligned} \|K^\lambda\|^2_{I_2(\mathcal{H}_\Sigma)} &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \operatorname{trace}[\gamma^0 k^\lambda(\mathbf{x}, \mathbf{y})^* \gamma^0 \Gamma(\mathbf{x}) k^\lambda(\mathbf{x}, \mathbf{y}) \Gamma(\mathbf{y})]\, d^3\mathbf{x}\, d^3\mathbf{y} \\ &\leqslant 4{\Gamma_{\max}}^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \|k^\lambda(\mathbf{x}, \mathbf{y})\|^2\, d^3\mathbf{x}\, d^3\mathbf{y} \\ &\leqslant 4{\Gamma_{\max}}^2 {C_6}^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{e^{-C_D(|\mathbf{y}-\mathbf{x}|+|\mathbf{x}|)}}{|\mathbf{y}-\mathbf{x}|^2}\, d^3\mathbf{x}\, d^3\mathbf{y} < \infty. \end{aligned} \tag{108}$$

This proves that $K^\lambda = |\Delta P^\lambda_\Sigma|^2$ is a Hilbert-Schmidt operator, and therefore, ΔP^λ_Σ is compact.

To prove part (iv) of Lemma 2.3, we assume $\lambda(x,y) = -\lambda(y,x)$ for all $x, y \in \Sigma$. From the symmetries $D(w^*) = D(w)^*$ and $D(-w) = D(w)$ for all $w \in \text{domain}(r)$ and $(\gamma^\mu)^* = \gamma^0\gamma^\mu\gamma^0$, we conclude

$$p^-(-w^*) = \gamma^0 p^-(w)\gamma^0, \tag{109}$$

and hence, using the assumed symmetry of λ,

$$\gamma^0 \left(e^{-i\lambda(y,x)} p_-(y - x + i\epsilon u)\right)^* \gamma^0 = e^{-i\lambda(x,y)} p_-(x - y + i\epsilon u) \tag{110}$$

for $x, y \in \Sigma$, $\epsilon > 0$ and $u \in \text{Past}$. Substituting this in the specification (34)-(35) of P^λ_Σ, it follows that P^λ_Σ is self-adjoint and concludes the proof. □

Proof of Theorem 2.4. To show the equivalence we need to control of the kernel of $P^\lambda_\Sigma - P^{\tilde\lambda}_\Sigma$ from above and from below. Let $\Delta\mathbf{A} : \mathbb{R}^3 \to \mathbb{R}^3$ be the vector field on $\mathbb{R}^3$ with

$$\Delta\mathbf{A}(\mathbf{x}) \cdot \mathbf{z} = (A_\mu(x) - \widetilde{A}_\mu(x)) z^\mu \tag{111}$$

for any $x = (x^0, \mathbf{x}) \in \Sigma$ and $z = (z^0, \mathbf{z}) \in T_x\Sigma$. Then for any $x = (x^0, \mathbf{x}) \in \Sigma$, $A(x)|_{T_x\Sigma} = \widetilde{A}(x)|_{T_x\Sigma}$ holds if and only if $\Delta\mathbf{A}(\mathbf{x}) = 0$. From $\lambda \in \mathcal{G}(A)$ and $\lambda \in \mathcal{G}(\widetilde{A})$, see Definition 2.2, we get the Taylor expansions

$$e^{-i\lambda(x,y)} = 1 + iA_\mu(x)(y^\mu - x^\mu) + O_\lambda(|x-y|^2)(1_K(x) \vee 1_K(y)), \tag{112}$$

$$e^{-i\tilde\lambda(x,y)} = 1 + i\widetilde{A}_\mu(x)(y^\mu - x^\mu) + O_{\tilde\lambda}(|x-y|^2)(1_K(x) \vee 1_K(y)), \tag{113}$$

$$y^0 - x^0 = \nabla t_\Sigma(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x}) + O_\Sigma(|\mathbf{x} - \mathbf{y}|^2) \tag{114}$$

for $y, x \in \Sigma$ from which we conclude

$$e^{-i\lambda(x,y)} - e^{-i\tilde\lambda(x,y)} = i\Delta\mathbf{A}(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x}) + r_1(\mathbf{x}, \mathbf{y}) \tag{115}$$

with an error term r_1 that fulfills for any $x, y \in \Sigma$

$$|r_1(\mathbf{x}, \mathbf{y})| \leqslant O_{\lambda,\tilde\lambda,V_{\max}}(|\mathbf{x} - \mathbf{y}|^2)\,(1_K(x) \vee 1_K(y))\,, \tag{116}$$

where we used $|x - y| = O_{V_{\max}}(|\mathbf{x} - \mathbf{y}|)$ due to (15). Note that the bound (116) holds not only locally near the diagonal but also *globally* for $x, y \in \Sigma$ because $e^{-i\lambda} - e^{-i\tilde\lambda}$ is bounded and λ and $\tilde\lambda$ vanish outside $K \times \mathbb{R}^4 \cup \mathbb{R}^4 \times K$ for some compact set $K \subset \mathbb{R}^4$. For $\phi, \psi \in \mathcal{H}_\Sigma$ formula (36) from Lemma 2.3 implies

$$\begin{aligned}
&\left\langle \phi, (P^\lambda_\Sigma - P^{\tilde\lambda}_\Sigma)\psi \right\rangle \\
&= \int_{x\in\Sigma} \overline{\phi}(x)\, i_\gamma(d^4x) \int_{y\in\Sigma} (e^{-i\lambda(x,y)} - e^{-i\tilde\lambda(x,y)}) p^-(y-x)\, i_\gamma(d^4y)\, \psi(y) \\
&= \int_{\mathbf{x}\in\mathbb{R}^3} \int_{\mathbf{y}\in\mathbb{R}^3} \phi(x)^* \gamma^0 \Gamma(\mathbf{x}) [t_1(x,y) + t_2(x,y)] \gamma^0 \Gamma(\mathbf{y}) \psi(y)\, d^3\mathbf{y}\, d^3\mathbf{x}
\end{aligned} \tag{117}$$

with

$$t_1(x,y) = i\Delta\mathbf{A}(\mathbf{x})\cdot(\mathbf{y}-\mathbf{x})p^-(y-x)\gamma^0, \tag{118}$$
$$t_2(x,y) = \ r_1(\mathbf{x},\mathbf{y})p^-(y-x)\gamma^0, \tag{119}$$

where we use the abbreviations $x = \pi_\Sigma(\mathbf{x})$, $y = \pi_\Sigma(\mathbf{y})$ again, and Γ is defined in (19). We have introduced two extra factors γ^0 in (117) in order to have a positive-definite weight $\gamma^0\Gamma$.

We claim that the kernel $t_2(x,y)\gamma^0$ gives rise to a Hilbert-Schmidt-operator T_2. Indeed, using the bound (20) for Γ, the bound (238) from Corollary A.1 in the appendix for p^-, and the bound (116) for r_1, we have

$$\begin{aligned}\|T_2\|^2_{I_2(\mathcal{H}_\Sigma)} &= \int_{\mathbf{x}\in\mathbb{R}^3}\int_{\mathbf{y}\in\mathbb{R}^3} \operatorname{trace}[t_2(x,y)^*\gamma^0\Gamma(\mathbf{x})t_2(x,y)\gamma^0\Gamma(\mathbf{y})]\, d^3\mathbf{y}\, d^3\mathbf{x}\\ &\leqslant C_7\int_{\mathbf{x}\in\mathbb{R}^3}\int_{\mathbf{y}\in\mathbb{R}^3}\left|\frac{e^{-C_D|\mathbf{y}-\mathbf{x}|^2}}{|\mathbf{y}-\mathbf{x}|}\right|^2 (1_K(x)+1_K(y))\, d^3\mathbf{y}\, d^3\mathbf{x} \leqslant C_8 < \infty\end{aligned} \tag{120}$$

for some constants C_7 and C_8 that depend on $\Sigma, \lambda, \tilde{\lambda}$.

If $A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}$ then $\Delta\mathbf{A} = 0$. This implies $t_1 = 0$ and therefore $P^\lambda_\Sigma - P^{\tilde{\lambda}}_\Sigma = T_2$ is a Hilbert-Schmidt operator. This proves the "$\Leftarrow$" part of the claim (40).

Conversely, let us assume that $A|_{T\Sigma} = \widetilde{A}|_{T\Sigma}$ does not hold. Then we can take some $x_0 \in \mathbb{R}^3$ with $\Delta\mathbf{A}(\mathbf{x}_0) \neq 0$. By continuity of $\Delta\mathbf{A}$, we have $\inf_{\mathbf{x}\in U}|\Delta\mathbf{A}(x)| > 0$ for some neighborhood U of $\mathbf{x}$. Furthermore there is a constant $C_9(V_{\max})$ such that $\gamma^0\Gamma(\mathbf{x}) - C_9$ is positive-semidefinite for all $x = (x^0,\mathbf{x}) \in \Sigma$. Consequently, we get the following bound for all $\mathbf{x}\in U$ and $\mathbf{y}\in\mathbb{R}^3$:

$$\begin{aligned}&\operatorname{trace}\left[t_1(\mathbf{x},\mathbf{y})^*\gamma^0\Gamma(\mathbf{x})t_1(\mathbf{x},\mathbf{y})\gamma^0\Gamma(\mathbf{y})\right] \geqslant {C_9}^2 \operatorname{trace}\left[t_1(\mathbf{x},\mathbf{y})^* t_1(\mathbf{x},\mathbf{y})\right]\\ &\geqslant C_{10}|\Delta\mathbf{A}(\mathbf{x})\cdot(\mathbf{y}-\mathbf{x})|^2\|p^-(y-x)\|^2 \geqslant C_{11}|\Delta\mathbf{A}(\mathbf{x})\cdot(\mathbf{y}-\mathbf{x})|^2\left(\frac{e^{-m|\mathbf{y}-\mathbf{x}|}}{|\mathbf{y}-\mathbf{x}|^3}\right)^2.\end{aligned} \tag{121}$$

with two positive constants C_{10} and C_{11} depending on $V_{\max}$. In the last step, we have used the lower bound (239) for $\|p^-\|$ from Corollary A.2 in the appendix. Because the lower bound given in (121) is not integrable over $(\mathbf{x},\mathbf{y}) \in U\times\mathbb{R}^4$, we conclude that T_1 is not a Hilbert-Schmidt operator. Because T_2 is a Hilbert-Schmidt operator, this implies that $P^\lambda_\Sigma - P^{\tilde{\lambda}}_\Sigma$ cannot be a Hilbert-Schmidt operator. Thus, we have proven part "$\Rightarrow$" of the Theorem. □

2.4 Proof of Theorem 2.8

This section contains the centerpiece of this work. The proof of Theorem 2.8 will be given at the end of this section. To show that the claimed equality (47) holds, we analyze the difference of matrix elements

$$\left\langle\phi,(P^A_{\Sigma_{t_1}} + S^A_{\Sigma_{t_1}})\psi\right\rangle - \left\langle\phi,(P^A_{\Sigma_{t_0}} + S^A_{\Sigma_{t_0}})\psi\right\rangle \tag{122}$$

for $\psi, \phi \in \mathcal{C}_A$. This is done in two steps. First, using Stokes' theorem, we provide a formula for the derivative w.r.t. the flow parameter of the family of Cauchy surfaces $(\Sigma_t)_{t\in T}$ in Lemma 2.11 and Corollary 2.12. Second, we give the relevant estimates on this derivative in Lemmas 2.13-2.15 which are summarized in Corollary 2.16, and conclude with the proof of Theorem 2.8.

For the first step, the following notations for the Dirac operators acting from the left and from the right, respectively, are convenient:

$$D^A\psi(x) = D^A_x\psi(x) := (i\partial\!\!\!/^x - A\!\!\!/(x) - m)\psi(x), \tag{123}$$

$$\overline{\phi(y)}\,\overleftarrow{D^A} = \overline{\phi(y)}\,\overleftarrow{D^A_y} := \overline{\phi(y)}(-i\overleftarrow{\partial\!\!\!/^y} - A\!\!\!/(y) - m) = \overline{D^A_y\phi(y)}, \tag{124}$$

where $f(y)\overleftarrow{\partial\!\!\!/^y} = f(y)\overleftarrow{\partial\!\!\!/} := \partial_\mu f(y)\gamma^\mu$.

Lemma 2.11. *Let $k : \mathbb{R}^4 \times \mathbb{R}^4 \to \mathbb{C}^{4\times 4}$ be a smooth function. Let $\phi, \psi \in \mathcal{C}_A$. Then for any $t \in T$ we have*

$$\begin{aligned}&\frac{d}{dt}\int_{x\in\Sigma_t}\int_{y\in\Sigma_t}\overline{\phi(x)}\,i_\gamma(d^4x)\,k(x,y)i_\gamma(d^4y)\,\psi(y)\\&= -i\int_{x\in\Sigma_t}\int_{y\in\Sigma_t}\overline{\phi(x)}\,i_\gamma(d^4x)\,\mathcal{D}^A_t k(x,y)i_\gamma(d^4y)\,\psi(y)\end{aligned} \tag{125}$$

with

$$\mathcal{D}^A_t k(x,y) := v_t(x)n\!\!\!/_t(x)D^A_x k(x,y) - k(x,y)\overleftarrow{D^A_y}v_t(y)n\!\!\!/_t(y). \tag{126}$$

Proof. Assume that $\phi', \psi' : \mathbb{R}^4 \to \mathbb{C}^4$ are smooth functions with $\operatorname{supp}\phi' \cap \operatorname{supp}\psi' \subseteq K +$ Causal for some compact set $K \subset \mathbb{R}^4$.

We set

$$\mathbf{\Sigma}_{t_0t_1} := \{(x,t) \in \mathbf{\Sigma} |\ t_0 \leqslant t \leqslant t_1\} \tag{127}$$

for any real numbers $t_0 \leqslant t_1$. By Stokes' theorem, we have:

$$\left(\int_{\Sigma_{t_1}} - \int_{\Sigma_{t_0}}\right)\overline{\phi'(x)}\,i_\gamma(d^4x)\,\psi'(x) = \int_{\mathbf{\Sigma}_{t_0t_1}} d[\overline{\phi'(x)}\,i_\gamma(d^4x)\,\psi'(x)]. \tag{128}$$

We calculate:

$$\begin{aligned}d[\overline{\phi'(x)}i_\gamma(d^4x)\psi'(x)] &= \partial_\mu(\overline{\phi'(x)}\gamma^\mu\psi'(x))\,d^4x\\&= (\partial_\mu\overline{\phi'(x)})\gamma^\mu\psi'(x)\,d^4x + \overline{\phi'(x)}\gamma^\mu\partial_\mu\psi'(x)\,d^4x\\&= \overline{\partial\!\!\!/\phi'(x)}\psi'(x)\,d^4x + \overline{\phi'(x)}\partial\!\!\!/\psi'(x)\,d^4x\\&= i\overline{D^A\phi'(x)}\psi'(x)\,d^4x - i\overline{\phi'(x)}D^A\psi'(x)\,d^4x,\end{aligned} \tag{129}$$

see also the calculation from (17) to (20) in [3]. Integration yields

$$\begin{aligned}&\left(\int_{\Sigma_{t_1}} - \int_{\Sigma_{t_0}}\right) \overline{\phi'(x)}\, i_\gamma(d^4x)\, \psi'(x)\\ &= i\int_{\mathbf{\Sigma}_{t_0t_1}} [\overline{D^A\phi'(x)}\psi'(x) - \overline{\phi'(x)}D^A\psi'(x)]\, d^4x\\ &= i\int_{t_0}^{t_1}\int_{\Sigma_t} [\overline{D^A\phi'(x)}\psi'(x) - \overline{\phi'(x)}D^A\psi'(x)]\, i_{v_tn_t}(d^4x)\, dt.\end{aligned} \tag{130}$$

Differentiating this with respect to the upper boundary t_1, we conclude

$$\begin{aligned}&\frac{d}{dt}\int_{\Sigma_t} \overline{\phi'(x)}\, i_\gamma(d^4x)\, \psi'(x)\\ &= i\int_{\Sigma_t} [\overline{D^A\phi'(x)}\psi'(x) - \overline{\phi'(x)}D^A\psi'(x)]\, i_{v_tn_t}(d^4x)\\ &= i\int_{\Sigma_t} [\overline{\phi'(x)}\,\overleftarrow{D^A} v_t(x)\not{n}_t(x) i_\gamma(d^4x)\psi'(x) - \overline{\phi'(x)} i_\gamma(d^4x) v_t(x)\not{n}_t(x) D^A\psi'(x)],\end{aligned} \tag{131}$$

using (19). In the special case $\phi' \in \mathcal{C}_A$ this boils down to

$$\frac{d}{dt}\int_{\Sigma_t} \overline{\phi'(x)}\, i_\gamma(d^4x)\, \psi'(x) = -i\int_{\Sigma_t} \overline{\phi'(x)}\, i_\gamma(d^4x)\, v_t(x)\not{n}_t(x)D^A\psi'(x), \tag{132}$$

while in the special case $\psi' \in \mathcal{C}_A$ it boils down to

$$\frac{d}{dt}\int_{\Sigma_t} \overline{\phi'(x)}\, i_\gamma(d^4x)\, \psi'(x) = i\int_{\Sigma_t} \overline{\phi'(x)}\,\overleftarrow{D^A} v_t(x)\not{n}_t(x)\, i_\gamma(d^4x)\, \psi'(x). \tag{133}$$

We consider the function

$$F : T \times T \to \mathbb{C}, \quad F(s,t) := \int_{x\in\Sigma_s}\int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x)\, k(x,y)\, i_\gamma(d^4y)\, \psi(y). \tag{134}$$

We apply (132) to $\phi' = \phi$ and $\psi'(x) = \int_{y\in\Sigma_t} k(x,y) i_\gamma(d^4y)\, \psi(y)$ to get

$$\frac{\partial}{\partial s}F(s,t) = -i\int_{x\in\Sigma_s}\int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x)\, v_s(x)\not{n}_s(x) D_x^A k(x,y)\, i_\gamma(d^4y)\, \psi(y). \tag{135}$$

Similarly, we apply (133) to $\overline{\phi'(y)} = \int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x)\, k(x,y)$ and $\psi' = \psi$ to get

$$\frac{\partial}{\partial t}F(s,t) = i\int_{x\in\Sigma_s}\int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x)\, k(x,y)\overleftarrow{D_y^A} v_t(y)\not{n}_t(y)\, i_\gamma(d^4y)\, \psi(y). \tag{136}$$

From the chain rule, claim (125) follows:

$$\begin{aligned}&\frac{d}{dt}F(t,t)\\ &= -i\int_{x\in\Sigma_s}\int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x)[v_t(x)\not{n}_t(x)D_x^A k(x,y) - k(x,y)\overleftarrow{D_y^A} v_t(y)\not{n}_t(y)]\, i_\gamma(d^4y)\, \psi(y).\end{aligned} \tag{137}$$

□

From formula (125) and the chain rule, we immediately get the following corollary.

Corollary 2.12. *For any smooth function* $k : \mathbb{R}^4 \times \mathbb{R}^4 \times T \to \mathbb{C}^{4\times 4}$, $(x, y, t) \mapsto k_t(x, y)$, *any* $\phi, \psi \in \mathcal{C}_A$, *and any* $t \in T$ *we have*

$$\begin{aligned}&\frac{d}{dt}\int_{x\in\Sigma_t}\int_{y\in\Sigma_t}\overline{\phi(x)}\, i_\gamma(d^4x)\, k_t(x,y) i_\gamma(d^4y)\,\psi(y)\\ &=\int_{x\in\Sigma_t}\int_{y\in\Sigma_t}\overline{\phi(x)}\, i_\gamma(d^4x)\left[-i\mathcal{D}_t^A k(x,y)+\frac{\partial k_t}{\partial t}(x,y)\right] i_\gamma(d^4y)\,\psi(y).\end{aligned} \tag{138}$$

This completes step one, and next, we turn to the relevant estimates. In the following calculations for fixed $t \in T$, we drop the index t in $v = v_t$ and $n = n_t$. Also, the t–dependence of the remainder terms $r_{\dots}$ is suppressed in the notation below, as we have uniformity in t of the error bounds. Recall from equation (42) that $E_\mu = F_{\mu\nu} n^\nu$ denotes the "electric field" of the electromagnetic field $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ with respect to the local Cauchy surface Σ.

Lemma 2.13. *For* $u \in \text{Past}$, $\epsilon > 0$, *and* $x, y \in \mathbb{R}^4$, *let*

$$p^{A,\epsilon u}(x,y) := e^{-i\lambda^A(x,y)} p^-(y-x+i\epsilon u) \tag{139}$$

with λ^A *defined in* (38). *Then for* $t \in T$, $x, y \in \Sigma_t$, $z = (z^0, \mathbf{z}) = y - x$, *and* $w = z + i\epsilon u$ *we have*

$$\begin{aligned}&\mathcal{D}_t^A p^{A,\epsilon u}(x,y)\\ =&\frac{1}{2}v(x)\not{n}(x)\gamma^\nu F_{\mu\nu}(x) z^\mu p^{A,\epsilon u}(x,y)+\frac{1}{2}p^{A,\epsilon u}(x,y)\gamma^\nu F_{\mu\nu}(y) z^\mu v(y)\not{n}(y) + r_2(x,y,\epsilon u) \qquad (140)\\ =&-\frac{i}{2m}v(x) z^\mu E_\mu(x)\not{\partial} D(w) + r_3(x,y,\epsilon u) + r_4(x,y,\epsilon u) \qquad (141)\end{aligned}$$

with error terms

$$r_2 = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x)\vee 1_K(y)], \tag{142}$$

$$r_3 = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x)\vee 1_K(y)], \tag{143}$$

$$r_4 = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)[1_K(x)\vee 1_K(y)] \tag{144}$$

for any compact set K *containing the support of* A. *For any two different points* $x \neq y$ *in* Σ_t, *the limit* $r_3(x, y, 0) := \lim_{\epsilon\downarrow 0} r_3(x, y, \epsilon u)$ *exists.*

Proof. We calculate for $x, y \in \Sigma_t$, $u \in \text{Past}$, and $\epsilon > 0$:

$$\begin{aligned}&D_x^A[e^{-i\lambda^A(x,y)}p^-(y-x+i\epsilon u)]\\ &=[\not{\partial}^x\lambda^A(x,y)-\not{A}(x)]e^{-i\lambda^A(x,y)}p^-(y-x+i\epsilon u)+e^{-i\lambda^A(x,y)}(i\not{\partial}^x-m)p^-(y-x+i\epsilon u)\\ &=[\not{\partial}^x\lambda^A(x,y)-\not{A}(x)]p^{A,\epsilon u}(x,y),\quad\text{because}\quad (i\not{\partial}^x-m)p^-(y-x+i\epsilon u)=0.\end{aligned} \tag{145}$$

Using the definition (38) of λ^A, we get

$$\begin{aligned}\not{\partial}^x \lambda^A(x,y) - \not{A}(x) &= \frac{1}{2}\gamma^\nu[A_\nu(y) - A_\nu(x) + (x^\mu - y^\mu)\partial_\nu^x A_\mu(x)] \\ &= \frac{1}{2}[\gamma^\nu F_{\mu\nu}(x)(y^\mu - x^\mu) + r_5(x,y)] \end{aligned} \tag{146}$$

with the Taylor rest term

$$\begin{aligned}&r_5(x,y) = \gamma^\nu[A_\nu(y) - A_\nu(x) - (y^\mu - x^\mu)\partial_\mu^x A_\nu(x)] = O_A(|x-y|^2)[1_K(x) \vee 1_K(y)] \\ &= O_A(|\mathbf{z}|^2)[1_K(x) \vee 1_K(y)] \text{ with } \mathbf{z} = \mathbf{y} - \mathbf{x}; \end{aligned} \tag{147}$$

cf. formula (28) in the appendix, which compares $|z|$ with $|\mathbf{z}|$. Recall that K denotes a compact set containing the support of A. Similarly, we find

$$\begin{aligned}&[e^{-i\lambda^A(x,y)}p^-(y-x+i\epsilon u)]\overleftarrow{D_y^A} \\ &= e^{-i\lambda^A(x,y)}p^-(y-x+i\epsilon u)[-\not{\partial}^y\lambda^A(x,y) - \not{A}(y)] + p^-(y-x+i\epsilon u)(-i\overleftarrow{\not{\partial}^y} - m)e^{-i\lambda^A(x,y)} \\ &= p^{A,\epsilon u}(x,y)[-\not{\partial}^y\lambda^A(x,y) - \not{A}(y)]. \end{aligned} \tag{148}$$

Using the symmetry $\lambda^A(x,y) = -\lambda^A(y,x)$ and interchanging x and y, equation (146) can be rewritten in the form

$$-\not{\partial}^y\lambda^A(x,y) - \not{A}(y) = \frac{1}{2}\left[-\gamma^\nu F_{\mu\nu}(y)(y^\mu - x^\mu) + r_5(y,x)\right]. \tag{149}$$

Combining this with the definition (126) of $\mathcal{D}_t^A$, we find for $x,y \in \Sigma_t$, $z = y - x$

$$\begin{aligned}&\mathcal{D}_t^A p^{A,\epsilon u}(x,y) \\ &= \frac{1}{2}v(x)\not{n}(x)[\gamma^\nu F_{\mu\nu}(x)z^\mu + r_5(x,y)]p^{A,\epsilon u}(x,y) \\ &\quad + \frac{1}{2}p^{A,\epsilon u}(x,y)[\gamma^\nu F_{\mu\nu}(y)z^\mu - r_5(y,x)]v(y)\not{n}(y) \\ &= \frac{1}{2}v(x)\not{n}(x)\gamma^\nu F_{\mu\nu}(x)z^\mu p^{A,\epsilon u}(x,y) + \frac{1}{2}p^{A,\epsilon u}(x,y)\gamma^\nu F_{\mu\nu}(y)z^\mu v(y)\not{n}(y) + r_2(x,y,\epsilon u) \end{aligned} \tag{150}$$

with the error term

$$\begin{aligned}r_2(x,y,\epsilon u) &= \frac{1}{2}v(x)\not{n}(x)r_5(x,y)p^{A,\epsilon u}(x,y) - \frac{1}{2}p^{A,\epsilon u}(x,y)r_5(y,x)v(y)\not{n}(y) \\ &= O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x) \vee 1_K(y)], \end{aligned} \tag{151}$$

for $t \in T$, $x,y \in \Sigma_t$, $\epsilon > 0$, $u \in$ Past. Here we used the bound (238) in Lemma A.1 in the appendix for p^-, the quadratic bound (147) for $r_5(x,y)$, and the fact that $|vn|$, being continuous, is bounded on compact sets. This proves the claim given in (140) with the error bound (142).

It remains to prove the claim given in (141) with the bounds (143) and (144). Recall the definitions of $p^{A,\epsilon u}$ and p^- given in (139) and (30), respectively. We have

$$p^{A,\epsilon u}(x,y) = -\frac{i}{2m}\partial\!\!\!/ D(w) + r_6(x,y,\epsilon u) \tag{152}$$

with the error term

$$r_6(x,y,\epsilon u) = \frac{1}{2}e^{-i\lambda^A(x,y)}D(w) + (e^{-i\lambda^A(x,y)}-1)p^-(z+i\epsilon u) = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^2}\right) \tag{153}$$

using the bounds (232), (238) from the appendix and the Taylor bound

$$|e^{-i\lambda^A(x,y)}-1| = O_A(|z|) \leqslant O_{A,\mathbf{\Sigma}}(|\mathbf{z}|), \tag{154}$$

which follows from $\lambda^A \in \mathcal{G}(A)$, cf. Definition 2.2 and, once more, from the estimate (28) in the appendix. Hence we get from (150)

$$\begin{aligned}
&\mathcal{D}_t^A p^{A,\epsilon u}(x,y) - r_2(x,y,\epsilon u) \\
&= \frac{1}{2}v(x)n\!\!\!/(x)\gamma^\nu F_{\mu\nu}(x)z^\mu p^{A,\epsilon u}(x,y) + \frac{1}{2}p^{A,\epsilon u}(x,y)\gamma^\nu F_{\mu\nu}(y)z^\mu v(y)n\!\!\!/(y) \\
&= -\frac{i}{4m}v(x)n\!\!\!/(x)\gamma^\nu F_{\mu\nu}(x)z^\mu\partial\!\!\!/ D(w) - \frac{i}{4m}\partial\!\!\!/ D(w)\gamma^\nu F_{\mu\nu}(y)z^\mu v(y)n\!\!\!/(y) + r_7(x,y,\epsilon u)
\end{aligned} \tag{155}$$

with the error term

$$r_7 = \frac{1}{2}v(x)n\!\!\!/(x)\gamma^\nu F_{\mu\nu}(x)z^\mu r_6 + \frac{1}{2}r_6\gamma^\nu F_{\mu\nu}(y)z^\mu v(y)n\!\!\!/(y) = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x)\vee 1_K(y)]. \tag{156}$$

We employ estimate (236) for ∂D from the appendix and the fact $\operatorname{supp} F_{\mu\nu} \subseteq K$ to find

$$v(x)n\!\!\!/(x)F_{\mu\nu}(x)\gamma^\nu z^\mu\partial\!\!\!/ D(w) = v(x)n\!\!\!/(x)F_{\mu\nu}(x)\gamma^\nu w^\mu\partial\!\!\!/ D(w) + r_8(x,y,\epsilon u) \tag{157}$$

$$\partial\!\!\!/ D(w)\gamma^\nu F_{\mu\nu}(y)z^\mu v(y)n\!\!\!/(y) = \partial\!\!\!/ D(w)\gamma^\nu F_{\mu\nu}(y)w^\mu v(y)n\!\!\!/(y) + r_9(x,y,\epsilon u) \tag{158}$$

with the error terms

$$r_8 = -v(x)n\!\!\!/(x)F_{\mu\nu}(x)\gamma^\nu i\epsilon u^\mu\partial\!\!\!/ D(w) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)1_K(x), \tag{159}$$

$$r_9 = -\partial\!\!\!/ D(w)\gamma^\nu F_{\mu\nu}(y)i\epsilon u^\mu v(y)n\!\!\!/(y) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)1_K(y). \tag{160}$$

Substituting this in (155), we conclude

$$\begin{aligned}
\mathcal{D}_t^A p^{A,\epsilon u}(x,y) = &-\frac{i}{4m}v(x)n\!\!\!/(x)\gamma^\nu F_{\mu\nu}(x)w^\mu\partial\!\!\!/ D(w) - \frac{i}{4m}\partial\!\!\!/ D(w)\gamma^\nu F_{\mu\nu}(y)w^\mu v(y)n\!\!\!/(y) \\
&+ (r_2+r_7+r_{10})(x,y,\epsilon u)
\end{aligned} \tag{161}$$

with the additional error term

$$r_{10} = -\frac{i}{4m}(r_8 + r_9) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)[1_K(x) \vee 1_K(y)]. \tag{162}$$

The following "Lorentz symmetry relation" will be used several times in the calculations below.

$$w_\nu \partial_\mu D(w) = w_\mu \partial_\nu D(w) \quad \text{for} \quad w \in \text{domain}(r). \tag{163}$$

Equation (163) can be seen as follows. Using $D = f \circ r$ with $f(\xi) = -m^3(2\pi^2)^{-1}K_1(m\xi)/(m\xi)$ from (31) and $\partial_\mu r(w) = -\frac{w_\mu}{r(w)}$, we obtain $w_\nu \partial_\mu D(w) = -\frac{w_\nu w_\mu}{r(w)} f'(r(w)) = w_\mu \partial_\nu D(w)$.

Using the anticommutator relation $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$ for the Dirac-matrices three times and the Lorentz symmetry relation (163), we calculate

$$\begin{aligned}
v(x)\not{n}(x)F_{\mu\nu}(x)\gamma^\nu w^\mu \not{\partial} D(w) &= [\not{n}(x)\gamma^\nu \not{w}]v(x)F_{\mu\nu}(x)\partial^\mu D(w)\\
=&[2n^\nu(x)\not{w} - 2\gamma^\nu n_\sigma(x)w^\sigma + 2w^\nu \not{n}(x) - \not{w}\gamma^\nu \not{n}(x)]v(x)F_{\mu\nu}(x)\partial^\mu D(w)\\
=&2n^\nu(x)\not{w}v(x)F_{\mu\nu}(x)\partial^\mu D(w) &(164)\\
&- 2\gamma^\nu n_\sigma(x)w^\sigma v(x)F_{\mu\nu}(x)\partial^\mu D(w) &(165)\\
&+ 2w^\nu \not{n}(x)v(x)F_{\mu\nu}(x)\partial^\mu D(w) &(166)\\
&- \not{w}\gamma^\nu \not{n}(x)v(x)F_{\mu\nu}(x)\partial^\mu D(w). &(167)
\end{aligned}$$

For the first term (164), using the Lorentz symmetry (163) again, we get

$$\begin{aligned}
(164) &= 2n^\nu(x)\not{w}v(x)F_{\mu\nu}(x)\partial^\mu D(w) = 2v(x)w^\mu E_\mu(x)\not{\partial} D(w)\\
&= 2v(x)z^\mu E_\mu(x)\not{\partial} D(w) + r_{11}(x, y, \epsilon u) &(168)
\end{aligned}$$

with the error term

$$r_{11} = 2v(x)i\epsilon u^\mu E_\mu(x)\not{\partial} D(w) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)1_K(x), \tag{169}$$

where in the last step we have used estimate (236) once more. For the second term (165), we use $n_\sigma(x)z^\sigma = O_{\mathbf{\Sigma}}(|\mathbf{z}|^2)$, which holds because of $x, y \in \Sigma_t$ and $n(x) \perp T_x\Sigma_t$, to get

$$(165) = -2\gamma^\nu n_\sigma(x)w^\sigma v(x)F_{\mu\nu}(x)\partial^\mu D(w) = r_{12}(x, y, \epsilon u) + r_{13}(x, y, \epsilon u) \tag{170}$$

with the error terms

$$r_{12} = -2\gamma^\nu n_\sigma(x)z^\sigma v(x)F_{\mu\nu}(x)\partial^\mu D(w) = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)1_K(x), \tag{171}$$

$$r_{13} = -2\gamma^\nu n_\sigma(x)i\epsilon u^\sigma v(x)F_{\mu\nu}(x)\partial^\mu D(w) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)1_K(x). \tag{172}$$

We have used the estimates (234) and, once more, (236). The contribution of the third term (166) is zero, i.e.

$$(166) = 2w^\nu \not{n}(x)v(x)F_{\mu\nu}(x)\partial^\mu D(w) = 0, \tag{173}$$

because of symmetry $w^\nu \partial^\mu D(w) = w^\mu \partial^\nu D(w)$, cf. (163), and antisymmetry $F_{\mu\nu} = -F_{\nu\mu}$. To express the fourth term (167), we use the Lorentz symmetry relation (163) again and replace x by y up to the following error term:

$$r_{14}(x,y) = F_{\mu\nu}(x)v(x)\not{n}(x) - F_{\mu\nu}(y)v(y)\not{n}(y) = O_{A,\mathbf{\Sigma}}(|\mathbf{z}|)[1_K(x) \vee 1_K(y)]. \tag{174}$$

We obtain for the fourth term (167):

$$\begin{aligned}(167) &= -\not{w}\partial^\mu D(w)\gamma^\nu \not{n}(x)v(x)F_{\mu\nu}(x) = -w^\mu \not{\partial} D(w)\gamma^\nu F_{\mu\nu}(x)v(x)\not{n}(x)\\ &= -\not{\partial} D(w)\gamma^\nu F_{\mu\nu}(y)w^\mu v(y)\not{n}(y) + r_{15}(x,y,\epsilon u)\end{aligned} \tag{175}$$

with the error term

$$r_{15} = w^\mu \not{\partial} D(w)\gamma^\nu r_{14} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x) \vee 1_K(y)]. \tag{176}$$

We have used estimate (235) from the appendix and the bound (174). The expressions (168), (170), (173) and (175) of the four terms (164)-(167) give

$$\begin{aligned}&v(x)\not{n}(x)F_{\mu\nu}(x)\gamma^\nu w^\mu \not{\partial} D(w) = (164) + (165) + (166) + (167) \qquad (177)\\ =&[2v(x)z^\mu E_\mu(x)\not{\partial} D(w) + r_{11}] + [r_{12} + r_{13}] + 0 + [-\not{\partial} D(w)\gamma^\nu F_{\mu\nu}(y)w^\mu v(y)\not{n}(y) + r_{15}],\end{aligned}$$

which can be rewritten in the form

$$\begin{aligned}&v(x)\not{n}(x)F_{\mu\nu}(x)\gamma^\nu w^\mu \not{\partial} D(w) + \not{\partial} D(w)\gamma^\nu F_{\mu\nu}(y)w^\mu v(y)\not{n}(y)\\ &= 2v(x)z^\mu E_\mu(x)\not{\partial} D(w) + r_{16}(x,y,\epsilon u) + r_{17}(x,y,\epsilon u)\end{aligned} \tag{178}$$

with the error terms

$$r_{16} = r_{12} + r_{15} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x) \vee 1_K(y)], \tag{179}$$

$$r_{17} = r_{11} + r_{13} = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)[1_K(x) \vee 1_K(y)]. \tag{180}$$

We have used the estimates (171) and (176) to bound r_{16} and the estimates (169) and (172) to bound r_{17}. Substituting this result in equation (161) together with the error bounds (151), (156) and (162), we infer

$$\begin{aligned}&\mathcal{D}_t^A p^{A,\epsilon u}(x,y)\\ =& -\frac{i}{4m}v(x)\not{n}(x)F_{\mu\nu}(x)\gamma^\nu w^\mu \not{\partial} D(w) - \frac{i}{4m}\not{\partial} D(w)\gamma^\nu F_{\mu\nu}(y)w^\mu v(y)\not{n}(y) + r_2 + r_7 + r_{10}\\ =& -\frac{i}{2m}v(x)z^\mu E_\mu(x)\not{\partial} D(w) + r_3 + r_4\end{aligned} \tag{181}$$

with the error terms

$$r_3(x,y,\epsilon u) = r_2 + r_7 - \frac{i}{4m}r_{16} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)[1_K(x) \vee 1_K(y)], \tag{182}$$

$$r_4(x,y,\epsilon u) = r_{10} - \frac{i}{4m}r_{17} = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right)[1_K(x) \vee 1_K(y)]. \tag{183}$$

This proves the claim given in (141) with the bounds (143), (144). Recall that despite the uniformity in ϵ of the bound given in (182), $r_3 = r_3(x, y, \epsilon u)$ depends on ϵ. To ensure existence of the limit $\lim_{\epsilon\downarrow 0} r_3(x, y, \epsilon u)$ for two different points $x, y \in \Sigma_t$ from the explicit form of r_3, we observe that $z = y - x$ is space-like, and hence $z \in \operatorname{domain} r$. As a consequence, the functions D and $\partial_\mu D$ are continuous at z, cf. Lemma 2.1, which implies the claim. □

In the following, we abbreviate $\partial_\mu = \partial/\partial w^\mu$. Recall the notation $r(w) = \sqrt{-w_\mu w^\mu}$ from (27).

Lemma 2.14. *For $w \in \operatorname{domain}(r)$ and $\mu = 0, 1, 2, 3$, one has*

$$\partial_\mu[r(w)^2 \partial\!\!\!/ D(w)] = 2w_\mu \partial\!\!\!/ D(w) - \gamma_\mu w^\nu \partial_\nu D(w) + w\!\!\!/ w_\mu m^2 D(w). \tag{184}$$

Proof. The function D fulfills the Klein-Gordon equation

$$(\Box + m^2) D(w) = 0, \quad w \in \operatorname{domain}(r). \tag{185}$$

Indeed, for $w \in \mathbb{R}^4 + i\,\mathrm{Past}$, this can be seen from the definition (31) of D as follows: Because of the fast convergence of e^{ipw} to 0 as $|p| \to \infty$, $p \in \mathcal{M}_-$, we can interchange the Klein-Gordon-operator with the integral in the following calculation:

$$\begin{aligned}(\Box + m^2) D(w) &= (2\pi)^{-3} m^{-1} \int_{\mathcal{M}_-} (\Box^w + m^2) e^{ipw}\, i_p(d^4p) \\ &= (2\pi)^{-3} m^{-1} \int_{\mathcal{M}_-} (-p^2 + m^2) e^{ipw}\, i_p(d^4p) = 0.\end{aligned} \tag{186}$$

By analytic continuation, the Klein-Gordon equation (185) follows for all $w \in \operatorname{domain}(r)$. Equation (184) is proven by the following calculation:

$$\begin{aligned}\partial_\mu[r(w)^2 \partial\!\!\!/ D(w)] &= -\partial_\mu[w^\nu w_\nu \partial\!\!\!/ D(w)] \\ &\overset{(163)}{=} -\partial_\mu[w^\nu w\!\!\!/ \partial_\nu D(w)] \\ &= -w\!\!\!/ \partial_\mu D(w) - w^\nu \gamma_\mu \partial_\nu D(w) - w^\nu w\!\!\!/ \partial_\mu \partial_\nu D(w) \\ &= -w\!\!\!/ \partial_\mu D(w) - w^\nu \gamma_\mu \partial_\nu D(w) - w\!\!\!/ \partial_\nu (w^\nu \partial_\mu D(w)) + w\!\!\!/ (\partial_\nu w^\nu) \partial_\mu D(w) \\ &= 3w\!\!\!/ \partial_\mu D(w) - w^\nu \gamma_\mu \partial_\nu D(w) - w\!\!\!/ \partial_\nu (w^\nu \partial_\mu D(w)) \\ &\overset{(163)}{=} 3w\!\!\!/ \partial_\mu D(w) - w^\nu \gamma_\mu \partial_\nu D(w) - w\!\!\!/ \partial_\nu (w_\mu \partial^\nu D(w)) \\ &= 2w\!\!\!/ \partial_\mu D(w) - w^\nu \gamma_\mu \partial_\nu D(w) - w\!\!\!/ w_\mu \Box D(w) \\ &\overset{(163),(185)}{=} 2w_\mu \partial\!\!\!/ D(w) - \gamma_\mu w^\nu \partial_\nu D(w) + w\!\!\!/ w_\mu m^2 D(w).\end{aligned} \tag{187}$$

□

Recall the definition of the helper object $s_\Sigma^{A,\epsilon u}(x, y) = [(n\!\!\!/ E\!\!\!/)(x)][(r^2 \partial\!\!\!/ D)(w)]/(8m)$ introduced in Definition 2.6. The properties of $s_\Sigma^{A,\epsilon u}(x, y)$ claimed in Lemma 2.7 follow analogously to the arguments used in (92)–(95), i.e., from the bound (233) given in Corollary A.1 in the appendix, the compact support of E, boundedness of $\partial(n\!\!\!/_t E\!\!\!/_t)/\partial t$, and the dominated convergence theorem.

Lemma 2.15. *For $t \in \mathbb{R}$, $x, y \in \Sigma_t$, $z = y - x$, $u \in$ Past, and $\epsilon > 0$ we have*

$$\mathcal{D}_t^A s_\Sigma^{A,\epsilon u}(x,y) = \frac{i}{2m} v_t(x) z^\mu E_\mu(x) \bar{\partial} D(w) + r_{18}(x,y,\epsilon u) + r_{19}(x,y,\epsilon u), \quad (188)$$

$$\mathcal{D}_t^A (p_\Sigma^{A,\epsilon u} + s_\Sigma^{A,\epsilon u})(x,y) = r_{20}(x,y,\epsilon u) + r_{21}(x,y,\epsilon u) \quad (189)$$

with error terms that fulfill the bounds

$$r_{18} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_{12}|\mathbf{z}|}}{|\mathbf{z}|}\right) 1_K(x), \qquad r_{19} = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_{12}|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right) 1_K(x), \quad (190)$$

$$r_{20} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_{12}|\mathbf{z}|}}{|\mathbf{z}|}\right) [1_K(x) \vee 1_K(y)], \qquad r_{21} = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_{12}|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right) [1_K(x) \vee 1_K(y)] \quad (191)$$

with some positive constant $C_{12}(\mathbf{\Sigma})$. Furthermore, for $x \neq y$ the following limit exists:

$$r_{20}(x,y,0) := \lim_{\epsilon \downarrow 0} r_{20}(x,y,\epsilon u) \quad (192)$$

Proof. In this proof, we abbreviate $w = y - x + i\epsilon u = z + iu\epsilon$. Moreover, we suppress the w dependence of $r(w)$, $D(w)$, ∂^w and again also the t-dependence of v, n, and of the remainder terms $r_{\dots}$ in the notation. Using the definition of $\mathcal{D}_t^A$ given in (126) of Lemma 2.11, we get

$$\begin{aligned}
&8m\mathcal{D}_t^A s_{\Sigma_t}^{A,\epsilon u}(x,y) \\
&= v(x) \not{n}(x) D_x^A [\not{n}(x) \not{E}(x) r^2 \bar{\partial} D] - [\not{n}(x)\not{E}(x) r^2 \bar{\partial} D] \overleftarrow{D_y^A} \not{n}(y) v(y) \\
&= v(x)\not{n}(x) i \bar{\partial}^x [\not{n}(x)\not{E}(x) r^2 \bar{\partial} D] - [\not{n}(x)\not{E}(x) r^2 \bar{\partial} D] \overleftarrow{\bar{\partial}^y} (-i) \not{n}(y) v(y) + r_{22}(x,y,\epsilon u) \\
&= iv(x)\not{n}(x)\gamma^\mu \not{n}(x)\not{E}(x) \partial_\mu^x [r^2 \bar{\partial} D] + i\not{n}(x)\not{E}(x) \partial_\mu^y [r^2 \bar{\partial} D] \gamma^\mu \not{n}(y) v(y) + r_{23}(x,y,\epsilon u) \\
&= -iv(x)\not{n}(x)\gamma^\mu \not{n}(x)\not{E}(x) \partial_\mu [r^2 \bar{\partial} D] + i\not{n}(x)\not{E}(x) \partial_\mu [r^2 \bar{\partial} D] \gamma^\mu \not{n}(x) v(x) + r_{24}(x,y,\epsilon u), \quad (193)
\end{aligned}$$

where the remainder terms are defined and estimated as follows:

(i) Recalling the definitions (123) and (124) of the Dirac operators D_A and $\overleftarrow{D^A}$ and the fact that A is compactly supported, the estimate (233) of Corollary A.1 in the appendix ensures

$$\begin{aligned}
r_{22} &= v(x)\not{n}(x)(-m - \not{A}(x))[\not{n}(x)\not{E}(x) r^2 \bar{\partial} D] - [\not{n}(x)\not{E}(x) r^2 \bar{\partial} D](-m - \not{A}(y))\not{n}(y) v(y) \\
&= O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right) 1_K(x) \quad (194)
\end{aligned}$$

for some compact set K containing the support of E.

(ii) Using once more that E has compact support and using the bound (233) again we have the analogous estimate

$$\begin{aligned}
r_{23} &= r_{22} + iv(x)\not{n}(x)\gamma^\mu \left(\partial_\mu^x [\not{n}(x)\not{E}(x)]\right) r^2 \bar{\partial} D + i \left(\partial_\mu^y [\not{n}(x)\not{E}(x)]\right) r^2 \bar{\partial} D \gamma^\mu \not{n}(y) v(y) \\
&= O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right) 1_K(x) \quad (195)
\end{aligned}$$

(iii) Using the signs coming from inner derivatives: $-\partial^x D(w) = \partial^y D(w) = \partial D(w)$ and the Taylor expansion

$$\not{n}(y)v(y) = \not{n}(x)v(x) + r_{25}(x,y) \quad \text{with} \quad r_{25} = O_{\mathbf{\Sigma}}(|\mathbf{z}|) \tag{196}$$

for $x, y \in \Sigma_t$ with $x \in K$ we find with the help of bound (237) in the appendix:

$$r_{24} = r_{23} + i\not{n}(x)\not{E}(x)\partial_\mu[r^2\not{\partial}D]\gamma^\mu r_{25} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right)1_K(x). \tag{197}$$

In the following calculations, we drop the argument x; thus, v, n, and E stand for $v(x)$, $n(x)$, and $E(x)$, respectively, but $r = r(w)$ and $D = D(w)$. Using Lemma 2.14, we get

$$\begin{aligned}
&-i\left(8m\mathcal{D}_t^A s_\Sigma^{A,\epsilon u}(x,y) - r_{24}\right) = -v\not{n}\gamma^\mu\not{n}\not{E}\partial_\mu[r^2\not{\partial}D] + \not{n}\not{E}\partial_\mu[r^2\not{\partial}D]\gamma^\mu\not{n}v \\
&= -v\not{n}\gamma^\mu\not{n}\not{E}[2w_\mu\not{\partial}D - \gamma_\mu w^\nu\partial_\nu D] + v\not{n}\not{E}[2w_\mu\not{\partial}D - \gamma_\mu w^\nu\partial_\nu D]\gamma^\mu\not{n} + r_{26}(x,y,\epsilon u) \\
&= T_1 + T_2 + T_3 + T_4 + r_{26}
\end{aligned} \tag{198}$$

with the four terms

$$\begin{aligned}
T_1 &= -2v\not{n}\not{w}\not{n}\not{E}\not{\partial}D, & T_2 &= v\not{n}\gamma^\mu\not{n}\not{E}\gamma_\mu w^\nu\partial_\nu D, \\
T_3 &= 2v\not{n}\not{E}\not{\partial}D\not{w}\not{n}, & T_4 &= -v\not{n}\not{E}\gamma_\mu\gamma^\mu\not{n}w^\nu\partial_\nu D,
\end{aligned} \tag{199}$$

and the remainder term

$$r_{26} = -v\not{n}\gamma^\mu\not{n}\not{E}\not{w}w_\mu m^2 D + v\not{n}\not{E}\not{w}w_\mu m^2 D\gamma^\mu\not{n} = O_{A,u,\mathbf{\Sigma}}\left(e^{-C_D|\mathbf{z}|}\right)1_K(x), \tag{200}$$

where the bound comes from (231) of Corollary A.1 in the appendix and from supp $E \subseteq K$. We evaluate the four terms T_j separately. Using the anticommutation rules $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$ for the Dirac matrices and $\not{n}^2 = 1$, we get

$$\begin{aligned}
T_1 &= -2v\not{n}[2w^\nu n_\nu - \not{n}\not{w}]\not{E}\not{\partial}D \\
&= -4v\not{n}w^\nu n_\nu\not{E}\not{\partial}D + 2v[2w^\mu E_\mu - \not{E}\not{w}]\not{\partial}D \\
&= -4v\not{n}w^\nu n_\nu\not{E}\not{\partial}D + 4vw^\mu E_\mu\not{\partial}D - 2v\not{E}w^\mu\partial_\mu D,
\end{aligned} \tag{201}$$

where in the last step we used the Lorentz symmetry (163) to compute

$$\begin{aligned}
\not{w}\not{\partial}D &= \gamma^\mu\gamma^\nu w_\mu\partial_\nu D = \frac{1}{2}\left(\gamma^\mu\gamma^\nu w_\mu\partial_\nu D + \gamma^\mu\gamma^\nu w_\nu\partial_\mu D\right) \\
&= \frac{1}{2}\left(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu\right)w_\mu\partial_\nu D = w^\mu\partial_\mu D.
\end{aligned} \tag{202}$$

Using the anticommutation rules again, the fact $\gamma^\mu\gamma_\mu = 4$, the definition $E_\mu = F_{\mu\nu}n^\nu$ given in (42), and the antisymmetry $F_{\mu\nu} = -F_{\nu\mu}$, we get

$$\begin{aligned}
\gamma^\mu\not{n}\not{E}\gamma_\mu &= (2n^\mu - \not{n}\gamma^\mu)(2E_\mu - \gamma_\mu\not{E}) = 4n^\mu E_\mu - 4\not{n}\not{E} + \not{n}\gamma^\mu\gamma_\mu\not{E} \\
&= 4n^\mu E_\mu = 4n^\mu F_{\mu\nu}n^\nu = 0
\end{aligned} \tag{203}$$

and therefore $T_2 = 0$. Using the same argument that was used to derive (202) we also find $\not\partial D(w)\not w = w^\mu \partial_\mu D$, and hence,

$$T_3 = 2v\not n \not E w^\mu \partial_\mu D \not n. \tag{204}$$

Finally, we have

$$T_4 = -4v\not n \not E \not n w^\nu \partial_\nu D, \tag{205}$$

which yields

$$T_3 + T_4 = -2v\not n \not E \not n w^\mu \partial_\mu D = 2v\not n^2 \not E w^\mu \partial_\mu D = 2v\not E w^\mu \partial_\mu D. \tag{206}$$

We have used that $\not n$ and $\not E$ anticommute because of $n^\mu E_\mu = n^\mu F_{\mu\nu} n^\nu = 0$. Together with the expression (201) for T_1 and $T_2 = 0$, we conclude

$$T_1 + T_2 + T_3 + T_4 = 4vw^\mu E_\mu \not\partial D + r_{27}(x, y, \epsilon u). \tag{207}$$

with the error terms

$$r_{27} = -4v\not n w^\nu n_\nu \not E \not\partial D = r_{28}(x, y, \epsilon u) + r_{29}(x, y, \epsilon u), \tag{208}$$

where using $w = z + i\epsilon u$

$$r_{28} = -4v\not n i\epsilon u^\nu n_\nu \not E \not\partial D, \qquad r_{29} = -4v\not n z^\nu n_\nu \not E \not\partial D. \tag{209}$$

Inequality (236) from the appendix and the fact $\operatorname{supp} E \subseteq K$ provide the bound

$$r_{28} = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right) 1_K(x). \tag{210}$$

For the next estimate, we observe $(\nabla t_{\Sigma_t}(\mathbf{x}) \cdot \mathbf{z}, \mathbf{z}) \in T_x\Sigma_t \perp n(x)$; recall the parametrization (13) of Σ_t. We obtain the Taylor expansion

$$z^\nu n_\nu = n_0(x)[t_{\Sigma_t}(\mathbf{y}) - t_{\Sigma_t}(\mathbf{x})] - \mathbf{n}(x) \cdot \mathbf{z} = n_0(x)\nabla t_{\Sigma_t}(\mathbf{x}) \cdot \mathbf{z} - \mathbf{n}(x) \cdot \mathbf{z} + O_{\mathbf{\Sigma}}(|\mathbf{z}|^2) = O_{\mathbf{\Sigma}}(|\mathbf{z}|^2) \tag{211}$$

uniformly for x in the compact set K. Using (234) from the appendix and the support property of E again, this implies

$$r_{29} = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right) 1_K(x). \tag{212}$$

Finally, we have from equation (207)

$$T_1 + T_2 + T_3 + T_4 - r_{27} = 4vw^\mu E_\mu \not\partial D = 4vz^\mu E_\mu \not\partial D + r_{30}(x, y, \epsilon u) \tag{213}$$

with the error term

$$r_{30} = 4vi\epsilon u^\mu E_\mu \not\partial D = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right) 1_K(x), \tag{214}$$

where once again we have used the bound (236) from the appendix and the fact supp $E \subseteq K$. Let us summarize: We use the equations (198), (213), and (208) to get the claimed formula

$$\mathcal{D}_t^A s_{\Sigma_t}^{A,\epsilon u}(x,y) = \frac{i}{2m} v z^\mu E_\mu \partial\!\!\!/ D + r_{18} + r_{19} \tag{188}$$

with the remainder terms

$$r_{18} := \frac{r_{24}}{8m} + \frac{i}{8m}(r_{26} + r_{29}) = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|} + e^{-C_D|\mathbf{z}|}\right) 1_K(x) = O_{A,u,\mathbf{\Sigma}}\left(\frac{e^{-C_{12}|\mathbf{z}|}}{|\mathbf{z}|}\right) 1_K(x) \tag{215}$$

$$r_{19} := \frac{i}{8m}(r_{28} + r_{30}) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right) 1_K(x) = O_{A,u,\mathbf{\Sigma}}\left(\sqrt{\epsilon}\frac{e^{-C_{12}|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right) 1_K(x) \tag{216}$$

with any positive constant $C_{12}(\mathbf{\Sigma}) < C_D(\mathbf{\Sigma})$. We have applied the error bounds (197), (200), and (212) for the first remainder term r_{18}, and the bounds (210) and (214) for the second remainder term r_{19}. Finally, we have weakened the bounds slightly to get a simpler notation. This shows the claimed error bounds in (190).

Combining this with Lemma 2.13 and setting $r_{20} = r_3 + r_{18}$, $r_{21} = r_4 + r_{19}$, equation (189) together with the corresponding error bounds (191) are immediate consequences.

To ensure existence of the limit of $r_{20}(x,y,\epsilon u)$ as $\epsilon \downarrow 0$ for $x, y \in \Sigma_t$ with $x \neq y$, we use the existence of the limits $\lim_{\epsilon\downarrow 0} r_3(x,y,\epsilon t)$ and $\lim_{\epsilon\downarrow 0} r_{18}(x,y,\epsilon u)$. The existence of the former limit was proven in Lemma 2.13, and existence of the latter limit follows by the same argument, i.e., from the fact that the functions D and $\partial_\mu D$ are continuous at z, and that r_{18} is explicitly given in terms of D and its derivative. This yields the claim. □

Corollary 2.16. *The error terms $r_{20}(\cdot,\cdot,\epsilon u)$ and $r_{21}(\cdot,\cdot,\epsilon u)$ in (189) give rise to bounded linear operators ${R_{20}}^{\epsilon u}(t), {R_{21}}^{\epsilon u}(t) : \mathcal{H}_{\Sigma_t} \circlearrowleft$ with matrix elements*

$$\langle \phi, {R_{20}}^{\epsilon u}(t)\psi\rangle = \int_{x\in\Sigma_t}\int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x)\, r_{20}(x,y,\epsilon u)\, i_\gamma(d^4y)\, \psi(y), \qquad \psi,\phi \in \mathcal{H}_{\Sigma_t} \tag{217}$$

and similarly for $r_{21}(x,y,\epsilon u)$, ${R_{21}}^{\epsilon u}(t)$. They fulfill:

(i) The operators ${R_{20}}^{\epsilon u}(t)$, $\epsilon \geqslant 0$, are Hilbert-Schmidt operators. There is a constant $C_{13}(A,u,\mathbf{\Sigma})$ such that $\sup_{t\in T,\epsilon>0} \|{R_{20}}^{\epsilon u}(t)\|_{I_2(\mathcal{H}_{\Sigma_t})} \leqslant C_{13}$. Furthermore,

$$\lim_{\epsilon\downarrow 0} \|{R_{20}}^{\epsilon u}(t) - {R_{20}}^{0}(t)\|_{I_2(\mathcal{H}_{\Sigma_t})} = 0. \tag{218}$$

(ii) $\sup_{t\in T} \|{R_{21}}^{\epsilon u}(t)\|_{\mathcal{H}_{\Sigma_t}\circlearrowleft} \leqslant O_{A,u,\mathbf{\Sigma}}(\sqrt{\epsilon})$.

Proof. (i) For $\psi, \phi \in \mathcal{H}_{\Sigma_t}$, using the bound (191) for r_{20}, we find uniformly for $\epsilon > 0$ and $t \in T$ that

$$\|{R_{20}}^{\epsilon u}(t)\|^2_{I_2(\mathcal{H}_{\Sigma_t})} = \int_{\mathbf{x}\in\mathbb{R}^3}\int_{\mathbf{y}\in\mathbb{R}^3} \operatorname{trace}\left[\gamma^0 r_{20}(x,y,\epsilon u)^* \gamma^0 \Gamma(\mathbf{x}) r_{20}(x,y,\epsilon u)\Gamma(\mathbf{y})\right] d^3\mathbf{y}\, d^3\mathbf{x} \tag{219}$$

$$\leqslant C_{14} \int_{\mathbf{x}\in\mathbb{R}^3}\int_{\mathbf{y}\in\mathbb{R}^3} \left[\frac{e^{-C_D|\mathbf{y}-\mathbf{x}|}}{|\mathbf{y}-\mathbf{x}|}\right]^2 (1_K(x) \vee 1_K(y))\, d^3\mathbf{y}\, d^3\mathbf{x} < \infty. \tag{220}$$

for some constant $C_{14}(A, u, \mathbf{\Sigma})$. The limit $R_{20}{}^{\epsilon u}(t) \xrightarrow{\epsilon \downarrow 0} R_{20}{}^{0}(t)$ in the $I_2(\mathcal{H}_{\Sigma_t})$ norm is implied by the point-wise convergence (192) stated in Lemma 2.15 and the point-wise bound (191), using dominated convergence.

(ii) For $\psi, \phi \in \mathcal{H}_{\Sigma_t}$, using the bound in (191) for r_{21} and the Cauchy-Schwarz inequality, we find analogously to the calculation (92)–(95):

$$|\langle \phi, R_{21}{}^{\epsilon u}(t)\psi \rangle| \leqslant O_{A,u,\mathbf{\Sigma}}(\sqrt{\epsilon}) \int_{\mathbf{x}\in\mathbb{R}^3} \int_{\mathbf{y}\in\mathbb{R}^3} |\phi(x)|\, |\Gamma(\mathbf{x})|\, d^3\mathbf{x}\, \frac{e^{-C_D|\mathbf{y}-\mathbf{x}|}}{|\mathbf{y}-\mathbf{x}|^{5/2}}\, |\Gamma(\mathbf{y})|\, d^3\mathbf{y}\, |\psi(y)| \quad (221)$$

$$\leqslant O_{A,u,\mathbf{\Sigma}}(\sqrt{\epsilon}) \int_{\mathbf{z}\in\mathbb{R}^3} \frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\, d^3\mathbf{z}\, \|\phi\|\, \|\psi\|, \quad (222)$$

which is finite and uniform in t.

The existence of the bounded linear operators $R_{20}{}^{\epsilon u}(t), R_{21}{}^{\epsilon u}(t) : \mathcal{H}_{\Sigma_t} \circlearrowleft$ follows. □

Finally, we prove the Theorem 2.8 with the collected ingredients.

Proof of Theorem 2.8. With justifications given below, we find that for $\phi, \psi \in \mathcal{C}_A$

$$\left\langle \phi|_{\Sigma_{t_1}}, (P^A_{\Sigma_{t_1}} + S^A_{\Sigma_{t_1}})\psi|_{\Sigma_{t_1}} \right\rangle - \left\langle \phi|_{\Sigma_{t_0}}, (P^A_{\Sigma_{t_0}} + S^A_{\Sigma_{t_0}})\psi|_{\Sigma_{t_0}} \right\rangle \quad (223)$$

$$= \lim_{\epsilon\downarrow 0} \left(\int_{x\in\Sigma_{t_1}} \int_{y\in\Sigma_{t_1}} - \int_{x\in\Sigma_{t_0}} \int_{y\in\Sigma_{t_0}} \right) \overline{\phi(x)}\, i_\gamma(d^4x)\, (p^{A,\epsilon u} + s^{A,\epsilon u}_{\Sigma_t})(x,y) i_\gamma(d^4y)\, \psi(y) \quad (224)$$

$$= \lim_{\epsilon\downarrow 0} \int_{t_0}^{t_1} \int_{x\in\Sigma_t} \int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x) \left[-i\mathcal{D}^A_t (p^{A,\epsilon u} + s^{A,\epsilon u}_{\Sigma_t}) + \frac{\partial s^{A,\epsilon u}_{\Sigma_t}}{\partial t} \right] (x,y) i_\gamma(d^4y)\, \psi(y)\, dt \quad (225)$$

$$= \lim_{\epsilon\downarrow 0} \int_{t_0}^{t_1} \int_{x\in\Sigma_t} \int_{y\in\Sigma_t} \overline{\phi(x)}\, i_\gamma(d^4x) \left[-ir_{20}(x,y,\epsilon u) - ir_{21}(x,y,\epsilon u) + \frac{\partial s^{A,\epsilon u}_{\Sigma_t}}{\partial t}(x,y) \right] \cdot i_\gamma(d^4y)\, \psi(y)\, dt \quad (226)$$

$$= \lim_{\epsilon\downarrow 0} \int_{t_0}^{t_1} \left[-i\langle \phi|_{\Sigma_t}, R_{20}{}^{\epsilon u}(t)\psi|_{\Sigma_t} \rangle - i\langle \phi|_{\Sigma_t}, R_{21}{}^{\epsilon u}(t)\psi|_{\Sigma_t} \rangle + \left\langle \phi|_{\Sigma_t}, \dot{S}^{A,\epsilon u}_{\Sigma_t}, \psi|_{\Sigma_t} \right\rangle \right] dt \quad (227)$$

In the first step from (223) to (224) we expressed the matrix elements of the operators $P^{\lambda_A}_{\Sigma}$ and S^A_Σ in terms of the respective integral kernels $p^{\epsilon u, \lambda_A}$ and $s^{\epsilon u, A}_\Sigma$ given in Lemma 2.3 and part (i) of Lemma 2.7. The step from (224) to (225) follows from Corollary 2.12. The step from (225) to (226) is a consequence of equation (189) in Lemma 2.15. Finally, in the step from (226) to (227) we have used that the integral kernels $r_{20}(\cdot,\cdot,\epsilon u)$, $r_{21}(\cdot,\cdot,\epsilon u)$, and $\partial s^{A,\epsilon u}_{\Sigma_t}/\partial t$ give rise to bounded operators $R_{20}{}^{\epsilon u}(t)$, $R_{21}{}^{\epsilon u}(t)$, and $\dot{S}^{A,\epsilon u}_{\Sigma_t}$ as ensured by Corollary 2.16 and part (ii) of Lemma 2.7.

Claim (ii) of Corollary 2.16 implies that $R_{21}{}^{\epsilon u}(t)$ converges to zero in operator norm as $\epsilon \downarrow 0$, uniformly in $t \in T$. Furthermore, claim (i) of Corollary 2.16 and part (ii) of Lemma 2.7 guarantee that $-iR_{20}{}^{\epsilon u}(t) + \dot{S}^{A,\epsilon u}_{\Sigma_t}$ converges in the $I_2(\mathcal{H}_{\Sigma_t})$ norm to a Hilbert-Schmidt operator $R(t) := -iR_{20}{}^{0}(t) + \dot{S}^{A,0}_{\Sigma_t}$ such that $\sup_{t\in T} \|R(t)\|_{I_2(\mathcal{H}_{\Sigma_t})} < \infty$. Calculation

(223)–(227) can now be rewritten in the form of claim (47):

$$\left\langle \phi|_{\Sigma_{t_1}}, (P^A_{\Sigma_{t_1}} + S^A_{\Sigma_{t_1}})\psi|_{\Sigma_{t_1}} \right\rangle - \left\langle \phi|_{\Sigma_{t_0}}, (P^A_{\Sigma_{t_0}} + S^A_{\Sigma_{t_0}})\psi|_{\Sigma_{t_0}} \right\rangle = \int_{t_0}^{t_1} \langle \phi|_{\Sigma_t}, R(t)\psi|_{\Sigma_t}\rangle \, dt \quad (228)$$

at first for $\phi, \psi \in \mathcal{C}_A$, but then extended by a density argument to $\phi, \psi \in \mathcal{H}_A$. Since the operators $U_{A\Sigma}$ are unitary, we get the estimate

$$\left\| U_{A\Sigma_{t_1}}(P^A_{\Sigma_{t_1}} + S^A_{\Sigma_{t_1}})U_{\Sigma_{t_1}A} - U_{A\Sigma_{t_0}}(P^A_{\Sigma_{t_0}} + S^A_{\Sigma_{t_0}})U_{\Sigma_{t_0}A} \right\|_{I_2(\mathcal{H}_A)} \quad (229)$$

$$\leqslant \int_{t_0}^{t_1} \|R(t)\|_{I_2(\mathcal{H}_{\Sigma_t})} \, dt < \infty. \quad (230)$$

This proves the claim. □

Proof of Theorem 2.5. As a consequence of Theorem 2.8 and Lemma 2.7 claim (41) holds for the special case $\lambda = \lambda^A$. For general $\lambda \in \mathcal{G}(A)$, Theorem 2.4 implies $P^A_\Sigma - P^\lambda_\Sigma \in I_2(\mathcal{H}_\Sigma)$ which concludes the proof for the general case. □

A Appendix

In this appendix we provide auxiliary estimates for the covariant functions D, its derivatives, and p^- needed in the proofs of the main results.

Lemma A.1 (Upper bounds). *Let u be a time-like four-vector. For all space-like $z \in \mathbb{R}^4$ with $|z^0| \leqslant V_{\max}|\mathbf{z}|$ and $\epsilon \geqslant 0$ with $w = z + i\epsilon u \neq 0$ we have the following bounds with the constant $C_D(V_{\max}) = \frac{m}{2}\sqrt{1 - {V_{\max}}^2}$, reading $1/0$ as $+\infty$:*

$$|w^\mu w^\nu D(w)| \leqslant O_{u,V_{\max}}\left(e^{-C_D|\mathbf{z}|}\right), \quad (231)$$

$$|D(w)| \leqslant O_{V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^2}\right), \quad (232)$$

$$\left|r(w)^2\partial_\mu D(w)\right| \leqslant O_{u,V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|}\right), \quad (233)$$

$$|\partial_\mu D(w)| \leqslant O_{u,V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^3 \vee \epsilon^3}\right), \quad (234)$$

$$|w^\nu \partial_\mu D(w)| \leqslant O_{u,V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^2 \vee \epsilon^2}\right), \quad (235)$$

$$|\epsilon u^\mu \partial_\nu D(w)| \leqslant O_{u,V_{\max}}\left(\frac{\sqrt{\epsilon}e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^{5/2}}\right), \quad (236)$$

$$\left|\partial_\nu\left[r(w)^2\partial_\mu D(w)\right]\right| \leqslant O_{u,V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^2}\right), \quad (237)$$

$$\left\|p^-(w)\right\| \leqslant O_{u,V_{\max}}\left(\frac{e^{-C_D|\mathbf{z}|}}{|\mathbf{z}|^3}\right). \quad (238)$$

For $\epsilon = 0$ one may take, e.g., $u = (-1, 0, 0, 0)$. In this case the u-dependence of the constants in (231)-(238) drops out.

Lemma A.2 (Lower Bound)**.** *For all space-like $z \in \mathbb{R}^4 \backslash \{0\}$ one has the lower bound*

$$\left\| p^-(z) \right\| \geqslant C_{15} \frac{e^{-m|\mathbf{z}|}}{|\mathbf{z}|^3} \tag{239}$$

with a positive numerical constant C_{15}.

The proofs have been carried out in [4]. However, they can also be inferred from the asymptotic behavior of the modified Bessel function K_1 and its derivative given in [1, Chapters 9.6 and 9.7].

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B Inhalt der Zielvereinbarung für das Habilitationsverfahren

Im Folgenden ist ein nicht unterschriebener Auszug der Zielvereinbarungen angehängt:

Zielvereinbarung für das Habilitationsverfahren
von Herrn Dr. Dirk - André Deckert

Die Mitglieder des Fachmentorats Prof. Dr. Francesca Biagini, Prof. Dr. Franz Merkl und Prof. Herbert Spohn beschließen im Einvernehmen mit dem Habilitanden Herrn Dr. Dirk - André Deckert einstimmig folgende Zielvereinbarung für die Feststellung der Befähigung des Habilitanden zur selbständigen Forschung und seiner pädagogischen Eignung.

Forschung: Entsprechend §12 der Habilitationsordnung weist der Kandidat seine Forschungsleistung in einer der folgenden Formen nach:

- Der Habilitand legt drei einschlägige wissenschaftliche Veröffentlichungen vor sowie eine Habilitationsschrift
- ODER der Habilitand legt insgesamt mindestens sechs einschlägige wissenschaftliche Veröffentlichungen vor zusammengebunden mit einem Bericht, in dem diese Arbeiten erläutert und in einen größeren wissenschaftlichen Zusammenhang gestellt werden.

Die unter Punkt 1. und 2. genannten wissenschaftlichen Veröffentlichungen dürfen nicht Teil der Promotionsschrift oder direkt in diese eingeflossen sein.

Lehre: Für den Nachweis der pädagogischen Eignung berücksichtigt das Fachmentorat die Lehrveranstaltungen, die Herr Deckert am Institut für Mathematik der LMU in selbständig abgehalten hat. Dazu zählen die Vorlesungen:

- Vorlesung “Lineare Algebra für Lehramt”, 4h Vorlesung, SS 18
- Vorlesung “Mathematics and Applications of Machine Learning”, 2h Vorlesung, 2h Übung, SS 18
- Hauptseminar “Advanced Topics in Machine Learning”, 2h, SS17
- Vorlesung “Mathematics and Applications of Machine Learning”, 2h Vorlesung, 2h Übung, WS 16/17,

Aufgrund dieser abgehaltenen Lehrveranstaltungen sehen die Fachmentoren die pädagogische Eignung nach § 14 der Habilitationsordnung als erfüllt an.

Herr Deckert und das Fachmentorat erklären einstimmig, dass die Erbringung der oben vereinbarten Leistungen in weniger als zwei Jahren abgeschlossen sein wird. Das Fachmentorat beschließt daher im Einvernehmen mit Herrn Deckert auf die Zwischenevaluierung zu verzichten.
