On domain, self-adjointness, and spectrum of Dirac operators for two interacting particles

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Abstract

Two-body Dirac operators, formally given by

$$H_{2\mathrm{BD}} = (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \beta m)\otimes \mathrm{id} + \mathrm{id}\otimes(-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}} + \beta m) + V_{\mathrm{ext}} + V_{\mathrm{int}},$$

find broad application in relativistic quantum chemistry and describe two via V_{int} interacting electrons in the external field V_{ext} of a nucleus. Contrary to Brown-Ravenhall operators, $H_{2\mathrm{BD}}$ is defined without spectral projections, and thus, not bounded from below. Despite the frequent use of $H_{2\mathrm{BD}}$ in relativistic quantum chemistry, only very few of its mathematical properties are known in the mathematical physics literature. This was brought to the attention of the mathematical physics community by Jan Dereziński in 2012. The present work addresses the questions of domain, self-adjointness, and spectrum of $H_{2\mathrm{BD}}$ in mathematically precise form.

For our main result, we assume two electrons with interaction of Coulomb type in the vicinity of an extended nucleus. We construct a self-adjoint extension of $H_{2\mathrm{BD}}$ which is uniquely distinguished by the criterion of finite potential energy. Since unbounded interaction potentials cannot be relatively bounded by the free two-body Dirac operator, we make use of a particular Frobenius-Schur factorization of $H_{2\mathrm{BD}}$ and infer self-adjointness as well as uniqueness from the Schur complement. The coupling constant of the interaction γ is restricted to values $|\gamma| < 2/\pi$.

Moreover, we show by means of explicit examples that elements of the domain $\mathcal{D}(\overline{H}_{2\mathrm{BD}})$ may exhibit infinite single particle kinetic energy. This unphysical phenomenon already occurs in the free case and is therefore no artifact of unbounded potentials. On the one hand, it vanishes when antisymmetric states are considered. On the other hand, initial states with finite single particle kinetic energy cannot evolve into states with infinite energy under the full time evolution.

As regards the spectrum of $H_{2\mathrm{BD}}$, we identify the essential spectrum as $\mathbb{R}$ and show absence of eigenvalues $|E| > 2m$, where m is the electron mass.

Zusammenfassung

Zwei-Teilchen Dirac-Operatoren $H_{2\mathrm{BD}}$, formal gegeben durch

$$H_{2\mathrm{BD}} = (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{x}} + \beta m) \otimes \mathrm{id} + \mathrm{id} \otimes (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{y}} + \beta m) + V_{\mathrm{ext}} + V_{\mathrm{int}},$$

kommen häufig in der relativistischen Quantenchemie zur Anwendung und beschreiben zwei mittels V_{int} wechselwirkende Elektronen im externen Feld V_{ext} eines Nukleus. Im Gegensatz zu Brown-Ravenhall-Operatoren wird $H_{2\mathrm{BD}}$ ohne Spektralprojektionen definiert und ist daher nicht von unten beschränkt. In der mathematischen Literatur sind—trotz der weiten Verbreitung in der relativistischen Quantenchemie—nur sehr wenige Eigenschaften von $H_{2\mathrm{BD}}$ bekannt. Diese Tatsache war von Jan Dereziński im Jahre 2012 an die Mathematische Physik Community herangetragen worden. Die vorliegende Arbeit geht der Frage nach Definitionsbereich, Selbstadjungiertheit und Spektrum von $H_{2\mathrm{BD}}$ in mathematisch präziser Form nach.

Für unser Hauptresultat nehmen wir Elektronen mit Coulomb-Wechselwirkung in der Nähe eines ausgedehnten Nukleus an. Es besteht in der Konstruktion einer selbstadjungierten Erweiterung von $H_{2\mathrm{BD}}$, die durch das Kriterium endlicher potentieller Energie eindeutig ausgezeichnet ist. Da ein unbeschränktes Wechselwirkungspotential nicht durch den freien Zweiteilchen-Dirac-Operator relativ beschränkt werden kann, greifen wir auf eine bestimmte Frobenius-Schur-Faktorisierung von $H_{2\mathrm{BD}}$ zurück und folgern sowohl Selbstadjungiertheit als auch Eindeutigkeit der Erweiterung aus dem Schurkomplement. Die Kopplungskonstante der Wechselwirkung γ ist auf Werte $|\gamma| < 2/\pi$ beschränkt.

Wir zeigen weiterhin anhand von explizit konstruierten Beispielen, dass Elemente des Definitionsbereiches $\mathcal{D}(\overline{H}_{2\mathrm{BD}})$ nicht notwendigerweise endliche kinetische Einteilchenenergie aufweisen. Dieser unphysikalische Umstand tritt bereits im freien Fall auf und ist daher kein Artefakt unbeschränkter Potentiale. Er kann zum einen durch Einschränkung auf antisymmetrische Zustände umgangen werden. Zum anderen können zwei wechselwirkende Elektronen mit endlicher kinetischer Einteilchenenergie nicht in Zustände mit unendlicher kinetischer Einteilchenenergie streuen.

Was die Untersuchung des Spektrums von $H_{2\mathrm{BD}}$ betrifft, so identifizieren wir das wesentliche Spektrum als $\mathbb{R}$ und zeigen, dass keine Eigenwerte im Bereich $|E| > 2m$ auftreten, wobei m die Elektronenmasse ist.

Contents

Eidesstattliche Versicherung

(Siehe Promotionsordnung vom 12.07.2011, §8, Abs. 2 Pkt. 5.)

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist.

Martin Johannes Oelker

München, den 25. März 2019

On contributing research

Some results that appear in this thesis are published with Dr. Dirk-André Deckert as co-author in [DO19]. M. Oelker essentially derived all results on the basis of many thorough and helpful discussions with D.-A. Deckert and his careful proof-reading. M. Oelker also drafted the major part of the manuscript. Although [DO19] is quoted verbatim in many places scattered across this thesis, it is not cited in the body of the thesis in order to increase the readability of the thesis. Instead, the chapters and sections in which results and paragraphs from [DO19] appear are listed in the following:

- **Chapter 2** contains, apart from minor modifications, the Sections 2, 3.1.1, and 3.1.3 from [DO19].
- **Chapter 3** contains, apart from minor modifications, the Section 3.1.2 and parts of Section 3.4 from [DO19].
- **Chapter 4** contains, apart from minor modifications, the Section 3.2 from [DO19].
- **Chapter 5** contains, apart from minor modifications, the Sections 3.3 and 3.5 as well as parts of Section 3.4 from [DO19].
- **Appendices A and B** match the corresponding Appendices from [DO19].

1. Introduction

1.1. Many-body Dirac operators

This thesis studies properties such as self-adjointness of two-body Dirac operators (2BD operators) and also investigates their domain and spectrum. 2BD operators are formally given by

$$\begin{aligned} H_{\mathrm{2BD}} &= H_0 + V_{\mathrm{ext}} + V_{\mathrm{int}} \\ &= (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \beta m)\otimes \mathrm{id} + \mathrm{id}\otimes(-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}} + \beta m) + V_{\mathrm{ext}} + V_{\mathrm{int}}, \end{aligned} \tag{1.1.1}$$

where H_0 denotes the free 2BD Dirac operator, V_{int} an interaction potential, and V_{ext} the external field. Before we summarize our results in the next section and define H_{2BD} rigorously in Section 2.1, we want to describe the context of their application and their status in the literature.

In contemporary relativistic quantum chemistry, 2BD operators[1] find broad application in the description of two electrons of mass m in an external field V_{ext} interacting via an interaction potential V_{int}. This models, e.g., the Helium atom. The main objective in the literature is the investigation of energy levels or spectral lines, i.e., the spectrum of H_{2BD}, via numerical simulations; see [Liu12] for an overview, and concerning spectral properties, e.g., [JBL97], [Liu12], [PBK06], [PBK07], [WNT07], and [WNT10]. There is, however, an ongoing debate concerning the nature of these spectral lines. Some authors believe, they correspond to true eigenvalues of H_{2BD} (see, e.g., [Liu12]), while others regard them as resonances (see, e.g., [PBK07], [PBK06], and [BPK08]). That this debate lacks a firm mathematical foundation was brought to the attention of the mathematical physics community by J. Dereziński in 2012. In [Der12], he reports on his correspondence with the chemist B. Jeziorski on this topic. In particular, Jeziorski notes that, although important properties such as self-adjointness or existence of eigenvalues of H_{2BD} are not proven, the "*Hamiltonian [H_{2BD}] is used by chemists in hundreds of papers every year ... with a tacit assumption that it has square integrable eigenfunctions*." Dereziński concludes that the lack of a rigorous mathematical study of H_{2BD} poses well-defined mathematical problems, which are of great interest for relativistic quantum chemistry. This thesis is one of the first works addressing these problems.

In contrast to many-body Schrödinger operators, the mathematical physics literature on many-body Dirac operators is rather sparse. This is on the one hand due to the widespread conviction among physicists that, in the relativistic realm, quantum field

[1] In the relativistic quantum chemistry literature, the notation H_{DC} is more common. It stands for Dirac-Coulomb Hamiltonian. Since in this thesis the Coulomb potential is not the only potential considered, we introduce the notation H_{2BD} which stands for two-body Dirac Hamiltonian.

theory, i.e., a description of many particles in terms of Fock spaces and creation and annihilation operators, is more adequate. "*On the other hand, the treatment of relativistic multi-particle quantum systems is notoriously difficult ... [even for] the naive Hamiltonian ... [H_0] ... of two non-interacting free Dirac particles ...*" (see [Sie06]).

One hardly encounters many-body Dirac operators of the form (1.1.1) in the literature. If they are mentioned at all, one often finds only the statement about the essential spectrum $\sigma_{\text{ess}}(H_{2\text{BD}}) = \mathbb{R}$, albeit without proof (see, e.g., [Mor08], [BES05]). Some rigorous works in the surroundings of many-body Dirac operators are, e.g., [HLS07] and [Sie06]. That in general not much is known in the literature on many-body Dirac operators regarding self-adjointness or spectrum, is the content of [Der12]. This problem also finds a mention in [Lev14]. The preprint [OKY14] is to our best knowledge the only article in the mathematical literature that attempts to treat Dirac operators of the form (1.1.1). The authors claim to have proven essential self-adjointness of $H_{2\text{BD}}$, where both external as well as interaction potential are of Coulomb type, absence of eigenvalues, as well as they claim to have identified the essential spectrum as $\mathbb{R}$. Unfortunately, their proof of essential self-adjointness comprises a gap. This gap also invalidates the proof of absence of eigenvalues. We discuss this gap and its implications in Section 5.4. The proof concerning the essential spectrum contains a different gap. While we could not fix the gap in the proof of essential self-adjointness, we were able to do so for the essential spectrum. We discuss our approach to the essential spectrum in Section 6 and how we fix the gap in the proof in [OKY14] in Remark 6.2.

The main objection of physicists to many-body Dirac operators is their unboundedness from below. Therefore, one often considers the so-called Brown-Ravenhall operators, i.e., many-body Dirac operators projected to the (carefully chosen) positive energy subspace. These operators are bounded from below and physically sufficiently reasonable in order to model atoms (see, e.g., [Tix97], [EPS96], [MV06], as well as [BE11], [SL10], and references therein). In these settings, mainly spectral questions are under investigation (see [MS10] and references therein).

We want to clearly distinguish the mathematical investigation of $H_{2\text{BD}}$ from considering $H_{2\text{BD}}$ as valid model for the Helium atom. The justification of a mathematical investigation is simply its frequent use in relativistic quantum chemistry and the corresponding mathematical questions concerning the spectrum. The traditional reservations of physicists (see, e.g., [BR51], [Suc80]) concerning the validity of $H_{2\text{BD}}$ as model for the Helium atom, however, are to our opinion at least partly justified but will not be our focus here. We reproduce in Section 7.3 the classical heuristic argument, the so-called Brown-Ravenhall disease, that $H_{2\text{BD}}$ might not have a stable eigenstates. We will see that this argument serves as substantial basis for future research on the spectrum of $H_{2\text{BD}}$.

The unboundedness from below of Dirac operators, i.e., the occurrence of negative energy states, can also be seen as virtue, namely when one wants to model the Dirac sea with the help of many-body Dirac operators. The Dirac sea is intimately connected to the so-called radiation catastrophe of Dirac electrons. In this scenario, an electron described by the Dirac equation is accelerated by some means. It thus emits radiation, i.e., loses energy. As the spectrum is not bounded from below, there is no mechanism preventing the electron from emitting more and more radiation, and thereby sinking deeper and deeper in the spectrum. In order to address this seemingly unphysical scenario, Dirac proposed the Dirac sea, i.e., that all negative energy states are occupied by electrons. The exclusion principle for fermions prevents any positive energy electron from transitions to negative energy states. On the one hand, this model of the vacuum proved very successful, as it correctly predicted the positron. It was also used in the proof of pair creation (see [PD08b] and [PD08a]). On the other hand, it poses interesting problems not only for a mathematically rigorous foundation of relativistic quantum mechanics. Besides the classic literature on, e.g., the external field problem in quantum electrodynamics (see [SS65], [Rui77a], [Rui77b], and [LM96]), some of these problems are also content of current research, such as [JMPP17], which investigates the invisibility of the Dirac sea due to its uniformity, [DDMS10] and [DM16], which study the time evolution of the Dirac sea, or [Fin06], which even generalizes the notion of the Dirac sea. As the Dirac sea is a relativistic many-fermion system with negative energies, it is natural to think of it as wedge product $\psi = \phi_1 \wedge \phi_2 \wedge \ldots \wedge \phi_N$, where each factor belongs to the negative energy spectrum. The antisymmetry of the wedge product reflects the fermionic character. One can then study the Dirac sea, either with finitely many particles or in the limit $N \to \infty$ as in [DDMS10]. Stability of the Dirac sea with finitely many particles is analogous to H_{2BD}, i.e., two electrons without radiation. One can think of scattering situations in which the particles move freely after a sufficiently long time. Since no radiation can escape to infinity, the free moving particles cannot lose energy, and thus, the system would indeed be stable in some sense. In any case, the relevance of (unprojected) many-body Dirac operators for it is clear: They are the natural candidates for generating the time evolution and their properties are most likely also reflected in the Dirac sea.

1.2. The results at a glance

The aim of this thesis is two-fold. First, the study of self-adjointness, i.e., existence of a unitary time evolution, and the spectrum of H_{2BD}. This investigation is suggested by the frequent use of H_{2BD} in the context of relativistic quantum chemistry, and is the first necessary step when addressing questions of physical relevance. Secondly, this thesis is concerned with regularity properties of the domain of H_{2BD} and the possibility of states with infinite single particle kinetic energy. This is suggested by explicit models of the Dirac sea. We have in mind the perspective of extending our results to N particles.

We outline very briefly our results. Our first main result proves the existence of a distinguished self-adjoint extension of H_{2BD}, denoted by $\widetilde{H}_{\mathrm{2BD}}$, under the assumption that the interaction potential V_{int} is of Coulomb type and the external field V_{ext} is bounded and symmetric. In the relativistic quantum chemistry literature mentioned above, this model describes two interacting point-like electrons in the vicinity of an extended nucleus. As regards the construction of $\widetilde{H}_{\mathrm{2BD}}$, we face two difficulties. First, the free two-body operator H_0 exhibits a non-trivial nullspace in the coordinate of the interaction. This nullspace is hidden in the standard representation of the Dirac matrices. Thus, an unbounded interaction potential cannot be relatively bounded by the free operator and a lot of standard perturbation techniques based on such a bound are not applicable. Instead, we use a Frobenius-Schur factorization based on this nullspace and its orthogonal complement and infer self-adjointness of the full two-body Dirac operator from self-adjointness of the Schur complement. The quadratic form techniques involved in this require the use of the theory of Calderón-Zygmund singular integrals. Second, $H_{2\mathrm{BD}}$ is not bounded from below, and thus, the existing machinery for finding and classifying self-adjoint extensions of semi-bounded operators does not apply immediately. Again, the Schur complement is of great help as it turns out that it is semi-bounded. Consequently, the self-adjoint extension of $H_{2\mathrm{BD}}$ we construct in this thesis is based on the Friedrichs extension of the Schur complement. This last step restricts the coupling constant γ to values $|\gamma| < 2/\pi$. Although inferring self-adjointness from the Schur complement in the context of one-particle Dirac operators has already been achieved in [EL08], this method has—to our best knowledge—never been applied to unbounded perturbations of linear operators with non-trivial nullspace.

In order to distinguish self-adjoint extensions in a physically sensible way, one usually provides a criterion. It is desirable that this criterion satisfies two conditions. First, it should have a clear physical meaning. Second, it should single out the extension uniquely. For $\tilde{H}_{2\mathrm{BD}}$, we adopt the criterion of finite potential energy and can show that it satisfies both of these conditions. This criterion is well-known from the one-particle Dirac operator in an external field.

The next group of important results concerns the domain of $H_{2\mathrm{BD}}$ and its operator closure $\overline{H}_{2\mathrm{BD}}$ in the presence of bounded external and interaction potentials. It derives its physical relevance ultimately from implications for explicit models of the Dirac sea. Although H_0 is a differential operator of first order, we find that $\mathcal{D}(\overline{H}_{2\mathrm{BD}})$ is not characterized by some kind of H^1-regularity. This is intimately connected to the presence of the non-trivial nullspace of H_0 in the coordinate of the interaction. If certain two-body states have parts in this nullspace, the regularity in the direction of the interaction, i.e., corresponding to this nullspace, can be relaxed. We show that existence of such nullspaces as well as the accompanying loss of H^1-regularity is generic for a broad class of sums of first order differential operators, including the natural candidates for relativistic many-body Hamiltonians. H^1- or $H^{1/2}$-regularity is typically associated with finite kinetic energy. That H^1- or $H^{1/2}$-regularity is no longer necessary, implies therefore that we can construct two-body states in $\mathcal{D}(\overline{H}_{2\mathrm{BD}})$ that have infinite single particle kinetic energy (infinite SPKE). Both particles exhibit infinite SPKE such that these energies cancel and the total kinetic energy remains finite. If however $\mathcal{D}(\overline{H}_{2\mathrm{BD}})$ is restricted to the antisymmetric subspace, this problem is circumvented as we can show that antisymmetric states always display finite SPKE. Our last result in this context treats scattering situations for smooth potentials. We show that, if the initial state exhibits finite SPKE, so does the scattered state for all fixed times $t \in \mathbb{R}$. In the literature on one-body Dirac operators with external field, the occurrence of infinite kinetic energies is also known (see, e.g., [ELS17]). There, the infinite kinetic energy is canceled by an infinite potential energy.

We conclude the thesis with two results that we consider as first steps towards a spectral analysis of $H_{2\mathrm{BD}}$. First, we prove $\sigma_{\mathrm{ess}}(H_{2\mathrm{BD}}) = \mathbb{R}$. Although this result has been anticipated in the literature, a complete proof seems to have been missing (cf. our discussion on [OKY14] above and Remark 6.2). Secondly, we show absence of large eigenvalues, i.e., we prove under a regularity assumption on possible eigenfunctions that no eigenvalues exist which are larger than twice the electron mass.

1.3. Structure of the thesis

The thesis is structured as follows. After this introduction, we give a detailed outline of the main results in Chapter 2. It is our attempt to help the reader understand within a few pages the main goals of the thesis and how we achieve these. Its first Section 2.1 provides the necessary notation and then states all main results. The second Section 2.2 is meant as a guided walk through the ideas and strategies which lie behind the main results. We also illustrate where some of the difficulties lie and how they are overcome in our proofs.

One of the very important and often employed objects, briefly introduced and motivated in Section 2.2, are the projections $P_\pm$. Chapter 3 is dedicated to a thorough study of $P_\pm$. Roughly speaking, P_+ projects onto that subspace, in which the two particles have the same sign of (relative) kinetic energy, and P_- onto that subspace, in which they have the opposite sign (see Section 3.2). They are not to be confused with the spectral projections of H_0. In Section 3.1, we define them properly and prove characteristic properties. An explicit integral kernel of $P_\pm$ is needed in the construction of the self-adjoint extension of $H_{2\mathrm{BD}}$. We rigorously compute it in Section 3.3 with the help of Calderón-Zygmund singular integrals. The last Section 3.4 provides a convenient characterization of what $P_\pm$ project onto.

After the rigorous introduction of $P_\pm$, we turn to the operator closure of H_0 and interesting physical properties of it that arise in that context. The closure is computed in Section 4.1 explicitly. In order to put the closure in a broader context, we give examples of more general sums of first order differential operators and their closure in Section 4.2. We illustrate that the interesting physical property of infinite single particle kinetic energy (infinite SPKE) is generic for such sums. States with infinite SPKE are discussed further in Section 4.3 by means of a series of explicit examples. That antisymmetrization of such states does not allow for infinite SPKE, is the content of Section 4.4. The invariance of finite SPKE states under the full time evolution is studied in Section 4.5, under the assumption of smooth potentials.

Chapter 4 treats the investigation of self-adjointness of $H_{2\mathrm{BD}}$ with unbounded interaction in Chapter 5. We first consider $H_{2\mathrm{BD}}$ with smooth potentials and its essential self-adjointness in Section 5.1, before we construct a self-adjoint extension under the assumption of Coulomb interaction in Section 5.2. We use ideas from the theory of matrix operators with unbounded entries, to which a brief introduction is given in Appendix A. In the subsequent Section 5.3, we provide the criterion for the just constructed self-adjoint extension. This criterion singles it out uniquely and in a physically sensible way. We conclude this chapter with a comment on an already existing proof of essential self-adjointness of $H_{2\mathrm{BD}}$ which—unfortunately—comprises a gap (Section 5.4).

The last regular Chapter 6 contains our results concerning the spectrum of $H_{2\mathrm{BD}}$. We prove in Section 6 that the essential spectrum of $H_{2\mathrm{BD}}$ comprises the entire real line as well as absence of eigenvalues for energies larger than twice the particles' mass.

Chapter 7 views this thesis as foundation for some topics of future research and indicates possible directions. These include a conjecture regarding infinite SPKE states and implications for stability, the incorporation of external Coulomb potentials when studying self-adjointness, as well as further investigations of the spectrum using physical insights and dilation methods.

For the reader's convenience, we included a List of Symbols. We tried to keep the notation consistent throughout the thesis, and it may thus be used as reference while reading.

As already practiced in the introduction, the first person plural will be used throughout this work since it is common in the mathematical physics literature.

2. Main results

In the following, we present a detailed outline of this thesis. The main goal of this chapter is to state the main results and to convey the strategy of their proof. Moreover, we list where the actual proofs can be found, give the motivation behind important steps in the proofs, and introduce often used notation. After a small paragraph on $H_{2\mathrm{BD}}$ and its domain, we state the three main theorems in Section 2.1: We begin with the result Theorem 1 on the domain, then turn to our main result Theorem 2 of this thesis on the distinguished self-extension of $H_{2\mathrm{BD}}$, and treat the result Theorem 3 on the spectrum in the end. In the same order, we provide the strategy of proof of these theorems in Section 2.2.

2.1. Statement of main results

The central object of study of this thesis is $H_{2\mathrm{BD}}$, the two-body Dirac operator (2BD operator) with interaction potential V_{int} in the presence of an external potential V_{ext}. The relevant Hilbert space is the twofold tensor product of the Hilbert space of $\mathbb{C}^4$-valued, square integrable functions on $\mathbb{R}^3$, i.e.,

$$\mathcal{H}_2 := L^2(\mathbb{R}^3,\, \mathrm{d}^3x) \otimes \mathbb{C}^4 \otimes L^2(\mathbb{R}^3,\, \mathrm{d}^3y) \otimes \mathbb{C}^4. \tag{2.1.1}$$

On $\mathcal{H}_2$, the symbolic expression of $H_{2\mathrm{BD}}$ takes the form

$$H_{2\mathrm{BD}} := H_0 + V_{\mathrm{ext}} + V_{\mathrm{int}}, \tag{2.1.2}$$

where the free two-body Dirac operator H_0 is given by

$$H_0 := (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \beta m_1) \otimes \mathrm{id} + \mathrm{id} \otimes (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}} + \beta m_2) \tag{2.1.3}$$

in units in which both the speed of light c and Planck's constant $\hbar$ equal one. Moreover, $m_1, m_2 \geq 0$ denote the masses of the two particles and $\nabla_{\boldsymbol{x}}$, $\partial/\partial x_i$, etc., denote the gradient with respect to $\boldsymbol{x} = (x_1, x_2, x_3)^\top \in \mathbb{R}^3$ and partial derivative with respect to x_i, $i = 1, 2, 3$, respectively. In places where the masses do not play a significant role we set $m_1 = m_2 = m$ or $m_1 = m_2 = 0$ without loss of generality. We denote by id_X the identity on the space X—however, whenever unambiguous, we usually drop the subscript X. As it is helpful to distinguish the identity on L^2 from the identity matrix on $\mathbb{C}^n$, we denote the latter by $\mathbf{1}_n$. Furthermore, the Hermitian matrices $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are the so-called Dirac matrices in standard representation

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{1}_2 & 0 \\ 0 & -\mathbf{1}_2 \end{pmatrix}, \tag{2.1.4}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.1.5}$$

The Dirac matrices obey the following anticommutation relations

$$\begin{aligned} &\alpha_k \alpha_l + \alpha_l \alpha_k = 2\delta_{kl} \mathbf{1}_4 , \quad k, l = 1, 2, 3, \\ &\alpha_i \beta + \beta \alpha_i = 0 , \quad i = 1, 2, 3, \\ &\beta^2 = \mathbf{1}_4, \end{aligned} \tag{2.1.6}$$

where the Kronecker delta satisfies $\delta_{kl} = 1$ if $k = l$, and zero else.

The canonical domain of H_0 as well as of H_{2BD} is

$$\mathcal{D}_0 := H^1(\mathbb{R}^3, \mathrm{d}^3x) \otimes \mathbb{C}^4 \otimes H^1(\mathbb{R}^3, \mathrm{d}^3y) \otimes \mathbb{C}^4, \tag{2.1.7}$$

where H^k denotes the k-th Sobolev space over L^2.

We now come to the main results. The proof ideas including detailed references to the actual proofs follow in the subsequent section. Our first main theorem concerns the domain of the closure of H_0. Some states from $\mathcal{D}(\overline{H}_0)$ may behave in a peculiar way, and so also some aspects of $\mathcal{D}(\overline{H}_0)$ with physical consequences are studied.

Theorem 1 (Domain)**.** *The following holds:*

a) H_0 *is essentially self-adjoint on* $\mathcal{D}_0$*, and the domain of the closure is*

$$\mathcal{D}(\overline{H}_0) = \left\{ f \in \mathcal{H}_2 \,\middle|\, \overline{H}_0 f \in \mathcal{H}_2 \right\}. \tag{2.1.8}$$

b) There exist states $f \in \mathcal{D}(\overline{H}_0)$ *such that* $E_{\mathrm{kin},1}[f] := \langle f, (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{x}} + \beta m_1) \otimes \mathrm{id} f \rangle$ *is ill-defined, and likewise for* $E_{\mathrm{kin},2}[f]$*.*

c) Let $\mathcal{H}_a := (L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes \mathbb{C}^4) \wedge (L^2(\mathbb{R}^3, \mathrm{d}^3y) \otimes \mathbb{C}^4)$*. For all* $f \in \mathcal{D}(\overline{H}_0) \cap \mathcal{H}_a$*, i.e.,* f *antisymmetric, we have*

$$|E_{\mathrm{kin},1}[f]| = |E_{\mathrm{kin},2}[f]| < \infty. \tag{2.1.9}$$

d) Let V_{ext}*,* V_{int} *be given as multiplication operators with smooth real functions, whose first and second order partial derivatives are bounded. Then, we have for all* $t \in \mathbb{R}$

$$\mathrm{e}^{-it\overline{H}_{\mathrm{2BD}}} \mathcal{D}_0 \subseteq \mathcal{D}_0, \tag{2.1.10}$$

where $\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}}$ *denotes the time evolution generated by* $\overline{H}_{2\mathrm{BD}}$.

From the point of view of dynamics, the second main theorem presented next is interesting as it guarantees existence of the full time evolution also for a class of unbounded pair interaction potentials, including the Coulomb type, by providing a distinguished self-adjoint extension of $H_{2\mathrm{BD}}$. In particular, our extension is distinguished uniquely by the criterion of finite potential energy.

Theorem 2 (Distinguished self-adjoint extension)**.** *Let* V_{ext} *be bounded and symmetric. Let, for almost all* $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$, V_{int} *be defined as the operator of multiplication by* $\gamma|\boldsymbol{x}-\boldsymbol{y}|^{-\kappa}$, *where* $0 < \kappa \leq 1$ *controls the strength of the singularity and* $\gamma \in \mathbb{R}$ *is the coupling constant. Moreover, let* $|\gamma| M_{\kappa/2}^2 < 1$, *where* $M_\kappa > 0$ *is given by*

$$M_\kappa := 2^{-\kappa} \frac{\Gamma\left(\frac{3}{4} - \frac{\kappa}{2}\right)}{\Gamma\left(\frac{3}{4} + \frac{\kappa}{2}\right)}. \tag{2.1.11}$$

a) There exists a self-adjoint extension of $H_{2\mathrm{BD}}$, *denoted by* $\tilde{H}_{2\mathrm{BD}}$, *with domain* $\mathcal{D}(\tilde{H}_{2\mathrm{BD}})$, *given in Eq.* (5.2.74).

b) $\tilde{H}_{2\mathrm{BD}}$ *is the unique self-adjoint extension that fulfills for all* $f \in \mathcal{D}(\tilde{H}_{2\mathrm{BD}})$ *the condition*

$$|E_{\mathrm{pot}}[f]| := |\langle f, (V_{\mathrm{ext}} + V_{\mathrm{int}})\, f\rangle| < \infty \tag{2.1.12}$$

and that can be split into a relative and a center-of-mass part, as it is made precise in Theorem 5.13, in particular, Eq. (5.3.1).

The third and last main theorem establishes that the essential spectrum of $H_{2\mathrm{BD}}$ comprises the entire real line. Moreover, we prove absence of eigenvalues $|E| > 2m$, under a condition on the eigenstates.

Theorem 3 (Essential spectrum/absence of large eigenvalues)**.** *Let* $\tilde{H}$ *denote any self-adjoint extension of* $H_{2\mathrm{BD}}$ *where* $V_{\mathrm{ext}} + V_{\mathrm{int}}$ *is the operator of multiplication with* $a|\boldsymbol{x}|^{-1} + a|\boldsymbol{y}|^{-1} + b|\boldsymbol{x}-\boldsymbol{y}|^{-1}$ *for* $a, b \in \mathbb{R}$ *and almost all* $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$. *Let* $m_1 = m_2 = m$.

a) Then, $\sigma_{\mathrm{ess}}(\tilde{H}) = \mathbb{R}$.

b) Assume further that all eigenstates of $\tilde{H}$ *lie in* $\mathcal{D}(\overline{H}_0) \cap \mathcal{D}(V_{\mathrm{ext}} + V_{\mathrm{int}})$. *Then,* $\tilde{H}$ *has no eigenvalues in* $(-\infty, -2m) \cup (2m, +\infty)$.

2.2. The ideas behind the proofs

Mathematical setting. We start with the mathematical setting that is common to all three main results, such as coordinate and Fourier transforms, Hilbert spaces, and the like. It is convenient to introduce a change of the coordinates $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ of the two particles to relative and center-of-mass coordinates by means of

$$\boldsymbol{r} := \boldsymbol{x} - \boldsymbol{y}\,, \quad \boldsymbol{R} := \frac{1}{2}(\boldsymbol{x} + \boldsymbol{y}). \tag{2.2.1}$$

Here, $\boldsymbol{r} \in \mathbb{R}^3$ is the relative coordinate (abbreviated by rel) and $\boldsymbol{R} \in \mathbb{R}^3$ the center-of-mass coordinate (com). Furthermore, we define with $\boldsymbol{X} := (\boldsymbol{x}, \boldsymbol{y})^\top$ and $\boldsymbol{Y} := (\boldsymbol{r}, \boldsymbol{R})^\top$ the transformation matrix $\mathrm{U} \colon \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3$ as

$$\mathrm{U}\boldsymbol{X} := \begin{pmatrix} 1 & -1 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{r} \\ \boldsymbol{R} \end{pmatrix} = \boldsymbol{Y}. \tag{2.2.2}$$

Since $\det \mathrm{U} = 1$, it induces a unitary transformation on the two-particle Hilbert space

$$U \colon \mathcal{H}_2 \to L^2(\mathbb{R}^3,\, \mathrm{d}^3R) \otimes \mathbb{C}^{16} \otimes L^2(\mathbb{R}^3,\, \mathrm{d}^3r) \tag{2.2.3}$$

given by $(Uf)(\boldsymbol{Y}) := f(\boldsymbol{X}) = f(\mathrm{U}^{-1}\boldsymbol{Y})$. We define the Hilbert spaces

$$\mathcal{H}^{\mathrm{rel}} := \mathbb{C}^{16} \otimes L^2(\mathbb{R}^3,\, \mathrm{d}^3r)\,, \quad \mathcal{H}^{\mathrm{com}} := L^2(\mathbb{R}^3,\, \mathrm{d}^3R) \otimes \mathbb{C}^{16}. \tag{2.2.4}$$

Remark 2.1. a) We want to point out that $U\mathcal{H}_2 \neq \mathcal{H}^{\mathrm{com}} \otimes \mathcal{H}^{\mathrm{rel}}$. Only the L^2-component of the center-of-mass motion is separated off of the relative motion. In the tensor factor $\mathbb{C}^{16}$, $\mathcal{H}^{\mathrm{rel}}$ and $\mathcal{H}^{\mathrm{com}}$ overlap.

b) In general, separating center-of-mass and relative motion is non-trivial in relativistic quantum mechanics (see, e.g., [Pry48]). This fact finds a manifestation in the non-commutativity of center-of-mass and relative Hamiltonian later on. Nevertheless, the coordinate transformation U can be applied to H_{2BD}. This simplifies the mathematical treatment of H_{2BD}. ■

The L^p-norm is as usually denoted by $\|\cdot\|_p$. In the case $p = 2$, the subscript is often dropped. The scalar product in all the Hilbert spaces we encounter is denoted by $\langle\cdot,\cdot\rangle$. In some cases, possible confusion is avoided by suitable subscripts. As an example, the scalar product on $\mathcal{H}^{\mathrm{rel}}$ of $f, g \in \mathcal{H}^{\mathrm{rel}}$ is defined as

$$\langle f, g\rangle := \int_{\mathbb{R}^3} f^\dagger(\boldsymbol{r})\, g(\boldsymbol{r})\, \mathrm{d}^3r = \int_{\mathbb{R}^3} \sum_{k=1}^{16} \overline{f^k(\boldsymbol{r})}\, g^k(\boldsymbol{r})\, \mathrm{d}^3r \tag{2.2.5}$$

and in analogy to that in the other Hilbert spaces. Here, f^k is the k-th component of the $\mathbb{C}^{16}$-spinor f. $\overline{z}$ denotes complex conjugation of $z \in \mathbb{C}$. Instead of $f(\boldsymbol{r})^\dagger f(\boldsymbol{r})$, we often write $|f(\boldsymbol{r})|^2$. When finite, $\|\cdot\|$ also denotes the norm of a linear operator. The context will always distinguish it from the L^2-norm. The operator closure of an arbitrary, but closable linear operator A is denoted by $\overline{A}$. No confusion with complex conjugation will arise. The adjoint of a linear operator A in Hilbert space is denoted by A^*. Since it is sometimes helpful to specify the variable associated to a particular L^2-space explicitly, we do that by writing, e.g., $L^2(\mathbb{R}^3,\, \mathrm{d}^3x)$ instead of $L^2(\mathbb{R}^3)$.

We define, as it is usually done for square-integrable, $\mathbb{C}$-valued functions, the following Fourier transform on $L^2(\mathbb{R}^3)$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ by

$$\hat{f}(\boldsymbol{p}) := (\mathcal{F}f)(\boldsymbol{p}) := L^2\text{-}\lim_{M\to\infty} \int_{|\boldsymbol{r}|\leq M} e^{-2\pi i \boldsymbol{r}\cdot\boldsymbol{p}} f(\boldsymbol{r})\, \mathrm{d}^3r \tag{2.2.6}$$

where the notation indicates that the limit is taken in the L^2-sense. In some cases, the notation $\mathcal{F}_{\boldsymbol{R}}$ and $\mathcal{F}_{\boldsymbol{r}}$ clarifies, whether the Fourier transform is taken with respect to the center-of-mass coordinate or the relative coordinate. This definition carries over to $L^2(\mathbb{R}^3) \otimes \mathbb{C}^n$ by applying the transformation component-wise. We introduce the notation for the relative momentum operator $\hat{\boldsymbol{p}} = -i\nabla_{\boldsymbol{r}}$ and the total momentum operator $\hat{\boldsymbol{P}} = -i\nabla_{\boldsymbol{R}}$. We remark with respect to this notation that it denotes both, the differential operators $-i\nabla_{\boldsymbol{R}}$ and $-i\nabla_{\boldsymbol{r}}$, respectively, when acting on f, as well as multiplication with $\boldsymbol{P} \in \mathbb{R}^3$ and $\boldsymbol{p} \in \mathbb{R}^3$, respectively, when acting on $\hat{f}$ in Fourier space. With p^2 we mean $|\boldsymbol{p}|^2$ for any $\boldsymbol{p} \in \mathbb{R}^3$. With $\hat{p}^2$, however, we denote the operator product $\hat{\boldsymbol{p}}^2$. Moreover, operators that are composed of $\hat{\boldsymbol{P}}$ or $\hat{\boldsymbol{p}}$ are defined with help of the Fourier transform. E.g., the operator $(\hat{p}^2+1)^{\kappa/2}$ that will occur in Section 5.2 is defined in Fourier space as multiplication by $(p^2+1)^{\kappa/2}$ with $\boldsymbol{p} \in \mathbb{R}^3$.

With the help of U, we can transform H_0 to relative and center-of-mass coordinates. Upon setting $m_1 = m_2 = 0$ for the moment, we obtain

$$\begin{aligned} T &:= U\Big((-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}}) \otimes \mathrm{id}_{L^2(\,\mathrm{d}^3x)\otimes\mathbb{C}^4} + \mathrm{id}_{L^2(\,\mathrm{d}^3y)\otimes\mathbb{C}^4} \otimes (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}})\Big)U^{-1} \\ &= \hat{\boldsymbol{P}}\cdot\mathbf{M}^+ \otimes \mathrm{id}_{L^2(\,\mathrm{d}^3r)} + \mathrm{id}_{L^2(\,\mathrm{d}^3R)} \otimes \mathbf{M}^-\cdot\hat{\boldsymbol{p}} \end{aligned} \tag{2.2.7}$$

where the 16×16-matrices $\mathbf{M}^\pm = \left(\mathrm{M}_1^\pm, \mathrm{M}_2^\pm, \mathrm{M}_3^\pm\right)$ are given by

$$\mathbf{M}^+ := \frac{1}{2}(\boldsymbol{\alpha}\otimes\mathbf{1}_4 + \mathbf{1}_4\otimes\boldsymbol{\alpha}) \tag{2.2.8}$$

and

$$\mathbf{M}^- := \boldsymbol{\alpha}\otimes\mathbf{1}_4 - \mathbf{1}_4\otimes\boldsymbol{\alpha}. \tag{2.2.9}$$

They are the coefficient matrices of center-of-mass momentum $\hat{\boldsymbol{P}}$ and relative momentum $\hat{\boldsymbol{p}}$, respectively. Unfortunately, they neither commute nor do they obey anticommutation relations similar to (2.1.6). Two things are to be noted in line (2.2.7). First, in the upper line, the identities have a spinor part, whereas in the lower line, they do not have a spinor part. This reflects the observation $U\mathcal{H}_2 \neq \mathcal{H}^{\mathrm{com}} \otimes \mathcal{H}^{\mathrm{rel}}$ from Remark 2.1. Secondly, our notation concerning hats is the following. Without hat, $\mathbf{M}^-\cdot\boldsymbol{p}$ means a $\mathbb{C}^{16\times16}$-matrix, whereas with hat, $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$ denotes an (unbounded) operator in Hilbert space.

The free relative Hamiltonian $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$ is defined in the underlying Hilbert space $\mathcal{H}^{\mathrm{rel}}$ with domain

$$\mathcal{D}(\mathbf{M}^-\cdot\hat{\boldsymbol{p}}) = \left\{f \in \mathcal{H}^{\mathrm{rel}} \,\middle|\, \mathbf{M}^-\cdot\hat{\boldsymbol{p}}f \in \mathcal{H}^{\mathrm{rel}}\right\}. \tag{2.2.10}$$

In the same manner, the free center-of-mass Hamiltonian $\hat{\boldsymbol{P}}\cdot\mathbf{M}^+$ is defined in the underlying Hilbert space $\mathcal{H}^{\mathrm{com}}$ with domain

$$\mathcal{D}(\hat{\boldsymbol{P}}\cdot\mathbf{M}^+) = \left\{f \in \mathcal{H}^{\mathrm{com}} \,\middle|\, \hat{\boldsymbol{P}}\cdot\mathbf{M}^+f \in \mathcal{H}^{\mathrm{com}}\right\}. \tag{2.2.11}$$

$\hat{\boldsymbol{P}}\cdot\mathbf{M}^+$ and $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$ inherit the non-commutativity of the matrices $\mathbf{M}^\pm = \left(\mathrm{M}_1^\pm, \mathrm{M}_2^\pm, \mathrm{M}_3^\pm\right)$.

Towards Theorem 1. Now, we come to the ideas that lie behind the proof of Theorem 1. The explicit form of the domain in part a) comes as no surprise. After all, H_0 is unitarily equivalent to an operator of multiplication with a Hermitian matrix for which $\mathcal{D}(\overline{H}_0)$ is the natural domain (see Theorem 4.1). In order to understand how single particle kinetic energy (SPKE) might diverge, we note one feature of the matrices $\mathbf{M}^- \cdot \boldsymbol{p}$ and $\boldsymbol{P} \cdot \mathbf{M}^+$, that has important consequences: They have a non-trivial nullspace. In Proposition 3.1, we will prove that $\mathrm{Ker}(\mathbf{M}^- \cdot \boldsymbol{p}) = \mathbb{C}^8$ which most importantly implies that

$$\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}) \simeq \mathbb{C}^8 \otimes L^2(\mathbb{R}^3). \tag{2.2.12}$$

The analogous statement for $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$ holds accordingly. Of course, elements from $\mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ that are mapped to zero by $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ do not need any H^1-regularity although $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ is a first order differential operator. This mechanism lies behind the proof of Theorem 1b): In order to construct states $f \in \mathcal{D}(\overline{H}_0)$ for which $E_{\mathrm{kin},1}[f] = \langle f, (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{x}} + \beta m_1) \otimes \mathrm{id} f \rangle$ diverges, one exploits the nullspaces of $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ or $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$ and constructs Uf in such a way that it has a part in, say, $\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ in which only L^2-regularity is required. With such an f, $E_{\mathrm{kin},1}[f]$ can be made divergent. In order to show this divergence, and thus, prove existence of infinite SPKE states, it suffices to give examples (see Examples 4.9 to 4.14).

Of course, these states with infinite energies are unphysical, and one may be tempted to dismiss a model predicting them. In order to shed some light on this situation, we included Section 4.2. There, we consider even more general sums of first order differential operators with two summands than H_0. Such operators are typical candidates for a many-body theory in the relativistic realm. Interestingly, we find that, if one requires these operators to describe two particles, nullspaces such as $\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$, and therefore also infinite SPKE states, are to be expected from such a model. This is simply due to their unboundedness from below.

We further discuss the physical relevance of infinite SPKE states in Theorem 1c). It is well-known that antisymmetrization of many-body states transforms pure tensor product states into a superposition of pure tensor product states, i.e., a wedge product state. Considering the energy of a single particle in an antisymmetric state, thus loses some of its intuitive appeal. This is reflected in the following fact which holds for all $\psi \in \mathcal{D}(\overline{H}_0)$

$$2 \cdot E_{\mathrm{kin},1}[\psi] = 2 \cdot E_{\mathrm{kin},2}[\psi] = E_{\mathrm{kin,tot}}[\psi] \tag{2.2.13}$$

where $E_{\mathrm{kin,tot}}[\psi]$ denotes the total kinetic energy of the state ψ (see Lemma 4.13). Since $|E_{\mathrm{kin,tot}}[\psi]| < \infty$ for all $\psi \in \mathcal{D}(\overline{H}_0)$ by definition, we can conclude that no infinite SPKE states exist which are antisymmetric.

Another issue pertaining to the physical relevance of infinite SPKE states is their behavior in scattering situations. In Theorem 1d), we answer the question if a finite SPKE state can scatter into an infinite SPKE state in the negative. If one starts out nice, one stays nice. Our way to show this is to prove invariance of the domain $\mathcal{D}_0$ under the full time evolution for all times $t \in \mathbb{R}$ (see Theorem 4.15).

Towards Theorem 2. In order to prepare everything we need for the distinguished self-adjoint extension of $H_{2\mathrm{BD}}$ from Theorem 2, we have to take the potentials V_{ext} and V_{int} into account, according to the conditions in Theorem 2. As V_{ext} is assumed to be symmetric and bounded, it plays no role for self-adjointness, and we can drop it. It can be restored later on by means of a small perturbation. The same holds for the mass term. For sake of concreteness, we assume that V_{int} is of Coulomb type. Transformed with U, it is the operator of multiplication with $\gamma|\boldsymbol{r}|^{-1}$ for almost all $\boldsymbol{r} \in \mathbb{R}^3$. The coupling constant $\gamma \in \mathbb{R}$ will be restricted later on to values $|\gamma| < 2/\pi$.

In relative and center-of-mass coordinates, $H_{2\mathrm{BD}}$ with zero masses has the form

$$UH_{2\mathrm{BD}}U^{-1} = \hat{\boldsymbol{P}} \cdot \mathbf{M}^{+} \otimes \mathrm{id}_{L^2(\,\mathrm{d}^3 r)} + \mathrm{id}_{L^2(\,\mathrm{d}^3 R)} \otimes \big(\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} + \frac{\gamma}{|\cdot|}\big). \tag{2.2.14}$$

We already dropped the mass term and V_{ext} as indicated above. Ultimately, we want to construct a self-adjoint extension of $H_{2\mathrm{BD}}$. As the interaction potential only acts in $\mathcal{H}^{\mathrm{rel}}$, it seems natural to prove self-adjointness of $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} + \gamma|\cdot|^{-1}$ first, and then infer self-adjointness of $\hat{\boldsymbol{P}} \cdot \mathbf{M}^{+} + \mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} + \gamma|\cdot|^{-1}$ from that. We note, however, the identities and the tensor product structure of $\mathcal{H}^{\mathrm{com}} = L^2(\mathbb{R}^3,\, \mathrm{d}^3 R) \otimes \mathbb{C}^{16}$ and $\mathcal{H}^{\mathrm{rel}} = \mathbb{C}^{16} \otimes L^2(\mathbb{R}^3,\, \mathrm{d}^3 r)$ again. Both share the tensor factor $\mathbb{C}^{16}$, and thus, also $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{P}} \cdot \mathbf{M}^{+}$ overlap in their spinor parts. Hence, it is not possible to write $H_{2\mathrm{BD}}$ in the form

$$A \otimes \mathrm{id}_Y + \mathrm{id}_X \otimes B \tag{2.2.15}$$

where A is a self-adjoint operator in the underlying Hilbert space $\mathcal{X}$ and B is a self-adjoint operator in the underlying Hilbert space $\mathcal{Y}$. In this simpler case, self-adjointness of A and B immediately implies essential self-adjointness of $A \otimes \mathrm{id}_{\mathcal{Y}} + \mathrm{id}_{\mathcal{X}} \otimes B$ by a standard result (see, e.g., [RS80, Corollary to Thm. VIII.33, pp. 300]). Unfortunately, this standard result does not apply to $H_{2\mathrm{BD}}$. Instead, we will make use of the method of direct fiber integrals in order to infer existence of a self-adjoint extension of $H_{2\mathrm{BD}}$ from existence of a self-adjoint extension of $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} + \gamma|\cdot|^{-1}$ (see Theorem 5.12).

Before we can construct a self-adjoint extension of $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} + \gamma|\cdot|^{-1}$, we come back to our earlier observation that $\mathrm{Ker}(\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}})$ is isomorphic to $\mathbb{C}^8 \otimes L^2(\mathbb{R}^3)$, and investigate its consequences regarding self-adjointness. An often used method is Kato-Rellich perturbation theory (see, e.g., [RS75, Theorem X.12]). It relies on the assumption that the potential is relatively bounded by the free Hamiltonian with relative bound smaller than one. Self-adjointness of the free Hamiltonian then implies self-adjointness of the full Hamiltonian. Now, as the nullspace of $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}}$ is non-trivial, Kato-Rellich perturbation theory is not applicable to $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} + \gamma|\cdot|^{-1}$. This is seen as follows. We can choose an $f \in \mathcal{D}(\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}})$ such that $f \in \mathrm{Ker}(\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}})$ but at the same time $f \notin \mathcal{D}(|\cdot|^{-1})$. This is possible as elements from the nullspace require only square-integrability and the interaction potential is unbounded. This implies $\mathcal{D}(\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}}) \nsubseteq \mathcal{D}(|\cdot|^{-1})$, and thus, $\gamma|\cdot|^{-1}$ cannot be relatively bounded by $\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}}$ at all (see Lemma 5.2).

In order to bypass Kato-Rellich perturbation theory, we focus on $\mathrm{Ker}(\mathbf{M}^{-} \cdot \hat{\boldsymbol{p}})$ and its orthogonal complement by splitting $\mathcal{H}^{\mathrm{rel}}$ correspondingly. To that end, we define the orthogonal projections $P_\pm$ in such a way that

$$\begin{aligned} P_+\mathcal{H}^{\mathrm{rel}} &= \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})^\perp = \mathcal{H}_+^{\mathrm{rel}} \\ P_-\mathcal{H}^{\mathrm{rel}} &= \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}) = \mathcal{H}_-^{\mathrm{rel}}, \end{aligned} \tag{2.2.16}$$

where $\mathcal{H}_\pm^{\mathrm{rel}}$ are themselves Hilbert spaces.

We want to point out that P_+ and P_- are *not* the spectral projections of H_0, i.e., *not* the operators that project onto the positive and negative part of the spectrum of H_0. By a heuristic argument given in Section 3.2, we can think of P_+ as projection on that subspace of $\mathcal{H}^{\mathrm{rel}}$ which contains the states describing particles with the same sign of kinetic energy, and of P_- as projection on that subspace which contains states describing particles with the opposite sign of kinetic energy.

The projections $P_\pm$ are thoroughly discussed in Chapter 3, where we define them in Definition 3.2, show that they indeed are the orthogonal projections from (2.2.16) in Proposition 3.3, and compute an explicit integral kernel in Theorem 3.8, which uses the Calderón-Zygmund theory of singular integrals.

As orthogonal projections, P_+ and P_- split $\mathcal{H}^{\mathrm{rel}}$ into two orthogonal subspaces, i.e., $\mathcal{H}^{\mathrm{rel}} = P_+\mathcal{H}^{\mathrm{rel}} \oplus P_-\mathcal{H}^{\mathrm{rel}} = \mathcal{H}_+^{\mathrm{rel}} \oplus \mathcal{H}_-^{\mathrm{rel}}$. This entails that we can recast the full relative Hamiltonian

$$H^{\mathrm{rel}} := \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + \frac{\gamma}{|\cdot|} \tag{2.2.17}$$

in matrix form as

$$\begin{aligned} H^{\mathrm{rel}} &= P_+H^{\mathrm{rel}}P_+ + P_+H^{\mathrm{rel}}P_- + P_-H^{\mathrm{rel}}P_+ + P_-H^{\mathrm{rel}}P_- \\ &=: \begin{pmatrix} \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + P_+\gamma|\cdot|^{-1}P_+ & P_+\gamma|\cdot|^{-1}P_- \\ P_-\gamma|\cdot|^{-1}P_+ & P_-\gamma|\cdot|^{-1}P_- \end{pmatrix} \end{aligned} \tag{2.2.18}$$

where we already applied $P_+\mathbf{M}^- \cdot \hat{\boldsymbol{p}}P_+ = \mathbf{M}^- \cdot \hat{\boldsymbol{p}}$, proven in Proposition 3.3. The domain of H^{rel} is

$$\mathcal{D}(H^{\mathrm{rel}}) = \mathcal{D}_+ \oplus \big(\mathcal{D}(|\cdot|^{-1}) \cap \mathcal{H}_-^{\mathrm{rel}}\big) \tag{2.2.19}$$

where

$$\mathcal{D}_+ := \big(\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3r)\big) \cap \mathcal{H}_+^{\mathrm{rel}}. \tag{2.2.20}$$

We note that $\mathcal{D}(H^{\mathrm{rel}})$ is dense in $\mathcal{H}^{\mathrm{rel}}$ (see Proposition 5.3).

That the projections $P_\pm$ split $\mathcal{H}^{\mathrm{rel}}$ into the subspaces $\mathcal{H}_\pm^{\mathrm{rel}}$ is very useful. One knows now, e.g., where to expect H^1-regularity (in $\mathcal{H}_+^{\mathrm{rel}}$; see Lemma 4.3). Moreover, by facilitating the matrix representation from line (2.2.18), they also point towards a strategy of proof, taken from the theory of matrix operators with unbounded entries (see Appendix A): The use of the Frobenius-Schur factorization and its so-called Schur complement. Before we go into more details, we define the bounded and symmetric operator $B := 2\beta \otimes \beta$ and modify with its help H^{rel}. The reason for that will be made clear in the following paragraphs. The modification of H^{rel} takes the form

$$H^{\mathrm{rel}} + P_+BP_+ = \begin{pmatrix} \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + P_+BP_+ + P_+\gamma|\cdot|^{-1}P_+ & P_+\gamma|\cdot|^{-1}P_- \\ P_-\gamma|\cdot|^{-1}P_+ & P_-\gamma|\cdot|^{-1}P_- \end{pmatrix}. \tag{2.2.21}$$

We introduce the abbreviations

$$A = A_0 + P_+\gamma|\cdot|^{-1}P_+ = \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + P_+BP_+ + P_+\gamma|\cdot|^{-1}P_+ \tag{2.2.22}$$

for the operator in the upper left corner of H^{rel} and compute (see Lemma 5.4)

$$A_0^2 = (\mathbf{M}^- \cdot \hat{\boldsymbol{p}} + P_+BP_+)^2 = 4(-\Delta + 1)P_+. \tag{2.2.23}$$

This means that A_0 and A share many properties with one-body Dirac operators, even though their coefficient matrices $\mathbf{M}^-$ do not obey the anticommutation relations from line (2.1.6). Therefore, if we restrict the coupling constant γ to values $|\gamma| < 1$, we obtain self-adjointness of A as well as existence and boundedness of A^{-1} (see Lemma 5.6). These properties are the reason for adding P_+BP_+ to H^{rel}. The Frobenius-Schur factorization is now well-defined and given by (see Lemma 5.7)

$$\begin{aligned} &H^{\mathrm{rel}} + P_+BP_+ = \\ &= \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ P_-\gamma|\cdot|^{-1}P_+A^{-1} & \mathrm{id} \end{pmatrix} \begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & S \end{pmatrix} \begin{pmatrix} \mathrm{id} & A^{-1}P_+\gamma|\cdot|^{-1}P_- \\ \mathbf{0} & \mathrm{id} \end{pmatrix} \end{aligned} \tag{2.2.24}$$

where the Schur complement $S\colon \mathcal{D}(S) \to \mathcal{H}_-^{\mathrm{rel}}$ of A is defined by

$$S := P_-\gamma|\cdot|^{-1}P_- - P_-\gamma|\cdot|^{-1}P_+A^{-1}P_+\gamma|\cdot|^{-1}P_- \tag{2.2.25}$$

with domain

$$\mathcal{D}(S) = \mathcal{D}(|\cdot|^{-1}) \cap \mathcal{H}_-^{\mathrm{rel}}. \tag{2.2.26}$$

The advantage of the Frobenius-Schur factorization is that it decomposes $H^{\mathrm{rel}}+P_+BP_+$ into a product of three matrix operators of which the first and the third factor are bounded and boundedly invertible (see Lemma A.2 in the Appendix A), while the second factor is diagonal. Now, the upper left operator of the diagonal matrix operator is self-adjoint as it behaves roughly like an ordinary one-body Dirac operator (see Lemma 5.6). Therefore, in order to obtain a self-adjoint extension of $H^{\mathrm{rel}} + P_+BP_+$, if suffices to construct a self-adjoint extension of the Schur complement S, the lower right operator of the diagonal matrix operator. Boundedness and bounded invertibility of the first and third factor imply self-adjointness of $H^{\mathrm{rel}} + P_+BP_+$ (see Theoremn 5.11).

In order to construct a self-adjoint extension of S, we use that $P_-|\cdot|^{-1}P_-$ is bounded from below and thus possesses a Friedrichs extension V_F. We show further that the remaining summand $P_-|\cdot|^{-1}P_+\gamma A^{-1}P_+|\cdot|^{-1}P_-$ is small in form sense with respect to V_F. The KLMN-theorem, which is the form analogue to Kato-Rellich perturbation theory, then yields a self-adjoint extension of S (see Lemma 5.10). The key estimate involved in the proof is

$$
\begin{aligned}
\Big| \big\langle f, \;\; & P_-|\cdot|^{-1}P_+\gamma A^{-1}P_+|\cdot|^{-1}P_- f\big\rangle_{\mathcal{H}_-^{\mathrm{rel}}}\Big| \\
&= \big|\big\langle |\cdot|^{-1/2}P_- f, \big(|\cdot|^{-1/2}P_+\gamma A^{-1}P_+|\cdot|^{-1/2}\big)\,|\cdot|^{-1/2}P_- f\big\rangle_{\mathcal{H}^{\mathrm{rel}}}\big| \\
&\le \big\||\cdot|^{-1/2}P_- f\big\|\,\big\||\cdot|^{-1/2}P_+\gamma A^{-1}P_+|\cdot|^{-1/2}\big\|\,\big\||\cdot|^{-1/2}P_- f\big\| \\
&= \big\||\cdot|^{-1/2}P_+\gamma A^{-1}P_+|\cdot|^{-1/2}\big\|\,\big\langle f, P_-|\cdot|^{-1}P_- f\big\rangle_{\mathcal{H}_-^{\mathrm{rel}}} \\
&= \big\||\cdot|^{-1/2}P_+\gamma A^{-1}P_+|\cdot|^{-1/2}\big\|\,\langle f, V_F f\rangle_{\mathcal{H}_-^{\mathrm{rel}}}
\end{aligned}
\tag{2.2.27}
$$

for all $f \in \mathcal{D}(S) = \mathcal{D}(|\cdot|^{-1}) \cap \mathcal{H}_-^{\mathrm{rel}}$. In order to apply the KLMN-theorem successfully, we need to establish the bound

$$
\big\||\cdot|^{-1/2}P_+\gamma A^{-1}P_+|\cdot|^{-1/2}\big\| < 1. \tag{2.2.28}
$$

This is possible if we restrict the coupling constant γ to values $|\gamma| < 2/\pi$ (see Lemma 5.9).

We need to have a closer look at the inequality from line (2.2.27). The KLMN-theorem actually requires that it holds for all $f \in \mathcal{D}(V_F)$. Our computation for all $f \in \mathcal{D}(S) = \mathcal{D}(|\cdot|^{-1}) \cap \mathcal{H}_-^{\mathrm{rel}}$ is not sufficient. However, we know from abstract results regarding Friedrichs extensions that $\mathcal{D}(V_F) = \mathcal{D}(|\cdot|^{-1/2}) \cap \mathcal{D}((P_-|\cdot|^{-1}P_-)^*)$. Moreover, we can prove (see Theorem 5.8) that for all $f \in \mathcal{D}(|\cdot|^{-1/2}) \cap \mathcal{H}_-^{\mathrm{rel}}$, there exists a sequence $(f_n)_{n\in\mathbb{N}} \subseteq \mathcal{D}(|\cdot|^{-1})$ such that

$$
\|P_-(f-f_n)\| + \big\||\cdot|^{-1/2}P_-(f-f_n)\big\| \xrightarrow{n\to\infty} 0, \tag{2.2.29}
$$

i.e., $\mathcal{D}(|\cdot|^{-1}) \cap \mathcal{H}_-^{\mathrm{rel}}$ is a form core and the estimate from line (2.2.27) extends to all $f \in \mathcal{D}(V_F)$. We found that the proof of this fact is by far not trivial as the projections split $\mathcal{H}^{\mathrm{rel}}$ corresponding to $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$, and the splitting is independent of the potential $|\cdot|^{-1}$. It is here in Theorem 5.8, where we need the explicit integral kernels of the projections $P_\pm$, computed in Theorem 3.8.

In conclusion, we constructed a self-adjoint extension of the Schur complement S, which we used as basis for a self-adjoint extension of H^{rel}. For this we needed the Frobenius-Schur factorization. By an argument using direct fiber integrals, we finally obtained the desired self-adjoint extension of $H_{2\mathrm{BD}}$ in Theorem 2a). We used in several places that bounded and symmetric operators can be added and subtracted without affecting self-adjointness.

A self-adjoint extension of a Hamiltonian considered only by itself is often meaningless since there might be infinitely many extensions. Therefore, one usually requires that self-adjoint extensions are uniquely distinguished by a physical criterion, i.e., there should exist only one extension that satisfies a certain criterion which is physically sensible. For $H_{2\mathrm{BD}}$ we adopt the criterion of finite potential energy in Theorem 2b). This criterion is well-accepted for one-body Dirac operators in an external field (see [Wü75]). For $H_{2\mathrm{BD}}$ it holds in the following sense. Let $\tilde{H}$ be any self-adjoint extension of $UH_{2\mathrm{BD}}U^{-1}$ which we assume to have the form

$$\tilde{H} = \hat{\boldsymbol{P}} \cdot \mathbf{M}^{+} \otimes \mathrm{id} + \mathrm{id} \otimes \tilde{H}^{\mathrm{rel}} + V_{\mathrm{ext}} + \beta \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta, \tag{2.2.30}$$

where $\tilde{H}^{\mathrm{rel}}$ is an arbitrary self-adjoint extension of $H^{\mathrm{rel}} = H_0 + \gamma|\cdot|^{-1}$. Then, $|\langle f, (V_{\mathrm{ext}} + V_{\mathrm{int}})f\rangle| < \infty$ for all $f \in \mathcal{D}(\tilde{H})$ if, and only if, $\tilde{H}$ coincides with our extension of H_{2BD} constructed above (see Theorem 5.13). The proof we found basically assumes the opposite and and shows that it implies a contradiction.

Remark 2.2. We want to remark on the strength of the singularity of V_{int}. In order to control this strength, we introduced the parameter $0 < \kappa \leq 1$ in Theorem 2. The smaller κ is chosen, the larger values of $|\gamma|$ are allowed. In the case of Coulomb interaction, i.e., $\kappa = 1$, we have $|\gamma| < 2/\pi$ for the coupling constant.

Towards Theorem 3. Our main result concerning the spectrum of H_{2BD} is Theorem 3. Its part a) identifies the essential spectrum. That the essential spectrum of H_{2BD} is $\mathbb{R}$, has been assumed, however, a complete proof seems to have been missing in the literature. The proof of $\sigma_{\mathrm{ess}}(H_{\mathrm{2BD}}) = \mathbb{R}$ we give here uses Weyl's criterion and applies to all self-adjoint extensions of H_{2BD} for which V_{ext} as well as V_{int} are of Coulomb type (see Theorem 6.1).

This result implies that no discrete spectrum exists, i.e., if eigenvalues exist at all, they are embedded into the continuous part of the spectrum. As this is a rare phenomenon, it has been conjectured that H_{2BD} does not possess any eigenvalues at all (see [Der12]). Theorem 3b) corroborates this conjecture in which we show absence of eigenvalues if $|E| > 2m$. Due to our method of proof, we assume that possible eigenstates lie in $\mathcal{D}(\overline{H}_0) \cap \mathcal{D}(V_{\mathrm{ext}} + V_{\mathrm{int}})$ (see Theorem 6.3).

3. The projections P_+ and P_- onto the spaces $\mathcal{H}_+^{\mathrm{rel}}$ and $\mathcal{H}_-^{\mathrm{rel}}$

3.1. Definition of the projections P_+ and P_-

This section defines in a rigorous way the projections P_+ and P_-, and therefore, also the spaces $\mathcal{H}_+^{\mathrm{rel}}$ and $\mathcal{H}_-^{\mathrm{rel}}$, respectively. As we mentioned briefly in Section 2.2, they are constructed in such a way that P_- projects onto $\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ and P_+ onto the orthogonal complement of $\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. They are crucial for the study of the relative Hamiltonian $H^{\mathrm{rel}} = \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + V_{\mathrm{int}}$ as they allow for the convenient matrix representation of H^{rel} from line (2.2.18).

Already at the beginning, we want to point out again that P_+ and P_- are *not* the spectral projections of H_0, i.e., *not* the operators that project onto the positive and negative part of the spectrum of H_0. We will elaborate on the physical meaning of $\mathcal{H}_\pm^{\mathrm{rel}}$ in the next section.

Before we state the first proposition of this section, we recall that $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ with hat denotes a linear operator on $\mathcal{H}^{\mathrm{rel}}$ whereas $\mathbf{M}^- \cdot \boldsymbol{p}$ without the hat is a 16×16-matrix for all $\boldsymbol{p} \in \mathbb{R}^3$, i.e., a linear operator on $\mathbb{C}^{16}$.

Proposition 3.1. *The following holds:*

a) For all $\boldsymbol{p} \in \mathbb{R}^3 \setminus \{0\}$*, we have* $\dim \mathrm{Ker}(\mathbf{M}^- \cdot \boldsymbol{p}) = 8$*.*

b) $\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ *is isomorphic to* $\mathbb{C}^8 \otimes L^2(\mathbb{R}^3, \mathrm{d}^3 r)$*.*

c) $\mathrm{Ker}(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+)$ *is isomorphic to* $L^2(\mathbb{R}^3, \mathrm{d}^3 R) \otimes \mathbb{C}^8$*.*

Proof. a) follows since for all $\boldsymbol{p} \in \mathbb{R}^3 \setminus \{0\}$ one finds that the Hermitian matrix $\mathbf{M}^- \cdot \boldsymbol{p}$ has the eigenvalue 0 with multiplicity 8.

b) Before we characterize all $f \in \mathcal{H}^{\mathrm{rel}}$ for which $\mathbf{M}^- \cdot \hat{\boldsymbol{p}} f = 0$ holds, we note the following. As $\mathbf{M}^- \cdot \boldsymbol{p}$ is a Hermitian matrix, there exists a unitary matrix $u(\boldsymbol{p})$ which diagonalizes $\mathbf{M}^- \cdot \boldsymbol{p}$. We find for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$u(\boldsymbol{p})\, \mathbf{M}^- \cdot \boldsymbol{p}\, u(\boldsymbol{p})^\dagger = \begin{pmatrix} -\mathbf{1}_4 |\boldsymbol{p}| & & \\ & \mathbf{1}_4 |\boldsymbol{p}| & \\ & & \mathbf{0}_8 \end{pmatrix}. \tag{3.1.1}$$

We further note that unitarity of $u(\hat{\boldsymbol{p}})$ implies that solving the equation $\mathbf{M}^- \cdot \hat{\boldsymbol{p}} f = 0$ in $L^2(\mathbb{R}^3)$ is equivalent to solving $u(\hat{\boldsymbol{p}})\, \mathbf{M}^- \cdot \hat{\boldsymbol{p}}\, u(\hat{\boldsymbol{p}})^* u(\hat{\boldsymbol{p}}) f = 0$ in $L^2(\mathbb{R}^3)$. In view of Eq. (3.1.1), we use that $\operatorname{Ker}(|\hat{\boldsymbol{p}}|) = \{0\}$ in $L^2(\mathbb{R}^3)$. Therefore, those eight components of $u(\hat{\boldsymbol{p}})f$, on which $|\hat{\boldsymbol{p}}|$ acts when solving $u(\hat{\boldsymbol{p}})\, \mathbf{M}^- \cdot \hat{\boldsymbol{p}}\, u(\hat{\boldsymbol{p}})^* u(\hat{\boldsymbol{p}}) f = 0$, are zero. The remaining eight components can be chosen linearly independent as the matrix $\mathbf{M}^- \cdot \boldsymbol{p}$ is Hermitian. Thus, $u(\hat{\boldsymbol{p}})$ establishes an isomorphism between $\operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ and $\mathbb{C}^8 \otimes L^2(\mathbb{R}^3, \mathrm{d}^3 r)$, which proves the statement.

c) Analogously to b). □

In order to give the definition of $P_\pm$, it is convenient to first define the Hermitian 16×16-matrix $\tau(\boldsymbol{p})$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ by

$$\tau(\boldsymbol{p}) := -\frac{\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p}}{p^2}. \tag{3.1.2}$$

We compute for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$\tau(\boldsymbol{p})^2 = \left(\frac{\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p}}{p^2} \right)^2 = \frac{(\boldsymbol{\alpha} \cdot \boldsymbol{p})^2 \otimes (\boldsymbol{\alpha} \cdot \boldsymbol{p})^2}{p^4} = \mathbf{1}_{16} \tag{3.1.3}$$

since $(\boldsymbol{\alpha} \cdot \boldsymbol{p})^2 = \mathbf{1}_4 p^2$ by the anticommutation relations (2.1.6) for the Dirac matrices. This implies that multiplication with $\tau(\boldsymbol{p})$ defines a bounded operator on all of $\mathcal{H}^{\mathrm{rel}}$ which we use in the following definition.

Definition 3.2. We define the operator $\tau \colon \mathcal{H}^{\mathrm{rel}} \to \mathcal{H}^{\mathrm{rel}}$ by its action on all $f \in \mathcal{H}^{\mathrm{rel}}$ and for almost all $\boldsymbol{r} \in \mathbb{R}^3$ by

$$(\tau f)(\boldsymbol{r}) := L^2\text{-}\lim_{M \to \infty} \int_{|\boldsymbol{p}| \le M} e^{2\pi i \boldsymbol{r} \cdot \boldsymbol{p}}\, \tau(\boldsymbol{p}) \hat{f}(\boldsymbol{p})\, \mathrm{d}^3 p. \tag{3.1.4}$$

We define the operators $P_\pm \colon \mathcal{H}^{\mathrm{rel}} \to \mathcal{H}^{\mathrm{rel}}_\pm$ by

$$P_\pm := \frac{1}{2} (\mathrm{id} \pm \tau) \tag{3.1.5}$$

where the spaces $\mathcal{H}^{\mathrm{rel}}_\pm$ are defined by

$$\mathcal{H}^{\mathrm{rel}}_\pm := P_\pm \mathcal{H}^{\mathrm{rel}}. \tag{3.1.6}$$

We also define for almost all $\boldsymbol{p} \in \mathbb{R}^3$ the 16×16-matrix

$$P_\pm(\boldsymbol{p}) := \frac{1}{2} \left(\mathbf{1}_{16} \pm \tau(\boldsymbol{p}) \right). \tag{3.1.7}$$

For the moment, the definition of $P_\pm$ as Fourier multiplier suffices. We will, however, derive integral kernels for τ and hence also for $P_\pm$ in Section 3.3.

Proposition 3.3. *The following holds:*

a) P_- *is the orthogonal projection onto* $\operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$*, i.e.,* $\mathcal{H}_-^{\mathrm{rel}} = \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$*.*

b) P_+ *is the orthogonal projection onto* $\operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})^\perp$*, i.e.,* $\mathcal{H}_+^{\mathrm{rel}} = \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})^\perp$*.*

c) $P_+ \mathbf{M}^- \cdot \hat{\boldsymbol{p}}\, P_+ f = \mathbf{M}^- \cdot \hat{\boldsymbol{p}} f$ *and* $P_- \mathbf{M}^- \cdot \hat{\boldsymbol{p}} f = 0$ *for all* $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$*.*

Furthermore, $\mathcal{H}^{\mathrm{rel}} = \mathcal{H}_+^{\mathrm{rel}} \oplus \mathcal{H}_-^{\mathrm{rel}}$*, and* $\mathcal{H}_\pm^{\mathrm{rel}}$ *are themselves Hilbert spaces.*

Proof. a) First, we prove that P_- is an orthogonal projection, i.e., $P_-^2 = P_-$, P_- is bounded, and $P_-^* = P_-$. Since $(\boldsymbol{\alpha} \cdot \boldsymbol{p})^2 = \mathbf{1}_4 p^2$ by the anticommutation relations (2.1.6) for the Dirac matrices and $\tau(\boldsymbol{p}) = \mathbf{1}_{16}$ by Eq. (3.1.3) hold, we obtain

$$P_-(\boldsymbol{p})^2 = \frac{1}{4}\left(\mathbf{1}_{16} - \tau(\boldsymbol{p})\right)^2 = \frac{1}{4}\left(\mathbf{1}_{16} - 2 \cdot \tau(\boldsymbol{p}) + \tau(\boldsymbol{p})^2\right) = P_-(\boldsymbol{p}) \tag{3.1.8}$$

for almost all $\boldsymbol{p} \in \mathbb{R}^3$. Thus, $P_-^2 = P_-$ follows. P_- is bounded with $\|P_-\| = 1$ since $P_-(\boldsymbol{p})$ is a Hermitian matrix with the only eigenvalues being 0 and 1. This also implies self-adjointness $P_-^* = P_-$.

In order to show that P_- projects onto $\operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$, we prove $\mathcal{H}_-^{\mathrm{rel}} = \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. We start with the inclusion $\mathcal{H}_-^{\mathrm{rel}} \subseteq \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ and compute for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$\begin{aligned}\mathbf{M}^- \cdot \boldsymbol{p}\, P_-(\boldsymbol{p}) &= (\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \mathbf{1}_4 - \mathbf{1}_4 \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p})\, \frac{1}{2}\left(\mathbf{1}_{16} + \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p}}{p^2}\right) \\ &= \frac{1}{2}\left(\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \mathbf{1}_4 - \mathbf{1}_4 \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p} + \frac{(\boldsymbol{\alpha} \cdot \boldsymbol{p})^2 \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p}}{p^2} - \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes (\boldsymbol{\alpha} \cdot \boldsymbol{p})^2}{p^2}\right) \\ &= 0\end{aligned} \tag{3.1.9}$$

where we used $(\boldsymbol{\alpha} \cdot \boldsymbol{p})^2 = \mathbf{1}_4 p^2$ once again. Therefore, we obtain $P_- f \in \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ for all $f \in \mathcal{H}^{\mathrm{rel}}$, i.e., $\mathcal{H}_-^{\mathrm{rel}} \subseteq \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$.

For the reverse inclusion $\operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}) \subseteq \mathcal{H}_-^{\mathrm{rel}}$, we show that for all $f \in \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ we have $P_- f = f$. Let $f \in \operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. From the proof of Proposition 3.1b), we know that the upper eight components of $u(\hat{\boldsymbol{p}})f$ are zero, where $u(\boldsymbol{p})$ diagonalizes $\mathbf{M}^- \cdot \boldsymbol{p}$ as introduced in line (3.1.1). We conjugate $P_-(\boldsymbol{p})$ with $u(\boldsymbol{p})$ and obtain

$$u(\boldsymbol{p}) P_-(\boldsymbol{p}) u(\boldsymbol{p})^\dagger = \begin{pmatrix} \mathbf{0}_8 & \\ & \mathbf{1}_8 \end{pmatrix} \tag{3.1.10}$$

for almost all $\boldsymbol{p} \in \mathbb{R}^3$. This implies that $u(\hat{\boldsymbol{p}}) P_- u(\hat{\boldsymbol{p}})^*$ acts as the zero operator on the upper eight components of $u(\hat{\boldsymbol{p}})f$ and as identity on the lower eight components of $u(\hat{\boldsymbol{p}})f$, i.e.,

$$u(\hat{\boldsymbol{p}}) P_- u(\hat{\boldsymbol{p}})^* u(\hat{\boldsymbol{p}}) f = u(\hat{\boldsymbol{p}}) f. \tag{3.1.11}$$

That $u(\hat{\boldsymbol{p}})$ is injective, allows us to conclude $P_- f = f$.

b) P_+ is an orthogonal projection by the same argument as for P_-. In order to show that P_+ projects on $\operatorname{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})^\perp$, we compute for almost all $\boldsymbol{p} \in \mathbb{R}^3$ $P_-(\boldsymbol{p}) P_+(\boldsymbol{p}) =$

$P_+(\boldsymbol{p})P_-(\boldsymbol{p}) = 0$, and therefore, for all $f, g \in \mathcal{H}^{\mathrm{rel}}$

$$\langle P_+ f, P_- g\rangle = \langle f, P_+ P_- g\rangle = 0. \tag{3.1.12}$$

c) follows since the relations

$$P_+(\boldsymbol{p})\mathbf{M}^- \cdot \boldsymbol{p} P_+(\boldsymbol{p}) = \mathbf{M}^- \cdot \boldsymbol{p} \tag{3.1.13}$$
$$P_-(\boldsymbol{p})\mathbf{M}^- \cdot \boldsymbol{p} = 0 \tag{3.1.14}$$

hold for almost all $\boldsymbol{p} \in \mathbb{R}^3$. This is shown by a direct computation.

Since the projections $P_\pm$ are closed, $\mathcal{H}^{\mathrm{rel}}_\pm$ are closed subspaces of $\mathcal{H}^{\mathrm{rel}}$. With the inherited inner product from $\mathcal{H}^{\mathrm{rel}}$, it follows that they are themselves Hilbert spaces. With [RS80, Theorem II.3], it follows that $\mathcal{H}^{\mathrm{rel}} = \mathcal{H}^{\mathrm{rel}}_+ \oplus \mathcal{H}^{\mathrm{rel}}_-$. □

3.2. Physical interpretation of $\mathcal{H}^{\mathrm{rel}}_+$ and $\mathcal{H}^{\mathrm{rel}}_-$

This section motivates the introduction of the spaces $\mathcal{H}^{\mathrm{rel}}_+$ and $\mathcal{H}^{\mathrm{rel}}_-$ from a physical point of view. The following arguments were presumably first made by Kemmer in [Kem37]. We will see that elements from $\mathcal{H}^{\mathrm{rel}}_+$ can be associated with two particles both of which have the same sign of energy, whereas elements from $\mathcal{H}^{\mathrm{rel}}_-$ correspond to two particles which have a different sign of energy. From this alone, one might already anticipate that states from $\mathcal{H}^{\mathrm{rel}}_-$ might cause difficulties in the presence of an interaction term as Dirac famously pointed out that "*the negative-energy electron will repel an ordinary positive-energy electron although it is itself attracted by the positive-energy electron*" (see [Dir30, p. 362]).

Since it simplifies the argument, we consider two particles of equal mass m, i.e., we set $m_1 = m_2 = m$. In Fourier space, H_0 is the operator of multiplication with the Hermitian 16×16-matrix $H_0(\boldsymbol{p_x}, \boldsymbol{p_y})$ defined by

$$H_0(\boldsymbol{p_x}, \boldsymbol{p_y}) := (\boldsymbol{\alpha} \cdot \boldsymbol{p_x} + \beta m_1) \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes (\boldsymbol{\alpha} \cdot \boldsymbol{p_y} + \beta m_2)\,, \tag{3.2.1}$$

where $\boldsymbol{p_x}, \boldsymbol{p_y} \in \mathbb{R}^3$ are the Fourier variables conjugate to $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$. We compute the eigenvalues of the matrix $H_0(\boldsymbol{p_x}, \boldsymbol{p_y})$, i.e., the energy of the two free particles, and find for all $\boldsymbol{p_x}, \boldsymbol{p_y} \in \mathbb{R}^3$

$$\lambda_1(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_4(\boldsymbol{p_x}, \boldsymbol{p_y}) = \sqrt{\boldsymbol{p_x}^2 + m^2} + \sqrt{\boldsymbol{p_y}^2 + m^2}, \tag{3.2.2a}$$

$$\lambda_5(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_8(\boldsymbol{p_x}, \boldsymbol{p_y}) = \sqrt{\boldsymbol{p_x}^2 + m^2} - \sqrt{\boldsymbol{p_y}^2 + m^2}, \tag{3.2.2b}$$

$$\lambda_9(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_{12}(\boldsymbol{p_x}, \boldsymbol{p_y}) = -\sqrt{\boldsymbol{p_x}^2 + m^2} + \sqrt{\boldsymbol{p_y}^2 + m^2}, \tag{3.2.2c}$$

$$\lambda_{13}(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_{16}(\boldsymbol{p_x}, \boldsymbol{p_y}) = -\sqrt{\boldsymbol{p_x}^2 + m^2} - \sqrt{\boldsymbol{p_y}^2 + m^2}\,. \tag{3.2.2d}$$

We see that the eigenvalues are just what one might have guessed: The sum of two single particle energies, albeit with all possible combinations of the energy sign.

As it is usually done for many-particle systems, we set the center-of-mass momentum $\boldsymbol{P} = \boldsymbol{p_x} + \boldsymbol{p_y}$ to zero. This yields $\boldsymbol{p_x} = -\boldsymbol{p_y}$, which in turn implies for the eigenvalues $\lambda_k(\boldsymbol{p_x}, \boldsymbol{p_y})$, $k = 1, 2, \ldots, 16$,

$$\lambda_1(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_4(\boldsymbol{p_x}, \boldsymbol{p_y}) = 2\sqrt{\boldsymbol{p_x}^2 + m^2}, \tag{3.2.3a}$$

$$\lambda_5(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_{12}(\boldsymbol{p_x}, \boldsymbol{p_y}) = 0, \tag{3.2.3b}$$

$$\lambda_{13}(\boldsymbol{p_x}, \boldsymbol{p_y}) = \ldots = \lambda_{16}(\boldsymbol{p_x}, \boldsymbol{p_y}) = -2\sqrt{\boldsymbol{p_x}^2 + m^2}\,. \tag{3.2.3c}$$

States that can be associated to the eigenvalue 0 lie in $\mathcal{H}_-^{\mathrm{rel}}$. The relation $\boldsymbol{p_x} = -\boldsymbol{p_y}$ has further implications on the relative momentum $\boldsymbol{p}$. We find

$$\boldsymbol{p} = \frac{1}{2}\left(\boldsymbol{p_x} - \boldsymbol{p_y}\right) = \boldsymbol{p_x}. \tag{3.2.4}$$

We transform $H_0(\boldsymbol{p_x}, \boldsymbol{p_y})$ to relative and center-of-mass coordinates, set $\boldsymbol{P} = 0$, and compute the eigenvalues of the resulting Hermitian matrix $\mathbf{M}^- \cdot \boldsymbol{p} + \beta m \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta m$. We find

$$\mu_1(\boldsymbol{p}) = \ldots = \mu_4(\boldsymbol{p}) = 2\sqrt{\boldsymbol{p}^2 + m^2}, \tag{3.2.5a}$$

$$\mu_5(\boldsymbol{p}) = \ldots = \mu_{12}(\boldsymbol{p}) = 0, \tag{3.2.5b}$$

$$\mu_{13}(\boldsymbol{p}) = \ldots = \mu_{16}(\boldsymbol{p}) = -2\sqrt{\boldsymbol{p}^2 + m^2}\,. \tag{3.2.5c}$$

After taking (3.2.4) into account, we can now compare (3.2.3) and (3.2.5). This allows for the following conclusion in the case of $\boldsymbol{P} = 0$:

1. If the kinetic energies of the two particles have the same sign, the corresponding state lies in $\mathcal{H}_+^{\mathrm{rel}}$.

2. If the kinetic energies of the two particles have the opposite sign, the corresponding state lies in $\mathcal{H}_-^{\mathrm{rel}}$.

3.3. Integral kernels of P_+ and P_-

The projections $P_\pm$ were naturally defined as Fourier multiplier on $\mathcal{H}^{\mathrm{rel}}$ in Definition 3.2. When one can work in Fourier space easily, this definition is sufficient. We saw, however, in the matrix representation of H^{rel} in line (2.2.18) that also the parts of the potential V_{int} in $\mathcal{H}_\pm^{\mathrm{rel}}$, i.e., $P_\pm V_{\mathrm{int}} P_\pm$ and $P_\pm V_{\mathrm{int}} P_\mp$, respectively, occur and we will see later on (see Theorem 5.8) that they have to be controlled. In order to do so, it turns out to be convenient to derive integral kernels of $P_\pm$ also in position space. This derivation is the content of this section.

Remark 3.4. Before we proceed, however, we want to remark on an alternative option, namely considering $P_\pm V_{\mathrm{int}} P_\pm$ and $P_\pm V_{\mathrm{int}} P_\mp$, respectively, in Fourier space. For simplicity, we write $V_{\mathrm{int}} = V$. V is then transformed to a convolution operator, of which many convolution kernels—the Coulomb case included—are well-known. This and the nice form of the projections $P_\pm$ in Fourier space might suggest this approach. However, a difficulty related to complex phases and oscillatory integrals becomes apparent when considering expressions of the form

$$\|Vf\|^2 \overset{(*)}{=} \left\|\hat{v} * \hat{f}\right\|^2 = \int_{\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \hat{v}(\boldsymbol{p}-\boldsymbol{k})\hat{f}(\boldsymbol{k})\,\mathrm{d}^3k \right|^2 \mathrm{d}^3p, \tag{3.3.1}$$

where f lies in $\mathcal{D}(V)$ and $\hat{v}$ is defined by $(*)$.

In order to highlight the possible oscillatory nature, we give a concrete example. For the remainder of this remark, we assume that $V \in L^2(\mathbb{R}^3)$ be given by multiplication with $V(\boldsymbol{r}) = \mathrm{e}^{-|\boldsymbol{r}|}|\boldsymbol{r}|^{-1}$ for almost all $\boldsymbol{r} \in \mathbb{R}^3$, define $g \in L^2(\mathbb{R}^3)$ by $g(\boldsymbol{r}) = \mathrm{e}^{-|\boldsymbol{r}|}|\boldsymbol{r}|^{-3/2+\varepsilon}$ for almost all $\boldsymbol{r} \in \mathbb{R}^3$ and an arbitrary $0 < \varepsilon < 1/2$, and look at $g_{\boldsymbol{a}} := g(\cdot - \boldsymbol{a})$ for a fixed $\boldsymbol{a} \in \mathbb{R}^3 \setminus \{0\}$. We see that on the one hand $Vg_{\boldsymbol{a}} \in L^2(\mathbb{R}^3)$, i.e., $g_a \in \mathcal{D}(V)$, as the singularities of $g_{\boldsymbol{a}}$ and V do not coincide. On the other hand, however, we have $Vg \notin L^2(\mathbb{R}^3)$, i.e., $g \notin \mathcal{D}(V)$. Now, standard theorems on convolutions and their Fourier transforms tell us that $Vg_a \in L^2(\mathbb{R}^3)$ implies that also the convolution $\hat{v} * \hat{g}_{\boldsymbol{a}}$ lies in $L^2(\mathbb{R}^3)$. Also from standard theorems, we know that $\hat{g}_{\boldsymbol{a}}(\boldsymbol{p}) = \mathrm{e}^{-2\pi i \boldsymbol{a}\cdot\boldsymbol{p}}\hat{g}(\boldsymbol{p})$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$. Moreover, one finds that $\hat{g}(\boldsymbol{p})$ is real-valued such that $\hat{g}(\boldsymbol{p}) > 0$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ as well as $\hat{g}(\boldsymbol{p}) \propto |\boldsymbol{p}|^{-3/2-\varepsilon}$ for large $|\boldsymbol{p}|$. We plug our choices of V and g_a into $\|Vg_{\boldsymbol{a}}\|^2$ and obtain

$$\|\hat{v} * \hat{g}_{\boldsymbol{a}}\|^2 = \int_{\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \frac{4\pi}{4\pi^2|\boldsymbol{p}-\boldsymbol{k}|^2+1} \mathrm{e}^{-2\pi i \boldsymbol{a}\cdot\boldsymbol{k}} \hat{f}(\boldsymbol{k})\,\mathrm{d}^3k \right|^2 \mathrm{d}^3p. \tag{3.3.2}$$

If now the absolute value was pulled into the d^3k-integral, the phase $\mathrm{e}^{-2\pi i \boldsymbol{a}\cdot\boldsymbol{k}}$ would vanish, and the remaining integrand would correspond to Vg whose L^2-norm, however, diverges as $Vg \notin L^2(\mathbb{R}^3)$ by construction:

$$\begin{aligned}
\|\hat{v} * \hat{g}_{\boldsymbol{a}}\|^2 &= \int_{\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \frac{4\pi}{4\pi^2|\boldsymbol{p}-\boldsymbol{k}|^2+1} \mathrm{e}^{-2\pi i \boldsymbol{a}\cdot\boldsymbol{k}} \hat{f}(\boldsymbol{k})\,\mathrm{d}^3k \right|^2 \mathrm{d}^3p \\
&\leq \int_{\mathbb{R}^3} \left(\int_{\mathbb{R}^3} \left| \frac{4\pi}{4\pi^2|\boldsymbol{p}-\boldsymbol{k}|^2+1} \hat{f}(\boldsymbol{k}) \right| \mathrm{d}^3k \right)^2 \mathrm{d}^3p \\
&\overset{(*)}{=} \int_{\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \frac{4\pi}{4\pi^2|\boldsymbol{p}-\boldsymbol{k}|^2+1} \hat{f}(\boldsymbol{k})\,\mathrm{d}^3k \right|^2 \mathrm{d}^3p \\
&= \left\|\hat{v} * \hat{f}\right\|^2,
\end{aligned} \tag{3.3.3}$$

which diverges due to $\hat{g}(\boldsymbol{p}) \propto |\boldsymbol{p}|^{-3/2-\varepsilon}$ for large $|\boldsymbol{p}|$. In $(*)$, we used that $\hat{g}(\boldsymbol{p})$ is real-valued and $\hat{g}(\boldsymbol{p}) > 0$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$.

Line (3.3.3) gives a diverging upper bound and is as such, of course, useless. The observation we are concerned with here, however, is the following: If one tries to get rid of complex phases by applying the triangle inequality, integrals may diverge at infinity. Therefore, one has to keep track of all complex phases. This makes the involved estimates quite unpractical in Fourier space. In position space, however, the strong singularity at the origin can be smoothed out by an estimate on the commutator $[V, P_\pm]$. We will see this in the proof of Theorem 5.8. ■

Since $P_\pm = 1/2(\mathrm{id} \pm \tau)$, it suffices to compute the integral kernel of the operator τ. In Definition 3.2, it was defined in Fourier space for almost all $\boldsymbol{p} \in \mathbb{R}^3$ as operator of multiplication with

$$\tau(\boldsymbol{p}) = -\frac{\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \boldsymbol{\alpha} \cdot \boldsymbol{p}}{p^2}, \tag{3.3.4}$$

i.e., for all $f \in \mathcal{H}^{\mathrm{rel}}$ and for almost all $\boldsymbol{r} \in \mathbb{R}^3$, we had

$$(\tau f)(\boldsymbol{r}) = L^2\text{-}\lim_{M\to\infty} \int_{|\boldsymbol{p}|\le M} \mathrm{e}^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}}\, \tau(\boldsymbol{p}) \hat{f}(\boldsymbol{p})\, \mathrm{d}^3 p. \tag{3.3.5}$$

Now, all entries of the matrix $\tau(\boldsymbol{p})$ are fractions. By expanding the Kronecker product in (3.3.4), one finds that the denominator of all of these fractions is p^2, whereas each numerator is given by combinations of the components of the form $p_i p_j$ for $i, j = 1, 2, 3$. Explicitly, each entry of the matrix $\tau(\boldsymbol{p})$ is one of the following expressions:

$$\frac{p_3^2}{p^2}, \quad \frac{(p_1 \pm i p_2) p_3}{p^2}, \quad \frac{(p_1 \pm i p_2)^2}{p^2}, \quad \frac{(p_1 - i p_2)(p_1 + i p_2)}{p^2}. \tag{3.3.6}$$

In order to control τ, it therefore suffices to control the (bounded) Fourier multiplier $p_i p_j / p^2$ for all $i, j = 1, 2, 3$. Hence, we define the operator T_{ij}, $i, j = 1, 2, 3$, for all $f \in L^2(\mathbb{R}^3, \mathrm{d}^3 r)$ and for almost all $\boldsymbol{r} \in \mathbb{R}^3$ by

$$(T_{ij} f)(\boldsymbol{r}) := L^2\text{-}\lim_{M\to\infty} \int_{|\boldsymbol{p}|\le M} \mathrm{e}^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}}\, \frac{p_i\, p_j}{p^2} \hat{f}(\boldsymbol{p})\, \mathrm{d}^3 p. \tag{3.3.7}$$

It is this operator T_{ij}, whose associated position space integral kernels we will compute.

Remark 3.5. This remark intends to address the fact that T_{ij} looks familiar from the more general viewpoint of Fourier analysis.

a) We consider the so-called Riesz transforms R_j, $j = 1, 2, 3$ (see, e.g., [Ste70]). They can be viewed as multiplier in Fourier space as well and are for all $f \in L^2(\mathbb{R}^3)$ and almost all $\boldsymbol{p} \in \mathbb{R}^3$ given by

$$(\mathcal{F} R_j f)(\boldsymbol{p}) = i \frac{p_j}{|\boldsymbol{p}|} \hat{f}(\boldsymbol{p}). \tag{3.3.8}$$

From the definition of T_{ij} in line (3.3.7), we see that

$$R_i R_j = -T_{ij}, \tag{3.3.9}$$

and so, up to a factor, T_{ij} is equal to the so-called double Riesz transform.

b) As Riesz transforms and similar Fourier multipliers are subject of intensive research, there do exist general theorems concerning multipliers and their associated integral kernel. Of particular interest for us is the following result ([SW71, Theorem 4.5, p. 164]). Suppose $P(\boldsymbol{x})$ is a *harmonic* polynomial on $\mathbb{R}^3$ that is homogeneous of degree $k \geq 1$, i.e., $P(\lambda \boldsymbol{x}) = \lambda^k P(\boldsymbol{x})$ for all real $k \geq 1$ and all $\boldsymbol{x} \in \mathbb{R}^3$. Then, $c_k P(\boldsymbol{p})/|\boldsymbol{p}|^k$ is the Fourier multiplier of the associated integral kernel $P(\boldsymbol{x})/|\boldsymbol{x}|^{3+k}$, where the constant $c_k \in \mathbb{C}$ depends on k only. This applies readily to T_{ij} if $i \neq j$. In the case $i = j$, however, the polynomial $P(\boldsymbol{p})$ is of the form p_i^2, and thus, *not* harmonic. Therefore, the integral kernel may have a different form.

Although T_{ij} is connected to the well-known Riesz transform, and the kernel for $i \neq j$ is known, no conclusions can be drawn from general results concerning the case $i = j$. Therefore, we compute the kernel explicitly. ■

As preparation, we cite two known results on the computation of such kernels. The first one is suggested by the factor $1/p^2$ and is the content of the following theorem. We cite it from [LL01] in the case of $\mathbb{R}^3$.

Theorem 3.6. *Let $\alpha \in \mathbb{R}^+$, and define $c_\alpha := \pi^{-\alpha/2}\Gamma(\alpha/2)$.*

a) Let f be a function in $C_c^\infty(\mathbb{R}^3)$ and let $0 < \alpha < 3$. Then,

$$c_\alpha \int_{\mathbb{R}^3} \mathrm{e}^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}} \frac{1}{p^\alpha} \hat{f}(\boldsymbol{p}) \, \mathrm{d}^3 p = c_{3-\alpha} \int_{\mathbb{R}^3} \frac{1}{|\boldsymbol{r}-\boldsymbol{y}|^{3-\alpha}} f(\boldsymbol{y}) \, \mathrm{d}^3 y. \tag{3.3.10}$$

b) If $0 < \alpha < 3/2$ and if $f \in L^p(\mathbb{R}^3, \mathrm{d}^3 r)$ with $p = 6/(3+2\alpha)$, then $\hat{f}$ exists in the sense of the Hausdorff-Young inequality (see [LL01, Theorem 5.7]). Moreover, defining the function g for almost all $\boldsymbol{r} \in \mathbb{R}^3$ by

$$g(\boldsymbol{r}) = c_{3-\alpha} \int_{\mathbb{R}^3} \frac{1}{|\boldsymbol{r}-\boldsymbol{y}|^{3-\alpha}} f(\boldsymbol{y}) \, \mathrm{d}^3 y, \tag{3.3.11}$$

we have $g \in L^2(\mathbb{R}^3, \mathrm{d}^3 r)$. Furthermore, for almost all $\boldsymbol{p} \in \mathbb{R}^3$, we obtain

$$c_\alpha |\boldsymbol{p}|^{-\alpha} \hat{f}(\boldsymbol{p}) = \hat{g}(\boldsymbol{p}). \tag{3.3.12}$$

Proof. a) See [LL01, Theorem 5.9].

b) See [LL01, Corollary 5.10]. □

It will turn out that the integral kernels $K_{ij}(\boldsymbol{y})$ exhibit a singularity at the origin. Since this singularity is of size $|\boldsymbol{y}|^{-3}$, it is not integrable. In order to address this problem, we will also need a result from the theory of Calderón-Zygmund singular integrals. For later reference, we state it in the following theorem in the case of $\mathbb{R}^3$.

Theorem 3.7. *If $K(\boldsymbol{y})$ is a homogeneous function of degree -3, i.e., $K(\lambda \boldsymbol{y}) = \lambda^{-3} K(\boldsymbol{y})$ for almost all $\boldsymbol{y} \in \mathbb{R}^3$ and for all $\lambda > 0$, and if $K(\boldsymbol{y})$ has in addition the following properties* *a) it has zero average on S^2, i.e., $\int_{S^2} K(\boldsymbol{y})\,\mathrm{d}\sigma(\boldsymbol{y}) = 0$, where S^2 denotes the surface of the unit ball and $\mathrm{d}\sigma$ the corresponding surface measure, and*

b) $\int_{S^2} |K(\boldsymbol{y}) + K(-\boldsymbol{y})| \log^+ |K(\boldsymbol{y}) + K(-\boldsymbol{y})| \,\mathrm{d}\sigma(\boldsymbol{y}) < \infty$, where $\log^+$ denotes the positive part of the logarithm,

then, if $f \in L^p(\mathbb{R}^3, \mathrm{d}^3 r)$, $1 < p < \infty$, the limit

$$\lim_{\varepsilon \to 0} \int_{|\boldsymbol{y}| > \varepsilon} K(\boldsymbol{y}) f(\boldsymbol{r} - \boldsymbol{y})\,\mathrm{d}^3 y \tag{3.3.13}$$

exists in L^p-sense and pointwise for almost all $\boldsymbol{r} \in \mathbb{R}^3$. Furthermore, there exists a constant $A > 0$, depending on p and K only, such that

$$\left\| \sup_{\varepsilon > 0} \left| \int_{|\boldsymbol{y}| > \varepsilon} K(\boldsymbol{y}) f(\cdot - \boldsymbol{y})\,\mathrm{d}^3 y \right| \right\| \leq A \, \|f\| \, . \tag{3.3.14}$$

Proof. See [CZ56, Theorem 1]. □

We point out the significance of assumption a) from Theorem 3.7 in Remark 3.9 below. We can now give the desired integral kernel of T_{ij}.

Theorem 3.8. *For all $f \in L^2(\mathbb{R}^3, \mathrm{d}^3 r)$, all $i, j = 1, 2, 3$, and almost all $\boldsymbol{r} \in \mathbb{R}^3$, the action of T_{ij}, defined in* (3.3.7)*, is given by*

$$\left(T_{ij} f\right)(\boldsymbol{r}) = \frac{\delta_{ij}}{3} f(\boldsymbol{r}) - \frac{1}{4\pi} \lim_{\varepsilon \to 0} \int_{|\boldsymbol{y}| > \varepsilon} K_{ij}(\boldsymbol{y}) f(\boldsymbol{r} - \boldsymbol{y})\,\mathrm{d}^3 y, \tag{3.3.15}$$

where δ_{ij} is the Kronecker delta. The integral kernels $K_{ij}(\boldsymbol{y})$ of T_{ij} are then for all $i, j = 1, 2, 3$ and all $|\boldsymbol{y}| > 0$ given by

$$K_{ij}(\boldsymbol{y}) := \frac{\partial^2}{\partial y_i \partial y_j} \frac{1}{|\boldsymbol{y}|} = \begin{cases} \dfrac{3 y_i y_j}{|\boldsymbol{y}|^5}\,, & i \neq j \\[2ex] \dfrac{3 y_i^2}{|\boldsymbol{y}|^5} - \dfrac{1}{|\boldsymbol{y}|^3}\,, & i = j. \end{cases} \tag{3.3.16}$$

Proof. First, we let $f \in C_c^\infty(\mathbb{R}^3)$ which denotes the set of smooth functions on $\mathbb{R}^3$ with compact support. Using (3.3.7), we calculate for all $\boldsymbol{r} \in \mathbb{R}^3$

$$
\begin{aligned}
-4\pi\,(T_{ij}f)(\boldsymbol{r}) &= -4\pi \int_{\mathbb{R}^3} e^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}}\,\frac{p_i\,p_j}{p^2}\hat{f}(\boldsymbol{p})\,\mathrm{d}^3p \\
&= \frac{1}{\pi}\int_{\mathbb{R}^3}\left(\frac{\partial^2}{\partial r_i \partial r_j}e^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}}\right)\frac{1}{p^2}\hat{f}(\boldsymbol{p})\,\mathrm{d}^3p \\
&\overset{\text{(i)}}{=} \frac{1}{\pi}\frac{\partial^2}{\partial r_i \partial r_j}\int_{\mathbb{R}^3} e^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}}\frac{1}{p^2}\hat{f}(\boldsymbol{p})\,\mathrm{d}^3p \\
&\overset{\text{(ii)}}{=} \frac{\partial^2}{\partial r_i \partial r_j}\int_{\mathbb{R}^3}\frac{1}{|\boldsymbol{y}|}f(\boldsymbol{r}-\boldsymbol{y})\,\mathrm{d}^3y \\
&\overset{\text{(iii)}}{=} \int_{\mathbb{R}^3}\frac{1}{|\boldsymbol{y}|}\frac{\partial^2 f(\boldsymbol{r}-\boldsymbol{y})}{\partial r_i \partial r_j}\,\mathrm{d}^3y \\
&= \int_{\mathbb{R}^3}\frac{1}{|\boldsymbol{y}|}(-1)^2\frac{\partial^2 f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_i \partial y_j}\,\mathrm{d}^3y
\end{aligned}
\tag{3.3.17}
$$

where we used dominated convergence to commute the derivatives with the integral in (i), Theorem 3.6a) for the Fourier integral in (ii), and the calculus of distributional convolutions and derivatives in (iii) (see [LL01, Lemma 6.8]). It applies since $|\cdot|^{-1} \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and since $f \in C_c^\infty(\mathbb{R}^3)$. In order to continue with integration by parts, we change the domain of integration to the set $B = \{\varepsilon < |\boldsymbol{y}| < R\}$, where $\varepsilon > 0$ is fixed and $R > 0$ is chosen sufficiently large such that $\mathrm{supp} f(\boldsymbol{r} - \cdot) \subset B_R(0)$. As $f \in C_c^\infty(\mathbb{R}^3)$, this is possible for all fixed $\boldsymbol{r} \in \mathbb{R}^3$. We obtain

$$
\begin{aligned}
&\int_B \frac{1}{|\boldsymbol{y}|}\frac{\partial^2 f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_i \partial y_j}\,\mathrm{d}^3y \\
&= -\int_B\left(\frac{\partial}{\partial y_i}\frac{1}{|\boldsymbol{y}|}\right)\left(\frac{\partial f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_j}\right)\mathrm{d}^3y + \int_{|\boldsymbol{y}|=\varepsilon}\frac{1}{|\boldsymbol{y}|}\frac{\partial f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_j}\,\nu^i\mathrm{d}\sigma(\boldsymbol{y}) \\
&= \int_B\left(\frac{\partial^2}{\partial y_j \partial y_i}\frac{1}{|\boldsymbol{y}|}\right)f(\boldsymbol{r}-\boldsymbol{y})\,\mathrm{d}^3y - \int_{|\boldsymbol{y}|=\varepsilon}\left(\frac{\partial}{\partial y_i}\frac{1}{|\boldsymbol{y}|}\right)f(\boldsymbol{r}-\boldsymbol{y})\,\nu^j\mathrm{d}\sigma(\boldsymbol{y}) \qquad (3.3.18a) \\
&\quad + \int_{|\boldsymbol{y}|=\varepsilon}\frac{1}{|\boldsymbol{y}|}\frac{\partial f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_j}\,\nu^i\mathrm{d}\sigma(\boldsymbol{y}), \qquad (3.3.18b)
\end{aligned}
$$

where ν^k denotes the k-th component of $\boldsymbol{\nu}$, the unit outward normal to B. Due to our choice of R, the boundary terms at $|\boldsymbol{y}| = R$ vanish.

In order to have equality of lines (3.3.17) and (3.3.18), we need to take the pointwise limits $\varepsilon \to 0$ and $R \to \infty$ in line (3.3.18). Existence of the latter follows from the compact support of f. For the former, we note that the derivative of $f \in C_c^\infty(\mathbb{R}^3)$ is uniformly bounded by a constant $C > 0$ independent of ε. We thus get for line (3.3.18b)

$$
\begin{aligned}
\left|\int_{|\boldsymbol{y}|=\varepsilon}\frac{1}{|\boldsymbol{y}|}\frac{\partial f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_j}\,\nu^i\mathrm{d}\sigma(\boldsymbol{y})\right| &\leq \int_{S^2}\frac{1}{\varepsilon}\left|\frac{\partial f(\boldsymbol{r}-\boldsymbol{y})}{\partial y_j}\right|\varepsilon^2\mathrm{d}\Omega \\
&\leq C\varepsilon\int_{S^2}\mathrm{d}\Omega \xrightarrow{\varepsilon\to 0} 0.
\end{aligned}
\tag{3.3.19}
$$

In the last summand of line (3.3.18a), we use the parametrization Φ of the boundary at $|\boldsymbol{y}| = \varepsilon$ with spherical coordinates and note that $\Phi(\nabla|\boldsymbol{y}|^{-1}) = \boldsymbol{\nu}/\varepsilon^2$. Thus,

$$
\begin{aligned}
&\lim_{\varepsilon\to 0}\int_{|\boldsymbol{y}|=\varepsilon}\left(\frac{\partial}{\partial y_i}\frac{1}{|\boldsymbol{y}|}\right) f(\boldsymbol{r}-\boldsymbol{y})\,\nu^j \mathrm{d}\sigma(\boldsymbol{y}) \\
&\quad = \lim_{\varepsilon\to 0}\int_{S^2}\frac{\nu^i}{\varepsilon^2} f(\boldsymbol{r}-\boldsymbol{y}(\varepsilon,\theta,\phi))\,\nu^j\,\varepsilon^2 \mathrm{d}\Omega \\
&\quad = \int_{S^2}\nu^i\nu^j \lim_{\varepsilon\to 0} f(\boldsymbol{r}-\boldsymbol{y}(\varepsilon,\theta,\phi))\,\mathrm{d}\Omega \\
&\quad = f(\boldsymbol{r})\int_{S^2}\nu^i\nu^j\,\mathrm{d}\Omega
\end{aligned}
\tag{3.3.20}
$$

follows from dominated convergence and continuity of f. Now, we need to distinguish the cases $i \neq j$ and $i = j$. We obtain by direct computation

$$
f(\boldsymbol{r})\int_{S^2}\nu^i\nu^j\,\mathrm{d}\Omega = \begin{cases} 0\,, & i \neq j, \\ \dfrac{4\pi}{3} f(\boldsymbol{r})\,, & i = j. \end{cases}
\tag{3.3.21}
$$

It remains to investigate the limit $\varepsilon \to 0$ for the first summand of (3.3.18a). This can be achieved with the help of Theorem 3.7 which, however, requires an analysis of the singular integral kernel $\partial^2/\partial y_i \partial y_j |\boldsymbol{y}|^{-1}$. By explicit computation, we obtain for $|\boldsymbol{y}| > 0$

$$
K_{ij}(\boldsymbol{y}) = \frac{\partial^2}{\partial y_i \partial y_j}\frac{1}{|\boldsymbol{y}|} = \begin{cases} \dfrac{3y_iy_j}{|\boldsymbol{y}|^5}\,, & i \neq j \\ \dfrac{3y_i^2}{|\boldsymbol{y}|^5} - \dfrac{1}{|\boldsymbol{y}|^3}\,, & i = j. \end{cases}
\tag{3.3.22}
$$

We check the conditions of Theorem 3.7 and observe first that $K_{ij}(\boldsymbol{y})$ is homogeneous of degree -3, i.e., $K_{ij}(\lambda\boldsymbol{y}) = \lambda^{-3}K_{ij}(\boldsymbol{y})$ for almost all $\boldsymbol{y} \in \mathbb{R}^3$ and for all $\lambda > 0$. Moreover, $K_{ij}(\boldsymbol{y})$ exhibits the following crucial property for all $i, j = 1, 2, 3$:

$$
\int_{S^2} K_{ij}(\boldsymbol{y})\,\mathrm{d}\sigma(\boldsymbol{y}) = 0.
\tag{3.3.23}
$$

Furthermore, since $K_{ij}(-\boldsymbol{y}) = K_{ij}(\boldsymbol{y})$, it suffices to estimate for all $i, j = 1, 2, 3$

$$
\int_{S^2} |K_{ij}(\boldsymbol{y})| \log^+ |K_{ij}(\boldsymbol{y})|\,\mathrm{d}\sigma(\boldsymbol{y}) \leq \int_{S^2} |K_{ij}(\boldsymbol{y})|^2\,\mathrm{d}\sigma(\boldsymbol{y}) < \infty
\tag{3.3.24}
$$

where $\log^+$ denotes the positive part of the logarithm. That the last integral is indeed finite can be seen by explicit calculation.

Hence, all conditions of Theorem 3.7 are met and we can conclude that the limit

$$
\lim_{\varepsilon\to 0}\int_{|\boldsymbol{y}|>\varepsilon} K_{ij}(\boldsymbol{y}) f(\boldsymbol{r}-\boldsymbol{y})\,\mathrm{d}^3y
\tag{3.3.25}
$$

exists pointwise for almost all $\boldsymbol{r} \in \mathbb{R}^3$ as well as in $L^2(\mathbb{R}^3, \mathrm{d}^3r)$. We have thus established for all $\boldsymbol{r} \in \mathbb{R}^3$ and $f \in C_c^\infty(\mathbb{R}^3)$

$$(T_{ij}f)(\boldsymbol{r}) = \frac{\delta_{ij}}{3} f(\boldsymbol{r}) - \frac{1}{4\pi} \lim_{\varepsilon \to 0} \int_{|\boldsymbol{y}|>\varepsilon} K_{ij}(\boldsymbol{y}) f(\boldsymbol{r}-\boldsymbol{y}) \, \mathrm{d}^3 y. \tag{3.3.26}$$

In order to extend the formula for the action of T_{ij} to all of $L^2(\mathbb{R}^3, \mathrm{d}^3r)$, we note that Theorem 3.7 also guarantees the existence of a constant $A > 0$ such that for all $f \in L^2(\mathbb{R}^3, \mathrm{d}^3r)$

$$\left\| \sup_{\varepsilon>0} \left| \int_{|\boldsymbol{y}|>\varepsilon} K_{ij}(\boldsymbol{y}) f(\cdot - \boldsymbol{y}) \, \mathrm{d}^3 y \right| \right\| \leq A \, \|f\| \, . \tag{3.3.27}$$

Choose now any $f \in L^2(\mathbb{R}^3, \mathrm{d}^3r)$ and fix a sequence $(f_n)_{n\in\mathbb{N}} \subset C_c^\infty(\mathbb{R}^3)$ such that $\|f - f_n\| \xrightarrow{n\to\infty} 0$. Then,

$$\begin{aligned} &\| \, T_{ij} \, (f - f_n) \| \\ &\quad \leq \frac{\delta_{ij}}{3} \, \|f - f_n\| + \frac{1}{4\pi} \left\| \sup_{\varepsilon>0} \left| \int_{|\boldsymbol{y}|>\varepsilon} K_{ij}(\boldsymbol{y}) \, (f(\cdot - \boldsymbol{y}) - f_n(\cdot - \boldsymbol{y})) \, \mathrm{d}^3 y \right| \right\| \\ &\quad \leq \left(\frac{\delta_{ij}}{3} + \frac{A}{4\pi} \right) \|f - f_n\| \xrightarrow{n\to\infty} 0. \end{aligned} \tag{3.3.28}$$

This proves the statement of the theorem. □

Remark 3.9. We continue with Remark 3.5 and look at T_{ij} in the context of Fourier analysis once more.

a) The Kronecker delta in line (3.3.15) is not surprising when one considers integral kernels associated to even more general multipliers $m \in C^\infty(\mathbb{R}^3 \setminus \{0\})$. In order to see this, we cite Theorem 4.13 from [Duo01]. Let $m \in C^\infty(\mathbb{R}^3 \setminus \{0\})$ be a homogeneous function of degree 0, and let T_m be the operator defined by $(\mathcal{F}T_m f)(\boldsymbol{p}) = m(\boldsymbol{p})\hat{f}(\boldsymbol{p})$ for all $f \in \mathcal{S}(\mathbb{R}^3)$ and almost all $\boldsymbol{p} \in \mathbb{R}^3$. Then, there exist $a \in \mathbb{C}$ and $\Omega \in C^\infty(S^2)$ with zero average (i.e. its surface integral over S^2 is zero) such that for any $f \in \mathcal{S}(\mathbb{R}^3)$ and almost all $\boldsymbol{x} \in \mathbb{R}^3$,

$$(T_m f)(\boldsymbol{x}) = a f(\boldsymbol{x}) + \lim_{\varepsilon\to 0} \int_{|\boldsymbol{y}|>\varepsilon} \frac{\Omega(\boldsymbol{y}/|\boldsymbol{y}|)}{|\boldsymbol{y}|^3} f(\boldsymbol{x}-\boldsymbol{y}) \, \mathrm{d}^3 y. \tag{3.3.29}$$

This theorem applies to T_{ij} and explains the occurrence of the Kronecker delta.

b) Taking an argument form [SW71], we want to point at one mechanism that shows why the zero surface integral of the singular integral kernel $K(\boldsymbol{y})$ is such an important assumption when checking existence of the pointwise limit

$$\lim_{\varepsilon\to 0} \int_{|\boldsymbol{y}|>\varepsilon} K(\boldsymbol{y}) f(\boldsymbol{x}-\boldsymbol{y}) \, \mathrm{d}^3 y \tag{3.3.30}$$

where $f \in \mathcal{S}(\mathbb{R}^3)$. To that end, we look at integral kernels of the form

$$K(\boldsymbol{y}) = \frac{\Omega(\boldsymbol{y}/|\boldsymbol{y}|)}{|\boldsymbol{y}|^3} \tag{3.3.31}$$

where $\Omega \in C^\infty(S^2)$, and for which the assumption of zero surface average, i.e.,

$$\int_{S^2} K(\boldsymbol{y})\, \mathrm{d}\sigma(\boldsymbol{y}) = 0 \tag{3.3.32}$$

holds. We can without loss of generality restrict the range of integration to $\varepsilon < |\boldsymbol{y}| < 1$ and obtain

$$\int_{\varepsilon<|\boldsymbol{y}|<1} K(\boldsymbol{y}) f(\boldsymbol{x}-\boldsymbol{y})\, \mathrm{d}^3 y = \int_{\varepsilon<|\boldsymbol{y}|<1} K(\boldsymbol{y}) \left(f(\boldsymbol{x}-\boldsymbol{y}) - f(\boldsymbol{x}) \right) \mathrm{d}^3 y. \tag{3.3.33}$$

But, one also has

$$|f(\boldsymbol{x}-\boldsymbol{y}) - f(\boldsymbol{x})| \leq |\boldsymbol{y}| \sup_{|\boldsymbol{z}|\leq 1} |(\nabla f)(\boldsymbol{z})|, \tag{3.3.34}$$

and thus, we finally obtain

$$\begin{aligned} \left| \int_{\varepsilon<|\boldsymbol{y}|<1} K(\boldsymbol{y})\; f(\boldsymbol{x}-\boldsymbol{y})\, \mathrm{d}^3 y \right| &= \left| \int_{\varepsilon<|\boldsymbol{y}|<1} K(\boldsymbol{y}) \left(f(\boldsymbol{x}-\boldsymbol{y}) - f(\boldsymbol{x}) \right) \mathrm{d}^3 y \right| \\ &\leq \sup_{|\boldsymbol{z}|\leq 1} |(\nabla f)(\boldsymbol{z})| \int_{|\boldsymbol{y}|\leq 1} \frac{\Omega(\boldsymbol{y}/|\boldsymbol{y}|)}{|\boldsymbol{y}|^2}\, \mathrm{d}^3 y < \infty \end{aligned} \tag{3.3.35}$$

uniformly in ε. Hence, the limit (3.3.30) exists. ■

3.4. A useful characterization of $\mathcal{H}_+^{\mathrm{rel}}$ and $\mathcal{H}_-^{\mathrm{rel}}$

We turn now to a useful characterization of elements in $\mathcal{H}_+^{\mathrm{rel}}$ and $\mathcal{H}_-^{\mathrm{rel}}$. This will help us in Section 4.3 on infinite energy states. To that end, we define the bounded operator $\mathcal{K}\colon \mathcal{H}^{\mathrm{rel}} \to \mathcal{H}^{\mathrm{rel}}$ by multiplication with the 16×16-matrix K (empty slots are filled with zeros)

$$
\mathrm{K} = \left(\begin{array}{c|c|c|c|c|c|c|c}
\begin{smallmatrix}1&0\\0&1\end{smallmatrix} & & & & & & & \\ \hline
 & & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} & & & & & \\ \hline
 & & & & & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} & & \\ \hline
 & & & & & & & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} \\ \hline
 & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} & & & & & & \\ \hline
 & & & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} & & & & \\ \hline
 & & & & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} & & & \\ \hline
 & & & & & & \begin{smallmatrix}1&0\\0&1\end{smallmatrix} &
\end{array}\right). \tag{3.4.1}
$$

As K is orthogonal with $\det \mathrm{K} = 1$, we know that $\mathcal{K}$ is unitary. We conjugate $P_\pm(\boldsymbol{p})$ with K and obtain for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$
\mathrm{K}\, P_\pm(\boldsymbol{p})\, \mathrm{K}^\dagger = \frac{1}{2}\left(\begin{array}{c|c}
\begin{matrix}\mathbf{1}_4 & \pm\kappa(\boldsymbol{p}) \\ \pm\kappa(\boldsymbol{p}) & \mathbf{1}_4\end{matrix} & \mathbf{0}_8 \\ \hline
\mathbf{0}_8 & \begin{matrix}\mathbf{1}_4 & \pm\kappa(\boldsymbol{p}) \\ \pm\kappa(\boldsymbol{p}) & \mathbf{1}_4\end{matrix}
\end{array}\right) =: \tilde{P}_\pm(\boldsymbol{p}) \tag{3.4.2}
$$

where the 4×4-matrix $\kappa(\boldsymbol{p})$ is for almost all $\boldsymbol{p} \in \mathbb{R}^3$ given by

$$
\kappa(\boldsymbol{p}) = -\frac{\boldsymbol{\sigma} \cdot \boldsymbol{p} \otimes \boldsymbol{\sigma} \cdot \boldsymbol{p}}{p^2} \tag{3.4.3}
$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the usual Pauli matrices from line (2.1.5). Following the definition of τ in Definition 3.2, we define κ for all $f \in \mathbb{C}^4 \otimes L^2(\mathbb{R}^3, \mathrm{d}^3 r)$ and almost all $\boldsymbol{r} \in \mathbb{R}^3$ by

$$
(\kappa f)(\boldsymbol{r}) := L^2\text{-}\lim_{M\to\infty} \int_{|\boldsymbol{p}|\le M} e^{2\pi i \boldsymbol{r}\cdot\boldsymbol{p}}\, \kappa(\boldsymbol{p}) \hat{f}(\boldsymbol{p})\, \mathrm{d}^3 p. \tag{3.4.4}
$$

We now view $\mathcal{H}^{\mathrm{rel}}$ as $\mathbb{C}^4 \otimes L^2(\mathbb{R}^3, \mathrm{d}^3 r; \mathbb{C}^4)$. $\tilde{P}_\pm$ acts on any $f = (f_1, f_2, f_3, f_4)^\top \in \mathbb{C}^4 \otimes L^2(\mathbb{R}^3, \mathrm{d}^3 r; \mathbb{C}^4)$, where $f_k \in L^2(\mathbb{R}^3, \mathrm{d}^3 r; \mathbb{C}^4)$ for $k = 1, 2, 3, 4$, as

$$
\tilde{P}_\pm f = \frac{1}{2}\begin{pmatrix} f_1 \pm \kappa f_2 \\ f_2 \pm \kappa f_1 \\ f_3 \pm \kappa f_4 \\ f_4 \pm \kappa f_3 \end{pmatrix}. \tag{3.4.5}
$$

This allows for the following characterization of $f \in \mathcal{H}_{\pm}^{\mathrm{rel}}$, namely

Theorem 3.10. *We have* $f \in \mathcal{H}_{\pm}^{\mathrm{rel}}$ *if, and only if, there exist* $f_k \in L^2(\mathbb{R}^3, \mathrm{d}^3r; \mathbb{C}^4)$, $k = 1, 2$, *such that*

$$\mathcal{K}f = \begin{pmatrix} f_1 \\ \pm\kappa f_1 \\ f_2 \\ \pm\kappa f_2 \end{pmatrix}. \tag{3.4.6}$$

Proof. We first assume $f \in \mathcal{K}\mathcal{H}_{\pm}^{\mathrm{rel}}$ and $f = (f_1, f_2, f_3, f_4)^\top$. This implies $\tilde{P}_{\pm} f = f$. With the help of (3.4.5), we compute

$$f = \frac{1}{2}\begin{pmatrix} f_1 \pm \kappa f_2 \\ f_2 \pm \kappa f_1 \\ f_3 \pm \kappa f_4 \\ f_4 \pm \kappa f_3 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} f_1 \pm \kappa f_2 \\ \pm\kappa(f_1 \pm \kappa f_2) \\ f_3 \pm \kappa f_4 \\ \pm\kappa(f_3 \pm \kappa f_4) \end{pmatrix}, \tag{3.4.7}$$

where we used $\kappa^2 = \mathrm{id}$ which follows from $\kappa(\boldsymbol{p})^2 = \mathbf{1}_4$. Setting $\tilde{f}_1 \equiv f_1 \pm \kappa f_2$ and $\tilde{f}_2 \equiv f_3 \pm \kappa f_4$, we have

$$f = \begin{pmatrix} \tilde{f}_1 \\ \pm\kappa \tilde{f}_1 \\ \tilde{f}_2 \\ \pm\kappa \tilde{f}_2 \end{pmatrix}. \tag{3.4.8}$$

For the reverse implication, we assume f to have the form

$$f = \begin{pmatrix} f_1 \\ \pm\kappa f_1 \\ f_2 \\ \pm\kappa f_2 \end{pmatrix}. \tag{3.4.9}$$

A straightforward calculation then shows $\tilde{P}_{\pm} f = f$ which proves the theorem. $\square$

We use the remainder of this section to give an example of a $\boldsymbol{p}$-independent eigenvector of $\kappa(\boldsymbol{p})$ and thus ultimately of $P_{\pm}$. We define η by

$$\eta = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} \tag{3.4.10}$$

and find for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$\kappa(\boldsymbol{p})\,\eta = \eta. \tag{3.4.11}$$

With its help, we further define

$$\tilde{\omega}_{+,1} = \frac{1}{2}\begin{pmatrix} \eta \\ \eta \\ \eta \\ \eta \end{pmatrix} \qquad \tilde{\omega}_{+,2} = \frac{1}{2}\begin{pmatrix} -\eta \\ -\eta \\ \eta \\ \eta \end{pmatrix} \tag{3.4.12}$$

$$\tilde{\omega}_{-,1} = \frac{1}{2}\begin{pmatrix} \eta \\ -\eta \\ \eta \\ -\eta \end{pmatrix} \qquad \tilde{\omega}_{-,2} = \frac{1}{2}\begin{pmatrix} \eta \\ -\eta \\ -\eta \\ \eta \end{pmatrix} \tag{3.4.13}$$

and find for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$\tilde{P}_{\pm}(\boldsymbol{p})\,\tilde{\omega}_{\pm,k} = \tilde{\omega}_{\pm,k} \quad \text{for} \quad k = 1, 2. \tag{3.4.14}$$

Thus, upon setting $\omega_{\pm,k} = \mathrm{K}^{\dagger}\tilde{\omega}_{\pm,k}$ for $k = 1, 2$, we obtain

$$P_{\pm}\,\omega_{\pm,k} \cdot \phi = \omega_{\pm,k} \cdot \phi \quad \text{for} \quad k = 1, 2 \tag{3.4.15}$$

for any $\phi \in L^2(\mathbb{R}^3)$.

4. The operator closure of $H_{2\mathrm{BD}}$ with bounded potentials

4.1. The domain of the closure

From one perspective, H_0 is a differential operator of first order. One could thus expect that the domain of its closure $\mathcal{D}(\overline{H}_0)$ is tied to some kind of H^1-regularity. In this section, however, we will see that this is not true. In the following Theorem 4.1, we consider the closure of H_0—as well as the closure of related operators for later reference—before we turn to the closure of $H_{2\mathrm{BD}}$ with bounded potentials in Theorem 4.2. Of course, bounded potentials do not alter the domain, and hence, $\mathcal{D}(\overline{H}_0) = \mathcal{D}(\overline{H}_{2\mathrm{BD}})$. Therefore, all arguments that work for $\overline{H}_0$ also apply to $\overline{H}_{2\mathrm{BD}}$. We also remark on unbounded potentials.

Theorem 4.1 (Claim a) of Theorem 1). *The following holds:*

a) $T = \hat{\boldsymbol{P}} \cdot \mathrm{M}^+ \otimes \mathrm{id} + \mathrm{id} \otimes \mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ *with domain* $\mathcal{D}(T) = \{f \in U\mathcal{H}_2 |\ Tf \in U\mathcal{H}_2\}$ *is self-adjoint.*

b) $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ *with domain* $\mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}) = \{f \in \mathcal{H}^{\mathrm{rel}} |\ \mathbf{M}^- \cdot \hat{\boldsymbol{p}} f \in \mathcal{H}^{\mathrm{rel}}\}$ *is self-adjoint.*

c) $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ *is essentially self-adjoint on* $\mathbb{C}^{16} \otimes H^2(\mathbb{R}^3)$.

d) $\hat{\boldsymbol{P}} \cdot \mathrm{M}^+$ *with domain* $\mathcal{D}(\hat{\boldsymbol{P}} \cdot \mathrm{M}^+) = \{f \in \mathcal{H}^{\mathrm{com}} |\ \hat{\boldsymbol{P}} \cdot \mathrm{M}^+ f \in \mathcal{H}^{\mathrm{com}}\}$ *is self-adjoint.*

e) H_0 *is essentially self-adjoint on* $\mathcal{D}_0$ *and*

$$\mathcal{D}(\overline{H}_0) = \left\{f \in \mathcal{H}_2 \,\middle|\, \overline{H}_0 f \in \mathcal{H}_2\right\} \tag{4.1.1}$$

Proof. Since self-adjointness of T, $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$, and $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$ is proven along the same lines, we only show it for T. Parts b) and d) and then follow. Of course, the proof follows the standard proof of self-adjointness for operators of multiplication with real-valued functions.

a) Since the Fourier transform is unitary, it suffices to prove self-adjointness in Fourier space. We therefore define the $\mathbb{C}^{16} \times \mathbb{C}^{16}$-matrix $\mathrm{T}(\boldsymbol{P}, \boldsymbol{p})$ for all $\boldsymbol{P}, \boldsymbol{p} \in \mathbb{R}^3$ by

$$\mathrm{T}(\boldsymbol{P}, \boldsymbol{p}) := \boldsymbol{P} \cdot \mathrm{M}^+ + \mathbf{M}^- \cdot \boldsymbol{p}. \tag{4.1.2}$$

Since $\mathrm{T}(\boldsymbol{P}, \boldsymbol{p})$ is Hermitian for all $\boldsymbol{P}, \boldsymbol{p} \in \mathbb{R}^3$, T is symmetric on $\mathcal{D}(T)$. Hence, it suffices to show $\mathcal{D}(T^*) \subseteq \mathcal{D}(T)$.

Let $f \in \mathcal{D}(T^*)$. Then, we obtain for all $g \in \mathcal{D}(T)$

$$\begin{aligned}\langle T^* f, g\rangle = \langle f, Tg\rangle &= \int_{\mathbb{R}^3\times\mathbb{R}^3} f(\boldsymbol{P},\boldsymbol{p})^\dagger\, \mathrm{T}(\boldsymbol{P},\boldsymbol{p}) g(\boldsymbol{P},\boldsymbol{p})\, \mathrm{d}^3p\, \mathrm{d}^3P \\ &= \int_{\mathbb{R}^3\times\mathbb{R}^3} [\mathrm{T}(\boldsymbol{P},\boldsymbol{p}) f(\boldsymbol{P},\boldsymbol{p})]^\dagger\, g(\boldsymbol{P},\boldsymbol{p})\, \mathrm{d}^3p\, \mathrm{d}^3P \end{aligned} \tag{4.1.3}$$

Since $(C_c^\infty(\mathbb{R}^3\times\mathbb{R}^3))^{\otimes 16}$ is contained in $\mathcal{D}(T)$, this holds in particular for all $g \in (C_c^\infty(\mathbb{R}^3\times\mathbb{R}^3))^{\otimes 16}$. This yields for almost all $\boldsymbol{P},\boldsymbol{p} \in \mathbb{R}^3$

$$\mathrm{T}(\boldsymbol{P},\boldsymbol{p}) f(\boldsymbol{P},\boldsymbol{p}) = (T^* f)\,(\boldsymbol{P},\boldsymbol{p}), \tag{4.1.4}$$

and thus, since $f \in \mathcal{D}(T^*)$, we get $Tf \in U\mathcal{H}_2$. Therefore, we can conclude $f \in \mathcal{D}(T)$.

c) For any $f \in \mathcal{H}^{\mathrm{rel}}$, we define the sequence $(f_n)_{n\in\mathbb{N}}$ as $f_n := \frac{n}{\hat{p}^2+n} f$. Then, $f_n \in \mathbb{C}^{16} \otimes H^2(\mathbb{R}^3)$ for every fixed $n \in \mathbb{N}$ since

$$\int_{\mathbb{R}^3} \left| (1+p^2)\frac{n}{p^2+n}\hat{f}(\boldsymbol{p})\right|^2 \mathrm{d}^3p \leq (1+n)\,\|f\|^2 < \infty. \tag{4.1.5}$$

Furthermore, $\|f_n - f\| \xrightarrow{n\to\infty} 0$ by dominated convergence. For $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$, we obtain similarly

$$\left\|\mathbf{M}^- \cdot \hat{\boldsymbol{p}}\,(f - f_n)\right\|^2 = \int_{\mathbb{R}^3} \left| \left(1 - \frac{n}{p^2+n}\right) \mathbf{M}^- \cdot \boldsymbol{p}\hat{f}(\boldsymbol{p})\right|^2 \mathrm{d}^3p \xrightarrow{n\to\infty} 0 \tag{4.1.6}$$

by dominated convergence. Hence, $\mathbb{C}^{16} \otimes H^2(\mathbb{R}^3,\, \mathrm{d}^3r)$ is a core for $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$.

e) That H_0 is essentially self-adjoint on $\mathcal{D}_0$, is well-known (see, e.g., [RS80, Corollary of Thm. VIII.33, pp. 300]). For the domain, we note that in the case $m_1 = 0 = m_2$ we have $H_0 f = U^{-1}TUf$ for all $f \in \mathcal{D}_0$. Unitarity of the coordinate transform U and closedness of T now imply (4.1.1). As the mass term $\beta m_1 \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta m_2$ is bounded and symmetric, this result carries over to the massive case $m_1, m_2 > 0$. □

Theorem 4.2. *Let V be a bounded and symmetric operator in $\mathcal{H}_2$. Then, $H_{\mathrm{2BD}} = H_0 + V$ is essentially self-adjoint on $\mathcal{D}_0$ and*

$$\mathcal{D}(\overline{H}_{\mathrm{2BD}}) = \mathcal{D}(\overline{H}_0) = \left\{ f \in \mathcal{H}_2 \,\middle|\, \overline{H}_0 f \in \mathcal{H}_2 \right\}. \tag{4.1.7}$$

Proof. The statement follows from boundedness of V and (4.1.1) by a standard Kato-Rellich perturbation argument. □

Of course, these two theorems come as no surprise. After all, H_0, T, $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$, and $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$ are each unitarily equivalent to multiplication with a Hermitian matrix, and the given domains are the natural domains of multiplication operators. However, H^1-regularity is not the distinguishing characteristic of these domains but escapes in some sense. Let us first sketch what happens before we bring the statement „H^1-regularity escapes in some sense“ into a mathematically rigorous form in Lemma 4.3.

To that end, we introduce an abbreviation for H_0

$$H_0 = (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \beta m)\otimes \mathrm{id} + \mathrm{id}\otimes(-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}} + \beta m) = D_1\otimes\mathrm{id} + \mathrm{id}\otimes D_2 \quad (4.1.8)$$

and notice that it was defined as operator sum on $\mathcal{D}_0 = H^1(\mathbb{R}^3,\,\mathrm{d}^3x)^{\otimes 4}\otimes H^1(\mathbb{R}^3,\,\mathrm{d}^3y)^{\otimes 4}$, i.e., each summand of H_0 is well-defined and can be considered separately. In $\mathcal{D}(\overline{H}_0)$ however, there are elements for which this is no longer true. Thus, the operator $\overline{H}_0$ might not be split into an operator sum; the notation $\overline{D_1\otimes\mathrm{id}+\mathrm{id}\otimes D_2}$ emphasizes this. More precisely, there are elements $f\in\mathcal{D}(\overline{H}_0)$ for which, e.g., $\|(D_1\otimes\mathrm{id})f\|$ diverges. Now, in order to have $f\in\mathcal{D}(\overline{H}_0)$, i.e., $\|\overline{H}_0 f\|<\infty$, also $\|(\mathrm{id}\otimes D_2)f\|$ has to diverge in such a way that the diverging contributions of $\|\overline{H}_0 f\|$ cancel.

The key ingredient in order to understand these cancellations is the coordinate transform U to relative and center-of-mass coordinates. In the massless case, it transforms $\overline{H}_0$ to $T = \hat{\boldsymbol{P}}\cdot\mathbf{M}^+\otimes\mathrm{id} + \mathrm{id}\otimes\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$, and does that in such a way that these elements that require cancellations correspond to those elements that lie in the nullspaces of $\hat{\boldsymbol{P}}\cdot\mathbf{M}^+$ or $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$, respectively. Now, each summand of T can again be evaluated against any element of $U\mathcal{D}(\overline{H}_0)$ as possibly infinite terms are mapped to zero.

This intuition is captured in the following Lemma 4.3. Part a) of it states that H^1-regulartiy is required only in $\mathcal{H}_+^{\mathrm{rel}}$, i.e., the orthogonal complement of the nullspace of $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$. Part b) shows that in $\mathcal{H}_+^{\mathrm{rel}}$ the domain of self-adjointness of $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$ is tied to H^1-regularity. We only state the lemma for $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$ in $\mathcal{H}^{\mathrm{rel}}$ and note that the corresponding statements for $\hat{\boldsymbol{P}}\cdot\mathbf{M}^+$ in $\mathcal{H}^{\mathrm{com}}$ also hold.

Lemma 4.3.

a) We have $f\in\mathcal{D}(\mathbf{M}^-\cdot\hat{\boldsymbol{p}})$ if, and only if,

$$\|-i\nabla_{\boldsymbol{r}}P_+f\| = \frac{1}{2}\left\|\mathbf{M}^-\cdot\hat{\boldsymbol{p}}\,f\right\| < \infty. \quad (4.1.9)$$

b) The restriction of $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}$ to $\mathcal{H}_+^{\mathrm{rel}}$, denoted by $\mathbf{M}^-\cdot\hat{\boldsymbol{p}}\restriction\mathcal{D}_+$, with domain $P_+\mathcal{D}(\mathbf{M}^-\cdot\hat{\boldsymbol{p}})$ is self-adjoint, and it holds that

$$P_+\mathcal{D}(\mathbf{M}^-\cdot\hat{\boldsymbol{p}}) = \mathcal{D}_+ = \left(\mathbb{C}^{16}\otimes H^1(\mathbb{R}^3,\,\mathrm{d}^3r)\right)\cap\mathcal{H}_+^{\mathrm{rel}}. \quad (4.1.10)$$

Proof. a) We first assume $f\in\mathcal{D}(\mathbf{M}^-\cdot\hat{\boldsymbol{p}})$ and show that relation (4.1.9) follows. A computation shows that for almost all $\boldsymbol{p}\in\mathbb{R}^3$ we have $(\mathbf{M}^-\cdot\boldsymbol{p})^2/4 = p^2P_+(\boldsymbol{p})$, and hence, $(\mathbf{M}^-\cdot\hat{\boldsymbol{p}})^2/4 = \hat{p}^2P_+$ holds on the intersection of their domains. Thus, for all

$g \in \mathbb{C}^{16} \otimes H^2(\mathbb{R}^3,\, \mathrm{d}^3 r)$ we have

$$
\begin{aligned}
\|{-i\nabla_{\boldsymbol{r}} P_+ g}\|^2 &= \langle -i\nabla_{\boldsymbol{r}} P_+ g, -i\nabla_{\boldsymbol{r}} P_+ g \rangle \\
&\overset{(*)}{=} \left\langle P_+ g, \hat{p}^2 P_+ g \right\rangle \\
&= \frac{1}{4} \left\langle P_+ g, \left(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}\right)^2 g \right\rangle \\
&\overset{(**)}{=} \frac{1}{4} \left\langle g, \left(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}\right)^2 g \right\rangle \\
&= \frac{1}{4} \left\|\mathbf{M}^- \cdot \hat{\boldsymbol{p}}\, g\right\|^2, \qquad (4.1.11)
\end{aligned}
$$

where we used in $(*)$ that the boundary terms vanish since $P_+ g \in \mathbb{C}^{16} \otimes H^2(\mathbb{R}^3,\, \mathrm{d}^3 r)$ and in $(**)$ that $P_+ \mathbf{M}^- \cdot \hat{\boldsymbol{p}}\, g = \mathbf{M}^- \cdot \hat{\boldsymbol{p}}\, g$.

Hence, claim a) already holds on $\mathbb{C}^{16} \otimes H^2(\mathbb{R}^3,\, \mathrm{d}^3 r)$, which however is a core for $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ by Theorem 4.1c). This means that for all $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ there exists a sequence $(f_n)_{n\in\mathbb{N}} \subset \mathbb{C}^{16} \otimes H^2(\mathbb{R}^3,\, \mathrm{d}^3 r)$ that converges to f in the graph norm of $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$. By Eq. (4.1.11), $(f_n)_{n\in\mathbb{N}}$ is then also a Cauchy sequence in the graph norm of $-i\nabla_{\boldsymbol{r}} P_+$. Now, the product of operators $-i\nabla_{\boldsymbol{r}} P_+ \colon \mathcal{D}(-i\nabla_{\boldsymbol{r}} P_+) \to \mathcal{H}^{\mathrm{rel}}$ with domain $\mathcal{D}(-i\nabla_{\boldsymbol{r}} P_+) = \{f \in \mathcal{H}^{\mathrm{rel}} |\, P_+ f \in \mathbb{C}^{16} \otimes H^1(\mathbb{R}^3,\, \mathrm{d}^3 r)\}$ is closed, as P_+ is bounded and both P_+ and $-i\nabla_{\boldsymbol{r}}$ are closed. Thus, $(f_n)_{n\in\mathbb{N}}$ converges then also to f with respect to the graph norm of $-i\nabla_{\boldsymbol{r}} P_+$. In conclusion, for all $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ we have

$$
\begin{aligned}
\frac{1}{4} \left\|\mathbf{M}^- \cdot \hat{\boldsymbol{p}} f\right\| &= \frac{1}{4} \lim_{n\to\infty} \left\|\mathbf{M}^- \cdot \hat{\boldsymbol{p}} f_n\right\| \\
&= \lim_{n\to\infty} \|{-i\nabla_{\boldsymbol{r}} P_+ f_n}\| = \|{-i\nabla_{\boldsymbol{r}} P_+ f}\|\,. \qquad (4.1.12)
\end{aligned}
$$

The reverse implication follows from the definition of $\mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$.

b) As the projections $P_\pm$ are tailor-made for $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$, we obtain in the same manner as for H^{rel} in line (2.2.18) the matrix representation

$$
\mathbf{M}^- \cdot \hat{\boldsymbol{p}} = \begin{pmatrix} \mathbf{M}^- \cdot \hat{\boldsymbol{p}} \restriction \mathcal{D}_+ & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}. \qquad (4.1.13)
$$

Now, by [Tre08, Prop. 2.6.3, p. 144], $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ is self-adjoint if, and only if, $\mathbf{M}^- \cdot \hat{\boldsymbol{p}} \restriction \mathcal{D}_+$ and $\mathbf{0}$ (that is, the operators in the upper left and lower right corner) are self-adjoint. Hence, self-adjointness of $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$, guaranteed by Theorem 4.1b), proves self-adjointness of $\mathbf{M}^- \cdot \hat{\boldsymbol{p}} \restriction \mathcal{D}_+$.

It remains to prove Eq. (4.1.10). Suppose $f \in P_+ \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. Then, $f = P_+ g$ for some $g \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. Since $g \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ and $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ and P_+ commute,

$$
\|\mathbf{M}^- \cdot \hat{\boldsymbol{p}} f\| = \|\mathbf{M}^- \cdot \hat{\boldsymbol{p}} P_+ g\| \leq \|\mathbf{M}^- \cdot \hat{\boldsymbol{p}} g\| < \infty \qquad (4.1.14)
$$

and so $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}) \cap \mathcal{H}_+^{\mathrm{rel}}$. By part a),

$$\| -i\nabla_{\boldsymbol{r}} f\| = \| -i\nabla_{\boldsymbol{r}} P_+ f\| = \|\frac{1}{2}\mathbf{M}^- \cdot \hat{\boldsymbol{p}} f\| < \infty \tag{4.1.15}$$

and so $f \in \mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r)$. Therefore, we have $f \in (\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r)) \cap \mathcal{H}_+^{\mathrm{rel}}$. Suppose conversely that $f \in (\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r)) \cap \mathcal{H}_+^{\mathrm{rel}}$. Then, $f = P_+ f$ and $f \in \mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r) \subseteq \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$, which implies $f \in P_+\mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. □

Lemma 4.3 allows for a concise characterization of $\mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ and $\mathcal{D}(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+)$ in the following corollary. Again, we only state it for $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$ but note that the corresponding statement for $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$ also holds.

Corollary. $\mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}}) = \mathcal{D}_+ \oplus \mathcal{H}_-^{\mathrm{rel}}$.

Proof. From Lemma 4.3, we know that in $\mathcal{H}_+^{\mathrm{rel}}$ one needs H^1-regularity, whereas in $\mathcal{H}_-^{\mathrm{rel}}$ L^2-regularity suffices. As the splitting $f = P_+ f + P_- f$ for any $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ is orthogonal, the statement follows. □

Remark 4.4. We can now address the question if the cases of singular V_{ext} or singular V_{int} affect the domain. Singular potentials are unbounded operators and as such only densely defined. E.g., in order to give meaning to $(\mathbf{M}^- \cdot \hat{\boldsymbol{p}} + V_{\mathrm{int}})f$, where $f \in \mathcal{H}_-^{\mathrm{rel}}$, one also needs $f \in \mathcal{D}(V_{\mathrm{int}})$. We give a heuristic argument that this restriction of the L^2-regularity of $f \in \mathcal{H}_-^{\mathrm{rel}}$ does not affect the domain $\mathcal{D}(\overline{H}_0)$ too much. Functions with L^2- but no $H^{1/2}$-regularity are, e.g., for almost all $\boldsymbol{r} \in \mathbb{R}^3$ given by $f(\boldsymbol{r}) = \mathrm{e}^{-|\boldsymbol{r}|}/|\boldsymbol{r}|^{\alpha}$, where $1 < \alpha < 3/2$ (see, e.g., [Ste70]). By considering its translations $f(\cdot - \boldsymbol{a})$ by a fixed $\boldsymbol{a} \in \mathbb{R}^3$, one can always move away from the singularities of V_{int} such that $f(\cdot - \boldsymbol{a})$ lies in the domain of V_{int}. Hence, we can conclude that, although considering singular potentials excludes some elements, translations of these elements are still in $\mathcal{D}(\overline{H}_0)$. How $\mathcal{D}(\overline{H}_0)$ is reduced explicitly, depends on the concrete form of V_{int}. ■

Before we finish this section, we see Lemma 4.3 at work in the following example.

Example 4.5. We saw in Proposition 3.1 that the matrix $\mathbf{M}^- \cdot \boldsymbol{p}$ has a non-trivial nullspace for all $\boldsymbol{p} \in \mathbb{R}^3$. Therefore, we can relax the regularity conditions in, let us say, p_1-direction on an $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ if the $\mathbb{C}^{16}$-part of this f lies in $\mathrm{Ker}(\mathrm{M}_1^-)$. Lemma 4.3a) now states that nevertheless we have $\| -i\nabla_{\boldsymbol{r}} P_+ f\| < \infty$, i.e. $P_+ f \in \mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r)$.

Choose, for concreteness, f such that

$$f(\boldsymbol{p}) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} f_1(p_1) f_2(p_2) f_3(p_3) \tag{4.1.16}$$

where $(1, 0, \cdots, 0, 1)^\top \in \mathrm{Ker}(\mathrm{M}_1^-)$. Now, we expect that f_1 can be freely chosen from all of $L^2(\mathbb{R}, \mathrm{d}p_1)$, whereas f_2 and f_3 need to have H^1-regularity in order to have $f \in \mathcal{D}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$. In order to probe this expectation, we compute $\mathbf{M}^- \cdot \boldsymbol{p} f(\boldsymbol{p})$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ and find

$$\mathbf{M}^- \cdot \boldsymbol{p} f(\boldsymbol{p}) = \left(M_2^- p_2 + M_3^- p_3 \right) f(\boldsymbol{p}) = f_1(p_1) \begin{pmatrix} 0 \\ 0 \\ -p_3 \\ -2ip_2 \\ 0 \\ 0 \\ 0 \\ -p_3 \\ p_3 \\ 0 \\ 0 \\ 0 \\ 2ip_2 \\ p_3 \\ 0 \\ 0 \end{pmatrix} f_2(p_2) f_3(p_3). \tag{4.1.17}$$

One can directly read off that f_2 and f_3 are multiplied by p_2 and p_3, respectively, but no multiplication with p_1 occurs. Thus, we need as expected $f_2 \in H^1(\mathbb{R}, \mathrm{d}p_2)$ and $f_3 \in H^1(\mathbb{R}, \mathrm{d}p_3)$, whereas f_1 can indeed be freely chosen from all of $L^2(\mathbb{R}, \mathrm{d}p_1)$ as it remains unchanged under the action of $\mathbf{M}^- \cdot \hat{\boldsymbol{p}}$.

The situation changes when we consider $P_+(\boldsymbol{p})f(\boldsymbol{p})$, which reads for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$P_+(\boldsymbol{p})f(\boldsymbol{p}) = \frac{1}{2p^2} \begin{pmatrix} 2p_2^2 + p_3^3 + 2ip_1p_2 \\ (p_1 - ip_2)p_3 \\ 0 \\ 0 \\ (p_1 - ip_2)p_3 \\ -p_3^2 \\ 0 \\ 0 \\ 0 \\ 0 \\ -p_3^2 \\ -(p_1 + ip_2)p_3 \\ 0 \\ 0 \\ -(p_1 + ip_2)p_3 \\ 2p_2^2 + p_3^2 - 2ip_1p_2 \end{pmatrix} f_1(p_1)f_2(p_2)f_3(p_3). \tag{4.1.18}$$

We compute $\mathbf{M}^- \cdot \boldsymbol{p}P_+(\boldsymbol{p})f(\boldsymbol{p})$ and find with Proposition 3.3

$$\mathbf{M}^- \cdot \boldsymbol{p}P_+(\boldsymbol{p})f(\boldsymbol{p}) = \mathbf{M}^- \cdot \boldsymbol{p}f(\boldsymbol{p}). \tag{4.1.19}$$

Therefore, we still need $f_2 \in H^1(\mathbb{R}, \mathrm{d}p_2)$ and $f_3 \in H^1(\mathbb{R}, \mathrm{d}p_3)$ as above in (4.1.17). In contrast to that, however, p_1 occurs as multiplication with p_1/p^2. Therefore, we also have $\hat{p}_1 P_+ f \in \mathcal{H}_+^{\mathrm{rel}}$ regardless of how f_1 behaves. Hence, we can conclude that projecting f to $\mathcal{H}_+^{\mathrm{rel}}$ has generated more regularity in p_1-direction, and so $P_+ f \in \mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3p)$.

For sake of completeness, we also compute $P_-(\boldsymbol{p})f(\boldsymbol{p})$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ and obtain

$$P_-(\boldsymbol{p})f(\boldsymbol{p}) = \frac{1}{2p^2} \begin{pmatrix} 2p_1^2 + p_3^3 - 2ip_1p_2 \\ -(p_1 - ip_2)p_3 \\ 0 \\ 0 \\ -(p_1 - ip_2)p_3 \\ p_3^2 \\ 0 \\ 0 \\ 0 \\ 0 \\ p_3^2 \\ (p_1 + ip_2)p_3 \\ 0 \\ 0 \\ (p_1 + ip_2)p_3 \\ 2p_1^2 + p_3^3 + 2ip_1p_2 \end{pmatrix} f_1(p_1)f_2(p_2)f_3(p_3). \tag{4.1.20}$$

We see that p_1 occurs as multiplication with p_1^2/p^2 and no extra regularity in p_1-direction is gained. ■

4.2. Remark on first order differential operators and their hidden nullspace structure

This section is a little detour, in which we investigate sums of two first order differential operators which are different from and even more general than H_0. It turns out that their domain of closedness again contains elements that require cancellations of the summands. Thus, the nullspace structure we encountered when studying H_0 is generic for operators that describe two particles and that are first order differential operators. The concluding remark of this section treats the semi-bounded case.

We take as underlying Hilbert space the Hilbert space tensor product

$$\mathcal{H} = L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes L^2(\mathbb{R}^3, \mathrm{d}^3y). \tag{4.2.1}$$

and define the coordinate transform W by

$$W\colon L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes L^2(\mathbb{R}^3, \mathrm{d}^3y) \to L^2(\mathbb{R}^3, \mathrm{d}^3R) \otimes L^2(\mathbb{R}^3, \mathrm{d}^3r) \tag{4.2.2}$$

of the coordinates $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ to coordinates $\boldsymbol{R}, \boldsymbol{r} \in \mathbb{R}^3$ by

$$\boldsymbol{r} := a\boldsymbol{x} + b\boldsymbol{y}\,, \quad \boldsymbol{R} := c\boldsymbol{x} + d\boldsymbol{y} \tag{4.2.3}$$

where $a, b, c, d \in \mathbb{R}$. We set $\boldsymbol{X} = (\boldsymbol{x}, \boldsymbol{y})^\top$ and $\boldsymbol{Y} = (\boldsymbol{r}, \boldsymbol{R})^\top$ and obtain the transformation matrix $\mathrm{W}\colon \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3$ as

$$\mathrm{W}\boldsymbol{X} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{r} \\ \boldsymbol{R} \end{pmatrix} = \boldsymbol{Y}. \tag{4.2.4}$$

We demand $\det \mathrm{W} \neq 0$, such that W be invertible and given by $(Wf)(\boldsymbol{Y}) = f(\boldsymbol{X}) = f(\mathrm{W}^{-1}\boldsymbol{Y})$.

We look at the operator sum

$$S_1 := -i\nabla_{\boldsymbol{x}} - i\nabla_{\boldsymbol{y}} = -i\nabla_{\boldsymbol{x}} \otimes \mathrm{id} - \mathrm{id} \otimes i\nabla_{\boldsymbol{y}}. \tag{4.2.5}$$

with domain

$$\mathcal{D}(S_1) = H^1(\mathbb{R}^3 \times \mathbb{R}^3, \mathrm{d}^3x\, \mathrm{d}^3y). \tag{4.2.6}$$

Clearly, each summand of S_1 is well-defined for all elements of $\mathcal{D}(S_1)$, and thus, S_1 is a well-defined operator sum on $\mathcal{D}(S_1)$. We set the entries of the matrix W to $a = -b = 1$ and $c = d = 1/2$ (such that W coincides with the coordinate transform U to relative and center-of-mass coordinates). Then, W is unitary, and S_1 is closed if, and only if,

WS_1W^{-1} is closed. We find

$$WS_1W^{-1} = -i\nabla_{\boldsymbol{R}} \otimes \mathrm{id} - \mathrm{id} \otimes (1-1)i\nabla_{\boldsymbol{r}} = -i\nabla_{\boldsymbol{R}} \tag{4.2.7}$$

as well as

$$W\mathcal{D}(S_1) = WH^1(\mathbb{R}^3 \times \mathbb{R}^3,\, \mathrm{d}^3x\,\mathrm{d}^3y) = H^1(\mathbb{R}^3 \times \mathbb{R}^3,\, \mathrm{d}^3R\,\mathrm{d}^3r). \tag{4.2.8}$$

The latter follows from orthogonality of W.

The need for cancellations when computing the closure comes about as follows. By standard arguments, we have that $-i\nabla_{\boldsymbol{R}}$ is closed on the domain

$$\mathcal{D}' = \left\{ f \in \mathcal{H} \,\middle|\, \nabla_{\boldsymbol{R}} f(\cdot, \boldsymbol{r}) \in \mathcal{H} \text{ for almost all } \boldsymbol{r} \in \mathbb{R}^3 \right\} \tag{4.2.9}$$

as $-i\nabla_{\boldsymbol{R}}$ is self-adjoint on $\mathcal{D}'$. However, $\mathcal{D}(S_1) = H^1(\mathbb{R}^3 \times \mathbb{R}^3,\, \mathrm{d}^3x\,\mathrm{d}^3y)$ is the largest set on which S_1 can be defined as operator sum. Therefore, it suffices to provide an $f \in \mathcal{D}' \setminus W\mathcal{D}(S_1)$ in order to prove that S_1 is not closed on $\mathcal{D}(S_1)$ and that cancellations occur. We define $f \in \mathcal{D}'$ by

$$f(\boldsymbol{R}, \boldsymbol{r}) = \frac{\mathrm{e}^{-|\boldsymbol{R}|^2}\,\mathrm{e}^{-|\boldsymbol{r}|^2}}{|\boldsymbol{r}|} \tag{4.2.10}$$

for almost all $\boldsymbol{R}, \boldsymbol{r} \in \mathbb{R}^3$. We first note that $\|\nabla_{\boldsymbol{R}} f\|$ is finite, and hence, we indeed have $f \in \mathcal{D}'$. Moreover, we note that $W\nabla_{\boldsymbol{x}}W^{-1} = \nabla_{\boldsymbol{R}}/2 + \nabla_{\boldsymbol{r}}$, and estimate

$$\left\|\nabla_{\boldsymbol{x}} W^{-1} f\right\| = \left\| \left(\frac{1}{2}\nabla_{\boldsymbol{R}} + \nabla_{\boldsymbol{r}} \right) f \right\| \geq \left| \frac{1}{2} \|\nabla_{\boldsymbol{R}} f\| - \|\nabla_{\boldsymbol{r}} f\| \right|. \tag{4.2.11}$$

As noted above, $\|\nabla_{\boldsymbol{R}} f\|$ is finite. However, $\|\nabla_{\boldsymbol{r}} f\|$ diverges since

$$\frac{\partial}{\partial r_k} \frac{\mathrm{e}^{-|\boldsymbol{r}|^2}}{|\boldsymbol{r}|} = \frac{-r_k}{|\boldsymbol{r}|}\,\mathrm{e}^{-|\boldsymbol{r}|^2} \left(\frac{1}{|\boldsymbol{r}|^2} + 1 \right) \tag{4.2.12}$$

and

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \left| \frac{\mathrm{e}^{-|\boldsymbol{R}|^2}\,\mathrm{e}^{-|\boldsymbol{r}|^2}}{|\boldsymbol{r}|^2} \right|^2 \mathrm{d}^3R\,\mathrm{d}^3r = \int_{\mathbb{R}^3} \mathrm{e}^{-2|\boldsymbol{R}|^2}\,\mathrm{d}^3R \int_{\mathbb{R}^3} \frac{\mathrm{e}^{-2|\boldsymbol{r}|^2}}{|\boldsymbol{r}|^4}\,\mathrm{d}^3r, \tag{4.2.13}$$

where the singularity $|\boldsymbol{r}|^{-4}$ is too strong for the d^3r-integral. Therefore, $\|\nabla_{\boldsymbol{x}} W^{-1} f\|$ diverges, and we find $f \notin W\mathcal{D}(S_1)$.

In conclusion, we encounter a loss of H^1-regularity in $\boldsymbol{r}$-direction when the operator closure $\overline{S}_1$ is computed. Thus, we have found another example of an operator whose closure depends on cancellation as in the previous section.

There is, however, a difference compared to H_0. For S_1 we chose real coefficients, whereas the coefficients of H_0 are Hermitian 16×16-matrices. In both cases, the coordinate transforms W and U, respectively, shed light on a nullspace structure that led to a certain loss of regularity in the respective domains of closedness. We see in line (4.2.7) that in the case of S_1, the coefficient of $-i\nabla_{\boldsymbol{r}}$ is $1-1=0$, i.e., the number of independent variables is reduced from six to three, and only the center-of-mass coordinate $\boldsymbol{R} \in \mathbb{R}^3$ remains. Such a reduction is not observed for H_0. In that sense, the hidden nullspace structure of S_1 is more severe.

In order to study the nullspace structure in an even more general setting, we consider another first order differential operator sum, namely

$$S_2 = -i(A_1 \otimes \mathbf{1}_n)\nabla_{\boldsymbol{x}} - i(\mathbf{1}_n \otimes A_2)\nabla_{\boldsymbol{y}} \tag{4.2.14}$$

where the coefficients A_1, A_2 are arbitrary, non-zero Hermitian $\mathbb{C}^{n\times n}$-matrices. As domain, we take

$$\mathcal{D}(S_2) = H^1(\mathbb{R}^3 \times \mathbb{R}^3,\, \mathrm{d}^3x\, \mathrm{d}^3y) \otimes \mathbb{C}^{n^2}. \tag{4.2.15}$$

A nullspace structure emerges if the entries $a, b, c, d \in \mathbb{R}$ of W are chosen carefully. In order to prove this, we compute

$$WS_2W^{-1} = -i(cA_1 \otimes \mathbf{1}_n + \mathbf{1}_n \otimes dA_2)\nabla_{\boldsymbol{R}} - i(aA_1 \otimes \mathbf{1}_n + \mathbf{1}_n \otimes bA_2)\nabla_{\boldsymbol{r}}. \tag{4.2.16}$$

Now, the matrices A_1 and A_2 are Hermitian and can thus be diagonalized. We denote the corresponding transformation matrices by u_1 and u_2, respectively. We use this in order to obtain

$$\mathrm{u}_1 \otimes \mathrm{u}_2\,(aA_1 \otimes \mathbf{1}_n + \mathbf{1}_n \otimes bA_2)\,\mathrm{u}_1^{-1} \otimes \mathrm{u}_2^{-1} = \begin{pmatrix} a\lambda_1 + b\mu_1 & & \\ & \ddots & \\ & & a\lambda_{n^2} + b\mu_{n^2} \end{pmatrix}, \tag{4.2.17}$$

where λ_k and μ_k, $k = 1, 2, \ldots, n^2$, denote the eigenvalues of $A_1 \otimes \mathbf{1}_n$ and $\mathbf{1}_n \otimes A_2$, respectively. Without loss of generality, we can assume $\mu_1 \neq 0 \neq \lambda_1$. Hence, the choice $a/b = -\mu_1/\lambda_1$ produces 0 as the first eigenvalue of $aA_1 \otimes \mathbf{1}_n + \mathbf{1}_n \otimes bA_2$. This implies that the coefficient matrix of $-i\nabla_{\boldsymbol{r}}$ has a non-trivial nullspace and all the arguments concerning loss of H^1-regularity etc. also apply to S_2.

This leads to the following conclusion. The nullspace structure of H_0 revealed by the coordinate transform U presents a rather unpleasant obstacle when, e.g., probing self-adjointness. However, as this section tries to argue, such a structure is to be expected if the Hamiltonian in question consists of a sum of first order differential operators with matrix coefficients, chosen as above. If the coefficients are real-valued, the number of independent variables might be reduced. This reduction implies that some degrees of freedom in the original Hamiltonian have no effect on the dynamics.

Remark 4.6. Before we proceed, we want to remark on the same situation as before, albeit for bounded below self-adjoint operators. Let $A \geq 0$ be a non-negative self-adjoint operator in the underlying Hilbert space $\mathcal{X}$, and $B \geq 0$ a non-negative self-adjoint operator in the Hilbert space $\mathcal{Y}$. Then, the domain of the closure of $A \otimes \mathrm{id}_{\mathcal{Y}} + \mathrm{id}_{\mathcal{X}} \otimes B$ does not contain elements with the above mentioned cancellations. We sketch the proof. Boundedness below and self-adjointness of A and of B imply that A is unitarily equivalent to multiplication with the non-negative function $a \geq 0$ and that B is unitarily equivalent to multiplication with the non-negative function $b \geq 0$. Hence, $A \otimes \mathrm{id}_{\mathcal{Y}} + \mathrm{id}_{\mathcal{X}} \otimes B$ is unitarily equivalent to multiplication with the function $a + b$. As a and b are non-negative, we obtain for suitable ϕ

$$\|(a+b)\phi\|^2_{\mathcal{X}\otimes\mathcal{Y}} = \|a\,\phi\|^2_{\mathcal{X}\otimes\mathcal{Y}} + \|b\,\phi\|^2_{\mathcal{X}\otimes\mathcal{Y}} + 2 \cdot \|a\,b\,\phi\|^2_{\mathcal{X}\otimes\mathcal{Y}} \,. \tag{4.2.18}$$

This shows that all ϕ which render the left-hand side of (4.2.18) finite also render the right-hand side finite, and thus, lie in the domain of $A \otimes \mathrm{id}_{\mathcal{Y}}$ and $\mathrm{id}_{\mathcal{X}} \otimes B$ at the same time. Therefore, no extra cancellation elements are added to the domain when taking the closure. ■

4.3. States with infinite single particle kinetic energy

In one-body problems, finite kinetic energy is usually associated with some kind of H^k-regularity: In the non-relativistic case with H^1-regularity, whereas in the relativistic case with $H^{1/2}$-regularity. In this section, we transfer this to the two-body case and explore what the loss of H^1- as well as $H^{1/2}$-regularity in the domain of H_0 means in view of states having finite or infinite single particle kinetic energy (finite or infinite SPKE). We do that by explicitly constructing various examples. We first consider examples of states with no H^k-regularity in $\boldsymbol{x}$- or $\boldsymbol{y}$-direction (Example 4.9), but finite single particle kinetic energy (Example 4.10). Next, we construct a state for which both single particle kinetic energies diverge (Example 4.11) and observe how these diverging contributions exactly cancel (Example 4.12). While this section simply gives examples of states with infinite single particle kinetic energy, further aspects of their physical relevance are discussed in the subsequent sections 4.4 and 4.5 as well as in the outlook in Section 7.2.

In order to make the association of H^k-regularity with kinetic energy precise, we first define single particle kinetic energy as well as total kinetic energy. To that end, we recall the notation of H_0 from line (4.1.8)

$$H_0 = (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{x}} + \beta m) \otimes \mathrm{id} + \mathrm{id} \otimes (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{y}} + \beta m) = D_1 \otimes \mathrm{id} + \mathrm{id} \otimes D_2. \tag{4.3.1}$$

Having in mind the non-relativistic two-particle system, the following definition of single particle kinetic energy might seem natural at first sight. However, as the subsequent Example 4.10 shows, this definition might not be satisfactory.

Definition 4.7. We define

a) the kinetic energy of the k-th particle in the state $\psi \in \mathcal{D}(\overline{H}_0)$ by

$$E_{\mathrm{kin},1}[\psi] = \langle \psi, D_1 \otimes \mathrm{id}\psi \rangle \;, \quad E_{\mathrm{kin},2}[\psi] = \langle \psi, \mathrm{id} \otimes D_2\psi \rangle \,, \tag{4.3.2}$$

b) the total kinetic energy of the state $\psi \in \mathcal{D}(\overline{H}_0)$ by

$$E_{\text{kin,tot}}[\psi] = \left\langle \psi, \overline{H}_0 \psi \right\rangle . \tag{4.3.3}$$

Remark 4.8. $E_{\text{kin},k}[\psi]$ for $k = 1, 2$ may be infinite for some $\psi \in \mathcal{D}(\overline{H}_0)$. After all, this is the main point of this section. Hence, $E_{\text{kin},k}[\psi]$ may not be well-defined. In that case, we simply write $|E_{\text{kin},1}[\psi]| = \infty$ and mean for an appropriate momentum cut-off $\Lambda \in \mathbb{R}^+$

i) $\|\psi - \psi_\Lambda\| \xrightarrow{\Lambda \to \infty} 0$,

ii) $E_{\text{kin},k}[\psi_\Lambda] < \infty \quad \text{for all fixed} \quad \Lambda > 0$,

iii) $\sup\limits_{\Lambda > 0} |E_{\text{kin},1}[\psi_\Lambda]| = \infty$. ■

Example 4.9. We construct a state $\psi_1 \in \mathcal{D}(\overline{H}_0)$ that exemplifies the possible loss of regularity when taking the closure and thus the emergence of infinite kinetic energy states. To that end, we define $\mathbf{S}_1 \in \mathbb{C}^4 \otimes \mathbb{C}^4$ by

$$\mathbf{S}_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \tag{4.3.4}$$

and with its help ψ_1 for almost all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ by

$$\psi_1(\boldsymbol{x}, \boldsymbol{y}) := \mathbf{S}_1\, f(\boldsymbol{x} + \boldsymbol{y})\, g(\boldsymbol{x} - \boldsymbol{y}). \tag{4.3.5}$$

A straightforward computation shows that $\mathbf{S}_1 f \in \mathcal{H}_-^{\text{com}} = \text{Ker}(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+)$ as well as $\mathbf{S}_1 g \in \mathcal{H}_+^{\text{rel}} = \text{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})^\perp$. This implies two things. First, it tells us that for $g \in H^1(\mathbb{R}^3)$ we have $\psi \in \mathcal{D}(\overline{H}_0)$. Secondly, no H^1-, not even $H^{1/2}$-regularity of f is needed in $\boldsymbol{x} + \boldsymbol{y}$-

direction, and thus, in $\boldsymbol{x}$-direction. We compute

$$
\begin{aligned}
\langle \psi_1, |\nabla_{\boldsymbol{x}}|\psi_1\rangle &= |\mathbf{S}_1|^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |\boldsymbol{p}_x|\, |f(p_{\boldsymbol{x}}+p_{\boldsymbol{y}})\, g(p_{\boldsymbol{x}}-p_{\boldsymbol{y}})|^2 \,\mathrm{d}^3p_{\boldsymbol{x}}\,\mathrm{d}^3p_{\boldsymbol{y}} \\
&= |\mathbf{S}_1|^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |\boldsymbol{P}/2+\boldsymbol{p}| \left|\hat{f}(\boldsymbol{P})\,\hat{g}(\boldsymbol{p})\right|^2 \,\mathrm{d}^3p\,\mathrm{d}^3P \\
&\geq |\mathbf{S}_1|^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{1}{\sqrt{2}}\sum_{k=1}^{3} |P_k/2+p_k| \left|\hat{f}(\boldsymbol{P})\,\hat{g}(\boldsymbol{p})\right|^2 \,\mathrm{d}^3p\,\mathrm{d}^3P \\
&\geq |\mathbf{S}_1|^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{1}{\sqrt{2}}\sum_{k=1}^{3} \Big|\, |P_k/2|-|p_k|\,\Big| \left|\hat{f}(\boldsymbol{P})\,\hat{g}(\boldsymbol{p})\right|^2 \,\mathrm{d}^3p\,\mathrm{d}^3P \\
&= |\mathbf{S}_1|^2 \frac{1}{\sqrt{2}}\sum_{k=1}^{3} \int_{\mathbb{R}^3} \left|\hat{f}(\boldsymbol{P})\right|^2 \int_{\mathbb{R}^3} \Big|\, |P_k/2|-|p_k|\,\Big|\, |\hat{g}(\boldsymbol{p})|^2 \,\mathrm{d}^3p\,\mathrm{d}^3P \\
&\geq |\mathbf{S}_1|^2 \frac{1}{2\sqrt{2}}\sum_{k=1}^{3} \int_{\mathbb{R}^3} |P_k| \left|\hat{f}(\boldsymbol{P})\right|^2 \,\mathrm{d}^3P \int_{\mathbb{R}^3} |\hat{g}(\boldsymbol{p})|^2 \,\mathrm{d}^3p \qquad (4.3.6a) \\
&\quad - |\mathbf{S}_1|^2 \frac{1}{\sqrt{2}}\sum_{k=1}^{3} \int_{\mathbb{R}^3} \left|\hat{f}(\boldsymbol{P})\right|^2 \,\mathrm{d}^3P \int_{\mathbb{R}^3} |p_k|\, |\hat{g}(\boldsymbol{p})|^2 \,\mathrm{d}^3p. \qquad (4.3.6b)
\end{aligned}
$$

Now, by our choice $g \in H^1(\mathbb{R}^3)$ from above, we see that the summand (4.3.6b) is finite. The minus sign in front of it can be compensated for by the summand (4.3.6a) and a suitable choice of f. Recall that no regularity conditions on f are needed as $\mathbf{S}_1 f \in \mathcal{H}_-^{\mathrm{com}} = \mathrm{Ker}(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+)$. Thus, f can be chosen such that (4.3.6a)-(4.3.6b) is positive and even diverges. Hence, ψ_1 need not have $H^{1/2}$-regularity in the single particle variable $\boldsymbol{x}$. For the variable $\boldsymbol{y}$, one proceeds analogously. ■

Example 4.10. We apply Definition 4.7a) to Example 4.9 and find

$$
E_{\mathrm{kin},1}[\psi_1] = \langle \psi_1, D_1 \otimes \mathrm{id}\psi_1\rangle = E_{\mathrm{kin},2}[\psi_1] = \langle \psi_1, \mathrm{id} \otimes D_2\psi_1\rangle = 0, \qquad (4.3.7)
$$

solely due to the spinor structure of $\mathbf{S}_1$, although nothing has been assumed concerning the distribution of the momenta. This result, however, is not generic for states with parts in $\mathrm{Ker}(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+)$ or $\mathrm{Ker}(\mathbf{M}^- \cdot \hat{\boldsymbol{p}})$ as the following example shows. ■

Example 4.11 (Claim b) of Theorem 1)**.** We present a state $\psi_2 \in \mathcal{D}(\overline{H}_0)$ for which $E_{\mathrm{kin},1}[\psi_2]$ as well as $E_{\mathrm{kin},2}[\psi_2]$ diverge. ψ_2 is for almost all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ defined by

$$
\psi_2(\boldsymbol{x},\boldsymbol{y}) := \left[\mathcal{K}^{-1} \begin{pmatrix} f \\ -\kappa f \\ f \\ -\kappa f \end{pmatrix}\right](\boldsymbol{x}-\boldsymbol{y}) \;\cdot h(\boldsymbol{x}+\boldsymbol{y}), \qquad (4.3.8)
$$

where $\mathcal{K}$ and κ are defined in (3.4.1) and (3.4.3), respectively. For h it suffices to specify $h \in H^1(\mathbb{R}^3)$ with $\|h\| = 1$. $f \in L^2(\mathbb{R}^3, \mathrm{d}^3r; \mathbb{C}^4)$ is defined in Fourier space and for almost all $\boldsymbol{p} \in \mathbb{R}^3$ given by

$$\hat{f}(\boldsymbol{p}) = \begin{pmatrix} \nu_+(\boldsymbol{p}) \cdot \hat{\varphi}(\boldsymbol{p}) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix} \tag{4.3.9}$$

where $\varphi \in L^2(\mathbb{R}^3, \mathrm{d}^3 r) \setminus H^{1/2}(\mathbb{R}^3, \mathrm{d}^3 r)$ and $\nu_+(\boldsymbol{p}) \in \mathbb{C}^2$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ with $\nu_+(\boldsymbol{p})^\dagger \nu_+(\boldsymbol{p}) = 1$ is defined by its property

$$\boldsymbol{\sigma} \cdot \boldsymbol{p}\, \nu_+(\boldsymbol{p}) = |\boldsymbol{p}|\, \nu_+(\boldsymbol{p}) \tag{4.3.10}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the usual Pauli matrices from line (2.1.5).

With Theorem 3.10, we conclude that $\psi_2 \in H^1(\mathbb{R}^3, \mathrm{d}^3 R) \otimes \mathcal{H}_-^{\mathrm{rel}}$ and therefore, $\psi_2 \in \mathcal{D}(\overline{H}_0)$.

It suffices to compute

$$\begin{aligned} &\langle \psi_2, -i\,(\boldsymbol{\alpha} \otimes \mathbf{1}_4) \cdot \nabla_{\boldsymbol{x}}\, \psi_2 \rangle = \langle U\psi_2, -i\,(\boldsymbol{\alpha} \otimes \mathbf{1}_4) \cdot (\nabla_{\boldsymbol{r}} + 1/2\, \nabla_{\boldsymbol{R}})\; U\psi_2 \rangle \\ &= \left\langle \mathcal{K}U\psi_2, -i\mathcal{K}\,(\boldsymbol{\alpha} \otimes \mathbf{1}_4) \cdot \nabla_{\boldsymbol{r}}\, \mathcal{K}^\dagger \mathcal{K} U\psi_2 \right\rangle + \langle U\psi_2, -i/2\,(\boldsymbol{\alpha} \otimes \mathbf{1}_4) \cdot\, \nabla_{\boldsymbol{R}}\, U\psi_2 \rangle\,. \end{aligned} \tag{4.3.11}$$

We compute $\mathcal{K}U\psi_2$ and find for almost all $\boldsymbol{r}, \boldsymbol{R} \in \mathbb{R}^3$

$$(\mathcal{K}U\psi_2)\,(\boldsymbol{r}, \boldsymbol{R}) = \begin{pmatrix} f(\boldsymbol{r}) \\ -(\kappa f)(\boldsymbol{r}) \\ f(\boldsymbol{r}) \\ -(\kappa f)(\boldsymbol{r}) \end{pmatrix} \cdot h(\boldsymbol{R}). \tag{4.3.12}$$

The last summand of (4.3.11) is finite, i.e., $\langle U\psi_2, -i/2\,(\boldsymbol{\alpha} \otimes \mathbf{1}_4) \cdot\, \nabla_{\boldsymbol{R}}\, U\psi_2 \rangle < \infty$ since $h \in H^1(\mathbb{R}^3)$. We drop it in the following. Recall the matrix K from (3.4.1). Using that

$$\mathrm{K}(\boldsymbol{\alpha} \cdot \boldsymbol{p} \otimes \mathbf{1}_4)\mathrm{K}^\dagger = \left(\begin{array}{c|c} \mathbf{0}_8 & \begin{matrix} \mathbf{0}_4 & \boldsymbol{\sigma} \cdot \boldsymbol{p} \otimes \mathbf{1}_2 \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} \otimes \mathbf{1}_2 & \mathbf{0}_4 \end{matrix} \\ \hline \begin{matrix} \mathbf{0}_4 & \boldsymbol{\sigma} \cdot \boldsymbol{p} \otimes \mathbf{1}_2 \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} \otimes \mathbf{1}_2 & \mathbf{0}_4 \end{matrix} & \mathbf{0}_8 \end{array}\right) \tag{4.3.13}$$

and

$$-(\sigma \cdot \boldsymbol{p} \otimes \mathbf{1}_2)\,\kappa(\boldsymbol{p}) = \mathbf{1}_2 \otimes \sigma \cdot \boldsymbol{p} = -\kappa(\boldsymbol{p})\,(\sigma \cdot \boldsymbol{p} \otimes \mathbf{1}_2) \tag{4.3.14}$$

hold for almost all $\boldsymbol{p} \in \mathbb{R}^3$, we obtain

$$
\begin{aligned}
\left\langle \mathcal{K}U\psi_2,\ -i\mathcal{K}\left(\boldsymbol{\alpha}\otimes\mathbf{1}_4\right)\cdot\nabla_{\boldsymbol{r}}\,\mathcal{K}^\dagger\mathcal{K}U\psi_2\right\rangle &= \int_{\mathbb{R}^3} |h(\boldsymbol{R})|^2\,\mathrm{d}^3R \quad \times \\
\int_{\mathbb{R}^3}\mathrm{d}^3p \begin{pmatrix} \hat{f}(\boldsymbol{p}) \\ -\kappa(\boldsymbol{p})\hat{f}(\boldsymbol{p}) \\ \hat{f}(\boldsymbol{p}) \\ -\kappa(\boldsymbol{p})\hat{f}(\boldsymbol{p}) \end{pmatrix}^\dagger & \mathrm{K}(\boldsymbol{\alpha}\cdot\boldsymbol{p}\otimes\mathbf{1}_4)\mathrm{K}^\dagger \begin{pmatrix} \hat{f}(\boldsymbol{p}) \\ -\kappa(\boldsymbol{p})\hat{f}(\boldsymbol{p}) \\ \hat{f}(\boldsymbol{p}) \\ -\kappa(\boldsymbol{p})\hat{f}(\boldsymbol{p}) \end{pmatrix} \\
&= 4\cdot\int_{\mathbb{R}^3} \hat{f}(\boldsymbol{p})^\dagger\left(\mathbf{1}_2\otimes\sigma\cdot\boldsymbol{p}\right)\hat{f}(\boldsymbol{p})\,\mathrm{d}^3p \\
&= 4\cdot\int_{\mathbb{R}^3} \begin{pmatrix} \nu_+(\boldsymbol{p})\cdot\hat{\varphi}(\boldsymbol{p}) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix}^\dagger \begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{p} & 0 \\ 0 & \boldsymbol{\sigma}\cdot\boldsymbol{p} \end{pmatrix} \begin{pmatrix} \nu_+(\boldsymbol{p})\cdot\hat{\varphi}(\boldsymbol{p}) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix} \mathrm{d}^3p \\
&= 4\cdot\int_{\mathbb{R}^3} \left[\nu_+(\boldsymbol{p})\cdot\hat{\varphi}(\boldsymbol{p})\right]^\dagger |\boldsymbol{p}|\left[\nu_+(\boldsymbol{p})\cdot\hat{\varphi}(\boldsymbol{p})\right]\,\mathrm{d}^3p \\
&= 4\cdot\int_{\mathbb{R}^3} |\boldsymbol{p}||\hat{\varphi}(\boldsymbol{p})|^2\,\mathrm{d}^3p = \infty, \qquad (4.3.15)
\end{aligned}
$$

which diverges by the definition of φ. In order to show that $E_{\text{kin},2}[\psi_2]$ is infinite, one proceeds analogously. ■

Example 4.12. We continue with Example 4.11 and show how the diverging contributions $E_{\text{kin},1}[\psi_2]$ and $E_{\text{kin},2}[\psi_2]$ to the total kinetic energy cancel each other. To that end, it suffices to note the minus sign in front of $\nabla_{\boldsymbol{r}}$

$$
U\left(-i\left(\mathbf{1}_4\otimes\boldsymbol{\alpha}\right)\cdot\nabla_{\boldsymbol{x}}\right)U^{-1} = -i\left(\mathbf{1}_4\otimes\boldsymbol{\alpha}\right)\cdot\left(-\nabla_{\boldsymbol{r}} + 1/2\,\nabla_{\boldsymbol{R}}\right). \qquad (4.3.16)
$$

This minus sign leads to

$$
\left\langle \mathcal{K}U\psi_2, i\mathcal{K}\left(\mathbf{1}_4\otimes\boldsymbol{\alpha}\right)\cdot\nabla_{\boldsymbol{r}}\,\mathcal{K}^\dagger\mathcal{K}U\psi_2\right\rangle = -4\cdot\int_{\mathbb{R}^3} |\boldsymbol{p}||\hat{\varphi}(\boldsymbol{p})|^2\,\mathrm{d}^3p \qquad (4.3.17)
$$

which cancels the corresponding term of $E_{\text{kin},1}[\psi_2]$ in line (4.3.15). Since we have $\psi_2 \in \mathcal{D}(\overline{H}_0)$, it follows that $E_{\text{kin,tot}}[\psi_2] = \left\langle \psi_2, \overline{H}_0\psi_2\right\rangle$ is finite. ■

4.4. The role of antisymmetry

In Section 4.3, we did not discuss the physical relevance of infinite single particle kinetic energy states, which we will address now. We do so by asking whether such states can occur if H_0 is supposed to describe two identical fermions. We will answer this question in the negative. For the fermionic case, we can restrict our considerations to states from that subspace of $\mathcal{H}_2$ which contains only antisymmetric wavefunctions and for which we write

$$\mathcal{H}_a := \left(L^2(\mathbb{R}^3,\, \mathrm{d}^3x) \otimes \mathbb{C}^4\right) \wedge \left(L^2(\mathbb{R}^3,\, \mathrm{d}^3y) \otimes \mathbb{C}^4\right). \tag{4.4.1}$$

We can immediately conclude that this has implications on the single particle kinetic energy from Definition 4.7. Let $\psi \in \mathcal{H}_a$ be of the form $\psi = \phi_1 \wedge \phi_2$ where $\phi_1, \phi_2 \in H^1(\mathbb{R}^3) \otimes \mathbb{C}^4$. Then,

$$\begin{aligned}
E_{\mathrm{kin},1}[\psi] &= \langle \phi_1 \wedge \phi_2, D_1 \otimes \mathrm{id}\, \phi_1 \wedge \phi_2 \rangle \\
&= \langle \phi_1 \otimes \phi_2 - \phi_2 \otimes \phi_1, D_1\phi_1 \otimes \phi_2 - D_1\phi_2 \otimes \phi_1 \rangle \\
&= \langle \phi_1, D_1\phi_1 \rangle \langle \phi_2, \phi_2 \rangle - \langle \phi_1, D_1\phi_2 \rangle \langle \phi_2, \phi_1 \rangle \\
&\quad - \langle \phi_2, D_1\phi_1 \rangle \langle \phi_1, \phi_2 \rangle + \langle \phi_2, D_1\phi_2 \rangle \langle \phi_1, \phi_1 \rangle \\
&= \langle \phi_2, \phi_2 \rangle \langle \phi_1, D_1\phi_1 \rangle - \langle \phi_2, \phi_1 \rangle \langle \phi_1, D_1\phi_2 \rangle \\
&\quad - \langle \phi_1, \phi_2 \rangle \langle \phi_2, D_1\phi_1 \rangle + \langle \phi_1, \phi_1 \rangle \langle \phi_2, D_1\phi_2 \rangle \\
&\overset{(*)}{=} \langle \phi_2 \otimes \phi_1 - \phi_1 \otimes \phi_2, \phi_2 \otimes D_2\phi_1 - \phi_1 \otimes D_2\phi_2 \rangle \\
&= \langle \phi_2 \wedge \phi_1, \mathrm{id} \otimes D_2\, \phi_2 \wedge \phi_1 \rangle \\
&= (-1)^2 \langle \phi_1 \wedge \phi_2, \mathrm{id} \otimes D_2\, \phi_1 \wedge \phi_2 \rangle = E_{\mathrm{kin},2}[\psi],
\end{aligned} \tag{4.4.2}$$

where we interchanged the integration variables $\boldsymbol{x}$ and $\boldsymbol{y}$ in $(*)$. Thus, we arrive at the following relation for $\psi = \phi_1 \wedge \phi_2$ with $\phi_1, \phi_2 \in H^1(\mathbb{R}^3) \otimes \mathbb{C}^4$

$$2 \cdot E_{\mathrm{kin},1}[\psi] = 2 \cdot E_{\mathrm{kin},2}[\psi] = E_{\mathrm{kin,tot}}[\psi] \tag{4.4.3}$$

which is finite. This allows us to conclude immediately that antisymmetry rules out states with infinite single particle kinetic energy of the form $\psi = \phi_1 \wedge \phi_2$. In particular, the cancellation mechanism observed in Example 4.12 is not effective in the antisymmetric subset of the domain since $E_{\mathrm{kin},1}[\psi]$ and $E_{\mathrm{kin},2}[\psi]$ have the same sign. That (4.4.3) extends to all $\psi \in \mathcal{D}(\overline{H}_0) \cap \mathcal{H}_a$, is the content of the following lemma.

Lemma 4.13 (Claim c) of Theorem 1)**.** *For all $\psi \in \mathcal{D}(\overline{H}_0) \cap \mathcal{H}_a$, we have*

$$E_{\mathrm{kin,tot}}[\psi] = 2 \cdot E_{\mathrm{kin},1}[\psi] = 2 \cdot E_{\mathrm{kin},2}[\psi], \tag{4.4.4}$$

which means in particular that $E_{\mathrm{kin},k}[\psi] < \infty$ for all $\psi \in \mathcal{D}(\overline{H}_0) \cap \mathcal{H}_a$ and $k = 1, 2$.

Proof. Let $\psi \in \mathcal{D}(\overline{H}_0) \cap \mathcal{H}_a$. We note that H_0 with domain $\mathcal{D}_0 \cap \mathcal{H}_a$ is essentially self-adjoint as H_0 leaves $\mathcal{H}_a$ invariant. The domain of the closure is given by $\mathcal{D}(\overline{H}_0) \cap \mathcal{H}_a$. Thus, we can choose a sequence $(\psi_n)_{n\in\mathbb{N}} \subset \mathcal{D}_0 \cap \mathcal{H}_a$ such that $\|\psi - \psi_n\| \xrightarrow{n\to\infty} 0$ and $\|\overline{H}_0(\psi - \psi_n)\| \xrightarrow{n\to\infty} 0$. Note that elements from $\mathcal{D}_0 \cap \mathcal{H}_a$ are of the form $\psi = \phi_1 \wedge \phi_2$

where $\phi_1, \phi_2 \in H^1(\mathbb{R}^3)$. Using the continuity of the scalar product twice, this implies

$$\begin{aligned}
2 \cdot E_{\mathrm{kin},1}[\psi] &= 2 \cdot \lim_{m\to\infty} \langle \psi_m, D_1 \otimes \mathrm{id}\psi \rangle \\
&= 2 \cdot \lim_{m\to\infty} \langle D_1 \otimes \mathrm{id}\psi_m, \psi \rangle \\
&= 2 \cdot \lim_{m\to\infty} \lim_{n\to\infty} \langle D_1 \otimes \mathrm{id}\psi_m, \psi_n \rangle \\
&= 2 \cdot \lim_{m\to\infty} \lim_{n\to\infty} \langle \psi_m, D_1 \otimes \mathrm{id}\psi_n \rangle \\
&\overset{(*)}{=} \lim_{m\to\infty} \lim_{n\to\infty} \langle \psi_m, (D_1 \otimes \mathrm{id} + \mathrm{id} \otimes D_2)\psi_n \rangle \\
&= \left\langle \psi, \overline{H}_0 \psi \right\rangle = E_{\mathrm{kin,tot}}[\psi] < \infty.
\end{aligned} \tag{4.4.5}$$

In $(*)$, we used the polarization identity in order to apply (4.4.3). In order to treat $E_{\mathrm{kin},2}[\psi]$, one proceeds analogously, which finishes the proof. □

One could think that (4.4.3) suggests that demanding antisymmetry from allowed wave-functions leads to higher regularity. After all, states like ψ_2 from Example 4.11 are ruled out. This, however, is in general not true as the next example shows.

Example 4.14. We continue Example 4.10. Recall the state $\psi_1(\boldsymbol{x}, \boldsymbol{y}) = \mathbf{S}_1 f(\boldsymbol{x}+\boldsymbol{y})g(\boldsymbol{x}-\boldsymbol{y})$. If one takes g to be an even function, then ψ_1 is antisymmetric by the choice of $\mathbf{S}_1$, yet f requires no other regularity than being square-integrable. ■

4.5. Time evolution generated by $\overline{H}_{\mathrm{2BD}}$

This section continues to address the question of physical relevance of states with infinite single particle kinetic energy (infinite SPKE). In Section 4.4, we restricted ourselves to antisymmetric states and found that then infinite SPKE cannot occur. In this section, however, we assume that the initial states are arbitrary states but with finite SPKE. We show that then for all finite times $t \in \mathbb{R}$ the single particle kinetic energy stays finite, where the time evolution we consider can be the free time evolution or the full time evolution, even including interaction, if the potentials obey a regularity condition. This is the content of the following theorem for which we recall $\mathcal{D}_0 = H^1(\mathbb{R}^3, \mathrm{d}^3x) \otimes \mathbb{C}^4 \otimes H^1(\mathbb{R}^3, \mathrm{d}^3y) \otimes \mathbb{C}^4$.

Theorem 4.15 (Claim d) of Theorem 1)**.** *Let V be the operator of multiplication with the smooth real-valued function $V \in C^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$. We assume that there exists a real constant $0 < M < \infty$ such that*

a) $\displaystyle\sup_{\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^3} \left| \left(\frac{\partial}{\partial x_i} V \right) (\boldsymbol{x}, \boldsymbol{y}) \right| \le M,$

b) $\displaystyle\sup_{\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^3} \left| \left(\frac{\partial}{\partial y_i} V \right) (\boldsymbol{x}, \boldsymbol{y}) \right| \le M,$

c) $\displaystyle\sup_{\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^3} \left| \left(\frac{\partial^2}{\partial x_i \partial y_j} V \right) (\boldsymbol{x}, \boldsymbol{y}) \right| \le M.$

Then,

a) the free time evolution generated by $\overline{H}_0$ leaves $\mathcal{D}_0$ invariant, i.e., for all $t \in \mathbb{R}$, we have

$$\mathrm{e}^{-it\overline{H}_0}\mathcal{D}_0 \subseteq \mathcal{D}_0, \tag{4.5.1}$$

b) the full time evolution generated by $\overline{H}_{2\mathrm{BD}} = \overline{H_0 + V}$ leaves $\mathcal{D}_0$ invariant, i.e., for all $t \in \mathbb{R}$, we have

$$\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}}\mathcal{D}_0 \subseteq \mathcal{D}_0. \tag{4.5.2}$$

Proof.

a) Recalling the notation of H_0 from line (4.1.8)

$$H_0 = (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{x}} + \beta m) \otimes \mathrm{id} + \mathrm{id} \otimes (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{y}} + \beta m) = D_1 \otimes \mathrm{id} + \mathrm{id} \otimes D_2, \tag{4.5.3}$$

we note that H_0 is the sum of two commuting operators. Thus,

$$\mathrm{e}^{-itD_1\otimes\mathrm{id}}\mathrm{e}^{-it\mathrm{id}\otimes D_2} = \mathrm{e}^{-it(D_1\otimes\mathrm{id}+\mathrm{id}\otimes D_2)} = \mathrm{e}^{-it\mathrm{id}\otimes D_2}\mathrm{e}^{-itD_1\otimes\mathrm{id}} \tag{4.5.4}$$

holds. This allows us to compute for all $i, j = 1, 2, 3$, all $t \in \mathbb{R}$, and all $f \in \mathcal{D}_0$

$$\begin{aligned} \|\partial_{x_i} \otimes \partial_{y_j} \mathrm{e}^{-it\overline{H}_0} f\| &= \|\partial_{x_i} \otimes \partial_{y_j} \mathrm{e}^{-it(D_1\otimes\mathrm{id}+\mathrm{id}\otimes D_2)} f\| \\ &= \|\mathrm{e}^{-itD_1\otimes\mathrm{id}}\mathrm{e}^{-it\mathrm{id}\otimes D_2}\partial_{x_i} \otimes \partial_{y_j} f\| \\ &= \|\partial_{x_i} \otimes \partial_{y_j} f\| < \infty, \end{aligned} \tag{4.5.5}$$

which finishes the proof.

b) We need to show for all $f \in \mathcal{D}_0$, all $i, j = 1, 2, 3$, and all $t \in \mathbb{R}$ that

$$\left\|\partial_{x_i} \otimes \partial_{y_j} \mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f\right\| < \infty. \tag{4.5.6}$$

We fix an $f \in \mathcal{D}_0$, set

$$T_n := \mathrm{e}^{-it\overline{H}_0/n}\mathrm{e}^{-itV/n}, \tag{4.5.7}$$

and define with its help the sequence $(f_n)_{n\in\mathbb{N}}$ by

$$f_n := T_n^n f. \tag{4.5.8}$$

Note that T_n is unitary due to the self-adjointness of $\overline{H}_0$ and of V. We will see in Theorem 5.1, that $H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3) \otimes \mathbb{C}^{16}$. Hence, we know from the Trotter product formula (see [RS80, Theorem VIII.31]) that

$$\lim_{n\to\infty} f_n = \lim_{n\to\infty} T_n^n f = \mathrm{e}^{-it\overline{H}_{\mathrm{2BD}}} f \tag{4.5.9}$$

for all $t \in \mathbb{R}$. Furthermore, we define the sequence $(g_n)_{n\in\mathbb{N}}$ by

$$g_n := \partial_{x_i} \otimes \partial_{y_j} f_n = \partial_{x_i} \otimes \partial_{y_j} T_n^n f. \tag{4.5.10}$$

It suffices to show that $(g_n)_{n\in\mathbb{N}}$ converges weakly in $\mathcal{H}_2$ to $\partial_{x_i} \otimes \partial_{y_j} \mathrm{e}^{-it\overline{H}_{\mathrm{2BD}}} f$ as this implies (4.5.6) using the lower semicontinuity of the L^2-norm (see (4.5.18) below).

To that end, we show that $\|\partial_{x_i} \otimes \partial_{y_j} T_n^n f\|$ is bounded uniformly in n. Therefore, we compute

$$\begin{aligned}
\|\partial_{x_i} &\otimes \partial_{y_j} T_n^n f\| = \left\|\partial_{x_i}\partial_{y_j}\mathrm{e}^{-it\overline{H}_0/n}\mathrm{e}^{-itV/n}T_n^{n-1}f\right\| \\
&= \left\|\mathrm{e}^{-it\overline{H}_0/n}\partial_{x_i}\partial_{y_j}\mathrm{e}^{-itV/n}T_n^{n-1}f\right\| \\
&= \left\|\partial_{x_i}\partial_{y_j}\mathrm{e}^{-itV/n}T_n^{n-1}f\right\| \\
&\leq \left\|\left(\partial_{x_i}\partial_{y_j}\mathrm{e}^{-itV/n}\right)T_n^{n-1}f\right\| + \left\|\mathrm{e}^{-itV/n}(\partial_{x_i}\partial_{y_j}T_n^{n-1}f)\right\| \\
&\quad + \left\|\left(\partial_{y_j}\mathrm{e}^{-itV/n}\right)(\partial_{x_i}T_n^{n-1}f)\right\| + \left\|\left(\partial_{x_i}\mathrm{e}^{-itV/n}\right)(\partial_{y_j}T_n^{n-1}f)\right\| \\
&= \left\|\left(\frac{t^2}{n^2}\mathrm{e}^{-itV/n}(\partial_{x_i}V)(\partial_{y_j}V) + \frac{t}{n}\mathrm{e}^{-itV/n}(\partial_{x_i}\partial_{y_j}V)\right)T_n^{n-1}f\right\| \\
&\quad + \left\|\left(\frac{t}{n}\mathrm{e}^{-itV/n}\partial_{y_j}V\right)(\partial_{x_i}T_n^{n-1}f)\right\| + \left\|\left(\frac{t}{n}\mathrm{e}^{-itV/n}\partial_{x_i}V\right)(\partial_{y_j}T_n^{n-1}f)\right\| \\
&\quad + \left\|\partial_{x_i}\partial_{y_j}T_n^{n-1}f\right\| \\
&\leq \left(\frac{t^2}{n^2}M^2 + \frac{t}{n}M\right)\left\|T_n^{n-1}f\right\| + \frac{t}{n}M\left(\left\|\partial_{x_i}T_n^{n-1}f\right\| + \left\|\partial_{y_j}T_n^{n-1}f\right\|\right) \\
&\quad + \left\|\partial_{x_i}\partial_{y_j}T_n^{n-1}f\right\| \\
&= \left(\frac{t^2}{n^2}M^2 + \frac{t}{n}M\right)\|f\| + \frac{t}{n}M\left(\left\|\partial_{x_i}T_n^{n-1}f\right\| + \left\|\partial_{y_j}T_n^{n-1}f\right\|\right) \\
&\quad + \left\|\partial_{x_i}\partial_{y_j}T_n^{n-1}f\right\|,
\end{aligned} \tag{4.5.11}$$

where we simplified the notation $\partial_{x_i} \otimes \partial_{y_j}$ to $\partial_{x_i}\partial_{y_j}$, used that $\mathrm{e}^{-itV/n} \in C^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$, and that $\|T_n^{n-1}f\| = \|f\|$ as T_n is unitary.

We consider $\|\partial_{x_i} T_n^{n-1} f\|$ separately and find

$$
\begin{aligned}
\left\|\partial_{x_i} T_n^{n-1} f\right\| &= \left\|\partial_{x_i} \mathrm{e}^{-it\overline{H}_0/n} \mathrm{e}^{-itV/n} T_n^{n-2} f\right\| \\
&= \left\|\mathrm{e}^{-it\overline{H}_0/n} \partial_{x_i} \mathrm{e}^{-itV/n} T_n^{n-2} f\right\| \\
&= \left\|\partial_{x_i} \mathrm{e}^{-itV/n} T_n^{n-2} f\right\| \\
&= \left\|\left(\frac{t}{n} \mathrm{e}^{-itV/n} \partial_{x_i} V\right) T_n^{n-2} f + \mathrm{e}^{-itV/n} \partial_{x_i} T_n^{n-2} f\right\| \\
&\leq \frac{t}{n} M \|f\| + \left\|\partial_{x_i} T_n^{n-2} f\right\|.
\end{aligned}
\tag{4.5.12}
$$

Upon noticing the recursive nature of inequality (4.5.12), we obtain

$$
\begin{aligned}
\left\|\partial_{x_i} T_n^{n-1} f\right\| &\leq \frac{t}{n} M \|f\| + \frac{t}{n} M \|f\| + \left\|\partial_{x_i} T_n^{n-3} f\right\| \\
&\leq \frac{(n-1)t}{n} M \|f\| + \|\partial_{x_i} f\| \\
&\leq tM \|f\| + \|\partial_{x_i} f\|.
\end{aligned}
\tag{4.5.13}
$$

As the same reasoning that led to inequality (4.5.13) also applies to $\|\partial_{y_j} T_n^{n-1} f\|$, line (4.5.11) can be estimated as

$$
\begin{aligned}
\left\|\partial_{x_i} \partial_{y_j}\ T_n^n f\right\| &\leq \left(\frac{t^2}{n^2} M^2 + \frac{t}{n} M\right) \|f\| + \frac{t}{n} M \left(2tM \|f\| + \|\partial_{x_i} f\| + \left\|\partial_{y_j} f\right\|\right) \\
&\quad + \left\|\partial_{x_i} \partial_{y_j} T_n^{n-1} f\right\| \\
&= \left(\frac{t^2(1+2n)}{n^2} M^2 + \frac{t}{n} M\right) \|f\| + \frac{t}{n} M \left(\|\partial_{x_i} f\| + \left\|\partial_{y_j} f\right\|\right) \\
&\quad + \left\|\partial_{x_i} \partial_{y_j} T_n^{n-1} f\right\| \\
&\overset{(*)}{\leq} \left(\frac{t^2(1+2n)}{n} M^2 + tM\right) \|f\| + tM \left(\|\partial_{x_i} f\| + \left\|\partial_{y_j} f\right\|\right) + \left\|\partial_{x_i} \partial_{y_j} f\right\| \\
&\leq \left(3t^2 M^2 + tM\right) \|f\| + tM \left(\|\partial_{x_i} f\| + \left\|\partial_{y_j} f\right\|\right) + \left\|\partial_{x_i} \partial_{y_j} f\right\|,
\end{aligned}
\tag{4.5.14}
$$

where we used recursion arguments in $(*)$ again. Line (4.5.14) is the desired uniform bound in n.

This bound implies that the sequence $(g_n)_{n \in \mathbb{N}}$ has a subsequence $(g_{n_k})_{k \in \mathbb{N}}$ which converges weakly to a $g \in \mathcal{H}_2$ (see [LL01, Theorem 2.18]), i.e., for all $h \in \mathcal{H}_2$ it holds that

$$
|\langle h, g_{n_k} - g \rangle| \xrightarrow{k \to \infty} 0. \tag{4.5.15}
$$

As this holds in particular for all $\varphi \in C_c^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4 \otimes C_c^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$, we can compute

$$\begin{aligned}\left|\left\langle \varphi, g_{n_k} - \partial_{x_i}\partial_{y_j}\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f\right\rangle\right| &= \left|\left\langle \varphi, \partial_{x_i}\partial_{y_j}(f_{n_k} - \mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f)\right\rangle\right| \\ &= \left|\left\langle \partial_{x_i}\partial_{y_j}\varphi, (f_{n_k} - \mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f)\right\rangle\right| \\ &\leq \left\|\partial_{x_i}\partial_{y_j}\varphi\right\| \left\|f_{n_k} - \mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f\right\| \xrightarrow{k\to\infty} 0. \end{aligned} \tag{4.5.16}$$

This implies

$$g = \partial_{x_i}\partial_{y_j}\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f. \tag{4.5.17}$$

Now, the lower semicontinuity of the L^2-norm (see [LL01, Theorem 2.11]) yields

$$\left\|\partial_{x_i}\partial_{y_j}\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}} f\right\| = \|g\| \leq \liminf_{k\to\infty} \|g_{n_k}\| < \infty, \tag{4.5.18}$$

where $\liminf_{k\to\infty}\|g_{n_k}\| < \infty$ holds by the uniform bound (4.5.14). □

Remark 4.16. Several remarks are in order.

a) We believe that the assumption $V \in C^\infty$ can be substantially relaxed. Smoothness of the potentials is assumed merely for technical reasons.

b) The same technique employed here can also be used to show invariance of $H^k(\mathbb{R}^3) \otimes \mathbb{C}^4 \otimes H^k(\mathbb{R}^3) \otimes \mathbb{C}^4$ for $k > 1$.

c) As $\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}}$ is boundedly invertible and Theorem 4.15b) also holds for the inverse, we see that also $\mathcal{D}(\overline{H}_{2\mathrm{BD}}) \setminus \mathcal{D}_0$ is left invariant by $\mathrm{e}^{-it\overline{H}_{2\mathrm{BD}}}$. Thus, the time evolution partitions $\mathcal{D}(\overline{H}_{2\mathrm{BD}})$ into two subsets that are disjoint in the sense that they cannot be mixed by the time evolution for finite times $t \in \mathbb{R}$.

d) This implies that finite SPKE states can reach infinite SPKE states only in the limit $t \to \infty$.

e) The converse of Theorem 4.15 is also true, i.e., a dense linear set $\tilde{\mathcal{D}}$ contained in the domain of a self-adjoint operator A is a core for A if for all $t \in \mathbb{R}$, $\mathrm{e}^{-itA}\tilde{\mathcal{D}} \subseteq \tilde{\mathcal{D}}$ (see [RS80, Theorem VIII.11]). ■

5. Self-adjointness of $H_{2\mathrm{BD}}$ with unbounded interaction

5.1. Essential self-adjointness of $H_{2\mathrm{BD}}$ with smooth potentials

Our first result concerning self-adjointness of $H_{2\mathrm{BD}}$ with unbounded interaction is presented in this section. We require a smooth potential and can then employ an elliptic regularity argument. In the case of one-body Dirac operators the analogous statement is well-known and can be found in [Tha92, Theorem 4.3]. The proof of this result extends to the N particle case. Therefore, we follow the proof of [Tha92, Theorem 4.3] closely, in some instances even verbatim.

Theorem 5.1. *Let the potential V be the operator of multiplication with a Hermitian matrix with entries $V_{ij} \in C^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$, $i, j = 1, 2, \ldots, 16$. Then, $H_{2\mathrm{BD}} = H_0 + V$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3 \times \mathbb{R}^3) \otimes \mathbb{C}^{16}$.*

Proof. Since V is multiplication with a Hermitian matrix, $H_{2\mathrm{BD}}$ is symmetric on $C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3) \otimes \mathbb{C}^{16}$. By the basic criterion for essential self-adjointness (see [RS75]), it thus suffices to show that $(H_{2\mathrm{BD}} \pm i)\psi = 0$ for some $\psi \in \mathcal{H}_2$ implies $\psi = 0$. The operator $H_{2\mathrm{BD}} \pm i$ is an elliptic differential operator of first order with variable C^∞- coefficients. By the local regularity property of elliptic operators, we conclude that any L^2-solution of $(H_{2\mathrm{BD}} + i)\psi = 0$ is infinitely differentiable. Let ψ be such a solution. Choose now a function $f \in C_c^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ with $f(\boldsymbol{x}, \boldsymbol{y}) = 1$ for $|\boldsymbol{x}|^2 + |\boldsymbol{y}|^2 \leq 1$ and set $f_n(\boldsymbol{x}, \boldsymbol{y}) = f(\frac{\boldsymbol{x}}{n}, \frac{\boldsymbol{y}}{n})$ for all $n \in \mathbb{N}$. Then, we find

$$(H_{2\mathrm{BD}} + i)\, f_n\psi = -i(\boldsymbol{\alpha} \otimes \mathbf{1}) \cdot \psi\nabla_{\boldsymbol{x}} f_n - i(\mathbf{1} \otimes \boldsymbol{\alpha}) \cdot \psi\nabla_{\boldsymbol{y}} f_n, \tag{5.1.1}$$

where we used $(H_{2\mathrm{BD}} + i)\psi = 0$. With $(\nabla f_n)(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{n}(\nabla f)(\frac{\boldsymbol{x}}{n}, \frac{\boldsymbol{y}}{n})$, we obtain

$$\begin{aligned}
\|f_n\psi\|^2 + \|H_{2\mathrm{BD}} f_n\psi\|^2 &= \|(H_{2\mathrm{BD}} + i)\, f_n\psi\|^2 \\
&= \|(\boldsymbol{\alpha} \otimes \mathbf{1}) \cdot \psi\nabla_{\boldsymbol{x}} f_n + (\mathbf{1} \otimes \boldsymbol{\alpha}) \cdot \psi\nabla_{\boldsymbol{y}} f_n\|^2 \\
&\leq \frac{2}{n^2} \sup_{\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^3} |(\nabla_{\boldsymbol{x}} f)(\boldsymbol{x}, \boldsymbol{y})|^2 \left\| \sum_{k=1}^{3} (\boldsymbol{\alpha}_k \otimes \mathbf{1})\psi \right\|^2 \\
&\quad + \frac{2}{n^2} \sup_{\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^3} |(\nabla_{\boldsymbol{y}} f)(\boldsymbol{x}, \boldsymbol{y})|^2 \left\| \sum_{k=1}^{3} (\mathbf{1} \otimes \boldsymbol{\alpha}_k)\psi \right\|^2 \xrightarrow{n\to\infty} 0,
\end{aligned} \tag{5.1.2}$$

which implies together with $\|f_n\psi\| \xrightarrow{n\to\infty} \|\psi\|$ that $\psi = 0$. The analogous argument for $(H_{2\mathrm{BD}} - i)\psi = 0$ finishes the proof of the theorem. $\square$

5.2. Self-adjoint extension of $H_{2\mathrm{BD}}$ with Coulomb interaction

This section is devoted to the proofs leading to our main result Theorem 2, and contains the construction of the self-adjoint extension of $H_{2\mathrm{BD}}$. In the subsequent section, we will complement this extension by a criterion that distinguishes it uniquely.

For the remainder of this chapter, we fix the interaction potential V_{int} and define with $\gamma \in \mathbb{R}$

$$V_{\mathrm{int}} := \gamma V, \tag{5.2.1}$$

where we assume that V is in the underlying Hilbert space $\mathcal{H}^{\mathrm{rel}}$ the operator of component-wise multiplication with $|\boldsymbol{r}|^{-\kappa}$ for almost all $\boldsymbol{r} \in \mathbb{R}^3$ and all $0 < \kappa \leq 1$ with domain

$$\mathcal{D}(V) = \left\{ f \in \mathcal{H}^{\mathrm{rel}} \,\middle|\, |\cdot|^{-\kappa} f \in \mathcal{H}^{\mathrm{rel}} \right\}. \tag{5.2.2}$$

It is well-known that V is positive and self-adjoint on $\mathcal{D}(V)$.

Before we proceed with the construction of the self-adjoint extension of $H_{2\mathrm{BD}}$, we want to understand why many standard techniques from the perturbation theory of self-adjoint operators are not helpful in finding such a self-adjoint extension: An unbounded interaction potential is not relatively bounded by $\overline{H}_0$.[1]

Lemma 5.2. *Let $\gamma \neq 0$ and let $0 < \kappa \leq 1$ be fixed. Then, V is not relatively bounded by $\overline{H}_0$.*

Proof. It suffices to provide an $f \in \mathcal{D}(\overline{H}_0)$ such that $f \notin \mathcal{D}(V)$. To that end, we fix $0 < \kappa \leq 1$ and chose a $\delta \in \mathbb{R}^+$ such that $0 < \delta < \kappa$. Next, we define f for almost all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ by

$$f(\boldsymbol{x}, \boldsymbol{y}) = \omega_{-,1} \cdot \frac{e^{-|\boldsymbol{x}-\boldsymbol{y}|^2}}{|\boldsymbol{x}-\boldsymbol{y}|^{3/2-\delta}} \cdot \phi(\boldsymbol{x}+\boldsymbol{y}) \tag{5.2.3}$$

for some $\phi \in \mathcal{S}(\mathbb{R}^3)$. We recall the definition of $\omega_{-,1}$ and its crucial property

$$P_{-}(\boldsymbol{p})\, \omega_{-,1} = \omega_{-,1} \tag{5.2.4}$$

from lines (3.4.13)-(3.4.15). This implies $\omega_{-,1} \in \mathrm{Ker}(\mathbf{M}^{-} \cdot \boldsymbol{p})$. Therefore, we obtain with help of the coordinate transform U

$$\left\|\overline{H}_0 f\right\| = \left\|\hat{\boldsymbol{P}} \cdot \mathbf{M}^{+} U f + \mathbf{M}^{-} \cdot \hat{\boldsymbol{p}} U f\right\| = \left\|\hat{\boldsymbol{P}} \cdot \mathbf{M}^{+} U f\right\| < \infty, \tag{5.2.5}$$

[1] This was first noticed by Julien Sabin and Jérémy Sok, private communication.

and can thus conclude that $f \in \mathcal{D}(\overline{H}_0)$. But $f \notin \mathcal{D}(|\cdot|^{-\kappa})$ as

$$\left\||\gamma|\cdot|^{-\kappa} f\right\|^2 = \int_{\mathbb{R}^3} \frac{\gamma^2}{|\boldsymbol{r}|^{3-2\delta+2\kappa}} e^{-2|\boldsymbol{r}|^2}\,\mathrm{d}^3 r \tag{5.2.6}$$

does not converge except for $\gamma = 0$. This proves the lemma. □

Before we can give domain and action of the self-adjoint extension of $H_{2\mathrm{BD}}$, we would like to recall from Section 2.2 the various steps (or layers of self-adjointness) involved in this construction, and hence, the corresponding proofs.

As first step, we note that H_0 does not separate into center-of-mass and relative Hamiltonian as one is used to since $U\mathcal{H}_2 \neq \mathcal{H}^{\mathrm{com}} \otimes \mathcal{H}^{\mathrm{rel}}$. Nevertheless, by employing direct fiber integrals, we can infer self-adjointness of $H_{2\mathrm{BD}}$ from self-adjointness of H^{rel}. Therefore, we look only for a self-adjoint extension of H^{rel}. This extension plus $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$ is then also a self-adjoint extension of $H_{2\mathrm{BD}}$. Since H^{rel} is a matrix operator, we have as second step the Frobenius-Schur factorization at our disposal. Therefore, we can use that important properties such as closedness and self-adjointness are encoded in the Schur complement. After a slight but important modification of H^{rel}, we see that the Schur complement possesses a self-adjoint extension, denoted by S_F. This, in turn, paves the way to H_F^{rel}, the self-adjoint extension of H^{rel}, and finally, to H_F which denotes the self-adjoint extension of $H_{2\mathrm{BD}}$ in relative and center-of-mass coordinates.

We start with the just mentioned slight but important modification of H^{rel}. We define the symmetric and bounded matrix

$$B := 2\beta \otimes \beta, \tag{5.2.7}$$

recall Eq. (2.1.4) for the definition of β. We now consider $H^{\mathrm{rel}} + P_+ B P_+$. Recalling the matrix representation of H^{rel} from line (2.2.18), we find

$$H^{\mathrm{rel}} + P_+ B P_+ = \begin{pmatrix} \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + P_+ B P_+ + P_+ \gamma V P_+ & P_+ \gamma V P_- \\ P_- \gamma V P_+ & P_- \gamma V P_- \end{pmatrix} \tag{5.2.8}$$

which is well-defined on

$$\mathcal{D}(H^{\mathrm{rel}}) = \mathcal{D}_+ \oplus (\mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}), \tag{5.2.9}$$

where $\mathcal{D}_+ = (\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r)) \cap \mathcal{H}_+^{\mathrm{rel}}$, introduced in (2.2.19). For sake of completeness, we prove that $\mathcal{D}(H^{\mathrm{rel}})$ is dense in $\mathcal{H}^{\mathrm{rel}}$.

Proposition 5.3. *$\mathcal{D}(H^{\mathrm{rel}})$ is dense in $\mathcal{H}^{\mathrm{rel}}$.*

Proof. The statement of the proposition follows if $\mathcal{D}_+$ is dense in $\mathcal{H}_+^{\mathrm{rel}}$ and $\mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$ is dense in $\mathcal{H}_-^{\mathrm{rel}}$ since the splitting of $\mathcal{H}^{\mathrm{rel}}$ is orthogonal. The former statement follows from density of H^1 in L^2, the latter holds then by Hardy's inequality. □

In the following lemma, we examine the properties of the combination of the matrices $P_+(\boldsymbol{p}) B P_+(\boldsymbol{p})$ and $\mathbf{M}^- \cdot \boldsymbol{p}$.

Lemma 5.4. *The following holds for almost all $\boldsymbol{p} \in \mathbb{R}^3$:*

a) $BP_+(\boldsymbol{p}) = P_+(\boldsymbol{p})B$,

b) $\left(\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})\right)^2 = 4\,(p^2+1)\,P_+(\boldsymbol{p})$, *and*

c) $|\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})| = 2\,(p^2+1)^{1/2}\,P_+(\boldsymbol{p})$.

Proof. a) We get by direct computation $BP_+(\boldsymbol{p}) = P_+(\boldsymbol{p})B$ for almost all $\boldsymbol{p} \in \mathbb{R}^3$ since $(\boldsymbol{\alpha}\cdot\boldsymbol{p})\beta = -\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})$ by Eq. (2.1.6).

b) Using $P_+(\boldsymbol{p})\mathbf{M}^- \cdot \boldsymbol{p} = \mathbf{M}^- \cdot \boldsymbol{p}P_+(\boldsymbol{p}) = \mathbf{M}^- \cdot \boldsymbol{p}$, we compute for almost all $\boldsymbol{p} \in \mathbb{R}^3$ $(\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p}))^2 = 4(p^2+1)P_+(\boldsymbol{p})$ where again we made use of the anticommutation relations in Eq. (2.1.6).

c) By part a), we have $P_+(\boldsymbol{p})BP_+(\boldsymbol{p}) = BP_+(\boldsymbol{p})$, and thus, $\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})$ is Hermitian. We compute for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$\begin{aligned} \left|\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})\right| &= \left(\left(\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})\right)^\dagger \left(\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})\right)\right)^{1/2} \\ &= \left(4\left(p^2+1\right)P_+(\boldsymbol{p})\right)^{1/2} \end{aligned} \tag{5.2.10}$$

where we used part b) in the last step. Now, $P_+(\boldsymbol{p})$ is a Hermitian matrix, and therefore, there exists a unitary matrix $u(\boldsymbol{p})$—the same matrix $u(\boldsymbol{p})$ as in lines (3.1.1) and (3.1.10)—such that we have for almost all $\boldsymbol{p} \in \mathbb{R}^3$

$$u(\boldsymbol{p})P_+(\boldsymbol{p})u(\boldsymbol{p})^\dagger = \begin{pmatrix} \mathbf{1}_8 & \\ & \mathbf{0}_8 \end{pmatrix}. \tag{5.2.11}$$

Then,

$$\begin{aligned} \left(4\left(p^2+1\right)P_+(\boldsymbol{p})\right)^{1/2} &= u(\boldsymbol{p})^\dagger\, 2\left(p^2+1\right)^{1/2} \begin{pmatrix} \mathbf{1}_8 & \\ & \mathbf{0}_8 \end{pmatrix} u(\boldsymbol{p}) \\ &= 2\left(p^2+1\right)^{1/2} P_+(\boldsymbol{p}) \end{aligned} \tag{5.2.12}$$

for almost all $\boldsymbol{p} \in \mathbb{R}^3$ which concludes the proof. □

In the following, we will make frequent use of the operator $\mathbf{M}^- \cdot \hat{\boldsymbol{p}} + BP_+$ in the underlying Hilbert space $\mathcal{H}_+^{\mathrm{rel}}$. Thus, we introduce the abbreviation

$$A_0 \equiv \mathbf{M}^- \cdot \hat{\boldsymbol{p}} + BP_+. \tag{5.2.13}$$

First, we want to relate the different interaction potentials, distinguished by the exponent $0 < \kappa \leq 1$, to A_0. Recall $\mathcal{D}_+ = (\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3r)) \cap \mathcal{H}_+^{\mathrm{rel}}$ from line (2.2.20).

Lemma 5.5. *Let $0 < \kappa \leq 1$ and let $M_\kappa > 0$ be given by*

$$M_\kappa = 2^{-\kappa}\frac{\Gamma\left(\frac{3}{4}-\frac{\kappa}{2}\right)}{\Gamma\left(\frac{3}{4}+\frac{\kappa}{2}\right)}. \tag{5.2.14}$$

a) For all $f \in \mathcal{D}_+$,

$$\big\| |\cdot|^{-\kappa} f \big\| \leq \frac{M_\kappa}{2} \, \|A_0 f\| \,. \tag{5.2.15}$$

b) For all $f \in (\mathbb{C}^{16} \otimes H^{1/2}(\mathbb{R}^3, \, \mathrm{d}^3 r)) \cap \mathcal{H}_+^{\mathrm{rel}}$,

$$\big\langle f, |\cdot|^{-\kappa} f \big\rangle \leq \frac{M_{\kappa/2}^2}{2} \, \langle f, |A_0| \, f \rangle \,. \tag{5.2.16}$$

Proof. a) By [Her77, Theorem 2.5], for all $h \in \mathbb{C}^{16} \otimes \mathcal{S}(\mathbb{R}^3)$ we have the bound

$$\big\| |\cdot|^{-\kappa} (\hat{p}^2 + 1)^{-\kappa/2} h \big\| \leq M_\kappa \|h\|. \tag{5.2.17}$$

This inequality extends to all $h \in \mathcal{H}_+^{\mathrm{rel}}$. Now, for all $f \in \mathcal{D}_+$, there exists a $g \in \mathcal{H}_+^{\mathrm{rel}}$ such that $f = (\hat{p}^2 + 1)^{-\kappa/2} g$. Thus, for all $f \in \mathcal{D}_+$ we can compute

$$\big\| |\cdot|^{-\kappa} f \big\| = \big\| |\cdot|^{-\kappa} (\hat{p}^2 + 1)^{-\kappa/2} g \big\| \leq M_\kappa \|g\| = M_\kappa \, \big\| (\hat{p}^2 + 1)^{\kappa/2} f \big\| \,. \tag{5.2.18}$$

With part c) of Lemma 5.4, for all $f \in \mathcal{D}_+$ we obtain

$$\begin{aligned} \big\| |\cdot|^{-\kappa} f \big\| &\leq \frac{M_\kappa}{2} \, \big\| 2(\hat{p}^2 + 1)^{\kappa/2} f \big\| \\ &\leq \frac{M_\kappa}{2} \, \big\| 2(\hat{p}^2 + 1)^{1/2} P_+ f \big\| \\ &= \frac{M_\kappa}{2} \, \big\| |\mathbf{M}^- \cdot \hat{\boldsymbol{p}} + B P_+| \, f \big\| \\ &= \frac{M_\kappa}{2} \, \|A_0 f\| \,, \end{aligned} \tag{5.2.19}$$

which proves the claim.

b) Due to (5.2.18), we find for all $f \in \mathcal{D}_+$

$$\begin{aligned} \big\langle f, |\cdot|^{-\kappa} f \big\rangle &= \big\| |\cdot|^{-\kappa/2} f \big\|^2 \\ &\leq M_{\kappa/2}^2 \, \big\| (\hat{p}^2 + 1)^{\kappa/4} P_+ f \big\|^2 \\ &= M_{\kappa/2}^2 \, \big\langle f, (\hat{p}^2 + 1)^{1/2} P_+ f \big\rangle \\ &= \frac{M_{\kappa/2}^2}{2} \, \big\langle f, 2(\hat{p}^2 + 1)^{1/2} P_+ f \big\rangle \\ &= \frac{M_{\kappa/2}^2}{2} \, \langle f, |A_0| \, f \rangle \,. \end{aligned} \tag{5.2.20}$$

Since $\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \, \mathrm{d}^3 r)$ is a core of $\langle \cdot, (\hat{p}^2 + 1)^{1/2} \cdot \rangle$ (see [LL01, Theorem 7.14]), this computation extends to all $f \in (\mathbb{C}^{16} \otimes H^{1/2}(\mathbb{R}^3, \, \mathrm{d}^3 r)) \cap \mathcal{H}_+^{\mathrm{rel}}$. $\square$

Part a) of Lemma 5.4 says that B leaves $\mathcal{H}_+^{\mathrm{rel}}$ invariant. Consequently, we can define the operator

$$A := A_0 + P_+\gamma V P_+ \tag{5.2.21}$$

in the underlying Hilbert space $\mathcal{H}_+^{\mathrm{rel}}$ with domain

$$\mathcal{D}(A) = \mathcal{D}_+ = \big(\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3, \mathrm{d}^3 r)\big) \cap \mathcal{H}_+^{\mathrm{rel}}. \tag{5.2.22}$$

The next lemma provides important properties of A in order to obtain a self-adjoint extension of $H^{\mathrm{rel}} + P_+BP_+$ later on in Theorem 5.11.

Lemma 5.6. *Let $0 < \kappa \leq 1$ and let M_κ be given as in Lemma 5.5. Moreover, let $|\gamma| M_\kappa < 2$. Then,*

a) A is self-adjoint on $\mathcal{D}_+$, and

b) $0 \in \rho(A)$.

Proof. a) Since BP_+ is symmetric and bounded, A_0 is self-adjoint on $\mathcal{D}_+$ by Lemma 4.3b). We have for all $f \in \mathcal{D}_+$

$$\|P_+\gamma V P_+ f\| \leq \|\gamma V f\| = \left\| \frac{\gamma}{|\cdot|^\kappa} f \right\| \leq \frac{|\gamma| M_\kappa}{2} \|A_0 f\| \tag{5.2.23}$$

where we used Lemma 5.5a) in the last estimate. For $|\gamma| M_\kappa < 2$, the Kato-Rellich theorem (see, e.g., [RS75, Theorem X.12]) now implies self-adjointness of A on $\mathcal{D}_+$.

b) First, we prove that A_0 has a bounded inverse $A_0^{-1} \colon \mathcal{H}_+^{\mathrm{rel}} \to \mathcal{D}_+$. For all $f \in \mathcal{H}_+^{\mathrm{rel}}$, we find $(\hat{p}^2 + 1)^{-1} f \in \mathbb{C}^{16} \otimes H^2(\mathbb{R}^3, \mathrm{d}^3 r)$ and $A_0(\hat{p}^2 + 1)^{-1} f \in \mathcal{D}_+$ with

$$\big\|A_0(\hat{p}^2 + 1)^{-1}\big\| = \sup_{\boldsymbol{p} \in \mathbb{R}^3} \left| \frac{\mathbf{M}^- \cdot \boldsymbol{p} + BP_+(\boldsymbol{p})}{p^2 + 1} \right| = 2 \tag{5.2.24}$$

By Lemma 5.4b), on $(\mathbb{C}^{16} \otimes H^2(\mathbb{R}^3, \mathrm{d}^3 r)) \cap \mathcal{H}_+^{\mathrm{rel}}$ we have $A_0^2 = 4(\hat{p}^2 + 1)P_+$. Hence, for all $f \in \mathcal{H}_+^{\mathrm{rel}}$

$$A_0 \left(\frac{1}{4} A_0 (\hat{p}^2 + 1)^{-1} f \right) = f \tag{5.2.25}$$

which together with Eq. (5.2.24) implies that $A_0^{-1} = {}^1\!/\!_4 A_0(\hat{p}^2 + 1)^{-1}$.

Moreover, for $|\gamma| M_\kappa < 2$, a theorem by Kato [Kat95, Theorem IV.1.16, p. 196] in combination with Eq. (5.2.23) gives the existence of a bounded inverse of A. The same theorem by Kato also implies that $A\mathcal{D}(A) = \mathcal{H}_+^{\mathrm{rel}}$ (see [Sch72, Lemma 1]), which in return implies $0 \in \rho(A)$. □

Next, we aim at the Frobenius-Schur factorization of $H^{\mathrm{rel}} + P_+BP_+$. Recalling the matrix representation of $H^{\mathrm{rel}} + P_+BP_+$ from line (5.2.8), we find

$$H^{\mathrm{rel}} + P_+BP_+ = \begin{pmatrix} A & P_+\gamma VP_- \\ P_-\gamma VP_+ & P_-\gamma VP_- \end{pmatrix} \tag{5.2.26}$$

with domains

$$\begin{aligned} A\colon \mathcal{D}_+ \to \mathcal{H}_+^{\mathrm{rel}}, \quad & P_+\gamma VP_-\colon \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}} \to \mathcal{H}_+^{\mathrm{rel}} \\ P_-\gamma VP_+\colon \mathcal{D}(V) \cap \mathcal{H}_+^{\mathrm{rel}} \to \mathcal{H}_-^{\mathrm{rel}}, \quad & P_-\gamma VP_-\colon \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}} \to \mathcal{H}_-^{\mathrm{rel}} \end{aligned} \tag{5.2.27}$$

and define the Schur complement $S\colon \mathcal{D}(S) \to \mathcal{H}_-^{\mathrm{rel}}$ of A by

$$S := P_-\gamma VP_- - P_-\gamma VP_+A^{-1}P_+\gamma VP_- \tag{5.2.28}$$

with domain

$$\mathcal{D}(S) = \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}. \tag{5.2.29}$$

That S is well-defined, and thus the Frobenius-Schur factorization of $H^{\mathrm{rel}}+P_+BP_+$ exists, is the content of the next lemma.

Lemma 5.7. *Let $0 < \kappa \leq 1$ and let $|\gamma|M_\kappa < 2$. Then, the matrix representation of $H^{\mathrm{rel}} + P_+BP_+$ is symmetric and its Frobenius-Schur factorization is given by*

$$\begin{aligned} &H^{\mathrm{rel}} + P_+BP_+ = \\ &\quad = \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ P_-\gamma VP_+A^{-1} & \mathrm{id} \end{pmatrix} \begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & S \end{pmatrix} \begin{pmatrix} \mathrm{id} & A^{-1}P_+\gamma VP_- \\ \mathbf{0} & \mathrm{id} \end{pmatrix}. \end{aligned} \tag{5.2.30}$$

Proof. We use the theory of unbounded matrix operators in Hilbert space from Appendix A. There we introduced the conditions **M1-M6**, which we need to check now:

M1 The entries $A, P_+\gamma VP_-, P_-\gamma VP_+$, and $P_-\gamma VP_-$ have dense domains by Proposition 5.3. As they are symmetric, A and $P_-\gamma VP_-$ are closable. $P_+\gamma VP_-$ is closable as $(P_-\gamma VP_+)^*$ is a closed extension of it which can be seen as follows. Suppose that $f \in \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$ and $g \in \mathcal{D}(V) \cap \mathcal{H}_+^{\mathrm{rel}}$. Then, we find

$$\langle f, P_-VP_+g\rangle = \langle f, Vg\rangle = \langle Vf, g\rangle = \langle P_+VP_-f, g\rangle\,, \tag{5.2.31}$$

and thus, $f \in \mathcal{D}((P_-\gamma VP_+)^*)$ holds. An analogous argument applies to $P_-\gamma VP_+$ and $(P_+\gamma VP_-)^*$.

M2 $\mathcal{D}(P_+\gamma VP_-) = \mathcal{D}(P_-\gamma VP_-)$ by definition in (5.2.27).

M3 The resolvent set of A is not empty as $0 \in \rho(A)$ by Lemma 5.6.

M4 $\mathcal{D}(A^*) = \mathcal{D}_+ \subset \mathcal{D}((P_+\gamma VP_-)^*)$ by definition in (5.2.27) and Hardy's inequality.

M5 $\mathcal{D}(A) \subset \mathcal{D}(P_-\gamma VP_+)$ by line (5.2.27) and Hardy's inequality.

M6 $\mathcal{D}(H^{\mathrm{rel}} + P_+ B P_+) = \mathcal{D}_+ \oplus (\mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}})$ which is dense in $\mathcal{H}^{\mathrm{rel}}$ by Proposition 5.3.

Symmetry follows from the criterion in Lemma A.1 for which we use self-adjointess of A from Lemma 5.6. Existence of the Frobenius-Schur factorization then follows from Theorem A.3. □

As outlined in Section 2.2 and briefly at the beginning of this section, the crucial ingredient in finding a self-adjoint extension of H_{2BD} is to find a self-adjoint extension of the Schur complement S. However, before we can present this extension in Lemma 5.10 below, we need to provide the technical results of Theorem 5.8 and Lemma 5.9.

Theorem 5.8. *Let $0 < \kappa \leq 1$. For every $f \in \mathcal{D}(V^{1/2}) \cap \mathcal{H}_-^{\mathrm{rel}}$, there exists a sequence $(f_n)_{n\in\mathbb{N}} \subset \mathcal{D}(V)$ such that*

$$\|f - P_- f_n\| + \left\|V^{1/2} P_-(f - f_n)\right\| \xrightarrow{n\to\infty} 0. \tag{5.2.32}$$

Proof. Let $f \in \mathcal{D}(V^{1/2}) \cap \mathcal{H}_-^{\mathrm{rel}}$. First, we define the Gaussian χ_n for all $n \in \mathbb{N}$ by

$$\chi_n(\boldsymbol{r}) := e^{-2^n \pi |\boldsymbol{r}|^2}, \tag{5.2.33}$$

and with its help the Gaussian cut-off $1 - \chi_n$ for f by $f_n := (1 - \chi_n)f$. By construction, $(f_n)_{n\in\mathbb{N}} \subset \mathcal{D}(V)$ for all $n \in \mathbb{N}$ since we have $(1 - \chi_n(\boldsymbol{r}))|\boldsymbol{r}|^{-\kappa} \to 0$ as $|\boldsymbol{r}| \to 0$ for all $n \in \mathbb{N}$.

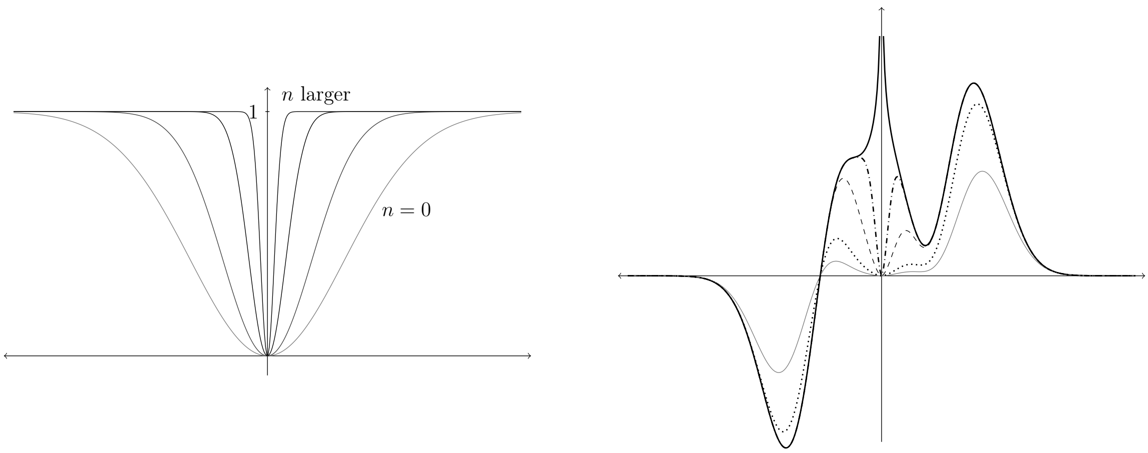

Figure 5.1.: The Gaussian cut-off function $1 - \chi_n$ for $n = 0$ and for n larger is depicted on the left. On the right, an arbitrary function f (solid line) with singularity in the origin and some of its cut-off versions $(1 - \chi_n)f$ (dashed lines) are shown. Notice that the cut-off versions all pass the origin.

Dominated convergence implies

$$\|f - f_n\|^2 = \|f - (1 - \chi_n)f\|^2 = \int_{\mathbb{R}^3} |\chi_n(\boldsymbol{r})|^2 \, |f(\boldsymbol{r})|^2 \, \mathrm{d}^3 r \xrightarrow{n\to\infty} 0 \tag{5.2.34}$$

since $|\chi_n(\boldsymbol{r})|^2 \leq 1$ and $|\chi_n(\boldsymbol{r})|^2 \xrightarrow{n\to\infty} 0$ for almost all $\boldsymbol{r} \in \mathbb{R}^3$, and therefore,

$$\|f - P_- f_n\| \; = \; \|P_- f - P_- f_n\| \leq \|P_-\| \|f - f_n\| \xrightarrow{n\to\infty} 0. \tag{5.2.35}$$

In order to show $\left\|V^{1/2}P_-(f-f_n)\right\| \xrightarrow{n\to\infty} 0$, we estimate

$$\begin{aligned}\left\|V^{1/2}P_-(f-f_n)\right\| &\leq \left\|P_-V^{1/2}\chi_n f\right\| + \left\|\left[V^{1/2},P_-\right]\chi_n f\right\| \\ &\leq \left\|P_-\right\|\left\|V^{1/2}\chi_n f\right\| + \left\|\left[V^{1/2},\tau\right]\chi_n f\right\|,\end{aligned} \tag{5.2.36}$$

where we used $P_- = 1/2\,(\mathrm{id}-\tau)$. Hence, using $f\in\mathcal{D}(V^{1/2})$, we get for the first summand of (5.2.36) by dominated convergence as above

$$\left\|V^{1/2}\chi_n f\right\| \xrightarrow{n\to\infty} 0. \tag{5.2.37}$$

In order to treat the second summand of (5.2.36), we note the following. In the paragraph leading to the definition of T_{ij} in line (3.3.7), we saw that in order to control τ, it suffices to control T_{ij}. Thus, denoting the spinor components of f by f^k, $k=1,2,\ldots,16$, it remains to show

$$\left\|\left[V^{1/2},T_{ij}\right]\chi_n f^k\right\| \xrightarrow{n\to\infty} 0 \tag{5.2.38}$$

for all $i,j=1,2,3$ and $k=1,2,\ldots,16$.

In the following, we will collect all numerical factors, which are independent of ε, $\boldsymbol{r}$, and $\boldsymbol{y}$, by the same symbol C. The exact value of C might therefore change from one line to the next.

Using that $V^{1/2}$ is multiplication with $|\cdot|^{-\kappa/2}$ and thus commutes with that summand of T_{ij} which contains the Kronecker delta δ_{ij}, we estimate for almost all $\boldsymbol{r}\in\mathbb{R}$ and for all i,j,k

$$\begin{aligned}&\left|\left(\left[|\cdot|^{-\kappa/2},T_{ij}\right]\chi_n f^k\right)(\boldsymbol{r})\right| \\ &= C\left|\lim_{\varepsilon\to0}\int_{|\boldsymbol{y}|>\varepsilon} K_{ij}(\boldsymbol{y})\left(\frac{1}{|\boldsymbol{r}|^{\kappa/2}}-\frac{1}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}}\right)\chi_n(\boldsymbol{r}-\boldsymbol{y})f^k(\boldsymbol{r}-\boldsymbol{y})\,\mathrm{d}^3y\right| \\ &\leq C\lim_{\varepsilon\to0}\int_{|\boldsymbol{y}|>\varepsilon}\frac{1}{|\boldsymbol{y}|^3}\left|\frac{1}{|\boldsymbol{r}|^{\kappa/2}}-\frac{1}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}}\right|\chi_n(\boldsymbol{r}-\boldsymbol{y})\left|f^k(\boldsymbol{r}-\boldsymbol{y})\right|\,\mathrm{d}^3y \\ &= C\lim_{\varepsilon\to0}\int_{|\boldsymbol{y}|>\varepsilon}\frac{1}{|\boldsymbol{y}|^3}\left|\frac{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}-|\boldsymbol{r}|^{\kappa/2}}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}|\boldsymbol{r}|^{\kappa/2}}\right|\chi_n(\boldsymbol{r}-\boldsymbol{y})\left|f^k(\boldsymbol{r}-\boldsymbol{y})\right|\,\mathrm{d}^3y \\ &\overset{(*)}{\leq} C\lim_{\varepsilon\to0}\int_{|\boldsymbol{y}|>\varepsilon}\frac{1}{|\boldsymbol{y}|^3}\frac{|\boldsymbol{y}|^{\kappa/2}}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}|\boldsymbol{r}|^{\kappa/2}}\chi_n(\boldsymbol{r}-\boldsymbol{y})\left|f^k(\boldsymbol{r}-\boldsymbol{y})\right|\,\mathrm{d}^3y \\ &= C\frac{1}{|\boldsymbol{r}|^{\kappa/2}}\lim_{\varepsilon\to0}\int_{|\boldsymbol{y}|>\varepsilon}\frac{1}{|\boldsymbol{y}|^{3-\kappa/2}}\frac{\chi_n(\boldsymbol{r}-\boldsymbol{y})\left|f^k(\boldsymbol{r}-\boldsymbol{y})\right|}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}}\,\mathrm{d}^3y \\ &= C\frac{1}{|\boldsymbol{r}|^{\kappa/2}}\int_{\mathbb{R}^3}\frac{1}{|\boldsymbol{y}|^{3-\kappa/2}}\frac{\chi_n(\boldsymbol{r}-\boldsymbol{y})\left|f^k(\boldsymbol{r}-\boldsymbol{y})\right|}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}}\,\mathrm{d}^3y\end{aligned} \tag{5.2.39}$$

where we used Theorem 3.6b) together with dominated convergence in the last step and

Lemma B.1 (Appendix B) in $(*)$. We define h_n for almost all $\boldsymbol{r} \in \mathbb{R}^3$ by

$$h_n(\boldsymbol{r}) := \int_{\mathbb{R}^3} \frac{1}{|\boldsymbol{y}|^{3-\kappa/2}} \frac{\chi_n(\boldsymbol{r}-\boldsymbol{y}) \left| f^k(\boldsymbol{r}-\boldsymbol{y}) \right|}{|\boldsymbol{r}-\boldsymbol{y}|^{\kappa/2}} \, \mathrm{d}^3 y. \tag{5.2.40}$$

Now, we exploit the Gaussian nature of the cut-off, i.e., the fact that χ_n from line (5.2.33) lies in $L^p(\mathbb{R}^3)$ for all $p \geq 1$. This implies $|\cdot|^{-\kappa/2}\chi_n|f^k| \in L^p(\mathbb{R}^3)$ for all $p \in [1,2]$ and $n \in \mathbb{N}$ as $|\cdot|^{-\kappa/2}|f^k| \in L^2(\mathbb{R}^3)$. With Theorem 3.6b), we can then conclude $h_n \in L^2(\mathbb{R}^3)$ for all $n \in \mathbb{N}$. Thus, h_n has a Fourier transform, which, also by Theorem 3.6b), is for almost all $\boldsymbol{p} \in \mathbb{R}^3$ given by

$$\hat{h}_n(\boldsymbol{p}) = \frac{C}{|\boldsymbol{p}|^{\kappa/2}} \mathcal{F}\left(\frac{\chi_n \left| f^k \right|}{|\cdot|^{\kappa/2}} \right)(\boldsymbol{p}). \tag{5.2.41}$$

A further consequence, known as Hardy-Littlewood-Sobolev theorem of fractional integration (see [Ste70, Chapter V, Theorem 1]), is the inequality

$$\|h_n\|_2 \leq C \left\| \frac{\chi_n \left| f^k \right|}{|\cdot|^{\kappa/2}} \right\|_{\frac{6}{3+\kappa}}. \tag{5.2.42}$$

Note the different L^p-norms. Since $\chi_n \leq \chi_1$ and χ_1 is a Gaussian and thus lies in $L^p(\mathbb{R}^3)$ for all $p \geq 1$, we can conclude with dominated convergence

$$\left\| \frac{\chi_n \left| f^k \right|}{|\cdot|^{\kappa/2}} \right\|_{\frac{6}{3+\kappa}} \xrightarrow{n\to\infty} 0. \tag{5.2.43}$$

Putting everything together then yields

$$\begin{aligned} \left\| \left[|\cdot|^{-\kappa/2}, T_{ij} \right] \chi_n f^k \right\| &\overset{\text{(i)}}{\leq} C \left\| |\cdot|^{-\kappa/2} h_n \right\| \\ &\overset{\text{(ii)}}{\leq} C \left\| \left(|\hat{\boldsymbol{p}}|^2 + 1 \right)^{\kappa/4} h_n \right\| \\ &\leq C \left(\left\| |\hat{\boldsymbol{p}}|^{\kappa/2} h_n \right\| + \|h_n\| \right) \\ &\overset{\text{(iii)}}{\leq} C \left\| \frac{\chi_n \left| f^k \right|}{|\cdot|^{\kappa/2}} \right\|_2 + C \left\| \frac{\chi_n \left| f^k \right|}{|\cdot|^{\kappa/2}} \right\|_{\frac{6}{3+\kappa}} \xrightarrow{n\to\infty} 0, \end{aligned} \tag{5.2.44}$$

where we used (5.2.39), (5.2.40) in (i), (5.2.18) from the proof of Lemma 5.5 in (ii), (5.2.41), (5.2.42) in (iii), and dominated convergence and line (5.2.43) for the convergence $n \to \infty$. This proves the statement. $\square$

Lemma 5.9. *Let* $0 < \kappa \le 1$ *and let* $|\gamma| M^2_{\kappa/2} < 1$*. Then, the operator*

$$(|\gamma| V)^{1/2} P_+ A^{-1} P_+ (|\gamma| V)^{1/2} \colon \mathcal{D}(V^{1/2}) \to \mathcal{H}^{\mathrm{rel}} \tag{5.2.45}$$

is bounded on the dense set $\mathcal{D}(V^{1/2})$ *with*

$$C := \|(|\gamma| V)^{1/2} P_+ A^{-1} P_+ (|\gamma| V)^{1/2}\| < 1. \tag{5.2.46}$$

Proof. As preparation, we prove that the operator $(|\gamma|V)^{1/2} P_+ |A_0|^{-1/2} \colon \mathcal{H}^{\mathrm{rel}}_+ \to \mathcal{H}^{\mathrm{rel}}$ is bounded with norm

$$\left\|(|\gamma| V)^{1/2} P_+ |A_0|^{-1/2}\right\| \le \sqrt{|\gamma|/2}\, M_{\kappa/2}. \tag{5.2.47}$$

This is equivalent to

$$\left\|(|\gamma| V)^{1/2} |A_0|^{-1/2}\right\| \le \sqrt{|\gamma|/2}\, M_{\kappa/2}, \tag{5.2.48}$$

as $|A_0|^{-1/2}$ maps into $\mathcal{H}^{\mathrm{rel}}_+$. By Lemma 5.5b), for all $f \in (\mathbb{C}^{16} \otimes H^{1/2}(\mathbb{R}^3, \mathrm{d}^3 r)) \cap \mathcal{H}^{\mathrm{rel}}_+$ we get

$$\langle f, |\gamma| V f\rangle = |\gamma| \left\langle f, |\cdot|^{-\kappa} f \right\rangle \le \frac{|\gamma| M^2_{\kappa/2}}{2} \langle f, |A_0|\, f\rangle \tag{5.2.49}$$

or equivalently

$$\left\|(|\gamma| V)^{1/2} f\right\| \le \sqrt{\frac{|\gamma|}{2}}\, M_{\kappa/2} \left\| |A_0|^{1/2}\, f \right\|. \tag{5.2.50}$$

As $|A_0|^{-1/2}$ maps $\mathcal{H}^{\mathrm{rel}}_+$ into $(\mathbb{C}^{16} \otimes H^{1/2}(\mathbb{R}^3, \mathrm{d}^3 r)) \cap \mathcal{H}^{\mathrm{rel}}_+$, this implies for all $g \in \mathcal{H}^{\mathrm{rel}}_+$

$$\left\|(|\gamma| V)^{1/2}\, |A_0|^{-1/2}\, g\right\| \le \sqrt{\frac{|\gamma|}{2}}\, M_{\kappa/2}\, \|g\|\,. \tag{5.2.51}$$

This also implies

$$\begin{aligned}\left\| |A_0|^{-1/2}\, P_+ (|\gamma| V)^{1/2} \right\| &= \left\| \left(|A_0|^{-1/2}\, P_+ (|\gamma| V)^{1/2} \right)^* \right\| \\ &= \left\| \left((|\gamma| V)^{1/2} \right)^* P_+^* \left(|A_0|^{-1/2} \right)^* \right\| \\ &= \left\| (|\gamma| V)^{1/2} P_+\, |A_0|^{-1/2} \right\| \le \sqrt{\frac{|\gamma|}{2}}\, M_{\kappa/2}. \end{aligned} \tag{5.2.52}$$

We use the polar decomposition $A_0 = U_{A_0} |A_0|$. Note that $\mathrm{Ker}(A_0) = \{0\}$, and hence,

U_{A_0} is unitary. We obtain

$$\begin{aligned}
\left\|(|\gamma|V)^{1/2}P_+A_0^{-1}P_+(|\gamma|V)^{1/2}\right\| &= \left\|(|\gamma|V)^{1/2}P_+\left(U_{A_0}|A_0|\right)^{-1}P_+(|\gamma|V)^{1/2}\right\| \\
&= \left\|(|\gamma|V)^{1/2}P_+|A_0|^{-1}U_{A_0}^{-1}P_+(|\gamma|V)^{1/2}\right\| \\
&= \left\|(|\gamma|V)^{1/2}P_+|A_0|^{-1/2}U_{A_0}^{-1}|A_0|^{-1/2}P_+(|\gamma|V)^{1/2}\right\| \\
&\le \left\|(|\gamma|V)^{1/2}P_+|A_0|^{-1/2}\right\|^2\left\|U_{A_0}^{-1}\right\| \\
&\le \frac{|\gamma|M_{\kappa/2}^2}{2}
\end{aligned} \tag{5.2.53}$$

where we used unitarity of $U_{A_0}^{-1}$ and the fact that $U_{A_0}^{-1}$ and $|A_0|^{-1/2}$ commute as both are functions of the self-adjoint operator A_0.

With the help of the resolvent identity we find

$$\begin{aligned}
&\left\|(|\gamma|V)^{1/2}P_+A^{-1}P_+(|\gamma|V)^{1/2}\right\| \\
&\le \left\|(|\gamma|V)^{1/2}P_+\left(A^{-1}-A_0^{-1}\right)P_+(|\gamma|V)^{1/2}\right\| + \left\|(|\gamma|V)^{1/2}P_+A_0^{-1}P_+(|\gamma|V)^{1/2}\right\| \\
&\le \left\|(|\gamma|V)^{1/2}P_+A^{-1}(A_0-A)A_0^{-1}P_+(|\gamma|V)^{1/2}\right\| + \frac{|\gamma|M_{\kappa/2}^2}{2} \\
&= \left\|(|\gamma|V)^{1/2}P_+A^{-1}P_+|\gamma|VP_+A_0^{-1}P_+(|\gamma|V)^{1/2}\right\| + \frac{|\gamma|M_{\kappa/2}^2}{2} \\
&= \left\|\left((|\gamma|V)^{1/2}P_+A^{-1}P_+(|\gamma|V)^{1/2}\right)\left((|\gamma|V)^{1/2}P_+A_0^{-1}P_+(|\gamma|V)^{1/2}\right)\right\| + \frac{|\gamma|M_{\kappa/2}^2}{2} \\
&\le \frac{|\gamma|M_{\kappa/2}^2}{2}\left\|(|\gamma|V)^{1/2}P_+A^{-1}P_+(|\gamma|V)^{1/2}\right\| + \frac{|\gamma|M_{\kappa/2}^2}{2}
\end{aligned} \tag{5.2.54}$$

which implies

$$C = \left\|(|\gamma|V)^{1/2}P_+A^{-1}P_+(|\gamma|V)^{1/2}\right\| \le \frac{|\gamma|M_{\kappa/2}^2}{2-|\gamma|M_{\kappa/2}^2}. \tag{5.2.55}$$

If $|\gamma|M_{\kappa/2}^2 < 1$, then $C < 1$. This concludes the proof. □

Lemma 5.10. *Let $0 < \kappa \le 1$ and let $|\gamma|M_{\kappa/2}^2 < 1$. Then, the form sum*

$$S_F := \gamma(V^{1/2}P_-)^*V^{1/2}P_- - P_-\gamma VP_+A^{-1}P_+\gamma VP_- \tag{5.2.56}$$

with domain

$$\mathcal{D}(S_F) = \mathcal{D}(V^{1/2}) \cap \mathcal{D}(S^*) \tag{5.2.57}$$

defines a self-adjoint extension of S.

Proof. In what follows, it is very useful to distinguish the different scalar products of the underlying Hilbert spaces $\mathcal{H}^{\mathrm{rel}}$ and $\mathcal{H}_-^{\mathrm{rel}}$, respectively. We define two forms that map from

$\mathcal{H}_{-}^{\mathrm{rel}} \times \mathcal{H}_{-}^{\mathrm{rel}}$ into $\mathbb{C}$. First, we define the form of $P_{-}VP_{-}$ by

$$\mathfrak{v}[f,g] := \langle f, P_{-}VP_{-}g\rangle_{\mathcal{H}_{-}^{\mathrm{rel}}}\ , \quad \mathcal{D}(\mathfrak{v}) = \mathcal{D}(V) \cap \mathcal{H}_{-}^{\mathrm{rel}}. \tag{5.2.58}$$

Second, we define the form $\mathfrak{t}$ by

$$\mathfrak{t}[f,g] := \left\langle V^{1/2}P_{-}f, V^{1/2}P_{-}g\right\rangle_{\mathcal{H}^{\mathrm{rel}}}\ , \quad \mathcal{D}(\mathfrak{t}) = \mathcal{D}(V^{1/2}) \cap \mathcal{H}_{-}^{\mathrm{rel}}. \tag{5.2.59}$$

Furthermore, we define the restriction of $V^{1/2}$ to $\mathcal{H}_{-}^{\mathrm{rel}}$. In order to clearly distinguish it from $V^{1/2}$, we write $V^{1/2}P_{-}$, i.e.,

$$V^{1/2}P_{-} \colon \mathcal{D}(V^{1/2}) \cap \mathcal{H}_{-}^{\mathrm{rel}} \to \mathcal{H}^{\mathrm{rel}}. \tag{5.2.60}$$

As it is a map from $\mathcal{H}_{-}^{\mathrm{rel}}$ to $\mathcal{H}^{\mathrm{rel}}$, its adjoint $(V^{1/2}P_{-})^{*}$ maps from $\mathcal{H}^{\mathrm{rel}}$ back to $\mathcal{H}_{-}^{\mathrm{rel}}$. We list a number of properties.

(i) $\mathfrak{v}$, $\mathfrak{t}$ are symmetric since V and $V^{1/2}$ are self-adjoint in the underlying Hilbert space $\mathcal{H}^{\mathrm{rel}}$.

(ii) $\mathfrak{v}$, $\mathfrak{t}$ are positive since V and $V^{1/2}$ are positive.

(iii) $V^{1/2}P_{-}$ is closed since $V^{1/2}$ and P_{-} are closed and P_{-} is bounded. Thus, $\mathfrak{t}$ is closed.

We claim that $\overline{\mathfrak{v}} = \mathfrak{t}$. For all $f, g \in \mathcal{D}(V) \cap \mathcal{H}_{-}^{\mathrm{rel}}$, we compute

$$\begin{aligned}\mathfrak{v}[f,g] &= \langle f, P_{-}VP_{-}g\rangle_{\mathcal{H}_{-}^{\mathrm{rel}}} = \langle P_{-}f, VP_{-}g\rangle_{\mathcal{H}^{\mathrm{rel}}} \\ &= \left\langle P_{-}f, V^{1/2}V^{1/2}P_{-}g\right\rangle_{\mathcal{H}^{\mathrm{rel}}} \\ &= \left\langle V^{1/2}P_{-}f, V^{1/2}P_{-}g\right\rangle_{\mathcal{H}^{\mathrm{rel}}} = \mathfrak{t}[f,g]\end{aligned} \tag{5.2.61}$$

where we used self-adjointness of P_{-} and $V^{1/2}$. Hence, $\mathfrak{v}$ coincides with $\mathfrak{t}$ on $\mathcal{D}(V) \cap \mathcal{H}_{-}^{\mathrm{rel}}$. Since $\mathcal{D}(V) \cap \mathcal{H}_{-}^{\mathrm{rel}}$ is a form core for $\mathfrak{t}$ by Theorem 5.8, we can conclude that $\overline{\mathfrak{v}} = \mathfrak{t}$.

Now, by [RS80, Theorem VIII.15], $\mathfrak{t}$ is the form of a unique self-adjoint operator, denoted by V_F with domain $\mathcal{D}(V_F)$. In particular, V_F is self-adjoint in the underlying Hilbert space $\mathcal{H}_{-}^{\mathrm{rel}}$. Since V is positive and self-adjoint on $\mathcal{D}(V)$, $P_{-}VP_{-}$ is positive and symmetric on $\mathcal{D}(V) \cap \mathcal{H}_{-}^{\mathrm{rel}}$. Therefore, also $\overline{\mathfrak{v}}$ is the form of a unique self-adjoint operator by [RS75, Theorem X.23]. By $\overline{\mathfrak{v}} = \mathfrak{t}$ from above, we know that the operator associated with $\overline{\mathfrak{v}}$ is V_F. V_F is the Friedrichs extension of $P_{-}VP_{-}$ and it is the unique self-adjoint extension whose domain is contained in $\mathcal{D}(\overline{\mathfrak{v}})$. Moreover, by [Sch12, Theorem 10.17], we have

$$\begin{aligned}\mathcal{D}(V_F) &= \mathcal{D}(\overline{\mathfrak{v}}) \cap \mathcal{D}((P_{-}VP_{-})^{*}) \\ &= \mathcal{D}(\mathfrak{t}) \cap \mathcal{D}((P_{-}VP_{-})^{*}) \\ &= \mathcal{D}(V^{1/2}) \cap \mathcal{D}((P_{-}VP_{-})^{*}).\end{aligned} \tag{5.2.62}$$

We compute V_F. For all $f \in \mathcal{D}(\mathfrak{t})$ and $g \in \mathcal{D}(V_F)$ we obtain

$$\left\langle V^{1/2}P_-f, V^{1/2}P_-g \right\rangle_{\mathcal{H}^{\mathrm{rel}}} = \mathfrak{t}[f,g] = \langle f, V_F g \rangle_{\mathcal{H}_-^{\mathrm{rel}}}\,. \tag{5.2.63}$$

Therefore, $V^{1/2}P_-g$ lies in $\mathcal{D}((V^{1/2}P_-)^*)$, and density of $\mathcal{D}(\mathfrak{t})$ implies $(V^{1/2}P_-)^*V^{1/2}P_-g = V_F g$ holds for all $g \in \mathcal{D}(V_F)$. We obtain $V_F \subseteq (V^{1/2}P_-)^*V^{1/2}P_-$. Self-adjointness of V_F and symmetry of $(V^{1/2}P_-)^*V^{1/2}P_-$ imply $V_F = (V^{1/2}P_-)^*V^{1/2}P_-$.

In order to connect the above to S, we estimate for all $f \in \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$

$$\begin{aligned}
&\left|\left\langle f, P_-VP_+\gamma A^{-1}P_+VP_-f \right\rangle_{\mathcal{H}_-^{\mathrm{rel}}}\right| \\
&= \left|\left\langle V^{1/2}P_-f, \left(V^{1/2}P_+\gamma A^{-1}P_+V^{1/2}\right)V^{1/2}P_-f \right\rangle_{\mathcal{H}^{\mathrm{rel}}}\right| \\
&\leq \left\|V^{1/2}P_-f\right\| \left\|V^{1/2}P_+\gamma A^{-1}P_+V^{1/2}\right\| \left\|V^{1/2}P_-f\right\| \\
&= C\,\langle f, P_-VP_-f \rangle_{\mathcal{H}_-^{\mathrm{rel}}} \\
&= C\,\langle f, V_F f \rangle_{\mathcal{H}_-^{\mathrm{rel}}}
\end{aligned} \tag{5.2.64}$$

where $C < 1$ holds by Lemma 5.9. Again by Theorem 5.8, we know that $\mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$ is a form core for $\mathfrak{t}$, and thus, the inequality (5.2.64) also holds for all $f \in \mathcal{D}(V_F)$.

The KLMN-theorem (see, e.g., [RS75, Theorem X.17]) guarantees that the form sum $V_F - P_-VP_+\gamma A^{-1}P_+VP_-$ is a self-adjoint operator with domain $\mathcal{D}(V_F)$. Moreover, as γ is real, we know that the form sum $S_F := \gamma V_F - P_-\gamma VP_+A^{-1}P_+\gamma VP_-$ with domain $\mathcal{D}(S_F) = \mathcal{D}(V_F)$ is a self-adjoint extension of S.

It remains to show that $\mathcal{D}(S_F) = \mathcal{D}(V^{1/2}) \cap \mathcal{D}(S^*)$. To that end, we introduce the abbreviation $K \equiv V - VP_+\gamma A^{-1}P_+V$ such that $S = P_-\gamma KP_-$. Next, we define the form $\mathfrak{k}$ by

$$\mathfrak{k}[f,g] := \langle f, P_-KP_-g \rangle_{\mathcal{H}_-^{\mathrm{rel}}}\,, \quad \mathcal{D}(\mathfrak{k}) = \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}. \tag{5.2.65}$$

From the inequality in line (5.2.64) and positivity of P_-VP_-, we conclude that $\mathfrak{k}[f,f] \geq 0$ for all $f \in \mathcal{D}(\mathfrak{k})$. Thus, by [Sch12, Proposition 10.4], $K \geq 0$ also holds. Self-adjointness of V on $\mathcal{D}(V)$ and the fact that $P_+A^{-1}P_+$ maps into $\mathcal{D}(V)$ imply symmetry of P_-KP_- on $\mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$. Therefore, we know that P_-KP_- has a self-adjoint extension, its Friedrichs extension, denoted by K_F with domain $\mathcal{D}(K_F) = \mathcal{D}(\bar{\mathfrak{k}}) \cap \mathcal{D}((P_-KP_-)^*)$. Since P_-KP_- and S differ only by the real multiple γ, we get $\mathcal{D}(K_F) = \mathcal{D}(\bar{\mathfrak{k}}) \cap \mathcal{D}(S^*)$.

Now, both $V_F - P_-VP_+\gamma A^{-1}P_+VP_-$ and K_F extend P_-KP_-. As they are uniquely distinguished by their respective form domains, we can conclude that they are equal if

$\mathcal{D}(\overline{\mathfrak{v}}) = \mathcal{D}(\overline{\mathfrak{k}})$. In order to prove precisely that, we compute for all $f \in \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$

$$\begin{aligned}
\mathfrak{v}[f,f] &\leq \langle f, P_- V P_- f\rangle \\
&\quad + \frac{1}{1-C}\left(C\,\langle f, P_- V P_- f\rangle - \left\langle f, P_- V P_+ \gamma A^{-1} P_+ V P_- f\right\rangle\right) \\
&= \frac{1}{1-C}\left(\langle f, P_- V P_- f\rangle - \left\langle f, P_- V P_+ \gamma A^{-1} P_+ V P_- f\right\rangle\right) \\
&= \frac{1}{1-C}\,\mathfrak{k}[f,f] \leq \frac{2}{1-C}\,\langle f, P_- V P_- f\rangle = \frac{2}{1-C}\,\mathfrak{v}[f,f]
\end{aligned} \tag{5.2.66}$$

where we used (5.2.64) in the first and second to last step. This shows that $\mathcal{D}(\overline{\mathfrak{v}}) = \mathcal{D}(\overline{\mathfrak{k}})$ and thus $K_F = V_F + P_- V P_+ \gamma A^{-1} P_+ V P_-$. We can now conclude

$$\mathcal{D}(S_F) = \mathcal{D}(K_F) = \mathcal{D}(\overline{\mathfrak{v}}) \cap \mathcal{D}(S^*) = \mathcal{D}(V^{1/2}) \cap \mathcal{D}(S^*), \tag{5.2.67}$$

which finishes the proof. □

Theorem 5.11. *Let* $0 < \kappa \leq 1$ *and* $|\gamma| M_{\kappa/2}^2 < 1$. *Then,*

$$H_F^{\mathrm{rel}} := \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ P_- \gamma V P_+ A^{-1} & \mathrm{id} \end{pmatrix} \begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & S_F \end{pmatrix} \begin{pmatrix} \mathrm{id} & \overline{A^{-1} P_+ \gamma V P_-} \\ \mathbf{0} & \mathrm{id} \end{pmatrix} - P_+ B P_+ \tag{5.2.68}$$

with domain

$$\mathcal{D}(H_F^{\mathrm{rel}}) = \left\{ \begin{pmatrix} f \\ g \end{pmatrix} \in \mathcal{H}_+^{\mathrm{rel}} \oplus \mathcal{H}_-^{\mathrm{rel}} \,\middle|\, \begin{array}{c} f + \overline{A^{-1} P_+ \gamma V P_-} g \in \mathcal{D}_+, \\ g \in \mathcal{D}(S_F) \end{array} \right\} \tag{5.2.69}$$

defines a self-adjoint extension of H^{rel}.

Proof. Since $P_+ B P_+$ is bounded and symmetric, it suffices to show self-adjointness of $H_F^{\mathrm{rel}} + P_+ B P_+$, for which we introduce the short-hand notation

$$\mathcal{R}\,\mathcal{S}_F\,\mathcal{T} \equiv \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ P_- \gamma V P_+ A^{-1} & \mathrm{id} \end{pmatrix} \begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & S_F \end{pmatrix} \begin{pmatrix} \mathrm{id} & \overline{A^{-1} P_+ \gamma V P_-} \\ \mathbf{0} & \mathrm{id} \end{pmatrix}. \tag{5.2.70}$$

where the three operators $\mathcal{R}$, $\mathcal{S}_F$, and $\mathcal{T}$ correspond to the three matrix operators on the right, respectively. We have already shown in the proof of Lemma 5.7 that the assumptions **M1-M6** from Appendix A are met. Hence, by Lemma A.2 from Appendix A, $\mathcal{R}$ and $\mathcal{T}$ are bounded and boundedly invertible as well as $\mathcal{R}^* = \mathcal{T}$ and $\mathcal{T}^* = \mathcal{R}$ hold. Moreover, self-adjointness of A (Lemma 5.6) and of S_F (Lemma 5.10) implies self-adjointness of $\mathcal{S}_F$. It is well-known that operator products with these properties are self-adjoint (see, e.g., [Sch12, Lemma 10.18]), and so, self-adjointness of H_F^{rel} follows. That H_F^{rel} extends H^{rel} follows from $\mathcal{D}(H^{\mathrm{rel}}) \subseteq \mathcal{D}(H_F^{\mathrm{rel}})$ and $S \subseteq S_F$ (Lemma 5.10). □

Theorem 5.12 (Claim a) of Theorem 2)**.** *Let* $0 < \kappa \leq 1$ *and* $|\gamma| M_{\kappa/2}^2 < 1$. *Moreover, let*

V_{ext} be bounded and symmetric. We define

$$H_F := \hat{\boldsymbol{P}} \cdot \mathbf{M}^+ \otimes \mathrm{id}_{L^2(\mathrm{d}^3 r)} + \mathrm{id}_{L^2(\mathrm{d}^3 P)} \otimes H_F^{\mathrm{rel}} \tag{5.2.71}$$

with domain

$$\mathcal{D}(H_F) = \left\{ f \in L^2(\mathbb{R}^3,\, \mathrm{d}^3 P; \mathcal{H}^{\mathrm{rel}}) \middle| \; f(\boldsymbol{P}) \in \mathcal{D}(H_F^{\mathrm{rel}}) \text{ for almost all } \boldsymbol{P} \in \mathbb{R}^3 \right.$$
$$\left. \text{and } \int_{\mathbb{R}^3} \left\| \left(\boldsymbol{P} \cdot \mathbf{M}^+ + H_F^{\mathrm{rel}} \right) f(\boldsymbol{P}) \right\|^2 \mathrm{d}^3 P < \infty \right\}. \tag{5.2.72}$$

Then, upon defining the unitary operator $\mathcal{W} := \mathcal{F}_{\boldsymbol{R}} U$, where U is the coordinate transform (2.2.3) *and $\mathcal{F}_{\boldsymbol{R}}$ is the Fourier transform with respect to the center-of-mass coordinate, it holds that*

$$\tilde{H}_{2\mathrm{BD}} := \mathcal{W}^{-1} H_F \mathcal{W} + V_{\text{ext}} + \beta m_1 \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta m_2 \tag{5.2.73}$$

with domain

$$\mathcal{D}(\tilde{H}_{2\mathrm{BD}}) = \mathcal{W}^{-1} \mathcal{D}(H_F) \tag{5.2.74}$$

defines a self-adjoint extension of $H_{2\mathrm{BD}}$.

Proof. First, we note that $\beta m_1 \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta m_2$ as well as V_{ext} are symmetric and bounded. Therefore, they can be added by means of a bounded perturbation. Moreover, the coordinate transformation U as well as the Fourier transform of the center-of-mass coordinate are unitary. Hence, self-adjointness of H_F implies self-adjointness of $\tilde{H}_{2\mathrm{BD}}$.

In order to prove self-adjointness of $H_F = \hat{\boldsymbol{P}} \cdot \mathbf{M}^+ \otimes \mathrm{id} + \mathrm{id} \otimes H_F^{\mathrm{rel}}$, we employ the method of direct fiber integrals. We define $H_F(\boldsymbol{P}) := \boldsymbol{P} \cdot \mathbf{M}^+ + H_F^{\mathrm{rel}}$ for a fixed $\boldsymbol{P} \in \mathbb{R}^3$ and so $\{H_F(\boldsymbol{P})\}_{\boldsymbol{P} \in \mathbb{R}^3}$ is a family of self-adjoint operators with common domain $\mathcal{D}(H_F^{\mathrm{rel}})$ in the underlying Hilbert space $\mathcal{H}^{\mathrm{rel}}$ by Theorem 5.11. The map $\boldsymbol{P} \mapsto H_F(\boldsymbol{P})$ from $\mathbb{R}^3$ into the self-adjoint operators on $\mathcal{H}^{\mathrm{rel}}$ is measurable as for all $f, g \in \mathcal{H}^{\mathrm{rel}}$ the map $\boldsymbol{P} \mapsto \langle f, (H_F(\boldsymbol{P}) + i)^{-1} g \rangle$ is continuous in $\boldsymbol{P}$:

$$\begin{aligned}
&\left| \left\langle f, (H_F(\boldsymbol{P}) + i)^{-1} g \right\rangle - \left\langle f, (H_F(\boldsymbol{P}') + i)^{-1} g \right\rangle \right| \\
&\overset{(*)}{=} \left| \left\langle f, (H_F(\boldsymbol{P}) + i)^{-1} \left(H_F(\boldsymbol{P}') - H_F(\boldsymbol{P}) \right) (H_F(\boldsymbol{P}') + i)^{-1} g \right\rangle \right| \\
&= \left| \left\langle f, (H_F(\boldsymbol{P}) + i)^{-1} (\boldsymbol{P}' - \boldsymbol{P}) \cdot \mathbf{M}^+ (H_F(\boldsymbol{P}') + i)^{-1} g \right\rangle \right| \\
&\leq \|f\| \left\| (H_F(\boldsymbol{P}') + i)^{-1} \right\|^2 \sum_{k=1}^{3} \left\| \mathrm{M}_k^+ \right\| |P_k' - P_k| \, \|g\| \xrightarrow{\boldsymbol{P} \to \boldsymbol{P}'} 0
\end{aligned} \tag{5.2.75}$$

since $\|(H_F(\boldsymbol{P}) + i)^{-1}\| \leq 1$. In $(*)$, we used the second resolvent identity.

Hence, due to [RS78, Theorem XIII.85], the direct fiber integral

$$H' = \int_{\mathbb{R}^3}^{\oplus} H_F(\boldsymbol{P})\,\mathrm{d}^3P \tag{5.2.76}$$

with domain

$$\begin{aligned}\mathcal{D}(H') = \Bigg\{ f \in L^2(\mathbb{R}^3,\, \mathrm{d}^3P; \mathcal{H}^{\mathrm{rel}}) \Bigg|\; & f(\boldsymbol{P}) \in \mathcal{D}(H_F^{\mathrm{rel}}) \text{ for almost all } \boldsymbol{P} \in \mathbb{R}^3 \\ & \text{and } \int_{\mathbb{R}^3} \|H_F(\boldsymbol{P})f(\boldsymbol{P})\|^2_{\mathcal{H}^{\mathrm{rel}}}\,\mathrm{d}^3P < \infty \Bigg\}\end{aligned} \tag{5.2.77}$$

defines a self-adjoint operator in the Hilbert space $L^2(\mathbb{R}^3,\, \mathrm{d}^3P; \mathcal{H}^{\mathrm{rel}})$ which acts for almost all $\boldsymbol{P} \in \mathbb{R}^3$ as $(H'f)(\boldsymbol{P}) = H_F(\boldsymbol{P})f(\boldsymbol{P})$. This is precisely the action of H_F. Since $\mathcal{D}_0 = H^1(\mathbb{R}^3,\, \mathrm{d}^3P) \otimes \mathbb{C}^{16} \otimes H^1(\mathbb{R}^3,\, \mathrm{d}^3r)$ is contained in $\mathcal{D}(H_F)$ and H_F^{rel} extends H^{rel}, we obtain $H_F \restriction \mathcal{D}_0 = \mathcal{W} H_{2\mathrm{BD}} \mathcal{W}^{-1}$. This proves the theorem. □

5.3. Criterion of finite potential energy

From a physical point of view, it is very desirable that a self-adjoint extension of a many-body Dirac operator is distinguished by a physical criterion. In this section, we introduce our criterion, as anticipated at the beginning of Section 5.2. This criterion should satisfy two requirements. First, it must have a clear physical meaning. This ensures that the extension is not only an abstract operator but has a chance to correspond to the physics the operator is supposed to describe. Secondly, it has to guarantee uniqueness in such a way that there exists only one extension that satisfies this criterion and hence provides a unique unitary time evolution.

We say that a state $\psi \in \mathcal{D}(H_F)$ has finite potential energy if $|E_{\mathrm{pot}}[\psi]| = |\langle f, (V_{\mathrm{ext}} + V_{\mathrm{int}})f\rangle| < \infty$. As physical criterion for a distinguished self-adjoint extension, we choose the one of finite potential energy. Although the physical status of $H_{2\mathrm{BD}}$ may remain unclear, finite potential energy is physically meaningful. As the following theorem shows, it also meets the second requirement since it singles out H_F uniquely. Recall that $\mathcal{D}_+ = (\mathbb{C}^{16} \otimes H^1(\mathbb{R}^3,\, \mathrm{d}^3r)) \cap \mathcal{H}_+^{\mathrm{rel}} \subset \mathcal{D}(V)$ by Hardy's inequality.

Theorem 5.13 (Claim b) of Theorem 2)**.** *Let $0 < \kappa \le 1$, $|\gamma| M_{\kappa/2}^2 < 1$, and let V_{ext} be bounded and symmetric. Moreover, let $\tilde{H}$ with domain $\mathcal{D}(\tilde{H})$ be any self-adjoint extension of $UH_{\mathrm{DC}}U^{-1}$ of the form*

$$\tilde{H} = \hat{\boldsymbol{P}} \cdot \mathbf{M}^+ \otimes \mathrm{id} + \mathrm{id} \otimes \tilde{H}^{\mathrm{rel}} + V_{\mathrm{ext}} + \beta \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta, \tag{5.3.1}$$

where $\tilde{H}^{\mathrm{rel}}$ is an arbitrary self-adjoint extension of $H^{\mathrm{rel}} = H_0 + V$ with domain $\mathcal{D}(\tilde{H}^{\mathrm{rel}})$. Then, $|\langle f, (V_{\mathrm{ext}} + V_{\mathrm{int}})f\rangle| < \infty$ for all $f \in \mathcal{D}(\tilde{H})$ if, and only if, $\tilde{H} = H_F$.

Proof. As V_{ext} is bounded, it suffices to consider V_{int}. We first prove $|\langle f, V_{\mathrm{int}} f\rangle| < \infty$ if $f \in \mathcal{D}(H_F)$. It suffices to show $|\langle f, V_{\mathrm{int}} f\rangle| \le \langle f, V f\rangle < \infty$ if $f \in \mathcal{D}(H_F^{\mathrm{rel}})$, since V_{int} acts as identity on $\mathcal{H}^{\mathrm{com}}$.

Let $f = (f_+, f_-)^\top \in \mathcal{D}(H_F^{\mathrm{rel}})$. Then, $f_- \in \mathcal{D}(S_F) = \mathcal{D}(V^{1/2}) \cap \mathcal{D}(S^*)$ by the definition of $\mathcal{D}(H_F^{\mathrm{rel}})$ in line (5.2.69) and Lemma 5.10. Hence, $\langle f_-, V f_- \rangle < \infty$ follows. As the cross terms $\langle f_\mp, V f_\pm \rangle$ can be recovered using the polarization identity, it remains to show $\langle f_+, V f_+ \rangle < \infty$ in order to prove $\langle f, V f \rangle < \infty$. We note that

$$\begin{aligned}\langle f_+, V f_+ \rangle^{1/2} = \left\| V^{1/2} f_+ \right\| \leq & \left\| V^{1/2}(f_+ + \overline{A^{-1} P_+ \gamma V P_-} f_-) \right\| \\ & + \left\| V^{1/2} \overline{A^{-1} P_+ \gamma V P_-} f_- \right\| . \end{aligned} \tag{5.3.2}$$

Since $f_+ + \overline{A^{-1} P_+ \gamma V P_-} f_- \in \mathcal{D}_+ \subset \mathcal{D}(V^{1/2})$, we see that $\langle f_+, V f_+ \rangle < \infty$ holds if $\| V^{1/2} \overline{A^{-1} P_+ \gamma V P_-} f_- \| < \infty$.

In order to show that, we use $\langle f_-, V f_- \rangle < \infty$ shown above. It allows us to apply Theorem 5.8. Hence, we know that there exists a sequence $(f_n)_{n \in \mathbb{N}} \subset \mathcal{D}(V) \cap \mathcal{H}_-^{\mathrm{rel}}$ with $\| f_- - f_n \| \xrightarrow{n \to \infty} 0$ such that $\left\| V^{1/2}(f_m - f_n) \right\| \xrightarrow{m,n \to \infty} 0$. With its help, we get

$$\begin{aligned} \Big\| & V^{1/2} \overline{A^{-1} P_+ \gamma V P_-} (f_m - f_n) \Big\| = \left\| V^{1/2} A^{-1} P_+ \gamma V P_- (f_m - f_n) \right\| \\ &= \left\| V^{1/2} P_+ \gamma A^{-1} P_+ V^{1/2} V^{1/2} (f_m - f_n) \right\| \\ &\leq \left\| V^{1/2} P_+ \gamma A^{-1} P_+ V^{1/2} \right\| \left\| V^{1/2} (f_m - f_n) \right\| \xrightarrow{m,n \to \infty} 0 \end{aligned} \tag{5.3.3}$$

where we used that $V^{1/2} P_+ \gamma A^{-1} P_+ V^{1/2}$ is bounded by Lemma 5.9. By Lemma A.2 (Appendix A), $\overline{A^{-1} P_+ V P_-}$ is bounded, and thus, $\| \overline{A^{-1} P_+ \gamma V P_-} (f_m - f_n) \| \xrightarrow{m,n \to \infty} 0$. Together with line (5.3.3), this now ensures that the sequence $(\overline{A^{-1} P_+ V P_-} f_n)_{n \in \mathbb{N}}$ is a Cauchy sequence in the graph norm of $V^{1/2}$. As $V^{1/2}$ is closed, this implies $\overline{A^{-1} P_+ \gamma V P_-} f_- \in \mathcal{D}(V^{1/2})$, i.e., $\| V^{1/2} \overline{A^{-1} P_+ \gamma V P_-} f_- \| < \infty$.

For the reverse implication, we assume $\langle f, V f \rangle < \infty$ for all $f \in \mathcal{D}(\tilde{H})$. Then, it suffices to show $\mathcal{D}(\tilde{H}^{\mathrm{rel}}) = \mathcal{D}(H_F^{\mathrm{rel}})$ in order to infer $\tilde{H} = H_F$, i.e., $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+ + \tilde{H}^{\mathrm{rel}} = \hat{\boldsymbol{P}} \cdot \mathbf{M}^+ + H_F^{\mathrm{rel}}$.

We first show $\mathcal{D}(\tilde{H}^{\mathrm{rel}}) \subseteq \mathcal{D}(H_F^{\mathrm{rel}})$, i.e., let $f \in \mathcal{D}(\tilde{H}^{\mathrm{rel}})$. In order to understand better what f might look like, we first note that $\mathcal{D}(\tilde{H}^{\mathrm{rel}}) \subseteq \mathcal{D}((H^{\mathrm{rel}} + P_+ B P_+)^*)$ as $P_+ B P_+$ is bounded. We compute $\mathcal{D}((H^{\mathrm{rel}} + P_+ B P_+)^*)$ with help of its Frobenius-Schur factorization. Recall the operators $\mathcal{R}$ and $\mathcal{T}$ from the proof of Theorem 5.11, line (5.2.70):

$$\mathcal{R} = \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ P_- \gamma V P_+ A^{-1} & \mathrm{id} \end{pmatrix}, \quad \mathcal{T} = \begin{pmatrix} \mathrm{id} & \overline{A^{-1} P_+ \gamma V P_-} \\ \mathbf{0} & \mathrm{id} \end{pmatrix}. \tag{5.3.4}$$

We note that one can rewrite this as $\mathcal{T} = \mathrm{id} + \overline{A^{-1} P_+ \gamma V P_-}$. We then have $\mathcal{T}^{-1} = \mathrm{id} - \overline{A^{-1} P_+ \gamma V P_-}$. In addition, we define

$$\mathcal{S} := \begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & S \end{pmatrix}, \quad \mathcal{D}(\mathcal{S}) = \mathcal{D}_+ \oplus \mathcal{D}(S). \tag{5.3.5}$$

This yields $(H^{\mathrm{rel}} + P_+ B P_+)^* = (\mathcal{R} \mathcal{S} \mathcal{T})^* = \mathcal{R} \mathcal{S}^* \mathcal{T}$ as $\mathcal{T} = \mathcal{R}^*$ and $\mathcal{R} = \mathcal{T}^*$ are bounded and boundedly invertible by Lemma A.2 (Appendix A). Theorem A.3 (Appendix A) provides the domain:

$$\mathcal{D}((\mathcal{R}\,\mathcal{S}\,\mathcal{T})^*) = \left\{ \left(\begin{array}{c} f \\ g \end{array} \right) \in \mathcal{H}_+^{\mathrm{rel}} \oplus \mathcal{H}_-^{\mathrm{rel}} \middle| \begin{array}{c} f + \overline{A^{-1}P_+\gamma VP_-}g \in \mathcal{D}_+, \\ g \in \mathcal{D}(S^*) \end{array} \right\}. \tag{5.3.6}$$

Therefore, it makes sense to again split $\mathcal{D}(\tilde{H}^{\mathrm{rel}})$ by the projections $P_\pm$. We thus write $f = (f_+, f_-)^\top$.

Now, as $\mathcal{T}$ is bounded and boundedly invertible, it is a one-to-one map between $\mathcal{D}((H^{\mathrm{rel}} + P_+BP_+)^*)$ and $\mathcal{D}_+ \oplus \mathcal{D}(S^*)$. Therefore, there exists a unique $\varphi = (\varphi_1, \varphi_2)^\top \in \mathcal{D}_+ \oplus \mathcal{D}(S^*)$ such that $f = \mathcal{T}^{-1}\varphi$, i.e.,

$$\begin{aligned} \mathcal{T}^{-1}\varphi &= \left(\begin{array}{cc} \mathrm{id} & -\overline{A^{-1}P_+\gamma VP_-} \\ \mathbf{0} & \mathrm{id} \end{array} \right) \left(\begin{array}{c} \varphi_1 \\ \varphi_2 \end{array} \right) \\ &= \left(\begin{array}{c} \varphi_1 - \overline{A^{-1}P_+\gamma VP_-}\varphi_2 \\ \varphi_2 \end{array} \right) = \left(\begin{array}{c} f_+ \\ f_- \end{array} \right). \end{aligned} \tag{5.3.7}$$

Since $\varphi_1 \in \mathcal{D}_+$ and $\varphi_2 \in \mathcal{D}(S^*)$, this form of f shows that f lies in

$$\mathcal{D}(H_F^{\mathrm{rel}}) = \left\{ \left(\begin{array}{c} f \\ g \end{array} \right) \in \mathcal{H}_+^{\mathrm{rel}} \oplus \mathcal{H}_-^{\mathrm{rel}} \middle| \begin{array}{c} f + \overline{A^{-1}P_+\gamma VP_-}g \in \mathcal{D}_+, \\ g \in \mathcal{D}(S_F) \end{array} \right\}, \tag{5.3.8}$$

if $f_- = \varphi_2 \in \mathcal{D}(S_F)$. Using $\mathcal{D}(S_F) = \mathcal{D}(V^{1/2}) \cap \mathcal{D}(S^*)$ by Lemma 5.10 and $f_- \in \mathcal{D}(S^*)$, we conclude that it suffices to show that $f_- \in \mathcal{D}(V^{1/2}) \cap \mathcal{H}_-^{\mathrm{rel}}$.

We want to remark at this point that it is not immediately clear that $\langle f, Vf \rangle < \infty$ implies $\langle f_-, Vf_- \rangle < \infty$ as, in principle, there could occur cancellations between the parts in $\mathcal{H}_+^{\mathrm{rel}}$ and $\mathcal{H}_-^{\mathrm{rel}}$. This, however, is not the case.

In the following, it will turn out to be useful to define the Gaussian χ_n for all $n \in \mathbb{N}$ by $\chi_n(\boldsymbol{r}) := e^{-2^n\pi|\boldsymbol{r}|^2}$ and with it the Gaussian cut-off $1 - \chi_n$ for f by $f_n := (1 - \chi_n)f$. Now, by the same reasoning as in the proof of Theorem 5.8, we know that $f_n \in \mathcal{D}(V)$ for all $n \in \mathbb{N}$, and moreover, we obtain $\|f - f_n\| \xrightarrow{n\to\infty} 0$, $\|f_\pm - P_\pm f_n\| \xrightarrow{n\to\infty} 0$, and $\|V^{1/2}(f - f_n)\| \xrightarrow{n\to\infty} 0$ by dominated convergence. This implies

$$\langle (f_m - f_n), V(f_m - f_n) \rangle \xrightarrow{m,n\to\infty} 0. \tag{5.3.9}$$

We express f in $f_n = (1 - \chi_n)f$ with $f = \mathcal{T}^{-1}\varphi$. In order to shorten the expressions, we introduce the abbreviations $\chi_{m,n} \equiv \chi_n - \chi_m$ and $f_{m,n} \equiv f_m - f_n$:

$$\begin{aligned} f_{m,n} &= \chi_{m,n}\,\mathcal{T}^{-1}\varphi \\ &= \chi_{m,n}\left(\varphi_1 - \overline{A^{-1}P_+\gamma VP_-}f_- + f_-\right) \\ &= \chi_{m,n}\left(\varphi_1 + (\mathrm{id} - \overline{A^{-1}P_+\gamma VP_-})f_-\right) \\ &= \chi_{m,n}\left(\varphi_1 + \mathcal{T}^{-1}f_-\right). \end{aligned} \tag{5.3.10}$$

As we have $f_{m,n} \in \mathcal{D}(V)$ for all $m, n \in \mathbb{N}$, we are allowed to expand the expression

$\langle f_{m,n}, Vf_{m,n}\rangle$ as follows:

$$\begin{aligned}\langle f_{m,n}, Vf_{m,n}\rangle &= \left\langle \chi_{m,n}\left(\varphi_1+\mathcal{T}^{-1}f_-\right), V\chi_{m,n}\left(\varphi_1+\mathcal{T}^{-1}f_-\right)\right\rangle \\ &= \langle \chi_{m,n}\varphi_1, V\chi_{m,n}\varphi_1\rangle + \left\langle \chi_{m,n}\varphi_1, V\chi_{m,n}\mathcal{T}^{-1}f_-\right\rangle \\ &\quad + \left\langle \chi_{m,n}\mathcal{T}^{-1}f_-, V\chi_{m,n}\varphi_1\right\rangle \\ &\quad + \left\langle \chi_{m,n}\mathcal{T}^{-1}f_-, V\chi_{m,n}\mathcal{T}^{-1}f_-\right\rangle. \end{aligned} \tag{5.3.11}$$

All summands containing a $\varphi_1 \in \mathcal{D}_+ \subset \mathcal{D}(V)$ are grouped together:

$$\begin{aligned} G_{m,n}(\varphi_1) := &\ \langle \chi_{m,n}\varphi_1, V\chi_{m,n}\varphi_1\rangle + \left\langle \chi_{m,n}\varphi_1, V\chi_{m,n}\mathcal{T}^{-1}f_-\right\rangle \\ &+ \left\langle \chi_{m,n}\mathcal{T}^{-1}f_-, V\chi_{m,n}\varphi_1\right\rangle. \end{aligned} \tag{5.3.12}$$

We first compute

$$\begin{aligned} \left|\left\langle \chi_{m,n}\varphi_1, V\chi_{m,n}\mathcal{T}^{-1}f_-\right\rangle\right| &= \left|\left\langle V\chi_{m,n}\varphi_1, \chi_{m,n}\mathcal{T}^{-1}f_-\right\rangle\right| \\ &\leq \|V\chi_{m,n}\varphi_1\| \left\|\chi_{m,n}\mathcal{T}^{-1}f_-\right\| \xrightarrow{m,n\to\infty} 0, \end{aligned} \tag{5.3.13}$$

where both factors tend to zero as $m,n\to\infty$ by dominated convergence. Note that here it is necessary that $\varphi_1 \in \mathcal{D}_+ \subset \mathcal{D}(V)$. In an analogous way, the convergence to zero of the remaining summands of $G_{m,n}(\varphi_1)$ is proven. Hence, we get $|G_{m,n}(\varphi_1)| \xrightarrow{m,n\to\infty} 0$. This, together with $\langle f_{m,n}, Vf_{m,n}\rangle \xrightarrow{m,n\to\infty} 0$, implies

$$\begin{aligned} \left\|V^{1/2}\chi_{m,n}\mathcal{T}^{-1}f_-\right\|^2 &= \left|\left\langle \chi_{m,n}\mathcal{T}^{-1}f_-, V\chi_{m,n}\mathcal{T}^{-1}f_-\right\rangle\right| \\ &\leq \langle f_{m,n}, Vf_{m,n}\rangle + |G_{m,n}(\varphi_1)| \xrightarrow{m,n\to\infty} 0. \end{aligned} \tag{5.3.14}$$

As we also have

$$\left\|(1-\chi_m)\mathcal{T}^{-1}f_- - (1-\chi_n)\mathcal{T}^{-1}f_-\right\| = \left\|\chi_{m,n}\mathcal{T}^{-1}f_-\right\| \xrightarrow{m,n\to\infty} 0 \tag{5.3.15}$$

by dominated convergence, we can conclude that $((1-\chi_n)\mathcal{T}^{-1}f_-)_{n\in\mathbb{N}}$ is a Cauchy sequence in the graph norm of $V^{1/2}$. Thus, $\mathcal{T}^{-1}f_- \in \mathcal{D}(V^{1/2})$ since $V^{1/2}$ is closed.

Since line (5.3.3) implies $\overline{A^{-1}P_+\gamma VP_-}\,\mathcal{D}(V^{1/2}) \subseteq \mathcal{D}(V^{1/2})$, we also get

$$(\mathrm{id} \pm \overline{A^{-1}P_+\gamma VP_-})\,\mathcal{D}(V^{1/2}) \subseteq \mathcal{D}(V^{1/2}), \tag{5.3.16}$$

i.e., $\mathcal{T}$ as well as $\mathcal{T}^{-1}$ map $\mathcal{D}(V^{1/2})$ into $\mathcal{D}(V^{1/2})$.

Now, we assume for the moment that $f_- \notin \mathcal{D}(V^{1/2})$ and aim at a contradiction. We already showed that $\mathcal{T}^{-1}f_- \in \mathcal{D}(V^{1/2})$, and from line (5.3.16) we know that $\mathcal{T}$ maps $\mathcal{D}(V^{1/2})$ into $\mathcal{D}(V^{1/2})$. Thus,

$$\mathcal{T}^{-1}f_- \in \mathcal{D}(V^{1/2}) \;\Rightarrow\; \mathcal{T}\mathcal{T}^{-1}f_- \in \mathcal{D}(V^{1/2}) \;\Rightarrow\; f_- \in \mathcal{D}(V^{1/2}). \tag{5.3.17}$$

This is a contradiction to our assumption $f_- \notin \mathcal{D}(V^{1/2})$ and thus, $f_- \in \mathcal{D}(V^{1/2})$. Therefore, $f_- \in \mathcal{D}(V^{1/2}) \cap \mathcal{D}(S^*) = \mathcal{D}(S_F)$ which implies $f \in \mathcal{D}(H_F^{\mathrm{rel}})$.

For the reverse inclusion $\mathcal{D}(H_F^{\mathrm{rel}}) \subseteq \mathcal{D}(\tilde{H}^{\mathrm{rel}})$, it suffices to note that

$$\mathcal{D}(H_F^{\mathrm{rel}}) = \mathcal{D}((H_F^{\mathrm{rel}})^*) \subseteq \mathcal{D}((\tilde{H}^{\mathrm{rel}})^*) = \mathcal{D}(\tilde{H}^{\mathrm{rel}}) \subseteq \mathcal{D}(H_F^{\mathrm{rel}}). \tag{5.3.18}$$

Therefore, $\mathcal{D}(\tilde{H}^{\mathrm{rel}}) = \mathcal{D}(H_F^{\mathrm{rel}})$, which concludes the proof. □

5.4. Comment on the article by Okaji et al. [OKY14]

We briefly comment on the article [OKY14] by Okaji et al. which was written in response to [Der12]. As already mentioned, the proof of their claim, i.e., essential self-adjointness of $H_{2\mathrm{BD}}$ (even including external Coulomb potentials) as operator in the underlying Hilbert space

$$\mathcal{H}_a = \big(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4\big) \wedge \big(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4\big) \tag{5.4.1}$$

comprises a gap. In the following, we want to lay out the missing step.

The authors employ an auxiliary operator which is denoted by H^+ and given by[2]

$$H^+ = \mathbf{1}_4 \otimes \boldsymbol{\alpha} \cdot (-i\nabla_{\boldsymbol{x}} - i\nabla_{\boldsymbol{y}}) + m(\beta \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes \beta) + V \tag{5.4.2}$$

where external potentials as well as the interaction potential are combined in V. Its domain is taken to be

$$\mathcal{D}_a = \big(C_c^\infty(\mathbb{R}^3; \mathbb{C}^4) \otimes C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)\big) \cap \mathcal{H}_a. \tag{5.4.3}$$

Now, $H_{2\mathrm{BD}}$ and H^+ coincide as quadratic form on $\mathcal{H}_a$ but not as operator, i.e., for all $\varphi, \psi \in \mathcal{D}_a$ one has

$$\langle \varphi, H_{2\mathrm{BD}}\psi \rangle = \big\langle \varphi, H^+\psi \big\rangle \tag{5.4.4}$$

but in general

$$H_{2\mathrm{BD}}\psi \neq H^+\psi. \tag{5.4.5}$$

The former is proven in [OKY14] in Theorem 5.4, the latter is seen as follows. Define ψ by

$$\psi(\boldsymbol{x}, \boldsymbol{y}) = \begin{pmatrix} 0 \\ f(\boldsymbol{x}) \\ 0 \\ f(\boldsymbol{x}) \end{pmatrix} \otimes \begin{pmatrix} f(\boldsymbol{y}) \\ 0 \\ f(\boldsymbol{y}) \\ 0 \end{pmatrix} - \begin{pmatrix} f(\boldsymbol{x}) \\ 0 \\ f(\boldsymbol{x}) \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ f(\boldsymbol{y}) \\ 0 \\ f(\boldsymbol{y}) \end{pmatrix} \tag{5.4.6}$$

where the function $f\colon \mathbb{R}^3 \to \mathbb{C}$ is chosen to be smooth and compactly supported. We see that ψ is antisymmetric, and therefore, $\psi \in \mathcal{D}_a$. That line (5.4.5) holds, is now a straightforward calculation.

[2] We give H^+ in the same $\mathbb{C}^{16}$-basis as $H_{2\mathrm{BD}}$ in Eq. (2.1.2). In [OKY14], a different basis is used.

Hence, from the essential self-adjointness of H^+ on $\mathcal{D}_a$ that was proven in [OKY14], it does not follow that $H_{2\mathrm{BD}}$ is essentially self-adjoint on $\mathcal{D}_a$. On the contrary, as this thesis shows, H_0 exhibits a non-trivial nullspace structure in the relative coordinate, i.e., the coordinate of the interaction, whereas one always has $\mathrm{Ker}(H^+) = \{0\}$.

We want to use this opportunity to add another remark on Eq. (5.4.4) and draw attention to an interesting implication. We denote by

$$P_a \colon \mathcal{H}_2 \to \mathcal{H}_a \tag{5.4.7}$$

the orthogonal projection on $\mathcal{H}_a$. An interesting fact is that P_a can also have a regularizing effect which we will outline briefly in the following without making the argument rigorous.

For the sake of our argument, it suffices to consider the free and massless case, i.e., all potentials and masses are set to zero. We will nevertheless keep the notation $H_{2\mathrm{BD}}$ and H^+ in order to maintain the distinction between the auxiliary operator H^+ and the actual operator $H_{2\mathrm{BD}}$. Then, $H_{2\mathrm{BD}}$ is the operator T from Section 2.2

$$H_{2\mathrm{BD}} = T = \hat{\boldsymbol{P}} \cdot \mathbf{M}^+ \otimes \mathrm{id} + \mathrm{id} \otimes \mathbf{M}^- \cdot \hat{\boldsymbol{p}} \tag{5.4.8}$$

and H^+ is in center-of-mass and relative coordinates of the form

$$H^+ = \mathbf{1}_4 \otimes \boldsymbol{\alpha} \cdot \hat{\boldsymbol{P}}. \tag{5.4.9}$$

We see now that in order to have $\|H^+ f\| < \infty$ for some f, this f must have at least $H^1(\mathbb{R}^3, \mathrm{d}^3 R)$-regularity. For $H_{2\mathrm{BD}}$ however, this is not the case because of the nullspace structure of $\hat{\boldsymbol{P}} \cdot \mathbf{M}^+$. E.g., using the ψ from line (5.4.6), it is possible to construct a less regular f with $\|H_{2\mathrm{BD}} f\| < \infty$ since $\psi \in \mathrm{Ker}(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+)$.

What the form equality Eq. (5.4.4) $\langle \varphi, H_{2\mathrm{BD}} \psi \rangle = \langle \varphi, H^+ \psi \rangle$ actually implies, is the operator equality $P_a H^+ P_a = H_{2\mathrm{BD}}$. However, $H_{2\mathrm{BD}}$ allows for less regular functions than H^+. Thus, we can conclude that the projection P_a has a regularizing effect on $H^+ P_a f$.

6. First results towards a spectral analysis of H_{2BD}

This section provides the first steps towards a spectral analysis of H_{2BD}. While it has been folklore knowledge for quite some time that the essential spectrum of H_{2BD} comprises the entire real line (see, e.g., the introduction of [Mor08]), a full proof has been missing. The one presented in [OKY14] is unfortunately incomplete. In Theorem 6.1, we prove that $\sigma_{\mathrm{ess}}(H_{\mathrm{2BD}}) = \mathbb{R}$ and remark on the proof given in [OKY14] subsequently. Furthermore, it has been conjectured that H_{2BD} does not possess any eigenvalues (see, e.g., [Der12]) as they would be embedded into the continuous part of the spectrum, which is, however, a rare phenomenon. We prove in Theorem 6.3 that no eigenvalues $|E| > 2m$ exist, where m is the particle's mass, under the assumption that possible eigenstates fulfill a very mild regularity condition.

Theorem 6.1 (Claim a) of Theorem 3)**.** *Let $\tilde{H}$ denote any self-adjoint extension of $H_{\mathrm{2BD}} = H_0 + V$ where V is the operator of multiplication with $a|\boldsymbol{x}|^{-1} + a|\boldsymbol{y}|^{-1} + b|\boldsymbol{x}-\boldsymbol{y}|^{-1}$ for $a, b \in \mathbb{R}$ and almost all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$. Then,*

$$\sigma_{\mathrm{ess}}(\tilde{H}) = \mathbb{R}. \tag{6.0.1}$$

Proof. Our proof is inspired by the proof of [Tha92, Theorem 4.20]. We construct a Weyl sequence for $\tilde{H}$ and every $E \in \mathbb{R}$, i.e., a sequence $(f_n)_{n\in\mathbb{N}} \subset \mathcal{D}(\tilde{H})$ such that for $E \in \mathbb{R}$, it holds that $\langle f_k, f_l \rangle = \delta_{kl}$ for all $k, l \in \mathbb{N}$ and $\|(\tilde{H} - E) f_n\| \xrightarrow{n\to\infty} 0$. Weyl's criterion (see, e.g., [HS96, Theorem 7.2]) then implies $E \in \sigma_{\mathrm{ess}}(\tilde{H})$. Before we can define this sequence, some preparations are needed. We recall the definition of the 16×16-matrix $H_0(\boldsymbol{p_x}, \boldsymbol{p_y})$ from line (3.2.1)

$$H_0(\boldsymbol{p_x}, \boldsymbol{p_y}) = (\boldsymbol{\alpha} \cdot \boldsymbol{p_x} + \beta m_1) \otimes \mathbf{1}_4 + \mathbf{1}_4 \otimes (\boldsymbol{\alpha} \cdot \boldsymbol{p_y} + \beta m_2), \tag{6.0.2}$$

and define with its help $\mathbf{S}_E(\boldsymbol{p_x}, \boldsymbol{p_y}) \in \mathbb{C}^{16}$ for almost all $\boldsymbol{p_x}, \boldsymbol{p_y} \in \mathbb{R}^3$ and all $E \in \mathbb{R}$ by

$$[H_0(\boldsymbol{p_x}, \boldsymbol{p_y}) - E]\, \mathbf{S}_E(\boldsymbol{p_x}, \boldsymbol{p_y}) = 0. \tag{6.0.3}$$

This is possible as $H_0(\boldsymbol{p_x}, \boldsymbol{p_y})$ is a Hermitian matrix with eigenvalues $\lambda_k(\boldsymbol{p_x}, \boldsymbol{p_y})$ for $k = 1, 2, \ldots, 16$ (see (3.2.2)) such that one can find $\boldsymbol{p_x}, \boldsymbol{p_y} \in \mathbb{R}^3$ and $k = 1, 2, \ldots, 16$ for each $E \in \mathbb{R}$ such that $\lambda_k(\boldsymbol{p_x}, \boldsymbol{p_y}) = E$.

Furthermore, we introduce for elements $\boldsymbol{X} \in \mathbb{R}^6$ the notation $\boldsymbol{X} = (\boldsymbol{x}, \boldsymbol{y})^\top$, where $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$. We fix the components such that the upper three components correspond to those of the first particle and the lower three components to those of the second particle.

The cone K is defined by

$$K := \left\{ \boldsymbol{X} \in \mathbb{R}^6 \middle|\ 0 \leq \measuredangle \left((1,1,1,-1,-1,-1)^\top, \boldsymbol{X} \right) \leq \pi/8 \right\} \tag{6.0.4}$$

In K, we define $(B_n)_{n\in\mathbb{N}} \subset K$ as the sequence of six-dimensional balls that are disjoint, have an ever increasing radius R_n, and whose centers are denoted by $\boldsymbol{X}_n \in \mathbb{R}^6$, i.e., we have for all $n \in \mathbb{N}$

$$B_n := \left\{ \boldsymbol{X} \in \mathbb{R}^6 \mid |\boldsymbol{X} - \boldsymbol{X}_n| \leq R_n \right\} \text{ such that } \begin{cases} B_n \subset K, \\ R_n \xrightarrow{n\to\infty} \infty, \\ B_k \cap B_l = \emptyset\,, \quad k \neq l. \end{cases} \tag{6.0.5}$$

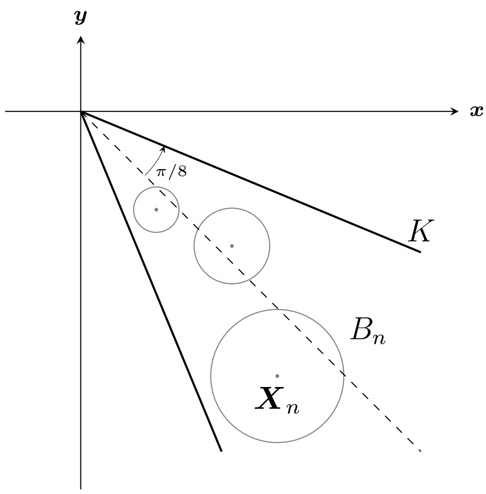

Figure 6.1.: Sketch of the cone K and the balls B_n.

We then define the smooth localization function $j_n \in C_c^\infty(\mathbb{R}^6)$ with $\operatorname{supp} j_n \subseteq B_n$ by

$$j_n(\boldsymbol{X}) := \begin{cases} 1\,, & |\boldsymbol{X} - \boldsymbol{X}_n| \leq R_n - 1\,, \\ 0\,, & |\boldsymbol{X} - \boldsymbol{X}_n| \geq R_n\,, \end{cases} \qquad 0 \leq j_n(\boldsymbol{X}) \leq 1 \quad \text{for all } \boldsymbol{X} \in \mathbb{R}^6, \tag{6.0.6}$$

such that there exists a finite constant $C > 0$ independent of $n \in \mathbb{N}$ such that for all $k = 1, 2, \ldots, 6$

$$\sup_{\boldsymbol{X}\in\mathbb{R}^6} \left| \left(\frac{\partial}{\partial X_k} j_n \right) (\boldsymbol{X}) \right| \leq C < \infty \quad \text{for all } n \in \mathbb{N}. \tag{6.0.7}$$

For the derivative of j_n, we obtain for all $k = 1, 2, \ldots, 6$

$$\left(\frac{\partial}{\partial X_k} j_n \right) (\boldsymbol{X}) = 0 \quad \text{if} \quad |\boldsymbol{X} - \boldsymbol{X}_n| \leq R_n - 1 \ \text{ or } \ |\boldsymbol{X} - \boldsymbol{X}_n| \geq R_n. \tag{6.0.8}$$

We are now in the position to define the sequence $(f_n)_{n\in\mathbb{N}}$ by

$$f_n(\boldsymbol{x},\boldsymbol{y}) = c_n\,\mathbf{S}_E(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})\,\mathrm{e}^{i\boldsymbol{p}_{\boldsymbol{x}}\cdot\boldsymbol{x}}\,\mathrm{e}^{i\boldsymbol{p}_{\boldsymbol{y}}\cdot\boldsymbol{y}}\,j_n(\boldsymbol{x},\boldsymbol{y}), \tag{6.0.9}$$

where c_n is the normalization constant such that $\|f_n\| = 1$ for all $n \in \mathbb{N}$. Smoothness of j_n guarantees $(f_n)_{n\in\mathbb{N}} \subset \mathcal{D}_0$. We proceed to prove that $(f_n)_{n\in\mathbb{N}}$ is indeed a Weyl sequence for $\tilde{H}$ and every $E \in \mathbb{R}$. First, we note that the disjoint support of j_k and j_l for all $k \neq l$ together with the normalization constant c_n implies orthonormality $\langle f_k, f_l\rangle = \delta_{kl}$. Next, we compute for all $E \in \mathbb{R}$

$$\begin{aligned}
\left\|(\tilde{H}-E)f_n\right\| &= \|(H_0+V_{\text{ext}}+V_{\text{int}}-E)\,f_n\| \\
&\leq \|(H_0(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})-E)\,f_n\| && (6.0.10a)\\
&\quad + c_n\,\|(\boldsymbol{\alpha}\otimes\mathbf{1})\cdot\nabla_{\boldsymbol{x}} j_n\,\mathbf{S}_E(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})\| && (6.0.10b)\\
&\quad + c_n\,\|(\mathbf{1}\otimes\boldsymbol{\alpha})\cdot\nabla_{\boldsymbol{y}} j_n\,\mathbf{S}_E(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})\| && (6.0.10c)\\
&\quad + \|(V_{\text{ext}}+V_{\text{int}})\,f_n\|\,. && (6.0.10d)
\end{aligned}$$

where we used $f_n \in \mathcal{D}_0$ in the first line. By the definition of $\mathbf{S}_E(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})$ in line (6.0.3), we have $(H_0(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})-E)\,f_n = 0$ for all $n \in \mathbb{N}$ and thus also

$$\|(H_0(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})-E)\,f_n\| = 0 \tag{6.0.11}$$

for all $n \in \mathbb{N}$.

In order to estimate lines (6.0.10b) and (6.0.10c), we recall the definition of j_n, in particular its derivative and its n-independent bound from lines (6.0.7) and (6.0.8). We further define $\tilde{B}_n := B_n \setminus B_{R_n-1}(\boldsymbol{X}_n)$ and obtain

$$\begin{aligned}
\int_{\mathbb{R}^6}\left|\left(\frac{\partial}{\partial X_k}j_n\right)(\boldsymbol{X})\right|^2\mathrm{d}^6X &= \int_{\tilde{B}_n}\left|\left(\frac{\partial}{\partial X_k}j_n\right)(\boldsymbol{X})\right|^2\mathrm{d}^6X\\
&\leq C\int_{\tilde{B}_n} R^5\,\mathrm{d}R\,\mathrm{d}\Omega\\
&= \frac{C\pi^3}{6}\left(R_n^6-(R_n-1)^6\right) \sim R_n^5.
\end{aligned} \tag{6.0.12}$$

However, we find for the normalization constant $c_n^2 \sim R_n^{-6}$ since

$$\begin{aligned}
\frac{\pi^3}{6}(R_n-1)^6 = \int_{B_{R_n-1}(\boldsymbol{X}_n)}\mathrm{d}^6X &\leq \int_{\mathbb{R}^6}|j_n(\boldsymbol{X})|^2\,\mathrm{d}^6X\\
&\leq \int_{B_{R_n}(\boldsymbol{X}_n)}\mathrm{d}^6X = \frac{\pi^3}{6}R_n^6.
\end{aligned} \tag{6.0.13}$$

Combining this with $R_n \xrightarrow{n\to\infty} \infty$ implies for (6.0.10b)

$$c_n\,\|(\boldsymbol{\alpha}\otimes\mathbf{1})\cdot\nabla_{\boldsymbol{x}} j_n\,\mathbf{S}_E(\boldsymbol{p}_{\boldsymbol{x}},\boldsymbol{p}_{\boldsymbol{y}})\| \xrightarrow{n\to\infty} 0 \tag{6.0.14}$$

and likewise for (6.0.10c).

In order to treat line (6.0.10d), we first note that $|\boldsymbol{x}-\boldsymbol{y}|$ is small if $\boldsymbol{x}$ lies in a neighborhood of $\boldsymbol{y}$. Within the cone K, however, $\boldsymbol{x}$ lies in the neighborhood of $-\boldsymbol{y}$. This together with $B_n \subset K$ for all $n \in \mathbb{N}$ implies

$$\begin{aligned} &\inf_{(\boldsymbol{x},\boldsymbol{y})\in B_n} |\boldsymbol{x}| \xrightarrow{n\to\infty} \infty \quad , \quad \inf_{(\boldsymbol{x},\boldsymbol{y})\in B_n} |\boldsymbol{y}| \xrightarrow{n\to\infty} \infty \\ &\inf_{(\boldsymbol{x},\boldsymbol{y})\in B_n} |\boldsymbol{x}-\boldsymbol{y}| \xrightarrow{n\to\infty} \infty. \end{aligned} \tag{6.0.15}$$

We can thus estimate

$$\begin{aligned} c_n^2 &\int_{\mathbb{R}^3\times\mathbb{R}^3} \left|\left(|\boldsymbol{x}|^{-1}+|\boldsymbol{y}|^{-1}+|\boldsymbol{x}-\boldsymbol{y}|^{-1}\right)\right|^2 |j_n(\boldsymbol{x},\boldsymbol{y})|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y \\ &\leq c_n^2 \int_{B_n} \left|\left(|\boldsymbol{x}|^{-1}+|\boldsymbol{y}|^{-1}+|\boldsymbol{x}-\boldsymbol{y}|^{-1}\right)\right|^2 |j_n(\boldsymbol{x},\boldsymbol{y})|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y \\ &\leq \sup_{(\boldsymbol{x},\boldsymbol{y})\in B_n} \left|\left(|\boldsymbol{x}|^{-1}+|\boldsymbol{y}|^{-1}+|\boldsymbol{x}-\boldsymbol{y}|^{-1}\right)\right|^2 \xrightarrow{n\to\infty} 0. \end{aligned} \tag{6.0.16}$$

This allows us to conclude that

$$\|(V_{\text{ext}}+V_{\text{int}})\, f_n\| \xrightarrow{n\to\infty} 0. \tag{6.0.17}$$

Putting (6.0.11), (6.0.14), and (6.0.17) together, shows that $(f_n)_{n\in\mathbb{N}}$ is a Weyl sequence for $\tilde{H}$ and every $E \in \mathbb{R}$, and thus, finishes the proof. □

Remark 6.2. We remark on the proof of $\sigma_{\text{ess}}(H_{2\text{BD}}) = \mathbb{R}$ given in [OKY14]. There, the authors also employ a Weyl sequence, denoted by $(w_n)_{n\in\mathbb{N}}$, which contains a smooth localization function, denoted by χ_n. However, when checking $\|(H_{2\text{BD}}-E)w_n\| \xrightarrow{n\to\infty} 0$, they do not control the convergence to zero of the terms corresponding to lines (6.0.10b) and (6.0.10c) in our proof, i.e., the derivatives of χ_n. In fact, their definition of χ_n is not sufficient to conclude said convergence. Our localization function j_n and the arguments leading to line (6.0.14) also fix the proof given in [OKY14]. ■

The next theorem shows absence of eigenvalues $|E| > 2m$ if possible eigenstates obey a mild regularity condition.

Theorem 6.3 (Claim b) of Theorem 3)**.** *Let $\tilde{H}$ denote any self-adjoint extension of $H_{2\text{BD}} = H_0 + V$ where V is the operator of multiplication with the real function V such that $V(a\boldsymbol{x}, a\boldsymbol{y}) = V(\boldsymbol{x},\boldsymbol{y})/a$ for all $a > 0$ and almost all $\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^3$. Assume further that all eigenstates of $\tilde{H}$ lie in $\mathcal{D}(\overline{H}_0) \cap \mathcal{D}(V)$. Then, $\tilde{H}$ has no eigenvalues in $(-\infty,-2m) \cup (2m,+\infty)$.*

Proof. We adapt the proof of [Wei80, Theorem 10.38] closely, in some instances even verbatim. Let $|E| > 2m$ and assume that $f \in \mathcal{D}(\tilde{H})$ satisfies $(\tilde{H} - E)f = 0$. By assumption, we can write $(\overline{H}_0 + V - E)f = 0$. We transform $\overline{H}_0 + V$ to relative and center-of-mass coordinates and find

$$U(\overline{H}_0+V)U^{-1} = \hat{\boldsymbol{P}}\cdot\mathbf{M}^+ + \mathbf{M}^-\cdot\hat{\boldsymbol{p}} + \beta m\otimes\mathbf{1} + \mathbf{1}\otimes\beta m + V(\boldsymbol{R},\boldsymbol{r}) \tag{6.0.18}$$

where we used the suggestive notation $V(\boldsymbol{R}, \boldsymbol{r})$ for UVU^{-1}. Note that U is induced by a linear transformation $\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3$. Therefore, we have for all $a > 0$ and almost all $\boldsymbol{R}, \boldsymbol{r} \in \mathbb{R}^3$

$$V(a\boldsymbol{R}, a\boldsymbol{r}) = V(\boldsymbol{R}, \boldsymbol{r})/a. \tag{6.0.19}$$

Upon defining $f_a(\boldsymbol{R}, \boldsymbol{r}) := f(a\boldsymbol{R}, a\boldsymbol{r})$, we compute for all $a > 0$ and almost all $\boldsymbol{R}, \boldsymbol{r} \in \mathbb{R}^3$

$$\begin{aligned}\left(U(\overline{H}_0 + V)\ U^{-1} f_a\right)(\boldsymbol{R}, \boldsymbol{r}) = a &\left(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+ f + \mathbf{M}^- \cdot \hat{\boldsymbol{p}} f\right)(a\boldsymbol{R}, a\boldsymbol{r}) \\ &+ \left(\beta m \otimes \mathbf{1} + \mathbf{1} \otimes \beta m + V(\boldsymbol{R}, \boldsymbol{r})\right) f(a\boldsymbol{R}, a\boldsymbol{r}) \\ = a &\left(\hat{\boldsymbol{P}} \cdot \mathbf{M}^+ f + \mathbf{M}^- \cdot \hat{\boldsymbol{p}} f + V(a\boldsymbol{R}, a\boldsymbol{r}) f\right)(a\boldsymbol{R}, a\boldsymbol{r}) \\ &+ \left(\beta m \otimes \mathbf{1} + \mathbf{1} \otimes \beta m\right) f(a\boldsymbol{R}, a\boldsymbol{r}) \\ = a &\left(U(\overline{H}_0 + V)U^{-1} f\right)(a\boldsymbol{R}, a\boldsymbol{r}) + (1-a)\left(\beta m \otimes \mathbf{1} + \mathbf{1} \otimes \beta m\right) f(a\boldsymbol{R}, a\boldsymbol{r}) \\ = a &E f_a(\boldsymbol{R}, \boldsymbol{r}) + (1-a)\left(\beta m \otimes \mathbf{1} + \mathbf{1} \otimes \beta m\right) f_a(\boldsymbol{R}, \boldsymbol{r}).\end{aligned} \tag{6.0.20}$$

This implies

$$\begin{aligned}0 &= \left\langle U(\overline{H}_0 + V)U^{-1} f, f_a\right\rangle - \left\langle f, U(\overline{H}_0 + V)U^{-1} f_a\right\rangle \\ &= E\left\langle f, f_a\right\rangle - aE\left\langle f, f_a\right\rangle - (1-a)\left\langle f, \left(\beta m \otimes \mathbf{1} + \mathbf{1} \otimes \beta m\right) f_a\right\rangle \\ &= (1-a)\left\langle f, \left(E - \beta m \otimes \mathbf{1} - \mathbf{1} \otimes \beta m\right) f_a\right\rangle.\end{aligned} \tag{6.0.21}$$

For $a \neq 1$, we can divide by $(1-a)$. Taking the limit $a \to 1$ gives

$$0 = \left\langle f, \left(E - \beta m \otimes \mathbf{1} - \mathbf{1} \otimes \beta m\right) f\right\rangle. \tag{6.0.22}$$

For $|E| > 2m$, the matrix $E - \beta m \otimes \mathbf{1} - \mathbf{1} \otimes \beta m$ is strictly positive or strictly negative. Thus, $|E| \leq 2m$ leads to a contradiction with (6.0.22). This finishes the proof. □

Remark 6.4. The assumption that all eigenstates f of $\tilde{H}$ lie in $\mathcal{D}(\overline{H}_0) \cap \mathcal{D}(V)$ ensures that we can evaluate f against each summand of $H_{2\mathrm{BD}}$ separately. This is needed for our method of proof. If a different method is employed, this assumption may be dropped. ■

7. Discussion and Outlook

7.1. External Coulomb potentials and essential self-adjointness

Since Stone's theorem links self-adjointness to the existence of a unitary time evolution, a proof of self-adjointness is a first step towards a rigorous investigation of the physical properties of the system at hand. In this respect, our main goal of this thesis is achieved. We provided a self-adjoint extension of $H_{2\mathrm{BD}}$ with Coulomb interaction, which is distinguished uniquely and, as we argue, in a physically sensible way by means of the criterion of finite potential energy. Hence, $H_{2\mathrm{BD}}$ generates a unitary time evolution for two interacting point-like electrons in the vicinity of an extended nucleus. However, we could not yet treat external potentials of Coulomb type. In our future research, we aim at including external Coulomb potentials as well. A positive result would be satisfying not only from a physical but also from a mathematical point of view.

In our strategy of proof, we relied on boundedness of external potentials in several places, in particular, when we constructed a self-adjoint extension of $H_{2\mathrm{BD}}$ from a self-adjoint extension of H^{rel} in Theorem 5.12. We see, however, the possibility of extending the method of direct fiber integrals we employed also to the more complex case when external Coulomb potentials are included.

Proving self-adjointness in the presence of unbounded external potentials might also be helpful for the extension to more than two particles with interaction potentials. It is well-known that the coordinates can always be chosen such that all but one tensor component feel the potential of that particular tensor component as external potential, in addition to the remaining interaction potentials.

Another direction of future research is towards essential self-adjointness of $H_{2\mathrm{BD}}$. We did not exclude this possibility. Theorem 5.8, in which we proved that $\mathcal{D}(V) \cap \mathcal{H}^{\mathrm{rel}}_{-}$ is a core for $V^{1/2}P_{-}$, points already in the right direction as regards essential self-adjointness of H^{rel}. If essential self-adjointness of H^{rel}—once proven—is to be extended to $H_{2\mathrm{BD}}$, one has to bear an important detail in mind. Operators constructed by direct fiber integrals rely on the notion of measurability of families of operators. This notion relies in turn on the closedness of the operators in such a family. Now, essentially self-adjoint operators are not closed, and essential self-adjointness of $H_{2\mathrm{BD}}$ can thus not be inferred from essential self-adjointness of H^{rel} immediately.

7.2. Infinite SPKE and radiation catastrophe

Relativistic quantum theories are, almost by their nature, plagued by infinities and divergences. In Chapter 4, we added one more infinity to the collection, which—to our best knowledge—has not been discussed in the literature so far, namely infinite single particle kinetic energy (infinite SPKE). We then found that, for fermions, these states cannot occur (see Section 4.4) as well as that infinite SPKE states cannot be reached by scattering processes involving finite SPKE states for all finite times $t \in \mathbb{R}$ (see Section 4.5).

We defined the kinetic energy of the first particle in the two-body state ψ by

$$E_{\mathrm{kin},1}[\psi] = \langle \psi, (-i\boldsymbol{\alpha} \cdot \nabla_{\boldsymbol{x}} + \beta m) \otimes \mathrm{id}\psi \rangle \tag{7.2.1}$$

in Definition 4.7 and analogously for the second particle. Due to the spinor structure of two-body states, it can happen that $E_{\mathrm{kin},1}[\psi] = E_{\mathrm{kin},2}[\psi] = 0$ although ψ may also contain high momenta, as shown in Example 4.10. This indicates that our definition of single particle kinetic energy by $E_{\mathrm{kin},1}[\psi]$ might not be satisfactory. However, Dirac's radiation catastrophe and the stability of (unprojected) relativistic many-body system partly rest on the notion of single particle kinetic energy. Therefore, a rigorous and physically meaningful definition of it lays the foundation of further investigations.

These further investigations can take several different directions. One particular interesting direction considers the connection of antisymmetric states and Dirac's radiation catastrophe, and is suggested by the absence of antisymmetric SPKE states. We modify the radiation catastrophe slightly such that it fits the context of $H_{2\mathrm{BD}}$. Originally, it consists of an electron that is accelerated by some means (in absence of the Dirac sea). This electron thus emits radiation. As the spectrum of the Dirac operator generically extends to $-\infty$, the electron can emit more and more radiation by falling deeper and deeper into the negative spectrum. Now, we no longer assume a radiation field with independent degrees of freedom, but simply a second particle. The two particles can interact. In this two-body universe, no energy can escape, i.e., energy is transferred from one particle to the other only. Precisely this situation is described by $H_{2\mathrm{BD}}$. If now one particle falls deeper and deeper in the spectrum, this has to be compensated for by the other particle which will attain higher and higher energies. In this heuristic picture, the two particles can reach positive, respectively, negative infinite energy only in infinite time.

In order to make now the connection to antisymmetric states, we first recast the modified radiation catastrophe in mathematical terms and conjecture that for each infinite SPKE state ψ_∞, there exists an initial state ψ_0 with finite SPKE such that

$$\psi_\infty = \lim_{t \to \infty} \mathrm{e}^{-itH_{2\mathrm{BD}}} \psi_0. \tag{7.2.2}$$

Maybe this limit can even be turned into an equivalence, i.e., if the time evolution $\mathrm{e}^{-itH_{2\mathrm{BD}}}\psi_0$ is such that the two particles move more and more apart in the spectrum, i.e., they exhibit the modified radiation catastrophe, then there exists an SPKE state to which they converge in the limit $t \to \infty$.

This conjectured equivalence of SPKE states and the modified radiation catastrophe in the limit $t \to \infty$ poses the question if absence of antisymmetric infinite SPKE states, as shown in Section 4.4, automatically entails stability of antisymmetric interacting relativistic two-body systems without radiation, or even more general, N-body systems. Put differently, is the Dirac sea, which is necessarily antisymmetric, automatically stable? Of course, answering this question rigorously hinges on satisfying and physically adequate notions of stability, single particle kinetic energy, and the like. We list a few questions:

Q1 Is it possible to explicitly construct an initial finite SPKE state ψ_0 for which it can be proven that $\lim_{t\to\infty} \mathrm{e}^{-itH_{\mathrm{2BD}}}\psi_0$ not only exists, but is an infinite SPKE state?

Q2 How can initial states be classified which are such that they drift apart in the spectrum under the time evolution, i.e., exhibit the modified radiation catastrophe after some time? Are they rare in some sense?

Q3 Does the restriction to antisymmetric two-body states rule out the modified radiation catastrophe completely, or only according to our notion of single particle kinetic energy?

Q4 What is a good notion of stability for unprojected many-body Dirac operators? Is the notion of asymptotic completeness adequate?

7.3. Brown-Ravenhall disease and the spectrum

Although identifying the essential spectrum of H_{2BD}, as we did in Chapter 6, is very important and generally regarded as one of the first steps towards any spectral analysis, what one is really interested in, of course, are eigenvalues and/or resonances. After all, using H_{2BD} as model for the Helium atom and investigating its spectral properties is the main motivation for the use of H_{2BD} in relativistic quantum chemistry. What makes the investigation of the point spectrum of H_{2BD} so interesting, however, is the absence of isolated eigenvalues. This is a reformulation of $\sigma_{\mathrm{ess}}(H_{\mathrm{2BD}}) = \mathbb{R}$ from Theorem 6.1. Before we shed light on some aspects concerning a further investigation of the spectrum of H_{2BD}, we describe the physical background of any spectral analysis of H_{2BD}.

The relevant phenomenon has been first described by G.E. Brown and D.G. Ravenhall in [BR51], and thus, goes under the name of «Brown-Ravenhall disease». The symptom of this disease is the non-existence of eigenvalues—including a lowest eigenvalue or physical ground state of H_{2BD}, i.e., the Helium atom—due to the possible interaction of particles with positive energy and negative energy. To be more precise, the Brown-Ravenhall disease is a direct consequence of the existence of the negative energy continuum, which is typical for Dirac operators, in combination with the interaction potential present in H_{2BD}.

Let us describe the mechanism that leads, according to Brown and Ravenhall, to the absence of eigenvalues. First, we consider H_{2BD} without interaction, i.e.,

$$\begin{aligned} H_0 + V_{\mathrm{ext}} = (&-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \beta m + V_{\mathrm{ext},\boldsymbol{x}}) \otimes \mathrm{id} \\ &+ \mathrm{id} \otimes (-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}} + \beta m + V_{\mathrm{ext},\boldsymbol{y}}), \end{aligned} \tag{7.3.1}$$

where $V_{\text{ext}} = V_{\text{ext},\boldsymbol{x}} + V_{\text{ext},\boldsymbol{y}}$. It is well-known that $H_0 + V_{\text{ext}}$ has eigenvalues E for which we can write $E = E_1 + E_2$, where E_1 is an eigenvalue of $-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{x}} + \beta m + V_{\text{ext},\boldsymbol{x}}$, and E_2 of $-i\boldsymbol{\alpha}\cdot\nabla_{\boldsymbol{y}} + \beta m + V_{\text{ext},\boldsymbol{y}}$ analogously. All eigenvalues E are embedded into the continuous part of the spectrum. This implies that for all energies E' arbitrarily close to E, there exist (uncountably many) eigenvalues $E_1' < -2m$ and $E_2' > 2m$, such that $E_1' + E_2' = E'$.

If the interaction is switched on, one expects a shift of the eigenvalue E to E'. Brown and Ravenhall now argue that Fermi's Golden Rule (see line (7.3.2) below) and the sheer abundance of energies $E_1' < -2m$ and $E_2' > 2m$ such that $E_1' + E_2' = E'$ imply that all eigenvalues vanish or turn into resonances. In the physics literature, one says that E dissolves into the continuum. The Brown-Ravenhall disease denotes exactly this continuum dissolution.

In conclusion, the direction of further research suggested by the Brown-Ravenhall disease is to show absence of embedded eigenvalues. There exists a canonical approach to this task, namely employing dilation methods. Applying the dilation transformation to $H_0 + V_{\text{ext}}$ has—under some conditions—the effect of isolating embedded eigenvalues. This makes standard Kato perturbation theory for eigenvalues applicable to the dilated operator. V_{int} is then considered as standard Kato perturbation of the dilated two-body Dirac operator without interaction, just as in the heuristic picture of the Brown-Ravenhall disease above. For the non-relativistic Helium atom, this approach is presented in great detail in [RS78]. In that scenario, eigenstates corresponding to embedded eigenvalues that turn into resonances when perturbed are called «Auger states». For the relativistic scenario, first results concerning complex dilated one-body Dirac operators were obtained in [Š88] and in [Wed73] which have been generalized considerably in [Hub09]. These references seem to be a promising starting point for applying dilation methods to $H_{2\text{BD}}$ due to the tensor product structure of $H_0 + V_{\text{ext}}$, and indeed, some arguments from the non-relativistic case also apply to $H_{2\text{BD}}$. We just want to mention one step from the presentation given in [RS78] that has to be substantially modified. The complex dilated two-body Dirac operator without interaction is not self-adjoint. Due to its unboundedness from below, eigenvalues cannot be directly read off from the tensor product structure, as in the non-relativistic case.

In, e.g., [Sim73], it is shown that there exists a formal connection between complex dilation methods and Fermi's Golden Rule. This formal connection can be made clear, if $H_0 + V_{\text{ext}}$ has continuum eigenstates. Let ψ_0 denote an eigenstate of $H_0 + V_{\text{ext}}$ with energy E_0, and let $\psi_\lambda(E)$ denote continuum eigenstates of $H_0 + V_{\text{ext}}$ with energy E, continuously parametrized by $\lambda \in \mathbb{R}$. The interaction potential V_{int} plays the role of the perturbation. When the interaction is turned on, the eigenstate ψ_0 turns into a resonance, if it has a non-zero decay width Γ, i.e.,

$$\Gamma = 2\pi \int_{\mathbb{R}} |\langle \psi_\lambda(E_0),\, V_{\text{int}}\, \psi_0 \rangle|^2 \, \mathrm{d}\lambda \neq 0. \tag{7.3.2}$$

This is precisely the mechanism leading to the Brown-Ravenhall disease cast into mathematical terms. Let us mention some literature relevant for this strategy of showing absence of embedded eigenvalues. Existence of continuum eigenstates, or generalized eigenfunctions, for one-particle Dirac operators in an external field has been treated rigorously by many authors, notably in [Nen75] and in [Yam76] as well as references therein. Explicit calculations of such eigenfunctions as well as bound states can be found in, e.g., [Gre00], [PG69], and [Ros61]. Due to its tensor product structure, these results carry over to $H_0 + V_{\text{ext}}$. In principle, showing absence of eigenvalues now reduces to plugging everything into (7.3.2), and carrying out all needed calculations. In the literature, these particular computations are acknowledged as formidable (see [Ros61]) as they involve, e.g., 16-component spinors, whose components can all lead to cancellations in the occurring scalar products and back and forth coordinate transformations. To our best knowledge, it has not been achieved, not even for simpler cases.

If absence of eigenvalues of H_{2BD} could be shown, this would be, of course, in stark contrast to the empirical evidence that Helium atoms are stable (provided that the lifetimes of possible resonances are not of the order of the age of the universe). Clearly, this would have strong negative implications for the validity of the H_{2BD}-model of Helium. Nevertheless, the two-body Dirac Hamiltonian is used in the relativistic quantum chemistry literature under the tacit assumption of, e.g., the existence of square-integrable eigenfunctions "*in hundreds of papers every year*" (see [Der12]). This makes an investigation of $\sigma(H_{\text{2BD}})$ in rigorous mathematical terms very relevant to current research.

A. Matrix operators with unbounded entries

This appendix gives a short introduction to the theory of matrix operators with unbounded entries. The goal is to derive the so-called Frobenius-Schur factorization of such operators in Theorem A.3. This factorization shows that important properties such as closedness or self-adjointness are—under some conditions—contained in the Schur complement, given in line (A.0.8). We apply this result to H^{rel}. A good general reference for matrix operators is [Tre08].

We introduce notation for this section only. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be closed subspaces of the Hilbert space $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ holds. We consider the matrix operator

$$\mathcal{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{A.0.1}$$

that acts naturally in the Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$. Its entries are unbounded operators with

$$\begin{aligned} &A\colon \mathcal{D}(A) \to \mathcal{H}_1, \quad B\colon \mathcal{D}(B) \to \mathcal{H}_1, \\ &C\colon \mathcal{D}(C) \to \mathcal{H}_2, \quad D\colon \mathcal{D}(D) \to \mathcal{H}_2 \end{aligned} \tag{A.0.2}$$

and they are throughout this section subject to the following conditions:

M1 A, B, C, and D are closable, possibly unbounded operators with dense domains

$$\mathcal{D}(A), \mathcal{D}(C) \subset \mathcal{H}_1\,, \quad \mathcal{D}(B), \mathcal{D}(D) \subset \mathcal{H}_2. \tag{A.0.3}$$

M2 $\mathcal{D}(B) = \mathcal{D}(D)$.

M3 The resolvent set of A is not empty, i.e. $\rho(A) \neq \emptyset$.

M4 $\mathcal{D}(A^*) \subset \mathcal{D}(B^*)$.

M5 $\mathcal{D}(A) \subset \mathcal{D}(C)$.

M6 $\mathcal{D}(\mathcal{A}) = \mathcal{D}(A) \oplus \mathcal{D}(D)$ which is dense in $\mathcal{H}$.

Lemma A.1. *The matrix operator $\mathcal{A}$ is symmetric if and only if*

$$A \subseteq A^*, \quad D \subseteq D^*, \quad C \restriction \mathcal{D}(A) \subseteq B^*, \quad B \subseteq C^*. \tag{A.0.4}$$

Proof. We follow [Tre08, Proposition 2.6.1]. □

Lemma A.2. *The following statements hold for all $\mu \in \rho(A)$:*

a) The operator $(A-\mu)^{-1}B$ is bounded on $\mathcal{D}(B)$.

b) The operator $C(A-\mu)^{-1}$ is bounded on all of $\mathcal{H}_1$.

c) The matrix operators $\mathcal{R}(\mu)\colon \mathcal{H} \to \mathcal{H}$ and $\mathcal{T}(\mu)\colon \mathcal{H} \to \mathcal{H}$, given by

$$\mathcal{R}(\mu) := \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ C(A-\mu)^{-1} & \mathrm{id} \end{pmatrix}, \quad \mathcal{T}(\mu) := \begin{pmatrix} \mathrm{id} & \overline{(A-\mu)^{-1}B} \\ \mathbf{0} & \mathrm{id} \end{pmatrix} \tag{A.0.5}$$

are bounded and boundedly invertible.

d) If $\mathcal{A}$ is symmetric with $A = A^*$, then $\mathcal{R}(\mu)^* = \mathcal{T}(\overline{\mu})$ and $\mathcal{T}(\mu)^* = \mathcal{R}(\overline{\mu})$ hold.

Proof. a) See [Tre08, Remark 2.2.15].

b) This follows from the closed graph theorem.

c) See [Tre08, Theorem 2.2.18].

d) With Lemma A.1 and $A = A^*$, we obtain

$$((A-\mu)^{-1}B)^* = B^*(A^*-\overline{\mu})^{-1} = B^*(A-\overline{\mu})^{-1} = C(A-\overline{\mu})^{-1} \tag{A.0.6}$$

and

$$(C(A-\mu)^{-1})^* \supseteq (A^*-\overline{\mu})^{-1}C^* = (A-\overline{\mu})^{-1}C^* \supseteq (A-\overline{\mu})^{-1}B. \tag{A.0.7}$$

Since the bounded linear transformation theorem gives a unique closed extension of $(A-\mu)^{-1}B$, and $(C(A-\mu)^{-1})^*$ is closed, it follows that $(C(A-\mu)^{-1})^* = \overline{(A-\overline{\mu})^{-1}B}$. Hence, equations (A.0.6) and (A.0.7) imply $\mathcal{R}(\mu)^* = \mathcal{T}(\overline{\mu})$ and $\mathcal{T}(\mu)^* = \mathcal{R}(\overline{\mu})$. □

The Schur complement of A is defined by

$$S(\mu) := D - \mu - C(A-\mu)^{-1}B \tag{A.0.8}$$

with domain $\mathcal{D}(S(\mu)) = \mathcal{D}(D)$ for all $\mu \in \rho(A)$.

Theorem A.3. *$\mathcal{A}$ is closable if and only if, for all $\mu \in \rho(A)$, $S(\mu)$ is closable in $\mathcal{H}_2$. The closure $\overline{\mathcal{A}}$ is given by the Frobenius-Schur factorization*

$$\overline{\mathcal{A}} = \mu + \begin{pmatrix} \mathrm{id} & \mathbf{0} \\ C(A-\mu)^{-1} & \mathrm{id} \end{pmatrix} \begin{pmatrix} A-\mu & \mathbf{0} \\ \mathbf{0} & \overline{S(\mu)} \end{pmatrix} \begin{pmatrix} \mathrm{id} & \overline{(A-\mu)^{-1}B} \\ \mathbf{0} & \mathrm{id} \end{pmatrix}, \tag{A.0.9}$$

independently of $\mu \in \rho(A)$, that is,

$$\mathcal{D}(\overline{\mathcal{A}}) = \left\{ \begin{pmatrix} f \\ g \end{pmatrix} \in \mathcal{H}_1 \oplus \mathcal{H}_2 \;\middle|\; \begin{array}{c} f + \overline{(A-\mu)^{-1}B}g \in \mathcal{D}(A), \\ g \in \mathcal{D}(\overline{S(\mu)}) \end{array} \right\} \tag{A.0.10}$$

$$\overline{\mathcal{A}}\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} (A-\mu)(f+\overline{(A-\mu)^{-1}B}g)+\mu f \\ C(f+\overline{(A-\mu)^{-1}B}g)+(\overline{S(\mu)}+\mu)g \end{pmatrix}. \tag{A.0.11}$$

Proof. See [Shk95, Theorem 1]. □

B. Auxiliary lemma

Lemma B.1. *Let* $0 < \kappa \leq 1$*. Then, for any* $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3$ *it holds that*

$$\left| |\boldsymbol{a} - \boldsymbol{b}|^{\kappa/2} - |\boldsymbol{a}|^{\kappa/2} \right| \leq |\boldsymbol{b}|^{\kappa/2}. \tag{B.0.1}$$

Proof. First, we assume $|\boldsymbol{a}-\boldsymbol{b}|^{\kappa/2} \geq |\boldsymbol{a}|^{\kappa/2}$. Then, with $|\boldsymbol{a}-\boldsymbol{b}| \leq |\boldsymbol{a}|+|\boldsymbol{b}|$ and monotonicity of exponentiation, we obtain

$$|\boldsymbol{a} - \boldsymbol{b}|^{\kappa/2} \leq (|\boldsymbol{a}| + |\boldsymbol{b}|)^{\kappa/2} \leq |\boldsymbol{a}|^{\kappa/2} + |\boldsymbol{b}|^{\kappa/2}, \tag{B.0.2}$$

where we used the equivalence of the $2/\kappa$-norm with the 1-norm in $\mathbb{R}^2$:

$$\begin{aligned}(|\boldsymbol{a}| + |\boldsymbol{b}|)^{\frac{1}{2/\kappa}} &= \left(|\boldsymbol{a}|^{\frac{2/\kappa}{2/\kappa}} + |\boldsymbol{b}|^{\frac{2/\kappa}{2/\kappa}}\right)^{\frac{1}{2/\kappa}} \\ &= \left\| \begin{pmatrix} |\boldsymbol{a}|^{\frac{1}{2/\kappa}} \\ |\boldsymbol{b}|^{\frac{1}{2/\kappa}} \end{pmatrix} \right\|_{2/\kappa} \leq \left\| \begin{pmatrix} |\boldsymbol{a}|^{\frac{1}{2/\kappa}} \\ |\boldsymbol{b}|^{\frac{1}{2/\kappa}} \end{pmatrix} \right\|_{1} = |\boldsymbol{a}|^{\frac{1}{2/\kappa}} + |\boldsymbol{b}|^{\frac{1}{2/\kappa}}.\end{aligned} \tag{B.0.3}$$

Inequality (B.0.2) then implies

$$|\boldsymbol{a} - \boldsymbol{b}|^{\kappa/2} - |\boldsymbol{a}|^{\kappa/2} \leq |\boldsymbol{b}|^{\kappa/2}. \tag{B.0.4}$$

Next, we assume $|\boldsymbol{a}|^{\kappa/2} \geq |\boldsymbol{a} - \boldsymbol{b}|^{\kappa/2}$. Then, with $|\boldsymbol{a}| \leq |\boldsymbol{a} - \boldsymbol{b}| + |\boldsymbol{b}|$ and monotonicity of exponentiation, we get

$$|\boldsymbol{a}|^{\kappa/2} \leq (|\boldsymbol{a} - \boldsymbol{b}| + |\boldsymbol{b}|)^{\kappa/2} \leq |\boldsymbol{a} - \boldsymbol{b}|^{\kappa/2} + |\boldsymbol{b}|^{\kappa/2} \tag{B.0.5}$$

which implies

$$|\boldsymbol{a}|^{\kappa/2} - |\boldsymbol{a} - \boldsymbol{b}|^{\kappa/2} \leq |\boldsymbol{b}|^{\kappa/2} \tag{B.0.6}$$

where we made again use of the inequality from line (B.0.3). This concludes the proof. □

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