On Quantum Mechanical Decay Processes

Robert Grummt

Dissertation
an der Fakultät für Mathematik, Informatik und Statistik
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Abstract

This thesis is concerned with quantum mechanical decay processes and their mathematical description. It consists out of three parts:

In the first part we look at Laser induced ionization, whose mathematical description is often based on the so-called dipole approximation. Employing it essentially means to replace the Laser's vector potential $\mathbf{A}(\mathbf{r}, t)$ in the Hamiltonian by $\mathbf{A}(0, t)$. Heuristically this is justified under usual experimental conditions, because the Laser varies only slowly in $\mathbf{r}$ on atomic length scales. We make this heuristics rigorous by proving the dipole approximation in the limit in which the Laser's length scale becomes infinite compared to the atomic length scale. Our results apply to N-body Hamiltonians.

In the second part we look at alpha decay as described by Skibsted (Comm. Math. Phys. 104, 1986) and show that Skibsted's model satisfies an energy-time uncertainty relation. Since there is no self-adjoint time operator, the uncertainty relation for energy and time can not be proven in the same way as the uncertainty relation for position and momentum. To define the time variance without a self-adjoint time operator, we will use the arrival time distribution obtained from the quantum current. Our proof of the energy-time uncertainty relation is then based on the quantitative scattering estimates that will be derived in the third part of the thesis and on a result from Skibsted. In addition to that, we will show that this uncertainty relation is different from the well known *linewidth-lifetime relation*.

The third part is about quantitative scattering estimates, which are of interest in their own right. For rotationally symmetric potentials having support in $[0, R_V]$ we will show that for $R \geq R_V$, the time evolved wave function $e^{-iHt}\psi$ satisfies

$$\|\mathbf{1}_R e^{-iHt}\psi\|_2^2 \leq c_1 t^{-1} + c_2 t^{-2} + c_3 t^{-3} + c_4 t^{-4}$$

with explicit quantitative bounds on the constants c_n in terms of the resonances of the S-Matrix. While such bounds on $\|\mathbf{1}_R e^{-iHt}\psi\|_2$ have

been proven before, the quantitative estimates on the constants c_n are new. These results are based on a detailed analysis of the S-matrix in the complex momentum plane, which in turn becomes possible by expressing the S-matrix in terms of the Jost function that can be factorized in a Hadamard product.

Zusammenfassung

Gegenstand dieser Arbeit ist die mathematische Beschreibung von quantenmechanischen Zerfallsprozessen.

Im ersten von drei Teilen, werden wir die durch Laser induzierte Ionisation von Atomen untersuchen, die üblicherweise mit Hilfe der sogenannten Dipolapproximation beschrieben wird. Bei dieser Approximation wird das Vektorpotential $\mathbf{A}(\mathbf{r}, t)$ des Lasers im Hamiltonoperator durch $\mathbf{A}(0, t)$ ersetzt, was oft dadurch gerechtfertigt ist, dass sich das Vektorpotential des Lasers auf atomaren Längenskalen in $\mathbf{r}$ kaum verändert. Ausgehend von dieser Heuristik werden wir die Dipolapproximation in dem Limes beweisen, in dem die Wellenlänge des Lasers im Verhältnis zur atomaren Längenskala unendlich groß wird. Unsere Resultate sind auf N-Teilchen Systeme anwendbar.

Im zweiten Teil wenden wir uns dem Alphazerfallsmodell von Skibsted (Comm. Math. Phys. 104, 1986) zu und beweisen, dass es eine Energie-Zeit Unschärfe erfüllt. Da kein selbstadjungierter Zeitoperator existiert, kann die Energie-Zeit Unschärfe nicht auf gleiche Weise wie die Orts-Impuls Unschärfe bewiesen werden. Um ohne einen selbstadjungierten Zeitoperator Zugriff auf die Zeitvarianz zu bekommen, werden wir mit Hilfe des quantenmechanischen Wahrscheinlichkeitsstroms eine Ankunftszeitverteilung definieren. Der Beweis der Energie-Zeit Unschärfe folgt dann aus einem Resultat von Skibsted und aus den quantitativen Streuabschätzungen, die im dritten Teil der Dissertation bewiesen werden. Darüber hinaus werden wir zeigen, dass diese Unschärfe von der *linewidth-lifetime relation* zu unterscheiden ist.

Hauptresultat des dritten Teils sind quantitative Streuabschätzungen, die als eigenständiges Resultat von Interesse sind. Für rotationssymmetrische Potentiale mit Träger in $[0, R_V]$ werden wir für alle $R \geq R_V$ die Abschätzung

$$\|\mathbf{1}_R e^{-iHt}\psi\|_2^2 \leq c_1 t^{-1} + c_2 t^{-2} + c_3 t^{-3} + c_4 t^{-4}$$

beweisen und darüber hinaus, das ist das Novum, quantitative Schranken

für die Konstanten c_n angeben, die von den Resonanzen der S-Matrix abhängen. Um zu diesen Schranken zu gelangen, werden wir die analytische Struktur der S-Matrix studieren, indem wir die Beziehung der S-Matrix zur Jost-Funktion ausnutzen und die wiederum in ein Hadamard-Produkt zerlegen.

Danksagung

Der wissenschaftliche Deckmantel dieser Arbeit soll nicht darüber hinweg täuschen, dass sie letztendlich das Resultat kostbarer persönlicher Einflüsse auf mich ist.

Den wundervollsten Einfluss auf mein Leben hat Carina. Durch sie habe ich gelernt worauf es wirklich ankommt: die Menschen. Jede Minute mit ihr ist ein Geschenk und es ist wundervoll zusammen mit ihr zu wachsen!

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Die vorliegenden Resultate sind vor allem aus der Zusammenarbeit mit Nicola Vona entstanden, die mir viel Freude bereitet hat. Durch ihn habe ich verstanden, wie wertvoll ein gutes Team ist.

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Chapter 1

Preface

Radioactivity was discovered in 1896 by Henri Becquerel and categorized into alpha-, beta- and gamma-radiation by Ernest Rutherford in 1899. In the wake of the discovery of Quantum Mechanics George Gamow [16] was able to explain alpha decay with the following insight. In contrast to Classical Mechanics where particles trapped by a potential barrier remain trapped, in Quantum Mechanics such particles can escape via tunneling through the barrier. Consider Uranium 238 for example. By assuming that some of the nucleons in Uranium formed an alpha particle moving with an energy $E > 0$ in an effective barrier potential (see Fig. 1.1) generated by the remaining nucleons, Gamow was able to explain the alpha decay of Uranium 238 with the help of this tunneling mechanism.

However, Gamow's explanation has a wider range of application than alpha decay. It has also been employed to understand the ionization of atoms due to Lasers. This process is governed by the Schrödinger

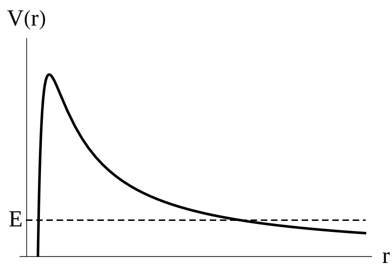

Figure 1.1: Gamow potential.

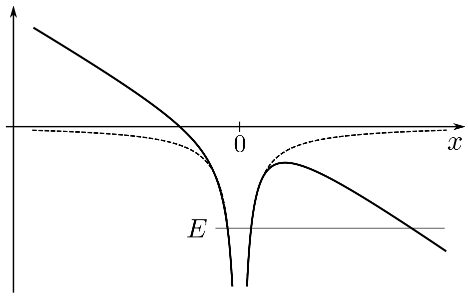

Figure 1.2: Plot of the Coulomb potential alone (dashed line) and of the Coulomb potential together with the electric potential $E\cos(\omega t)x$ of a continuous wave Laser at time $t = 0$ (solid line).

equation

$$i\hbar\frac{\partial}{\partial t}\psi = \left[\frac{1}{2m}(-i\hbar\nabla - \tfrac{e}{c}\mathbf{A}_\lambda(\mathbf{r},t))^2 - \frac{e^2}{r}\right]\psi, \tag{1.1}$$

where $\mathbf{A}_\lambda$ is the vector potential that describes the Laser with wave length λ in Coulomb gauge ($\nabla \cdot \mathbf{A}_\lambda = 0$). If we then simplify Eq. (1.1) using the so-called dipole approximation, which in essence replaces the vector potential $\mathbf{A}_\lambda(\mathbf{r},t)$ by $\mathbf{A}_\lambda(0,t)$, we arrive after a simple gauge transformation at

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\Delta - \frac{e^2}{r} - e\mathbf{E}(0,t)\cdot\mathbf{r}\right]\psi, \tag{1.2}$$

where $\mathbf{E} = -\frac{1}{c}\partial_t\mathbf{A}_\lambda$ is the electric field of the Laser. Heuristically this approximation is justified by the fact that the Laser's vector potential under usual experimental conditions varies only slowly in $\mathbf{r}$ on atomic length scales. Now we can plot the total potential in Eq. (1.2) that governs the motion of the electron (see Fig. 1.2), if we assume a continuous wave Laser, for which $\mathbf{E}(0,t)\cdot\mathbf{r}$ is given by $E\cos(\omega t)x$ with ω denoting the Laser's frequency and E denoting its field strength. We see that the Laser deforms the Coulomb potential in such a way that the previously bound electron can escape via tunneling. In Chapter 2 we will turn the heuristic justification for the dipole approximation given above into a proof.

A central parameter of decay processes is the lifetime, say for example of the Uranium 238 nucleus. It is believed (see e.g. [50]) that the energy-time uncertainty relation gives a handle on that, i.e. by measuring the energy variance of the decay product one obtains the lifetime of the nucleus using this relation. But due to the fact that there is no self-adjoint time operator (see [39]), the energy-time uncertainty relation requires a completely different justification than the well known position-momentum uncertainty relation. In Chapter 4 we will look at the alpha decay model used in [56] that is based on Gamow's ideas and we will show that this model satisfies an energy-time uncertainty relation. But we will also show that this relation gives poor control over the lifetime. This is due to the fact that the energy-time uncertainty relation is different from the well known *linewidth-lifetime relation*, an observation already made by Fock and Krylov [28].

I should like to thank V. Bach, M. Goldberg, W. Schlag, E. Skibsted, and M. Zworski for helpful correspondence. Financial support by the Studienstiftung des deutschen Volkes is gratefully acknowledged.

Chapter 2

On the Proof of the Dipole Approximation

2.1 Introduction

The interaction of atoms with Lasers is governed by the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}U_\lambda(t,t_0) = \left[\frac{1}{2m}(-i\hbar\nabla - \tfrac{e}{c}\mathbf{A}_\lambda(\mathbf{r},t))^2 + V(\mathbf{r})\right]U_\lambda(t,t_0), \tag{2.1}$$

where V is the atomic binding potential and $\mathbf{A}_\lambda$ is the vector potential that describes the Laser with wave length λ in Coulomb gauge ($\nabla\cdot\mathbf{A}_\lambda = 0$). However, in the mathematical as well as the physical literature the analysis of atoms interacting with Lasers is very often based on

$$i\hbar\frac{\partial}{\partial t}U_D(t,t_0) = \left[-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) - e\mathbf{E}(0,t)\cdot\mathbf{r}\right]U_D(t,t_0), \tag{2.2}$$

where $\mathbf{E} = -\frac{1}{c}\partial_t\mathbf{A}_\lambda$, rather than Eq. (2.1).

Heuristically, one arrives at Eq. (2.2) by applying the dipole approximation to Eq. (2.1), which we will explain now using the example of a Coulomb potential $V(r) = -e^2/r$ interacting with a continuous wave Laser described by the electric field

$$\mathbf{E}(\mathbf{r},t) = E\cos\left(\frac{2\pi}{\lambda}\hat{k}\cdot\mathbf{r} - \omega t\right)\hat{\varepsilon}. \tag{2.3}$$

Here E denotes the electric field strength, $\hat{k}$ the normalized vector pointing in propagation direction and $\hat{\varepsilon}$ the normalized vector pointing in polar-

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ization direction. For $\mathbf{E}$ to satisfy the sourceless Maxwell equations, we further need $\hat{k}\cdot\hat{\varepsilon} = 0$ and $\omega = 2\pi c/\lambda$. In natural units Eq. (2.1) then reads

$$i\frac{\partial}{\partial t}U_\lambda(t,t_0) = \left[\left(-i\nabla - \frac{ea_0E}{\hbar\omega}\sin\left(2\pi\frac{a_0}{\lambda}\hat{k}\cdot\mathbf{r} - \tau\omega t\right)\right)^2 - \frac{2}{r}\right]U_\lambda(t,t_0), \tag{2.4}$$

where a_0 is the characteristic length scale of an atom (Bohr radius) and $\tau = 2ma_0^2/\hbar$ is the characteristic time scale. Defining the characteristic velocity by $v = a_0/\tau$, the Dipole approximation of Eq. (2.4) is obtained by taking the scaling limits $a_0/\lambda \to 0$ and $v/c \to 0$ in such a way that $\omega = 2\pi c/\lambda$ remains constant. Performing these limits on Eq. (2.4), we obtain

$$i\frac{\partial}{\partial t}U_\infty(t,t_0) = \left[\left(-i\nabla + \frac{ea_0E}{\hbar\omega}\sin(\tau\omega t)\right)^2 - \frac{2}{r}\right]U_\infty(t,t_0), \tag{2.5}$$

which upon gauge transformation yields Eq. (2.2) in natural units.

The purpose of this Chapter is to prove that in the scaling limits $a_0/\lambda \to 0$ and $v/c \to 0$ with ω kept constant the dipole approximation is exact, in the sense that the time evolution generated by Eq. (2.1) is the same as the one generated by Eq. (2.2), up to gauge equivalence. In the rest of the Chapter we will use units, where $\hbar = e = 1$ and $m = 1/2$. Our main result is the following

Theorem 2.1. *Assume that the potential $V \in L^2_{loc}(\mathbb{R}^n)$ is infinitesimally $-\Delta$-bounded and that $\mathbf{A}_\lambda(\mathbf{r},t) = \frac{c}{\omega}\mathbf{a}(\frac{\mathbf{r}}{\lambda},\omega t)$, where $\mathbf{a} \in C^2(\mathbb{R}^{n+1})^n$ is independent of λ,ω,c and satisfies $\nabla\cdot\mathbf{a}(\mathbf{r},t) = 0$ as well as $\|\partial_t^j a^i(\cdot,t)\|_\infty \le C$ for some $C < \infty$ uniformly in t, $i = 1,\dots,n$ and $j = 0,1,2$. Then*

1) the operators

$$H_\lambda(t) = (-i\nabla - \tfrac{1}{c}\mathbf{A}_\lambda(\mathbf{r},t))^2 + V(\mathbf{r}) \quad \textit{and} \tag{2.6}$$

$$H_\infty(t) = (-i\nabla - \tfrac{1}{\omega}\mathbf{a}(0,\omega t))^2 + V(\mathbf{r}). \tag{2.7}$$

with common domain $\mathcal{D}(H_\lambda(t)) = \mathcal{D}(H_\infty(t)) = W^{2,2}(\mathbb{R}^n)$ are self-adjoint and generate unitary evolution operators $(U_\lambda(t,t_0))_{0\le t_0\le t}$

and $(U_\infty(t,t_0))_{0\le t_0\le t}$, *respectively.* $U_\lambda(t,t_0)$ *and* $U_\infty(t,t_0)$ *are strongly continuous in* t *as well as* t_0 *and leave* $W^{2,2}(\mathbb{R}^n)$ *invariant.*

2) *Further, for every* $\psi \in L^2(\mathbb{R}^n)$ *and* $0 < t_0 \le t < \infty$,

$$\|(U_\lambda(t,t_0) - U_\infty(t,t_0))\psi\| \to 0 \tag{2.8}$$

as $\lambda \to \infty$ *and* $c \to \infty$ *such that* ω *remains constant.*

There are two difficulties in proving this Theorem. Firstly, the Hamiltonian is time dependent. Time *in*dependent Hamiltonians H generate time evolution operators $U(t,t_0)$, which are given by $e^{-iH(t-t_0)}$. So if we have a series of Hamiltonians $\{H_n\}_{n=0}^{\infty}$ with $H_n \to H$ as $n \to \infty$ in strong resolvent sense, we know that the time evolution operators $e^{-iH_n(t-t_0)}$ converge to $e^{-iH(t-t_0)}$. This is a consequence of the Spectral Theorem (see [46, Theorem VIII.21] for details). In contrast, time evolution operators generated by time dependent Hamiltonians that do not commute at different instances of time can not be expressed as functions of the Hamiltonian. Hence, the Spectral Theorem is not applicable to the time evolution operator. To show that $U_\lambda(t,t_0) \to U_\infty(t,t_0)$ as $\lambda \to \infty$ and $c \to \infty$ with ω constant, we will therefore use Cook's argument. This allows us to express the difference between time evolution operators in terms of the difference between their respective generators:

$$\begin{aligned}
&U_\lambda(t,t_0) - U_\infty(t,t_0) \\
&\quad = -i\int_{t_0}^{t} U_\lambda(t,s)(H_\lambda(s) - H_\infty(s))U_\infty(s,t_0)\,ds && (2.9)\\
&\quad = -i\int_{t_0}^{t} U_\lambda(t,s)(2i(\tfrac{1}{c}\mathbf{A}_\lambda(\mathbf{r},s) - \tfrac{1}{\omega}\mathbf{a}(0,\omega s))\cdot\nabla \\
&\qquad\qquad + (\tfrac{1}{c^2}\mathbf{A}_\lambda(\mathbf{r},s)^2 - \tfrac{1}{\omega^2}\mathbf{a}(0,\omega s)^2))U_\infty(s,t_0)\,ds && (2.10)\\
&\quad = -i\int_{t_0}^{t} U_\lambda(t,s)(\tfrac{2i}{\omega}(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda},\omega s) - \mathbf{a}(0,\omega s))\cdot\nabla \\
&\qquad\qquad + \tfrac{1}{\omega^2}(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda},\omega s)^2 - \mathbf{a}(0,\omega s)^2))U_\infty(s,t_0)\,ds. && (2.11)
\end{aligned}$$

Since $\mathbf{a}(\frac{\mathbf{r}}{\lambda},\omega s) - \mathbf{a}(0,\omega s)$ and $\mathbf{a}(\frac{\mathbf{r}}{\lambda},\omega s)^2 - \mathbf{a}(0,\omega s)^2$ tend pointwise to zero as $\lambda \to \infty$, the main task is now to show that the Theorem of Dominated Convergence applies to Eq. (2.11). The second and main difficulty in proving the Theorem is seen from Eq. (2.11): we need control over $\nabla U_\infty(s, t_0)$. If the first order term did not appear in Eq. (2.11), we would only deal with bounded operators, in which case the application of the Dominated Convergence Theorem is trivial. However, since ∇ is an unbounded operator the application of the Dominated Convergence Theorem needs careful justification.

We want to stress that physically, time dependent vector potentials are very important, because they describe Lasers. In fact proofs of ionization such as [10, 62, 19, 33, 14], which rely on the time dependence of the Laser field and make use of the dipole approximation, have been the main motivation for this work. Ionization also has been studied in the framework of non-relativistic QED (Pauli equation coupled to the second quantized vector potential), see e.g. [20]. In this paper the authors show that the ionization probability given by formal time-dependent perturbation theory is rigorously justified. As the vector potential only enters the ionization probability via $\mathbf{A}(0, t)$ their result also justifies the dipole approximation, but in a weaker sense than our Theorem 2.1. The use of the dipole approximation in non-relativistic QED dates back at least to a paper of Pauli and Fierz [40] and in [1] this use is justified regarding the Hamiltonians. Here we justify the dipole approximation directly for the time evolution.

The conditions on the vector potential in Theorem 2.1 are very general. They are fulfilled e.g. by continuous wave Lasers and also by Laser pulses (in this case λ is the central wave length), to mention two important examples. To see that, we discuss these cases in more detail.

Example 1. *Continuous wave Laser*

From Eq. (2.3), we see that the vector potential for a continuous wave

Laser in $\mathbb{R}^3$ is given by

$$\mathbf{A}_\lambda(\mathbf{r},t) = c\frac{E}{\omega}\sin\left(\frac{2\pi}{\lambda}\hat{k}\cdot\mathbf{r} - \omega t\right)\hat{\varepsilon} = \frac{c}{\omega}\mathbf{a}(\tfrac{\mathbf{r}}{\lambda},\omega t) \quad \text{with} \tag{2.12}$$

$$\mathbf{a}(\mathbf{r},t) = E\sin\left(2\pi\hat{k}\cdot\mathbf{r} - t\right)\hat{\varepsilon}, \tag{2.13}$$

which evidently satisfies the assumptions of Theorem 2.1.

Example 2. *Laser pulses*

An example for a Laser pulse with Gaussian shape in $\mathbb{R}^3$ is

$$\mathbf{E}(\mathbf{r},t) = Ee^{-\left(\frac{2\pi}{\lambda}\hat{k}\cdot\mathbf{r}-\omega t\right)^2}\cos\left(\frac{2\pi}{\lambda}\hat{k}\cdot\mathbf{r} - \omega t\right)\hat{\varepsilon}. \tag{2.14}$$

The parameters have the same physical meaning as for the continuous wave Laser and as before we need $\hat{k}\cdot\hat{\varepsilon} = 0$ and $\omega = 2\pi c/\lambda$ for $\mathbf{E}$ to satisfy the sourceless Maxwell equations. Now we have

$$\mathbf{A}_\lambda(\mathbf{r},t) = -c\int_{-\infty}^{t}\mathbf{E}(\mathbf{r},s)\,ds = \tfrac{c}{\omega}\mathbf{a}(\tfrac{\mathbf{r}}{\lambda},\omega t) \quad \text{with} \tag{2.15}$$

$$\mathbf{a}(\mathbf{r},t) = -\int_{-\infty}^{t} Ee^{-(2\pi\hat{k}\cdot\mathbf{r}-s)^2}\cos(2\pi\hat{k}\cdot\mathbf{r} - s)\hat{\varepsilon}\,ds \tag{2.16}$$

and since

$$a^i(\mathbf{r},t) = E\int_{\infty}^{2\pi\hat{k}\cdot\mathbf{r}-t} e^{-s^2}\cos(s)\hat{\varepsilon}\,ds, \tag{2.17}$$

it is evident that $\partial_t^j\mathbf{a} \in C^2(\mathbb{R}^{3+1})^3$ for $j = 0, 1, 2$ and

$$\nabla\cdot\mathbf{a}(\mathbf{r},t) = 2\pi Ee^{-(2\pi\hat{k}\cdot\mathbf{r}-t)^2}\cos(2\pi\hat{k}\cdot\mathbf{r} - t)\hat{k}\cdot\hat{\varepsilon} = 0. \tag{2.18}$$

Moreover, $\|\partial_t^j a^i(\cdot,t)\|_\infty$ is bounded uniformly in i, j and t, so that the vector potential of our Laser pulse with Gaussian shape satisfies the conditions of Theorem 2.1.

In [33] the dipole approximation is used to prove ionization for a two-body Schrödinger equation. Theorem 2.1 applies to N-body Schrödinger equations, too. Let us illustrate that with the following

Example 3. *N-body Hamiltonian*

An atom with N electrons interacting with a Laser described by the vector potential $\mathbf{A}_\lambda$ is described by the Hamiltonian

$$H_\lambda^N(t) = \sum_{k=1}^{N}(-i\nabla_k - \tfrac{1}{c}\mathbf{A}_\lambda(\mathbf{r}_k, t))^2 - \sum_{k=1}^{N} \frac{2N}{|\mathbf{r}_k|} + \sum_{k<l}^{N} \frac{2}{|\mathbf{r}_k - \mathbf{r}_l|}. \tag{2.19}$$

$H_\lambda^N(t)$ can be rewritten in the form given in Theorem 2.1 via the definitions

$$\mathcal{A}_\lambda(\mathbf{r}, t) \equiv (\mathbf{A}_\lambda(\mathbf{r}_1, t), \mathbf{A}_\lambda(\mathbf{r}_2, t), \ldots, \mathbf{A}_\lambda(\mathbf{r}_N, t))^t, \tag{2.20}$$

$$V(\mathbf{r}) \equiv -\sum_{k=1}^{N} \frac{2N}{|\mathbf{r}_k|} + \sum_{k<l}^{N} \frac{2}{|\mathbf{r}_k - \mathbf{r}_l|}, \tag{2.21}$$

$$\nabla \equiv (\nabla_1, \nabla_2, \ldots, \nabla_N)^t, \tag{2.22}$$

$$\mathbf{r} \equiv (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)^t. \tag{2.23}$$

Clearly $\mathcal{A}_\lambda$ satisfies the assumptions of Theorem 2.1 if $\mathbf{A}_\lambda$ does and [44, Theorem X.16] shows that $V \in L^2_{loc}(\mathbb{R}^{3N})$ is infinitesimally $-\Delta$-bounded, where $-\Delta$ denotes the Laplacian on $\mathbb{R}^{3N}$.

2.2 Proof

Proof. (Theorem 2.1) Assertion one is in fact well known, but we include these results for completeness. Since V is infinitesimally $-\Delta$-bounded and $\|a^i(\cdot, t)\|_\infty < C$ uniformly in i and t,

$$W_\lambda(\mathbf{r}, t) := \tfrac{2i}{c}\mathbf{A}_\lambda(\mathbf{r}, t) \cdot \nabla + \tfrac{1}{c^2}\mathbf{A}_\lambda(\mathbf{r}, t)^2 + V(\mathbf{r}) \tag{2.24}$$

$$= \tfrac{2i}{\omega}\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega t) \cdot \nabla + \tfrac{1}{\omega^2}\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega t)^2 + V(\mathbf{r}) \quad \text{and} \tag{2.25}$$

$$W_\infty(\mathbf{r}, t) := \tfrac{2i}{\omega}\mathbf{a}(0, \omega t) \cdot \nabla + \tfrac{1}{\omega^2}\mathbf{a}(0, \omega t)^2 + V(\mathbf{r}) \tag{2.26}$$

satisfy

$$\|W_{\lambda/\infty}(t)\psi\|^2 \le C\Big(\|\psi\|^2 + \sum_{i=1}^{n} \|\partial_i\psi\|^2 + \|V\psi\|^2\Big) \le \varepsilon\| - \varDelta\psi\|^2 + C_\varepsilon\|\psi\|^2 \tag{2.27}$$

for every $\psi \in W^{2,2}(\mathbb{R}^n)$ and suitable constants C, C_ε. This implies self-adjointness of $H_\lambda(t)$ and $H_\infty(t)$ on $\mathcal{D}(H_\lambda(t)) = \mathcal{D}(H_\infty(t)) = W^{2,2}(\mathbb{R}^n)$. The existence of the unitary evolution operators, their strong continuity and the fact that they leave the domain invariant follow from Theorem X.70 in [44]. Lemma 2.1 below proves that the assumptions of Theorem X.70 are fulfilled.

Now, we prove assertion two. In view of Eq. (2.11), we note that the differences $\mathbf{a}(\frac{\mathbf{r}}{\lambda}, \omega s)^2 - \mathbf{a}(0, \omega s)^2$ and $\mathbf{a}(\frac{\mathbf{r}}{\lambda}, \omega s) - \mathbf{a}(0, \omega s)$ converge pointwise to zero as $\lambda \to \infty$ and $c \to \infty$ such that $\omega = 2\pi c/\lambda$ remains constant. We will make use of this by employing the Theorem of dominated convergence: Due to Eq. (2.11), we have

$$\|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi\| \tag{2.28}$$

$$\le \frac{2}{\omega} \int_{t_0}^{t} \|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega s) - \mathbf{a}(0, \omega s)) \cdot \nabla U_\infty(s, t_0)\psi\| \, ds \tag{2.29}$$

$$+ \frac{1}{\omega^2} \int_{t_0}^{t} \|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega s)^2 - \mathbf{a}(0, \omega s)^2) U_\infty(s, t_0)\psi\| \, ds. \tag{2.30}$$

Assertion two is proven once we have shown that we can pull the combined limit $\lambda \to \infty$ and $c \to \infty$ with $\omega = 2\pi c/\lambda$ kept fixed into the s-integral and into the $\mathbf{r}$-integral due to the norm $\|\cdot\|$. Note that Eqs. (2.29) and (2.30) depend on c only through ω, which is why the limit $c \to \infty$ only needs to be taken in order to keep ω fixed.

Consider Eq. (2.30) first. By assumption $\|\mathbf{a}(\cdot, \omega s)^2 - \mathbf{a}(0, \omega s)^2\|_\infty \le C$. Therefore, we get an integrable dominating function for the s-integral from

$$\|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega s)^2 - \mathbf{a}(0, \omega s)^2) U_\infty(s, t_0)\psi\| \le C \tag{2.31}$$

and similarly for the **r**-integral, from

$$|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega s)^2 - \mathbf{a}(0, \omega s)^2) U_\infty(s, t_0)\psi(\mathbf{r})|^2 \leq C |U_\infty(s, t_0)\psi(\mathbf{r})|^2. \tag{2.32}$$

So the Theorem of Dominated Convergence applies to Eq. (2.30).

For Eq. (2.29), we have

$$\|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega s) - \mathbf{a}(0, \omega s)) \cdot \nabla U_\infty(s, t_0)\psi\| \leq C \sum_{i=1}^{n} \|\partial_i U_\infty(s, t_0)\psi\|, \tag{2.33}$$

$$|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda}, \omega s) - \mathbf{a}(0, \omega s)) \cdot \nabla U_\infty(s, t_0)\psi(\mathbf{r})|^2 \leq Cn \sum_{i=1}^{n} |\partial_i U_\infty(s, t_0)\psi(\mathbf{r})|^2, \tag{2.34}$$

using the assumption that $\|a^i(\cdot, t)\|_\infty$ is bounded uniformly in i and t. It remains to control $\partial_i U_\infty(s, t_0)\psi$. For this purpose, we will use a side result in the proof of Theorem X.70 in [44], which states that if $P(s)$ denotes the generator of the unitary group $U(s, t_0)$ with $0 \in \rho(P(s))$ for all s, then $P(s)U(s, t_0)P(t_0)^{-1}$ is bounded. We bring $\partial_i U_\infty(s, t_0)$ in this form by observing that

$$\sum_{i=1}^{n} \|\partial_i U_\infty(s, t_0)\psi\| \leq \sum_{i=1}^{n} (1 + \|\partial_i U_\infty(s, t_0)\psi\|^2) \leq C \|U_\infty(s, t_0)\psi\|^2_{W^{2,2}(\mathbb{R}^n)}, \tag{2.35}$$

because $U_\infty(s, t_0)$ leaves $W^{2,2}(\mathbb{R}^n)$ invariant. Using Lemma 2.2, we can now show that

$$\|U_\infty(s, t_0)\psi\|^2_{W^{2,2}(\mathbb{R}^n)} \leq C(\|\psi\|^2 + \|H_\infty(s)U_\infty(s, t_0)\psi\|^2), \tag{2.36}$$

which is exactly what we need. However, Theorem X.70 in [44] requires $0 \in \rho(P(s))$. Clearly, this does not hold if $P(s) = H_\infty(s)$, but Lemma 2.1 shows that $H_\infty(s) + \alpha$ fulfills this requirement as long as $\alpha \in \mathbb{R}$ is big enough. Therefore, we write

$$\|U_\infty(s,t_0)\psi\|_{W^{2,2}(\mathbb{R}^n)} = \|e^{-i\alpha s}U_\infty(s,t_0)\psi\|_{W^{2,2}(\mathbb{R}^n)} = \|\tilde{U}_\infty(s,t_0)\psi\|_{W^{2,2}(\mathbb{R}^n)}, \tag{2.37}$$

where $\tilde{U}_\infty(s,t_0)$ is generated by $H_\infty(s)+\alpha$. Due to Lemma 2.2 there is a constant C such that

$$\begin{aligned}
&\|\tilde{U}_\infty(s,t_0)\psi\|^2_{W^{2,2}(\mathbb{R}^n)} \\
&\quad \le C(\|\psi\|^2 + \|(H_\infty(s)+\alpha)\tilde{U}_\infty(s,t_0)\psi\|^2) && (2.38)\\
&\quad = C(\|\psi\|^2 + \|(H_\infty(s)+\alpha)\tilde{U}_\infty(s,t_0)(H_\infty(t_0)+\alpha)^{-1}(H_\infty(t_0)+\alpha)\psi\|^2). && (2.39)
\end{aligned}$$

Choosing $P(s) = H_\infty(s)+\alpha$ and $U(s,t_0) = \tilde{U}_\infty(s,t_0)$ in Theorem X.70 in [44] we then obtain

$$\sum_{i=1}^{n} \|\partial_i U_\infty(s,t_0)\psi\| \le C(\|\psi\|^2 + C'\|(H_\infty(t_0)+\alpha)\psi\|^2) < \infty. \tag{2.40}$$

Thereby we get an integrable dominating function for the s-integral in Eq. (2.29) from

$$\|(\mathbf{a}(\tfrac{\mathbf{r}}{\lambda},\omega s) - \mathbf{a}(0,\omega s))\cdot\nabla U_\infty(s,t_0)\psi\| \le C \tag{2.41}$$

and for the $\mathbf{r}$-integral due to $\|\cdot\|$, we can directly use Eq. (2.34).

Having proven that we can use the Theorem of Dominated Convergence in Eqs. (2.29) and (2.30), we get

$$\|(U_\lambda(t,t_0) - U_\infty(t,t_0))\psi\| \to 0 \tag{2.42}$$

for all $\psi \in W^{2,2}(\mathbb{R}^n)$ in the limit $\lambda\to\infty$ and $c\to\infty$ such that ω is kept constant.

To extend the assertion to $\psi \in L^2(\mathbb{R}^n)$, we observe that for every $\psi \in L^2(\mathbb{R}^n)$ there exists $\psi_k \in W^{2,2}(\mathbb{R}^n)$ such that $\|\psi - \psi_k\| \le 1/k$. Using the triangle inequality and the fact that the evolution operators $U_\lambda(t,t_0)$ and

$U_\infty(t, t_0)$ are unitary operators we conclude

$$
\begin{aligned}
&\|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi\| && (2.43)\\
&\leq \|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi_k\| + \|(U_\lambda(t, t_0) - U_\infty(t, t_0))(\psi - \psi_k)\| && (2.44)\\
&\leq \|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi_k\| + 2\|\psi - \psi_k\| && (2.45)\\
&\leq \|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi_k\| + \frac{2}{k}. && (2.46)
\end{aligned}
$$

This shows that for every $k \in \mathbb{N}$ we have $\|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi\| \leq 2/k$ as $\lambda \to \infty$ and $c \to \infty$ such that ω remains constant. □

Lemma 2.1. *For large enough $\alpha \in \mathbb{R}$, $H_\infty(t) + \alpha$ satisfies the assumptions of [44, Theorem X.70]: Let $a, b \in \mathbb{R}$ and $P(t) \equiv H_\infty(t) + \alpha$. For each $t \in [a, b]$, $P(t)$ is the generator of a unitary group on $L^2(\mathbb{R}^n)$ and $0 \in \rho(P(t))$. Define $C(t, s) = P(t)P(s)^{-1} - 1$ and assume further that*

(a) $\mathcal{D}(P(t)) \equiv \mathcal{D}$ is independent of t and dense in $L^2(\mathbb{R}^n)$,

(b) For each $\psi \in L^2(\mathbb{R}^n)$, $(t - s)^{-1}C(t, s)\psi$ is uniformly strongly continuous and bounded with bound M uniformly in $s, t \in [a, b]$ for $t \neq s$,

(c) For each $\psi \in L^2(\mathbb{R}^n)$, $C(t)\psi \equiv \lim_{s \nearrow t}(t - s)^{-1}C(t, s)\psi$ exists uniformly for $t \in [a, b]$ and $C(t)$ is bounded and strongly continuous in t.

Proof. Since $P(t)$ is self-adjoint for all $\alpha \in \mathbb{R}$ and each $t \in [a, b]$, it is a generator of a unitary group. Clearly, $0 \in \rho(P(t))$ for all t when α is large enough. That $\mathcal{D}(P(t))$ is independent of t follows from assertion one in Theorem 2.1.

Now we will prove condition (b). To see that $(t - s)^{-1}C(t, s)$ is uniformly bounded in s and t, we write

$$
\begin{aligned}
&(t-s)^{-1}C(t,s) && (2.47)\\
&= (t-s)^{-1}(P(t)-P(s))P(s)^{-1} && (2.48)\\
&= (t-s)^{-1}(2i(\mathbf{A}(0,t)-\mathbf{A}(0,s))\cdot\nabla + (\mathbf{A}(0,t)^2-\mathbf{A}(0,s)^2))P(s)^{-1} && (2.49)\\
&= 2i\Big(\partial_t\mathbf{A}(0,s) + (t-s)^{-1}\int_s^t \partial_t^2\mathbf{A}(0,\xi)(t-\xi)\,d\xi\Big)\cdot\nabla P(s)^{-1}\\
&\quad + \Big(\partial_t\mathbf{A}(0,s)^2 + (t-s)^{-1}\int_s^t \partial_t^2\mathbf{A}(0,\xi)^2(t-\xi)\,d\xi\Big)P(s)^{-1}, && (2.50)
\end{aligned}
$$

where we have used the Taylor expansion of $\mathbf{A}(0,t)$ and $\mathbf{A}(0,t)^2$ in t. Uniform boundedness of the second term in Eq. (2.50) follows from the boundedness of $\mathbf{A}(0,t)$ as well as its derivatives and the uniform boundedness of $P(s)^{-1}$. To prove the latter, observe that

$$
\begin{aligned}
P(s)^{-1} &= (H_\infty(t)+\alpha)^{-1} = (-\varDelta + W(s)+\alpha)^{-1} && (2.51)\\
&= \big[(1+W(s)(-\varDelta+\alpha)^{-1})(-\varDelta+\alpha)\big]^{-1} && (2.52)\\
&= (-\varDelta+\alpha)^{-1}\big[1+W(s)(-\varDelta+\alpha)^{-1}\big]^{-1}, && (2.53)
\end{aligned}
$$

where $W(s) \equiv 2i\mathbf{A}(0,s)\cdot\nabla + \mathbf{A}(0,s)^2 + V$. Due to the fact that V is infinitesimally $-\varDelta$-bounded and the boundedness of $\mathbf{A}(0,s)$, we have

$$
\begin{aligned}
\|W(s)(-\varDelta+\alpha)^{-1}\psi\| &\le \varepsilon\|-\varDelta(-\varDelta+\alpha)^{-1}\psi\| + C_\varepsilon\|(-\varDelta+\alpha)^{-1}\psi\| && (2.54)\\
&\le \varepsilon\|(1-\alpha(-\varDelta+\alpha)^{-1})\psi\| + \tfrac{C_\varepsilon}{\alpha}\|\psi\| && (2.55)\\
&\le (2\varepsilon + \tfrac{C_\varepsilon}{\alpha})\|\psi\| && (2.56)
\end{aligned}
$$

for all $\psi \in L^2(\mathbb{R}^n)$. For α large enough $(2\varepsilon + \frac{C_\varepsilon}{\alpha}) < 1$ and hence

$$
P(s)^{-1} = (-\varDelta+\alpha)^{-1}\sum_{n=0}^{\infty}\big[-W(s)(-\varDelta+\alpha)^{-1}\big]^n. \qquad (2.57)
$$

This implies uniform boundedness of $P(s)^{-1}$. Uniform boundedness of the first term in Eq. (2.50) follows from the boundedness of $\mathbf{A}(0,t)$ as well as its derivatives and from the estimate

$$
\begin{aligned}
&\|\partial_i P(s)^{-1}\psi\| && (2.58)\\
&\leq \|P(s)^{-1}\psi\| + \|-\Delta P(s)^{-1}\psi\| && (2.59)\\
&= \|P(s)^{-1}\psi\| + \|-\Delta(-\Delta+\alpha)^{-1}[1+W(s)(-\Delta+\alpha)^{-1}]^{-1}\psi\| && (2.60)\\
&= \|P(s)^{-1}\psi\| + \|(1-\alpha(-\Delta+\alpha)^{-1})[1+W(s)(-\Delta+\alpha)^{-1}]^{-1}\psi\| && (2.61)\\
&\leq (\tfrac{1}{\alpha}+2)\sum_{n=0}^{\infty}(2\varepsilon+\tfrac{C_\varepsilon}{\alpha})^n\|\psi\| && (2.62)\\
&\leq C\|\psi\|, && (2.63)
\end{aligned}
$$

which holds for all i. The strong continuity of $(t-s)^{-1}C(t,s)$ in t is immediately evident from Eq. (2.50) and the fact that $P(s)^{-1}$ as well as $\partial_i P(s)^{-1}$ are uniformly bounded. Strong continuity in s follows from Eq. (2.50) and the strong continuity of $P(s)^{-1}$. The latter can be seen from Eq. (2.53) and the fact that $\sum_{n=0}^{\infty}\big[-W(s)(-\Delta+\alpha)^{-1}\big]^n$ is strongly continuous, which is a consequence of $[-W(s)(-\Delta+\alpha)^{-1}]^n$ being strongly continuous for all n (proof by induction) and $\|[-W(s)(-\Delta+\alpha)^{-1}]^n\psi\| \leq q^n\|\psi\|$ with $q<1$, so that

$$\lim_{s\to s'}\sum_{n=0}^{\infty}\big[-W(s)(-\Delta+\alpha)^{-1}\big]^n\psi = \sum_{n=0}^{\infty}\lim_{s\to s'}\big[-W(s)(-\Delta+\alpha)^{-1}\big]^n\psi. \quad (2.64)$$

Next we will prove condition (c). Due to Eq. (2.50) and the strong continuity of the right hand side we get

$$C(t)\psi \equiv \lim_{s\nearrow t}(t-s)^{-1}C(t,s)\psi = 2i(\dot{\mathbf{A}}(0,t)\cdot\nabla + \dot{\mathbf{A}}(0,t)^2)P(t)^{-1}\psi. \quad (2.65)$$

Uniform boundedness and strong continuity of $C(t)$ now follow from same arguments as used for $(t-s)^{-1}C(t,s)$. □

Lemma 2.2. *Let $P(t) \equiv H_\infty(t)+\alpha$ with $\alpha, t \in \mathbb{R}$. Then the graph norm $\|\cdot\|_{P(t)} \equiv \|\cdot\| + \|P(t)\cdot\|$ of $P(t)$ and $\|\cdot\|_{W^{2,2}(\mathbb{R}^n)}$ are equivalent.*

Proof. The proof is standard, we include it only for convenience of the reader. Due to assertion one in Theorem 2.1, $P(t)$ is self-adjoint on $W^{2,2}(\mathbb{R}^n)$. Hence, $W^{2,2}(\mathbb{R}^n)$ is closed not only under the Sobolev norm, but also under the graph norm of $P(t)$. Define the map

$$T : (W^{2,2}(\mathbb{R}^n), \|\cdot\|_{W^{2,2}(\mathbb{R}^n)}) \to (W^{2,2}(\mathbb{R}^n), \|\cdot\|_{P(t)}) \qquad (2.66)$$
$$\psi \mapsto \psi.$$

Clearly T is bijective and Eq. (2.27) implies $\|T\cdot\|_{P(t)} = \|\cdot\|_{P(t)} \leq D\|\cdot\|_{W^{2,2}(\mathbb{R}^n)}$ for some D. By the Inverse Mapping Theorem we then know that T^{-1} is continuous and thereby bounded. Thus, for some C

$$\|\cdot\|_{W^{2,2}(\mathbb{R}^n)} = \|T^{-1}\cdot\|_{W^{2,2}(\mathbb{R}^n)} \leq C\|\cdot\|_{P(t)}. \qquad (2.67)$$

□

Chapter 3

Description of the Alpha Decay Model

The theoretical study of alpha decay goes back to Gamow [16], whose model is based on the one dimensional Schrödinger equation. We will summarize his key insight for the three dimensional Schrödinger equation

$$i\partial_t \Psi = (-\Delta + V)\Psi =: H\Psi, \tag{3.1}$$

with rotationally symmetric V having compact support in $[0, R_V]$ because in the following we will work in this setting. We will only be concerned with the case of zero angular momentum to avoid the angular momentum barrier potential, which would not have compact support. In this case the three dimensional Schrödinger equation is equivalent to the one dimensional problem

$$i\partial_t \psi = \left(-\partial_r^2 + V\right)\psi =: H\psi \qquad \text{with} \quad \Psi(r, \theta, \phi) = \frac{\psi(r)}{r}. \tag{3.2}$$

Gamow's key insight was that eigenfunctions $f(k_0, r)$ of the stationary Schrödinger equation

$$\left(-\partial_r^2 + V(r)\right) f(k_0, r) = k_0^2 f(k_0, r) \tag{3.3}$$

that satisfy the boundary conditions $f(k_0, r) = e^{ik_0 r}$ for $r \geq R_V$ and $f(k_0, 0) = 0$ have complex eigenvalues that with the definition

$$k_0 = \alpha_0 - i\beta_0, \tag{3.4}$$

Note: The discussion given in this Chapter has been partly published in [13].

for some $\alpha_0, \beta_0 > 0$ read

$$k_0^2 = \alpha_0^2 - \beta_0^2 - i2\alpha_0\beta_0 =: E - i\frac{\gamma}{2}. \tag{3.5}$$

So, the function $f(k_0, r)$ yields a solution

$$f_t(k_0, r) := e^{-ik_0^2 t} f(k_0, r) \tag{3.6}$$

to the time-dependent Schrödinger equation

$$i\partial_t f_t(k_0, r) = \left(-\partial_r^2 + V(r)\right) f_t(k_0, r) = \left(E - i\frac{\gamma}{2}\right) f_t(k_0, r) \tag{3.7}$$

which decays exponentially in time with lifetime $1/\gamma$ since

$$|f_t(k_0, r)|^2 = e^{-\gamma t} |f(k_0, r)|^2. \tag{3.8}$$

In the sequel we will also refer to $f(k_0, r)$ as Gamow function. Note that both boundary conditions on the Gamow function are natural: the condition $f(k_0, r) = e^{ik_0 r}$ for $r \geq R_V$ means that $f(k_0, r)$ is purely outgoing which is reasonable for states describing decay and the condition $f(k_0, 0) = 0$ means that no probability should enter the region $r < 0$ which is the standard condition on physical states expressed in spherical coordinates.

Gamow's description does not immediately connect with Quantum Mechanics. While Eq. (3.3) appears there, too, in Quantum Mechanics eigenvalues are real and wave functions are square integrable. The Gamow function $f(k_0, r)$, on the other hand, belongs to complex eigenvalues and is not square integrable. In fact, it is readily seen from the purely outgoing behavior of $f(k_0, r)$ and $k_0 = \alpha_0 - i\beta_0$ having negative imaginary part, that $f(k_0, r)$ has exponentially growing tails. Such a function is not square integrable. So the question is: How does Gamow's description of alpha decay connect with Quantum Mechanics?

There are numerous mathematical articles concerned with this question, e.g. [9, 30, 56, 57]. From the articles it is, unfortunately, often not so easy to extract the clear and straightforward answer to that question. It is this:

$f(k_0, r)$ is approximately a quantum mechanical generalized eigenfunction (i.e. scattering state). Since generalized eigenfunctions govern the time evolution of square integrable wave functions which are orthogonal to all bound states, there are special initial wave functions, namely those which are approximated by $f(k_0, r)$ and which therefore approximately undergo exponential decay in time.

Of course, this answer needs a bit of elaboration. We need to qualify the various "approximations": First, generalized eigenfunctions do not have exponentially growing tails. Therefore, $f(k_0, r)$ approximates generalized eigenfunctions only locally, e.g. on the support of the potential. The physical wave function, which undergoes approximate exponential decay must be square integrable and therefore can only be locally given by $f(k_0, r)$, too. Finally, approximate exponential decay in time means that neither for very small nor for very large times exponential decay holds. It only holds on an intermediate time regime.

Remark 3.1. A square integrable wave function can not decay exponentially for small times because of the unitarity of the time evolution operator e^{-iHt}. Using the unitarity, we can conclude for the survival probability $P_\psi(t) = |\langle \psi, e^{-iHt}\psi \rangle|^2$ that $P_\psi(t) \leq P_\psi(0)$. Since the survival probability is differentiable and symmetric $P_\psi(-t) = P_\psi(t)$, this shows that $\frac{d}{dt}P_\psi(0) = 0$. Hence, exponential decay is impossible for very small times and that it is impossible for very large times, too, is due to the well known fact that the scattering behavior of wave functions ψ without bound state components is such that $e^{-iHt}\psi$ decays polynomially as $t \to \infty$ (see e.g. [23]).

Except for Ref. [17], the pedagogical accounts on Gamow's description of alpha decay we are aware of, usually only sketch its connection to the quantum mechanical description based on square integrable wave functions [5, 7, 11, 15, 22]. The purpose of this Chapter is to explain this connection in more detail. Compared to Ref. [17], which is a fairly complete discussion for a particular potential, we will stress the general principles underlying the connection between Gamow's description and the quantum mechanical description in a way which seems the most straightforward one.

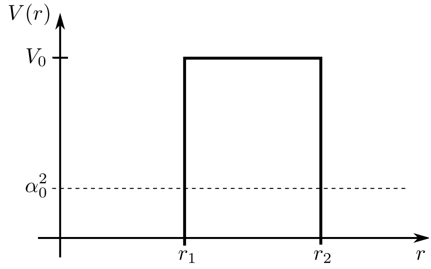


Figure 3.1: Plot of the barrier potential.

Gamow had the right intuition, "eigenfunctions" corresponding to complex "eigenvalues" do give rise to long lived square integrable states, which decay exponentially in time and thereby serve to describe alpha decay. However, their presence becomes only apparent in special physical situations. The prototype of a potential that creates such a situation is the barrier potential sketched in Fig. 3.1. Wave functions initially localized in $[0, r_1]$ are long lived if the wells are high, because at the potential steps they are partially transmitted and partially reflected; if the steps are high, reflection outweighs transmission. At each time of transmission, it is natural to view the transmitted portion as being proportional to what is left inside the double well and thus exponential decay appears naturally.

This point of view shows that exponential decay is not at all a tunneling phenomenon, as it is often intuitively assumed. For a metastable state to occur, it suffices that a potential has steps at which a wave is partially reflected. The rectangular potential well $V_0\mathbf{1}_{r_1}$ is thus another example, which allows for unstable but long lived states that decay exponentially in time. Here $\mathbf{1}_{r_1}(r)$ denotes the indicator function on $[0, r_1]$. If V_0 is large, states initially localized on top of the rectangular potential well will be metastable and will decay exponentially in time (see [21, 17]).

Assume that the barrier potential in Fig. 3.1 allows for a Gamow type solution $f(k_0, r)$ to Eq. (3.3), then the truncated version of it, namely $f_R(r) := \mathbf{1}_R f(k_0, r)$ for some $R \geq r_1$ yields a long lived square integrable initial wave function and we will now explain that it decays exponentially on intermediate time scales. We will give a two step argument, which shows that f_R decays exponentially in time when evolved according to the time dependent Schrödinger equation (3.2). In the first step we will establish a generic connection between the time evolution of any square integrable wave function and $f(k_0, r)$. In the second step we will use this connection to show that $e^{-iHt} f_R$ decays exponentially in time. Since decay is a genuine scattering phenomenon, we assume in this Chapter for simplicity that V does not have bound states.

So, how does $e^{-iHt} f_R$ evolve in time? To find an answer, we need a method that makes the time evolution palpable. For this purpose, we will use the method of expansions in generalized eigenfunctions $\psi^+(k, r)$, which applied to an arbitrary square integrable wave function ψ yields

$$\psi(r) = \int_0^\infty \hat{\psi}(k)\psi^+(k, r)\, dk \quad \text{with} \tag{3.9}$$

$$\hat{\psi}(k) = \int_0^\infty \psi(r)\bar{\psi}^+(k, r)\, dr. \tag{3.10}$$

These generalized eigenfunctions are bounded, but not square integrable solutions to the stationary Schrödinger equation

$$H\psi^+(k, r) = (-\partial_r^2 + V(r))\psi^+(k, r) = k^2\, \psi^+(k, r). \tag{3.11}$$

An expansion in terms of $\psi^+(k, r)$ diagonalizes H in a completely analogous way as the Fourier transform diagonalizes $-\frac{d^2}{dr^2}$. The time evolved ψ can thereby be expressed in a very concrete analytical way as

$$e^{-iHt}\psi(r) = \int_0^\infty \hat{\psi}(k)\psi^+(k, r)e^{-ik^2 t}\, dk. \tag{3.12}$$

Why should the time evolution expressed in terms of an expansion in generalized eigenfunctions (3.12) be related in any way to the Gamow function $f(k_0, r)$? Because both, the generalized eigenfunctions $\psi^+(k, r)$ as well as the $f(k_0, r)$, solve the stationary Schrödinger equation (3.11); the Gamow function for complex $k_0^2 = E - i\gamma/2$ with $E, \gamma > 0$ and the generalized eigenfunctions for real $k^2 \geq 0$. This suggests that in some sense $\psi^+(k,r) \approx f(k_0,r)$, when the complex "eigenvalue" is close to the real axis ($\gamma \ll 1$). According to Eq. (3.11) generalized eigenfunctions behave like plane waves in regions where the potential is zero. Therefore, combining plane wave behavior and "near Gamow function behavior", we make the ansatz

$$\psi^+(k,r) \approx \eta(k)\mathbf{1}_R f(k_0,r) + e^{ikr}. \tag{3.13}$$

We need to determine η. Plugging Eq. (3.13) into Eq. (3.11), we find

$$\Big(-\frac{d^2}{dr^2} + V(r)\Big)(\eta(k)\mathbf{1}_R f(k_0,r) + e^{ikr}) \approx k^2\,(\eta(k)\mathbf{1}_R f(k_0,r) + e^{ikr}). \tag{3.14}$$

Now, $H\mathbf{1}_R f(k_0,r) \approx k_0^2\mathbf{1}_R f(k_0,r)$ and $-\frac{d^2}{dr^2}e^{ikr} = k^2 e^{ikr}$, so we can rearrange the above equation, putting $h(k,r) = V(r)e^{ikr}$, such that

$$\eta(k)\mathbf{1}_L G(r) \approx \frac{h(k,r)}{k^2 - k_0^2}. \tag{3.15}$$

Integrating both sides with respect to r, entails that

$$\eta(k) \approx \frac{\tilde{h}(k)}{k^2 - (E - i\gamma/2)}, \tag{3.16}$$

where $\tilde{h}$ is some analytic function. We find that the complex "eigenvalue" $E - i\gamma/2$ causes the generalized eigenfunctions $\psi^+(k,r)$ to have a pole, when continued to the complex k-plane and the Gamow function $f(k_0,r)$ is the corresponding residue. This was the first step of our heuristic argument.

In the second step, we will use Eq. (3.16) in Eq. (3.13) to show that $e^{-iHt}f_R$ decays exponentially in time. We only need to calculate the integral in the eigenfunction expansion (3.12). The heart of this calculation lies in the fact that the first summand on the right hand side of (3.13) dominates

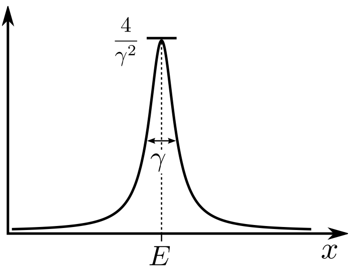


Figure 3.2: Plot of the Breit-Wigner function $\frac{1}{(x-E)^2+\gamma^2/4}$.

when $\gamma \ll 1$, because $|\eta(k)|$ is much larger than $|e^{ikr}|$ for $k \approx \alpha_0$. Therefore,

$$\psi^+(k,r) \approx \eta(k)\mathbf{1}_R f(k_0,r) = \eta(k) f_R(r) \tag{3.17}$$

and hence

$$\hat{f}_R(k) \approx \int_0^\infty f_R(r)\bar{\eta}(k)\bar{f}_R(r)\,dr \approx c\,\overline{\eta}(k), \tag{3.18}$$

$$e^{-iHt} f_R(r) \approx c\int_0^\infty \bar{\eta}(k)\eta(k) f_R(r) e^{-ik^2 t}\,dk \tag{3.19}$$

$$= c\, f_R(r)\int_0^\infty \frac{|\tilde{h}(k)|^2}{|k^2-(E-i\gamma/2)|^2} e^{-ik^2 t}\,dk. \tag{3.20}$$

To solve the integral notice that it is essentially the Fourier transformation of the Breit-Wigner function $1/[(k^2-E)^2+\gamma^2/4]$. They differ only by the appearance of an additional function $|\tilde{h}(k)|^2$ and the fact that in Eq. (3.20) we integrate over k instead of k^2. Therefore, we change the integration variable

$$e^{-iHt} f_R(r) \approx c\, f_R(r)\int_0^\infty \frac{|\tilde{h}(k)|^2}{|k^2-(E-i\gamma/2)|^2} e^{-ik^2 t}\,dk \tag{3.21}$$

$$= c\, f_R(r)\int_0^\infty \frac{|\tilde{h}(\sqrt{x})|^2}{(x-E)^2+\gamma^2/4} e^{-ixt}\,\frac{dx}{2\sqrt{x}}. \tag{3.22}$$

Due to the fact that the Breit-Wigner function is strongly peaked at $x = E$ if $\gamma \ll 1$ (see Fig. 3.2), the integrand in Eq. (3.22) is localized about $E > 0$. Hence, we can replace $\tilde{h}(\sqrt{x})$ and $1/\sqrt{x}$ by their respective values at $x = E$, so that

$$e^{-iHt} f_R(r) \approx c\, f_R(r) \frac{|\tilde{f}(\sqrt{E})|^2}{2\sqrt{E}} \int_0^\infty \frac{1}{(x-E)^2 + \gamma^2/4} e^{-ixt}\, dx \tag{3.23}$$

$$\approx c'\, f_R(r)\, e^{-\gamma t/2}, \tag{3.24}$$

where we have used that the Fourier transformation of the Breit-Wigner function is the exponential function. Thus, $e^{-iHt} f_R$ decays exponentially in time whenever $\gamma \ll 1$.

What we just showed heuristically has been analyzed rigorously by Skibsted in [56] for three dimensional, rotationally symmetric, and compactly supported potentials. He proved the following

Lemma 3.1 (Lemma 3.5 of [56]). *Let the three dimensional potential V be rotationally symmetric, compactly supported in $[0, R_V]$, with $\|rV(r)\|_1 < \infty$, and let it have no bound states. Moreover, let $t \geq 0$, $R \geq R_V$, $R_2(t) = 2\alpha_0 t + R$, and*

$$f_R(r) := \mathbf{1}_R f(k_0, r). \tag{3.25}$$

Then,

$$\|e^{-iHt} f_R - e^{-ik_0^2 t} f_{R_2(t)}\|_2 \leq K(\alpha_0, \beta_0, t) \|f_R\|_2, \tag{3.26}$$

$$K(\alpha_0,\beta_0,t) = \frac{4}{\sqrt{\pi}} \left[\left(\frac{\beta_0}{\alpha_0}\right)^{\frac{1}{2}} + \left(\frac{\beta_0}{\alpha_0}\right)^{\frac{1}{4}} \left[\frac{3\pi}{16} \sqrt{\gamma t} \left(\frac{1 + 20\left(\frac{\beta_0}{\alpha_0}\right)^{\frac{1}{2}}}{1 + 10\left(\frac{\beta_0}{\alpha_0}\right)^{\frac{1}{2}}} \right)^2 + \frac{3}{40} \right]^{\frac{1}{2}} \right]. \tag{3.27}$$

If $\beta_0 \ll \alpha_0$, we see that $K(\alpha_0, \beta_0, t) \ll 1$ for several lifetimes $1/\gamma$. So for this time span Eq. (3.26) implies that $e^{-iHt} f_R$ undergoes approximate exponential decay, because

$$e^{-iHt} f_R \approx e^{-ik_0^2 t} f_{R_2(t)}. \tag{3.28}$$

Chapter 4

On the Energy-Time Uncertainty Relation

4.1 Introduction

A central feature of wave dynamics is that it satisfies so-called uncertainty relations. Quantum systems are governed by Schrödinger's wave equation, therefore they obey the uncertainty relation

$$\operatorname{Var} A \operatorname{Var} B \geq \frac{1}{4}|\langle [A, B] \rangle|^2, \tag{4.1}$$

where A, B are self-adjoint operators, $\operatorname{Var} A$, $\operatorname{Var} B$ are their variances, and $\langle A \rangle$, $\langle B \rangle$ their means. When applied for example to position and momentum, this formula gives the famous Heisenberg uncertainty relation

$$\operatorname{Var} X \operatorname{Var} P \geq \frac{\hbar^2}{4}. \tag{4.2}$$

Equally famous is the analogous *energy-time uncertainty relation*

$$\operatorname{Var} E \operatorname{Var} T \geq \frac{\hbar^2}{4}, \tag{4.3}$$

whose status is nevertheless much different from that of Eq. (4.2). Contrary to Eq. (4.2), the relation (4.3) cannot be derived from the general formula (4.1), as no self-adjoint time operator exists [39]. The description of time measurements in the framework of quantum mechanics is a debated topic, and many proposals have been put forward. Different

Note: The results in this Chapter were developed in collaboration with Nicola Vona. Nicola Vona and I contributed equally to the work that led to the present Chapter.

approaches have produced a number of relations having the form of (4.3), but a general understanding of the energy-time uncertainty relation is still missing (see for example [6, 34, 35]). For instance, the results in [58, 25, 18, 61] rest on the assumption that the detection happens on the whole time interval $(-\infty, \infty)$, which is appropriate for describing scattering experiments, but cannot be applied in general. In particular, for alpha decay one has a sample containing unstable nuclei, surrounded by detectors waiting for the decay product to hit them. The setting is prepared at time zero and the number of decay events is counted starting at that time, so one can not consider the detection window to extend to $-\infty$. In this case the mentioned results do not apply, and the uncertainty relation (4.3) could in principle be violated. This circumstance is indeed general (see [29]) and easily understood by looking at a particle in a box in an eigenstate of the momentum, for which $\operatorname{Var} P = 0$, while $\operatorname{Var} X$ cannot exceed the size of the box, thereby violating the position-momentum uncertainty relation. Nevertheless, the energy-time uncertainty relation is often used for alpha decay (see for example [50]) to connect the energy spread of the alpha particle to the lifetime of the nucleus.

In the present Chapter we study the energy-time uncertainty relation (4.3) for alpha decay. We will start from Gamow's model [16], where the alpha particle at time zero is trapped inside a barrier potential but subsequently escapes via tunneling and then hits a detector. We calculate $\operatorname{Var} E$ exactly, obtain an approximation for $\operatorname{Var} T$, and estimate the error made with this approximation. For potentials with long lifetimes the error is small enough to check the validity of the energy-time uncertainty relation (4.3), and we find that it holds. To calculate $\operatorname{Var} T$ we used the flux of the probability current through the detecting surface as probability density function for the arrival time of the alpha particle at the detector. The flux of the probability current in general does not have the needed properties to be a probability density function. Nevertheless, its use in this case is justified by the fact that the distance between the detector and the decaying nucleus is much bigger than the nucleus itself, therefore the measurement is practically performed under scattering conditions.[1]

[1] For a general discussion of the role of the probability current in the description of time measurements see [59, 60].

We also compare the energy-time uncertainty (4.3) with the so-called *linewidth-lifetime relation*, which, letting τ denote the lifetime of the unstable nucleus and Γ the full width at half maximum of the probability density function of the energy of the decay product, reads

$$\Gamma\tau = \hbar. \tag{4.4}$$

This relation is a fundamental feature of exponentially decaying systems and therefore also of nuclei that undergo alpha decay. Since Γ expresses an uncertainty on energy and τ on time, Eq. (4.4) is often presented as an instance of the energy-time uncertainty relation (4.3) (see for example [50]). However, Fock and Krylov [28] argued that Eqs. (4.3) and (4.4) are unrelated. We will give a rigorous proof for that, by calculating Γ and τ for Gamow's model and comparing them to $\operatorname{Var} E$ and $\operatorname{Var} T$. We find that it is possible to adjust the potential and the initial state in such a way that the product $\Gamma\tau$ gets arbitrarily close to $\hbar$, while at the same time the product $\operatorname{Var} E \operatorname{Var} T$ gets arbitrarily large.

Because we have explicit control over $\operatorname{Var} E$ and $\operatorname{Var} T$ for Gamow's model of alpha decay, the question arises whether their values can be calculated for physical systems. In principle this is possible, but for physically reasonable lifetimes our error bounds are not good enough. As mentioned above, we determine an approximation of $\operatorname{Var} T$ and calculate the error made with this approximation. The error estimates decrease with growing lifetime and if we calculate it for the longest lived element, i.e. Bismuth 209 (1.16×10^{-27} s^{-1}, see [12]), we see that the error is too big for the approximation on $\operatorname{Var} T$ to be reliable or to check Eq. (4.3). However, for even longer lived systems that are not physical the error becomes small enough for us to check the validity of the energy-time uncertainty relation (4.3). The relation between the error and the lifetime is of technical nature, therefore there is no apparent physical explanation for this.

4.2 Assumptions and Definitions

Throughout this Chapter we will work in the setting introduced in Chapter 3, recall in particular Eqs. (3.1) and (3.2). In the following we use units in which $\hbar = 1$, the mass $m = 1/2$, and we will also assume that

$$R \geq R_V, \tag{4.5}$$

where R_V was introduced in Chapter 3 as the radius of the potential's support. Moreover, for ease of notation we introduce for a function ϕ

$$\phi'(k,r) := \partial_r \phi(k,r) \quad \text{and} \quad \dot{\phi}(k,r) := \partial_k \phi(k,r). \tag{4.6}$$

4.2.1 Alpha Decay Model

Because of Lemma 3.1, we would like to use f_R as model for the decaying state, but $\operatorname{Var} E$ is not defined for it. Let us show why, assuming that V does not have bound states. Consider the mean energy

$$\langle f_R, H f_R \rangle = \|H^{\frac{1}{2}} f_R\|_2^2 = \|k \hat{f}_R\|_2^2, \tag{4.7}$$

where $\hat{f}_R$ is the generalized Fourier transform of f_R. From Lemma 3.2 in [56] we know that

$$\hat{f}_R = -\frac{1}{2}\left[\frac{e^{i(k_0-k)R}}{k-k_0}\bar{S}(k) + \frac{e^{i(k_0+k)R}}{k+k_0}\right], \tag{4.8}$$

where S is the S-matrix. Multiplied with k this function is not square integrable and therefore neither the mean energy $\langle f_R, H f_R \rangle$ nor the energy variance is defined for f_R. In fact this argument shows that f_R is not in the form domain of H, because for this to be the case, $\langle f_R, H f_R \rangle$ needs to be finite. While this is completely unproblematic for Skibsted in [56], it presents a problem for us, since we want to calculate $\operatorname{Var} E$.

Clearly the sharp truncation of f_R causes the tails of the generalized Fourier transform to be so slow in decay that $k\hat{f}_R(k)$ is not square integrable. We can solve the problem by using a Gaussian cutoff, which is why we will work with the initial wave function

$$\psi(r) := f(k_0, r)\left[\mathbf{1}_R + \mathbf{1}_{[R,\infty)} \exp\left(-\frac{(r-R)^2}{2\sigma^2}\right)\right] \tag{4.9}$$

for some $\sigma > 0$. Note that we do not normalize the Gaussian, because we want the wave function to be continuous at $r = R$. For notational convenience we introduce

$$g_R(r) := f(k_0, r)\mathbf{1}_{[R,\infty)} \exp\left(-\frac{(r-R)^2}{2\sigma^2}\right), \tag{4.10}$$

so that

$$\psi(r) = f_R(r) + g_R(r). \tag{4.11}$$

Clearly, for σ small enough $\|g_R\|_2$ is small and the result of Lemma 3.1 carries over to $e^{-iHt}\psi$, i.e.

$$e^{-iHt}\psi \approx e^{-ik_0^2 t} f_{R_2(t)} \tag{4.12}$$

for several lifetimes.

The following Lemma proves that $H\psi \in L^2(\mathbb{R}^+)$ so that $\operatorname{Var} E$ exists and is finite for the wave function ψ.

Lemma 4.1. *Let the three dimensional potential V be rotationally symmetric with $\|V\|_2 < \infty$. Then ψ lies in the domain of self-adjointness of H.*

Proof. We start by determining the domain of self-adjointness of H via the Kato-Rellich Theorem [44, Theorem X.12]. For this purpose define

$$H_0 := -\frac{d^2}{dr^2} \tag{4.13}$$

on $\{\phi \in L^2(\mathbb{R}^+) \,|\, \phi(0) = 0\}$ and let $\mathcal{D}(H_0)$ denote its domain of self-adjointness. From [44, p. 144] we get

$$\mathcal{D}(H_0) = \{\phi \in L^2(\mathbb{R}^+) \,|\, \phi(0) = 0, \phi' \in L^2(\mathbb{R}^+),$$
$$\phi' \text{ abs. continuous}, \phi'' \in L^2(\mathbb{R}^+)\}. \qquad (4.14)$$

From the proof of Lemma 5.1 we see that $\mathcal{D}(H_0) \subset Q(H_0)$, so that by Eq. (5.25) we have

$$\|\phi\|_\infty \leq \sqrt{2\|\phi\|_2\|\phi'\|_2} \qquad (4.15)$$

for all $\phi \in \mathcal{D}(H_0)$. With the help of the fact that for arbitrary $A, B > 0$ and all $\varepsilon > 0$ there is a $c_\varepsilon > 0$ such that

$$\sqrt{AB} = A\sqrt{B/A} \leq \varepsilon B + c_\varepsilon A, \qquad (4.16)$$

we then arrive at

$$\|\phi\|_\infty \leq \varepsilon\|\phi'\|_2 + c_\varepsilon\|\phi\|_2. \qquad (4.17)$$

Using this, Cauchy-Schwarz, and Eq. (4.16) again, we obtain

$$\begin{aligned} \|V\phi\|_2 &\leq \|V\|_2\|\phi\|_\infty && (4.18)\\ &\leq \varepsilon\|\phi'\|_2 + c_\varepsilon\|\phi\|_2 && (4.19)\\ &\leq \varepsilon\sqrt{\|\phi\|_2\|H_0\phi\|_2} + c_\varepsilon\|\phi\|_2 && (4.20)\\ &\leq \varepsilon\|H_0\phi\|_2 + c_\varepsilon\|\phi\|_2, && (4.21) \end{aligned}$$

thereby proving that V is infinitesimally H_0-bounded. The Kato-Rellich Theorem [44, Theorem X.12] then shows that H is self-adjoint on $\mathcal{D}(H_0)$.

To prove that $\psi \in \mathcal{D}(H_0)$, recall that $f(k_0, r)$ is the solution of the stationary Schrödinger equation (3.3), which satisfies the boundary conditions $f(k_0, r) = e^{ik_0 r}$ for $r \geq R_V$ and $f(k_0, 0) = 0$ with $k_0 = \alpha_0 - i\beta_0$ for some $\alpha_0, \beta_0 > 0$. For notational convenience set

$$\chi(r) := \mathbf{1}_R + \mathbf{1}_{[R,\infty)} \exp\left(-\frac{(r-R)^2}{2\sigma^2}\right), \qquad (4.22)$$

so that $\psi(r) = f(k_0, r)\chi(r)$. The boundary conditions on f imply that

$$\psi(0) = f(k_0, 0) = 0. \tag{4.23}$$

Now,

$$\psi'(r) = f'(k_0, r)\chi(r) + f(k_0, r)\chi'(r), \tag{4.24}$$

$$\chi'(r) = -\mathbf{1}_{[R,\infty)} \frac{(r-R)}{\sigma^2} \exp\left(-\frac{(r-R)^2}{2\sigma^2}\right) \tag{4.25}$$

and from Theorem XI.57 in [45] we know that $f'(k_0, r)$ is continuous in r. This and the boundary conditions on $f(k_0, r)$ yield the estimate

$$\begin{aligned} \|\psi'\|_2 &\le \|f'(k_0, r)\chi(r)\|_2 + \|f(k_0, r)\chi'(r)\|_2 && (4.26) \\ &\le \|\mathbf{1}_R f'(k_0, r)\|_\infty R + |k_0| \left\| \mathbf{1}_{[R,\infty)} \exp\left(ik_0 r - \frac{(r-R)^2}{2\sigma^2}\right)\right\|_2 \\ &\quad + \left\| \mathbf{1}_{[R,\infty)} \frac{(r-R)}{\sigma^2} \exp\left(ik_0 r - \frac{(r-R)^2}{2\sigma^2}\right)\right\|_2 && (4.27) \\ &< \infty. && (4.28) \end{aligned}$$

In order to show the absolute continuity of ψ', it is sufficient to ensure that for all $r \in \mathbb{R}^+$

$$\psi'(r) = \psi'(R) + \int_R^r \psi''(r')\, dr'. \tag{4.29}$$

Observe that f' and f'' exist for all $r \in \mathbb{R}^+$ because f is a solution of the Schrödinger equation in the ordinary sense. Moreover, χ' exists and is continuous for all $r \in \mathbb{R}^+$, but it is not differentiable in $r = R$, so χ'' and ψ'' exist in the weak sense for all $r \in \mathbb{R}^+$ and in the ordinary sense for $r \neq R$. Now consider the function

$$\phi(x, r) := \psi'(x) + \int_x^r \psi''(r')\, dr', \tag{4.30}$$

defined for $x, r < R$ and for $x, r > R$. Consider $r > R$, then

$$\phi(x, r) = \psi'(r) \quad \forall x > R, \tag{4.31}$$

therefore

$$\lim_{x \to R^+} \phi(x, r) = \psi'(r) \quad \forall r > R. \tag{4.32}$$

Similarly, one gets

$$\lim_{x \to R^-} \phi(x, r) = \psi'(r) \quad \forall r < R. \tag{4.33}$$

Due to the continuity of ψ', from the definition of ϕ we have

$$\lim_{x \to R^\pm} \phi(x, r) = \psi'(R) + \int_R^r \psi''(r')\, dr', \tag{4.34}$$

from which we get the absolute continuity of ψ'.

It remains to show that $\|\psi''\|_2 < \infty$. Clearly,

$$\|\psi''\|_2 \leq \|f''(k_0, r)\chi(r)\|_2 + 2\|f'(k_0, r)\chi'(r)\|_2 + \|f(k_0, r)\chi''(r)\|_2. \tag{4.35}$$

The same arguments which led to $\|\psi'\|_2 < \infty$ can be applied to show the square integrability of $f'\chi'$. In the weak sense,

$$\chi''(r) = \mathbf{1}_{[R,\infty)} \left[\frac{(r - R)^2}{\sigma^4} - \frac{1}{\sigma^2} \right] \exp\left(-\frac{(r - R)^2}{2\sigma^2} \right), \tag{4.36}$$

that together with the boundary conditions on $f(k_0, r)$ gives $\|f(k_0, \cdot)\chi''\|_2 < \infty$. To handle $\|f''(k_0, r)\chi(r)\|_2$, we use the fact that $f(k_0, r)$ satisfies the Schrödinger equation (3.3), which gives

$$\begin{aligned} \|f''(k_0, r)\chi(r)\|_2 &\leq \|V(r)f(k_0, r)\chi(r)\|_2 + |k_0|^2 \|f(k_0, r)\chi(r)\|_2 && (4.37)\\ &\leq \|V\|_2 \|\psi\|_\infty + |k_0|^2 \|\psi\|_2 && (4.38)\\ &< \infty. && (4.39) \end{aligned}$$

Thus we see that $\|\psi''\|_2 < \infty$, which finishes the proof. □

4.2.2 Assumptions on the Potential

Throughout this Chapter we require the potential V to satisfy the assumptions stated in Section 5.2.1. For convenience we repeat them here: we consider a non-zero, three-dimensional, rotationally symmetric potential $V = V(r)$, that is real, with support contained in $[0, R_V]$, such that $\sup(\operatorname{supp} V) = R_V$, and $\|V\|_1 < \infty$ (note that this implies $\|rV(r)\|_1 < \infty$). We also assume that the potential admits the asymptotic expansion

$$V(r) \sim \sum_{n=0}^{M} d_n (R_V - r)^{\delta_n}, \qquad \text{as } r \to R_V^-, \tag{4.40}$$

with $0 \leq M < \infty$, $-1 < \delta_0 < \cdots < \delta_N$, and $d_n \in \mathbb{R}$ and not all zero.

In addition to the assumptions of Section 5.2.1 we will assume that $\|V\|_2 < \infty$ and that the potential has no bound states, nor virtual states, nor a zero resonance.[2] We also assume that among all resonances $k_n = \alpha_n - i\beta_n$, k_0 is such that α_0 and β_0 are the minimal ones. For notational convenience we introduce

$$\beta := \beta_0, \quad \alpha := \alpha_0, \text{ and } \quad \gamma := 4\alpha\beta. \tag{4.41}$$

4.2.3 Time Distribution

The time variance will be calculated using the flux of the quantum current through the detector surface, which we consider to be a sphere of radius R around the origin. Note that the cut-off radius R is equal to the detector radius, that is a good choice to model all experiments in which one starts with a bulk of material, and the only information available is that the decay products did not hit the detector yet. Setting

$$\Psi_t(r, \theta, \phi) := e^{-iHt}\Psi(r, \theta, \phi) \qquad \text{and} \qquad \psi_t(r) := e^{-iHt}\psi(r), \tag{4.42}$$

[2] In presence of bound states, the current can be a constant, and its use as arrival time statistic is not reasonable. Moreover, if the potential has a zero-resonance, then the probability that the particle is in the interior of the detector surface decays as t^{-1} (see [23]), and the probability current through the detector has then no variance nor mean.

the probability current is

$$\mathbf{J}(r,t) = \frac{2}{\|\Psi\|_2^2}\,\mathrm{Im}\left[\bar{\Psi}_t(r,\theta,\phi)\nabla\Psi_t(r,\theta,\phi)\right] \tag{4.43}$$

$$= \frac{2}{4\pi\|\psi\|_2^2}\,\mathrm{Im}\left[\frac{\bar{\psi}_t(r)}{r}\nabla\left(\frac{\psi_t(r)}{r}\right)\right], \tag{4.44}$$

hence it is zero in the angular directions, while in the radial direction

$$J_r(r,t) = \frac{1}{2\pi\|\psi\|_2^2}\,\mathrm{Im}\left[\frac{\bar{\psi}_t(r)}{r}\partial_r\left(\frac{\psi_t(r)}{r}\right)\right] \tag{4.45}$$

$$= \frac{1}{2\pi\|\psi\|_2^2 r^2}\,\mathrm{Im}\left(\bar{\psi}_t(r)\partial_r\psi_t(r)\right) - \frac{1}{2\pi\|\psi\|_2^2 r^3}\,\mathrm{Im}\left(|\psi_t(r)|^2\right) \tag{4.46}$$

$$= \frac{1}{2\pi\|\psi\|_2^2 r^2}\,\mathrm{Im}\left(\bar{\psi}_t(r)\partial_r\psi_t(r)\right). \tag{4.47}$$

Let

$$j(r,t) := \frac{2}{\|\psi\|_2^2}\,\mathrm{Im}\left(\bar{\psi}_t(r)\partial_r\psi_t(r)\right), \tag{4.48}$$

then the flux of the probability current $\mathbf{J}(r,t)$ through the detector is simply

$$4\pi R^2\, J_r(R,t) = j(R,t). \tag{4.49}$$

The arrival time probability density Π_T, being defined as the flux (4.49) through the detector surface normalized to one on the time interval $(0,\infty)$, then reads

$$\Pi_T(t) = \frac{j(R,t)}{\int_0^\infty j(R,t')dt'}. \tag{4.50}$$

Now, the mean arrival time is

$$\langle t\rangle := \int_0^\infty t\,\Pi_T(t)\,dt \tag{4.51}$$

and the time variance is

$$\operatorname{Var} T := \int_0^\infty (t - \langle t \rangle)^2 \Pi_T(t)\, dt. \tag{4.52}$$

We further simplify the expressions for $\langle t \rangle$ and $\operatorname{Var} T$ in the following Lemma, which shows that rather than Π_T, the relevant object is

$$\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}, \tag{4.53}$$

which we will call *non-escape probability*.

Lemma 4.2. *Let $t > 0$, then*

$$\Pi_T(t) = -\partial_t \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}. \tag{4.54}$$

Moreover,

$$\langle t \rangle = \int_0^\infty \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}\, dt, \tag{4.55}$$

$$\operatorname{Var} T = 2 \int_0^\infty t \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}\, dt - \langle t \rangle^2. \tag{4.56}$$

Proof. With the help of the continuity equation for the probability, which reads

$$\partial_r j(r,t) + \partial_t \frac{|\psi_t(r)|^2}{\|\psi\|_2^2} = 0, \tag{4.57}$$

and the fact that $j(0,t) = 0$ for all times, the current can be written as

$$j(R,t) = \int_0^R \partial_r j(r,t) dr = -\int_0^R \partial_t \frac{|\psi_t(r)|^2}{\|\psi\|_2^2} dr = -\partial_t \frac{\|\mathbf{1}_R \psi_t\|_2^2}{\|\psi\|_2^2}. \tag{4.58}$$

This together with Theorem 5.3 gives

$$\int_0^\infty j(R,t)dt = -\left[\frac{\|\mathbf{1}_R\psi_t\|_2^2}{\|\psi\|_2^2}\right]_0^\infty = \frac{\|\mathbf{1}_R\psi\|_2^2}{\|\psi\|_2^2}. \tag{4.59}$$

Plugging Eqs. (4.58) and (4.59) into Eq. (4.50) for the arrival time probability density, we obtain Eq. (4.54).

Using integration by parts we obtain

$$\langle t\rangle = \int_0^\infty t\,\Pi_T(t)\,dt = -\left[t\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right]_0^\infty + \int_0^\infty \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\,dt. \tag{4.60}$$

The boundary term clearly vanishes for $t = 0$ and for $t \to \infty$ it vanishes because of Theorem 5.3, which proves Eq. (4.55).

The variance can be expressed as

$$\operatorname{Var} T = \langle t^2\rangle - \langle t\rangle^2. \tag{4.61}$$

Using integration by parts we get

$$\begin{aligned}\langle t^2\rangle &= \int_0^\infty t^2\Pi_T(t)\,dt \\ &= -\left[t^2\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right]_0^\infty + 2\int_0^\infty t\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\,dt,\end{aligned} \tag{4.62}$$

where the boundary terms vanish for the same reasons as before. This proves Eq. (4.56). □

Remark 4.1. For a sample of radioactive matter initially containing N_0 atoms, the number of non-decayed atoms $N(t)$ in the sample at time t is equal to N_0 times the non-escape probability, i.e.

$$N(t) = N_0\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}, \tag{4.63}$$

therefore the activity $-dN/dt$ is equal to $N_0 \Pi_T$.

4.3 Main Results

4.3.1 Approximate Time Distribution

Due to Eq. (4.12), an approximate time variance is obtained from the approximate arrival time density

$$\Pi_T^0(t) := -\partial_t \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}, \tag{4.64}$$

that corresponds to the non-escape probability

$$\frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}. \tag{4.65}$$

We call the approximate time variance $\mathrm{Var}_0\, T$ and the approximate mean time $\langle t \rangle_0$. Analogously to Lemma 4.2 we get

$$\langle t \rangle_0 = \int_0^\infty \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}\, dt, \tag{4.66}$$

$$\mathrm{Var}_0\, T = 2 \int_0^\infty t \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}\, dt - \langle t \rangle_0^2. \tag{4.67}$$

To get an estimate on the error that we make by approximating $\mathrm{Var}\, T$ with $\mathrm{Var}_0\, T$ we will use Lemma 3.1, but this will only work up to several lifetimes. To control the long-time behavior of the wave function, we will use the quantitative bounds given in the next Corollary. Since it is simply the application of the general estimates from Theorem 5.3 to the particular situation we are looking at right now, we shift its proof to the Appendix. To state the Corollary we will at first define some shorthands for certain compositions of the constants given in Section 5.2.2.

Definition 4.1. *For $K > 0$ let*

$$M_{K,\infty}(0) := e^{\beta R}\left[\frac{2}{\alpha} + \frac{\sigma}{\sqrt{2}}E_{\beta,\sigma/\sqrt{2}}\right], \tag{4.68}$$

$$\begin{aligned} M_{K,\infty}(1) := e^{\beta R}\Big[&\frac{2^2}{\alpha^2} + \frac{2R + C_{1,K}}{\alpha} + \sigma^2 \\ &+ \left(R + \beta\sigma^2 + \frac{C_{1,K}}{2}\right)\frac{\sigma}{\sqrt{2}}E_{\beta,\sigma/\sqrt{2}}\Big], \end{aligned} \tag{4.69}$$

$$\begin{aligned} M_{K,\infty}(2) := e^{\beta R}\Big[&\frac{2^4}{\alpha^3} + \frac{2^2(2R + C_{1,K})}{\alpha^2} + \left(R^2 + RC_{1,K} + \frac{C_{2,K}}{2}\right)\frac{2}{\alpha} \\ &+ \sigma^2\left(2R + C_{1,K} + \beta\sigma^2\right) + \Big(\frac{C_{2,K}}{2} \\ &+ C_{1,K}(R + \beta\sigma^2) + \sigma^2 + (R + \beta\sigma^2)^2\Big)\frac{\sigma}{\sqrt{2}}E_{\beta,\sigma/\sqrt{2}}\Big], \end{aligned} \tag{4.70}$$

$$M_1(0) := e^{\beta R}\left[2\log\left(\frac{2}{\beta}\right) + \frac{\pi}{2} + \frac{\pi\sigma}{2^{3/2}}E_{\beta,\sigma/\sqrt{2}}\right], \tag{4.71}$$

$$\begin{aligned} M_1(1) := e^{\beta R}\Big[&\left(2\log\left(\frac{2}{\beta}\right) + \frac{\pi}{2}\right)\left(R + \frac{C_1}{2s}\right) + \frac{\pi}{\beta} \\ &+ \frac{\pi\sigma^2}{2} + \left(R + \beta\sigma^2 + \frac{C_1}{2s}\right)\frac{\pi\sigma}{2^{3/2}}E_{\beta,\sigma/\sqrt{2}}\Big], \end{aligned} \tag{4.72}$$

$$\begin{aligned} M_1(2) := e^{\beta R}\Big[&\left(2\log\left(\frac{2}{\beta}\right) + \frac{\pi}{2}\right)\left(R^2 + \frac{C_1}{s}R + \frac{C_2}{2s^2}\right) + \frac{\pi}{\beta}\left(2R + \frac{C_1}{s}\right) \\ &+ \frac{4}{\beta^2} + \frac{\pi\sigma^2}{2}\left(2R + \frac{C_1}{s} + \beta\sigma^2\right) + \Big(\frac{C_2}{2s^2} \\ &+ \frac{C_1}{s}(R + \beta\sigma^2) + \sigma^2 + (R + \beta\sigma^2)^2\Big)\frac{\pi\sigma}{2^{3/2}}E_{\beta,\sigma/\sqrt{2}}\Big], \end{aligned} \tag{4.73}$$

$$\begin{aligned} \tilde{c}_3 := {}&27\frac{2^{10}}{\alpha^5}M_{K,\infty}^2(0)z_{ac,K}^2(2) + 23\pi^2\frac{2^6}{\alpha^3}M_{K,\infty}^2(1)z_{ac,K}^2(1) \\ &+ 27\frac{2^2}{\alpha}M_{K,\infty}^2(2)z_{ac,K}^2(0), \end{aligned} \tag{4.74}$$

$$\begin{aligned}\tilde{c}_4 &:= 276\frac{M_1^2(0)}{s^5}\left(1+\frac{2^4}{\alpha^2}\right)^4\left(z_{ac}^2(2)+s^2z_{ac}^2(1)+s^4z_{ac}^2(0)\right)\\&+304\frac{M_1^2(1)}{s^3}\left(1+\frac{2^4}{\alpha^2}\right)^3\left(z_{ac}^2(1)+s^2z_{ac}^2(0)\right)\\&+14\frac{M_1^2(2)}{s}\left(1+\frac{2^4}{\alpha^2}\right)^2 z_{ac}^2(0).\end{aligned} \tag{4.75}$$

Corollary 4.1. *Let $t>0$, $K=\alpha/4$, and $s<K\leq 1$. Then, for $n=0,1,2$*

$$s_K = 1, \tag{4.76}$$

$$\|\mathbf{1}_K\hat{\psi}^{(n)}\|_\infty \leq M_{K,\infty}(n), \tag{4.77}$$

$$\|\hat{\psi}^{(n)}w\|_1 \leq M_1(n), \tag{4.78}$$

$$\|\mathbf{1}_R e^{-iHt}\psi\|_2^2 \leq \tilde{c}_3 t^{-3} + \tilde{c}_4 t^{-4}. \tag{4.79}$$

Lemma 3.1 and Corollary 4.1 allow us to estimate the error on the variance of time. The result is given in the following Lemma, which is proven in Section 4.5.

Lemma 4.3. *Let $A>0$,*

$$E_{\beta,\sigma} := \sqrt{\pi}e^{\beta^2\sigma^2}\left(1+\mathrm{Erf}(\beta\sigma)\right), \tag{4.80}$$

$$\begin{aligned}\omega_{(0,A)} &:= \left(2+\sqrt{E_{\beta,\sigma}\beta\sigma}\right)\left[\frac{4\sqrt{54\beta}}{5}A^{5/4}\right.\\&\left.+\left(\frac{\sqrt{6}\beta^{1/4}}{\sqrt{5\pi}\alpha^{1/4}}+\frac{4\sqrt{\beta}}{\sqrt{\pi\alpha}}+\sqrt{E_{\beta,\sigma}\beta\sigma}\right)A\right],\end{aligned} \tag{4.81}$$

$$\omega_{[A,\infty)} := 2\beta e^{-2\beta R}\left(\frac{\tilde{c}_3}{2}A^{-2}+\frac{\tilde{c}_4}{3}A^{-3}\right)+\frac{e^{-\gamma A}}{\gamma}, \tag{4.82}$$

$$\begin{aligned}\zeta_{(0,A)} &:= \left(2+\sqrt{E_{\beta,\sigma}\beta\sigma}\right)\left[\frac{4\sqrt{54\beta}}{9}A^{9/4}\right.\\&\left.+\frac{1}{2}\left(\frac{\sqrt{6}\beta^{1/4}}{\sqrt{5\pi}\alpha^{1/4}}+\frac{4\sqrt{\beta}}{\sqrt{\pi\alpha}}+\sqrt{E_{\beta,\sigma}\beta\sigma}\right)A^2\right],\end{aligned} \tag{4.83}$$

$$\zeta_{[A,\infty)} := 2\beta e^{-2\beta R}\left(\tilde{c}_3 A^{-1} + \frac{\tilde{c}_4}{2} A^{-2}\right) + \frac{e^{-\gamma A}}{\gamma^2}(1+\gamma A), \tag{4.84}$$

and

$$\omega := \omega_{(0,A)} + \omega_{[A,\infty)}, \tag{4.85}$$

$$\zeta := \zeta_{(0,A)} + \zeta_{[A,\infty)}, \tag{4.86}$$

$$\varepsilon_T := 2\zeta + \omega^2 + \frac{2}{\gamma}\omega. \tag{4.87}$$

Then, for the wave function ψ the following error estimates hold

$$|\langle t\rangle - \langle t\rangle_0| \leq \omega, \tag{4.88}$$

$$|\mathrm{Var}\, T - \mathrm{Var}_0\, T| \leq \varepsilon_T. \tag{4.89}$$

4.3.2 Validity of the uncertainty relation

We will now see that there are β and σ values for which the error estimate ε_T is sufficiently small to check if the uncertainty relation holds. For these values we will find that the uncertainty relation is satisfied. We start by defining

$$P_0 := \mathrm{Var}\, E\, \mathrm{Var}_0\, T, \qquad \varepsilon_P := \mathrm{Var}\, E\, \varepsilon_T, \tag{4.90}$$

so that

$$|\mathrm{Var}\, E\, \mathrm{Var}\, T - P_0| \leq \varepsilon_P. \tag{4.91}$$

Then, we have the following possibilities:

$P_0 - \varepsilon_P \geq 1/4$: this implies that $\mathrm{Var}\, E\, \mathrm{Var}\, T \geq 1/4$ and we can state that the uncertainty relation holds;

$P_0 + \varepsilon_P < 1/4$: this implies that $\mathrm{Var}\, E\, \mathrm{Var}\, T < 1/4$ and we can state that the uncertainty relation is violated;

$1/4 \in (P_0 - \varepsilon_P, P_0 + \varepsilon_P]$: in this case we are not able to check the validity of the uncertainty relation.

This situation is summarized in the following

Definition 4.2. *We say that the error* ε_P *on the product* $\mathrm{Var}\, E\, \mathrm{Var}\, T$ *for the wave function* ψ *is small enough to allow us to make statements on the validity of the uncertainty relation if* $P_0 - \varepsilon_P \geq 1/4$ *or* $P_0 + \varepsilon_P < 1/4$.

We will need the next hypothesis, whose validity will be discussed in Section 4.4. Recall that $\nu_{\tilde{K}}$ was introduced in Definition 5.2 as the smallest non-negative integer such that $\alpha_n \geq 2\tilde{K} = 12\|V\|_1$ for all $n \geq \nu_{\tilde{K}}$.

Definition 4.3. *Let* C_V *be the set of all one-parameter families of potentials* $\{V_b\}_{b\in[0,\infty)}$ *satisfying the properties:*

1. *For every finite* $b \geq 0$ *the potential* V_b *satisfies the assumptions of Section 4.2.2.*
2. *There are two constants* $c_{1,2} > 0$ *so that* $c_1 \leq \alpha(b) \leq c_2$ *for all* $b \geq 0$.
3. $\lim_{b\to\infty} \beta(b) = 0$.
4. $r_0(b) = \sum_{n=0}^{\infty} \frac{5\beta_n(b)}{\alpha_n^2(b)+\beta_n^2(b)} = O(1)$ *as* $b \to \infty$.
5. $\nu_{\tilde{K}} = O\left((\log \beta(b))^2\right)$ *as* $b \to \infty$.

Hypothesis 4.1. *The set* C_V *is not empty.*

Physically, the most important thing is Property 3 of Definition 4.3, that means that it is possible to consider potentials that give rise to resonances with arbitrary long lifetime. For simplicity we give also the following

Definition 4.4. *By* $\lim_{\beta\to 0}$ *we denote the following: pick any family of potentials* $\{V_b\}_{b\in[0,\infty)} \in C_V$ *and calculate the limit* $\lim_{b\to\infty}$.

Using this notation, we can rewrite Property 5 of Definition 4.3 as

$$\nu_{\tilde{K}} = O\left((\log \beta)^2\right), \qquad \text{as } \beta \to 0. \tag{4.92}$$

We can now state our Theorem.

Theorem 4.1. *Let the assumptions of Corollary 4.1 be satisfied and consider the wave function ψ.*

1. *Let the error ε_P be small enough to allow us to make statements on the validity of the uncertainty relation (cf. Definition 4.2), then*

$$\operatorname{Var} E \operatorname{Var} T \geq 1/4. \tag{4.93}$$

2. *Let moreover $\sigma = \beta$ and Hypothesis 4.1 be satisfied, then*

$$\lim_{\beta \to 0}(P_0 - \varepsilon_P) = \infty. \tag{4.94}$$

The second statement of the Theorem implies that there actually exist values of β and σ for which $P_0 - \varepsilon_P \geq 1/4$ and therefore our error estimate is small enough to check the validity of the uncertainty relation. Unfortunately, as we mentioned in the Introduction, this range of parameters requires β to be smaller than the value corresponding to the longest lived physical element, i.e. Bismuth (recall that the lifetime is connected with β by $1/(4\alpha\beta)$).

4.3.3 The energy time uncertainty relation and the linewidth-lifetime relation are different

The linewidth-lifetime relation (4.4) has been verified in many experiments, and its validity is often explained making reference to the time-energy uncertainty relation (see e.g. [50]). In the following we will see that, with $\sigma = \beta$, it is possible to find values of β such that the product of the linewidth and the lifetime is arbitrarily close to 1, while at the same time the product of $\operatorname{Var} E$ and $\operatorname{Var} T$ is arbitrarily large and hence far from $1/4$. Therefore, the validity of the linewidth-lifetime relation cannot be a consequence of the validity of the time-energy uncertainty relation, as asserted by Fock and Krylov [28].

In order to prove this statement, we have at first to give a precise definition for the lifetime and for the linewidth of a generic state.

Definition 4.5 (Lifetime). *Let $\mathbb{P}(T \leq t)$ be the arrival time cumulative distribution function, i.e. the probability that the decay product reaches the detector at a time T not later than t, and let it be continuous. The lifetime is the time τ such that*

$$\mathbb{P}(T \leq \tau) = 1 - \frac{1}{e}. \tag{4.95}$$

In other words, the lifetime is the time at which a fraction $1/e$ of the initial sample has decayed. In the usual case in which $\mathbb{P}(T \leq t) = 1 - e^{-\nu t}$, then $\tau = 1/\nu$.

Definition 4.6 (Linewidth). *Let Π_E be the probability density function of the energy of the decay product, let it be continuous, and let M be its maximal value. The linewidth Γ is the distance between those solutions of the equation*

$$\Pi_E(E) = \frac{M}{2} \tag{4.96}$$

that lie furthest apart.

If Π_E has just one peak, then Γ is its full width at half maximum; in particular, if Π_E is of Breit-Wigner shape, i.e.

$$\Pi_E \propto \frac{1}{(E - E_0)^2 + G^2}, \tag{4.97}$$

then $\Gamma = G$.

With these definitions we can state the following

Theorem 4.2. *Let $\sigma = \beta$, the assumptions of Corollary 4.1 and Hypothesis 4.1 be satisfied, then for the wave function ψ*

$$\lim_{\beta \to 0} \Gamma\tau = 1, \tag{4.98}$$

while

$$\lim_{\beta \to 0} \operatorname{Var} E \operatorname{Var} T = \infty. \tag{4.99}$$

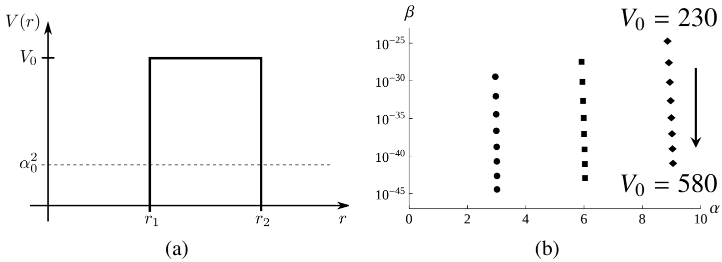


Figure 4.1: (a) Example of barrier potential. (b) The plot shows how the first three resonances (●, ■, and ◆) of the barrier potential shown in Fig. 4.1a for $r_1 = 1$ and $r_2 = 2$ move as V_0 is increased from 230 to 580 in steps of 50.

4.4 Discussion of Hypothesis 4.1

Hypothesis 4.1 holds if the requirements in Definition 4.3 are satisfied. Therefore, we will now give arguments why there exist potentials that satisfy them.

4.4.1 Properties 1-3 in Definition 4.3

Consider the simple barrier potential shown in Fig. 4.1a as a family parametrized by $V_0 \geq 1$; Property 1 is then immediate, except for the fact that α and β are both minimal for all $V_0 \geq 1$.

This potential is simple enough to allow us to calculate its Jost function explicitly, that will also be parametrized by $V_0 \geq 1$ (see Eq. (5.100)). Using this explicit formula we have numerically calculated the location of the first three resonances for eight increasing values of V_0 and depicted them in Fig. 4.1b. We found that their real parts change negligibly, while their imaginary parts tend to zero. Moreover, $k_0(V_0)$ always has the smallest imaginary and real part. Thus, Properties 2 and 3 of Definition 4.3

appear to be fulfilled. From the physical point of view the reason for this is that when the barrier is high enough then the resonances get close to the bound states of the infinitely high barrier.

4.4.2 Property 4 in Definition 4.3

The scattering length a is defined as (see [45, page 136])

$$a = \frac{\dot{S}(0)}{2iS(0)}. \tag{4.100}$$

From Eq. (5.80) we see that for potentials without bound and virtual states

$$|a| = \left| R_V - \frac{2}{5} r_0 \right| \geq \frac{2}{5} r_0 - R_V. \tag{4.101}$$

For the barrier potential, using the explicit form of the Jost function and the relation $S(k) = F(-k)/F(k)$ one gets

$$\lim_{V_0 \to \infty} a(V_0) = -r_2, \tag{4.102}$$

which together with Eq. (4.101) shows that Property 4 is satisfied.

4.4.3 Property 5 in Definition 4.3

According to Definition 5.2, we have that $\nu_{\tilde{K}}$ is the number of resonances that lie in the stripe $\{z \in \mathbb{C} \,|\, 0 \leq \operatorname{Re} z \leq 12\|V\|_1, \operatorname{Im} k \leq 0\}$. Clearly, this number depends on the distribution of the zeros of the Jost function. Unfortunately, results from inverse scattering theory like [27, 32] suggest that there are little restrictions on this distribution: Korotyaev for example proves in [27] that resonances and potentials are in one-to-one correspondence, so that one can interpret resonances as variables which fix the potential. Hence, they can be put essentially everywhere and the potential just changes accordingly. On the other hand, Zworski proved a formula [Theorem 6 in 63] for the location of the n-th resonance that holds up to an error that becomes small for growing n; however, no bound on the error is given. According to this formula we would have

$$\nu_{\tilde{K}} \approx C\|V\|_1 \tag{4.103}$$

with the constant $C > 0$ depending only on the size of the potential's support and on the behavior of the potential at $r = R_V$ (see [63]). Assuming Property 1 of Definition 4.3 and Eq. (4.103) to be satisfied, then $\nu_{\tilde{K}}$ changes only through $\|V\|_1$ when $\beta \to 0$, and we have to study how $\|V\|_1$ behaves in this limit.

A relation between the inverse of the lifetime $\gamma = 4\alpha\beta$ and an integral of the potential was famously obtained by G. Gamow [16, 54]. He found the following formula (see [54, Chapter 7])

$$\gamma = 4\alpha\beta = \frac{\alpha}{R_N} \exp\left(-2\int_{r_1}^{r_2} \sqrt{V(r) - (\alpha^2 - \beta^2)}\, dr\right), \tag{4.104}$$

where $V(r)$ is assumed to be shaped like a barrier through which the alpha particle needs to tunnel in order for alpha decay to occur, and $\alpha^2 - \beta^2$ is the energy of the alpha particle. The radii r_1 and r_2 are such that $V(r) - (\alpha^2 - \beta^2) \geq 0$ if $r \in [r_1, r_2]$ and R_N denotes the nuclear radius. Applying Eq. (4.104) to the barrier potential shown in Fig. 4.1a and assuming that $V_0 - (\alpha^2 - \beta^2) \geq V_0/4$ as well as $r_2 - r_1 \geq \sqrt{r_2 - r_1}$, which is justified by the fact that in physical examples the barrier is very thick and much higher than the energy of the alpha particle, we get

$$\log\frac{1}{\beta} = \log(4R_N) + 2\sqrt{V_0 - (\alpha^2 - \beta^2)}(r_2 - r_1) \geq \sqrt{\|V\|_1}, \tag{4.105}$$

Hence, Gamow's formula, Eq. (4.104), suggests that

$$\|V\|_1 \leq \left(\log\frac{1}{\beta}\right)^2 = (\log\beta)^2, \tag{4.106}$$

that together with Eq. (4.103) gives exactly Property 5 in the form of Eq. (4.92).

To transform the previous argument into a proof one needs an explicit bound on $\nu_{\tilde{K}}$ in the form of Eq. (4.103), and a rigorous version of Eq. (4.104). We see two ways to derive the former. First, by modification of the proof of Levinson's Theorem (see [45]), which connects the number of bound states N with the Jost function F. In this proof the number of bound states is calculated via the complex contour integral

$$N = \frac{1}{2\pi i} \int_C \frac{\dot{F}(z)}{F(z)}\, dz, \tag{4.107}$$

where the contour C is a closed semi circle in the upper half plane that encloses all bound states. The bound states are zeros of F and thereby poles of the integrand, so that Eq. (4.107) is a direct consequence of the Residue Theorem. For the purposes of getting a handle on $\nu_{\tilde{K}}$, we can use Eq. (4.107), but choose as contour the boundary of the region $\{z \in \mathbb{C} \,|\, 0 \leq \operatorname{Re} z \leq 12\|V\|_1, \operatorname{Im} k \leq 0\}$. The difficulty is now to derive bounds for $\dot{F}(z)/F(z)$ along this contour, which yield bounds for $\nu_{\tilde{K}}$. The second way we can think of to derive a rigorous bound on $\nu_{\tilde{K}}$ is via a well known result from inverse scattering theory, namely the Marchenko equation (see [27]). Using this equation, one can calculate the potential from the S-matrix and thereby from the resonances. Thus, it might be possible to characterize the potential class for which the resonances in $\{z \in \mathbb{C} \,|\, 0 \leq \operatorname{Re} z \leq 12\|V\|_1, \operatorname{Im} k \leq 0\}$ only have imaginary parts above a certain value. Then one can employ the bounds on the number of resonances $n(r)$ in a ball of radius r, obtained in Lemma 5.2, to get a bound for $\nu_{\tilde{K}}$.

The proof of Eq. (4.104) is, to our knowledge, still an open problem. Moreover, Eq. (4.106) will not hold for general potentials, but only for barrier-like ones as considered by Gamow. For other potentials, Eq. (4.104) is not satisfied, so that the relation between $\|V\|_1$ and β might be different. For example, in [21] it was shown that the resonances of the one-dimensional "potential table" $V(x) = V_0 \mathbf{1}_{[-a,a]}(x)$ satisfy

$$k_n = \sqrt{V_0 + \frac{(n+1)^2\pi^2}{4a^2}} - i \frac{(n+1)^2\pi^2}{4a^3\sqrt{V_0^2 + V_0\frac{(n+1)^2\pi^2}{4a^2}}} + O(V_0^{-3/2}). \quad (4.108)$$

Using $\|V\|_1 = 2aV_0$ and assuming that V_0 is large, we have for $\beta = -\operatorname{Im} k_0$ that

$$\|V\|_1^2 + \|V\|_1 \frac{\pi^2}{2a} \approx \frac{\pi^4}{4a^4\beta^2}, \quad (4.109)$$

which is a completely different relationship between $\|V\|_1$ and β than Eq. (4.106). Note that this difference is not due to the fact that we are looking at a one-dimensional potential rather than a three-dimensional one with rotational symmetry. Indeed, in the one-dimensional situation the resonances satisfy the equation [21]

$$\exp\left(i4a\sqrt{k^2 - V_0}\right) = \left(\frac{k + \sqrt{k^2 - V_0}}{k - \sqrt{k^2 - V_0}}\right)^2 \quad (4.110)$$

and in the analogous three-dimensional situation, where the potential reads $V(r) = V_0 \mathbf{1}_a(r)$, following [21] it is easy to verify that the resonances satisfy

$$\exp\left(i2a\sqrt{k^2 - V_0}\right) = \frac{k + \sqrt{k^2 - V_0}}{k - \sqrt{k^2 - V_0}}. \quad (4.111)$$

Hence, every resonance of the three-dimensional potential appears also in the one-dimensional situation, so that there is a n for which Eq. (4.108) captures the location of the first resonance of the three-dimensional potential.

4.5 Energy- and Time-Variance

In this Section we explicitly calculate the variance of energy and time that will be extensively used in the proofs of Theorems 4.1 and 4.2.

Lemma 4.4. *Let $E_{\beta,\sigma}$ be defined as in Eq.* (4.80). *Then, for the wave function ψ*

$$\operatorname{Var} E = \frac{2\alpha^2\beta^2 E_{\beta,\sigma}^2 + \frac{\beta^2}{2\sigma^2}(1 + E_{\beta,\sigma}^2) + \frac{\beta}{2\sigma}\left(\beta^2 + 4\alpha^2 + \frac{3}{2\sigma^2}\right) E_{\beta,\sigma}}{\left(1 + \beta\sigma E_{\beta,\sigma}\right)^2}. \tag{4.112}$$

Proof. Note that

$$\operatorname{Var} E = \frac{\langle\psi, H^2\psi\rangle}{\|\psi\|^2} - \frac{\langle\psi, H\psi\rangle^2}{\|\psi\|^4}. \tag{4.113}$$

First look at

$$\langle\psi, H\psi\rangle = \langle\psi, \mathbf{1}_R H\psi\rangle + \langle\psi, \mathbf{1}_{[R,\infty)} H\psi\rangle \tag{4.114}$$

$$= k_0^2 \|f_R\|_2^2 - \langle\psi, \mathbf{1}_{[R,\infty)}\psi''\rangle. \tag{4.115}$$

From Lemma 3.1 in [56] we have

$$\|f_R\|_2^2 = \frac{e^{2\beta R}}{2\beta} \tag{4.116}$$

and since for $r \geq R$

$$-\psi''(r) = \left[\frac{1}{\sigma^2} - \left(ik_0 - \frac{r-R}{\sigma^2}\right)^2\right] \exp\left(ik_0 r - \frac{(r-R)^2}{2\sigma^2}\right) \tag{4.117}$$

in the weak sense, the second summand in Eq. (4.115) is readily calculated. One finds elementary error function integrals, which is why we omit the details and directly give the result

$$\langle\psi, H\psi\rangle = \frac{e^{2\beta R}}{2\beta}\left(\alpha^2 + \frac{\beta}{2\sigma}(1 + 2\alpha^2\sigma^2)\sqrt{\pi}e^{\beta^2\sigma^2}(1 + \mathrm{Erf}(\beta\sigma))\right). \quad (4.118)$$

Now,

$$\langle\psi, H^2\psi\rangle = \langle H\psi, H\psi\rangle = \langle H\psi, \mathbf{1}_R H\psi\rangle + \langle H\psi, \mathbf{1}_{[R,\infty)} H\psi\rangle \quad (4.119)$$

$$= |k_0|^4 \|f_R\|_2^2 + \langle\psi'', \mathbf{1}_{[R,\infty)}\psi''\rangle. \quad (4.120)$$

The first summand is again obtained from Eq. (4.116) and the second one by integrating the modulus square of Eq. (4.117) over $[R, \infty)$, yielding error function integrals again. Omitting the details, one arrives at

$$\langle\psi, H^2\psi\rangle = \frac{e^{2\beta R}}{2\beta}\Big[\frac{1}{2\sigma^2}(\beta^2 + 2\alpha^4\sigma^2) + \frac{\beta}{4\sigma^3}(3 + 12\alpha^2\sigma^2 + 4\alpha^4\sigma^4)\sqrt{\pi}e^{\beta^2\sigma^2}(1 + \mathrm{Erf}(\beta\sigma))\Big]. \quad (4.121)$$

Moreover, using the fact that $f(k_0, r) = e^{ik_0 r}$ for $r \geq R$, we have

$$\|g_R\|_2^2 = \int_R^\infty \exp\left(2\beta r - \frac{(r-R)^2}{\sigma^2}\right) dr = \frac{\sigma}{2} e^{2\beta R} E_{\beta,\sigma} \quad (4.122)$$

and this together with Eq. (4.116) gives us

$$\|\psi\|_2^2 = \|f_R\|_2^2 + \|g_R\|_2^2 = \frac{e^{2\beta R}}{2\beta}\left[1 + \beta\sigma E_{\beta,\sigma}\right]. \quad (4.123)$$

Plugging $\langle\psi, H^2\psi\rangle, \langle\psi, H\psi\rangle$ and $\|\psi\|_2^2$ into the formula for the variance, Eq. (4.113), we obtain the assertion of the Lemma. □

In contrast to the energy variance, $\mathrm{Var}\, T$ can not be calculated directly. We will approximate it by $\mathrm{Var}_0\, T$, which is defined in Eq. (4.67) and determined in the next Lemma. Recall that $\gamma = 4\alpha\beta$.

Lemma 4.5. *The probability density*

$$\Pi_T^0(t) = -\partial_t \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R \psi\|_2^2}, \tag{4.124}$$

has the mean

$$\langle t \rangle_0 = \frac{1}{\gamma} \tag{4.125}$$

and the variance

$$\operatorname{Var}_0 T = \frac{1}{\gamma^2}. \tag{4.126}$$

Proof. Due to the fact that

$$\|\mathbf{1}_R \psi\|_2^2 = \|f_R\|_2^2, \qquad \|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2 = e^{-\gamma t}\|f_R\|_2^2 \tag{4.127}$$

we have

$$\Pi_T^0(t) = -\partial_t \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R \psi\|_2^2} = -\partial_t e^{-\gamma t} = \gamma e^{-\gamma t}. \tag{4.128}$$

Using integration by parts, the mean then calculates to

$$\int_0^\infty t\,\gamma e^{-\gamma t} dt = \int_0^\infty e^{-\gamma t} dt = \frac{1}{\gamma}, \tag{4.129}$$

and the variance

$$\begin{aligned} \operatorname{Var}_0 T &= \langle t^2 \rangle_0 - \langle t \rangle_0^2 \\ &= 2\int_0^\infty t\, e^{-\gamma t} dt - \frac{1}{\gamma^2} \\ &= \frac{1}{\gamma^2}. \end{aligned} \tag{4.130}$$

□

To estimate the error on the time variance made by using $\operatorname{Var}_0 T$ as approximation, we start by estimating in the following Lemma the pointwise difference between the true non-escape probability Π_T and Π_T^0. For early times, say $t \in (0, A)$, we will control this difference using the results of Skibsted given in Lemma 3.1. At late times, i.e. for $t \in [A, \infty)$, we can use the scattering estimates of Corollary 4.1.

Lemma 4.6. *Let $t > 0$ and*

$$\xi_{(0,A)}(t) := \left(2 + \sqrt{E_{\beta,\sigma}\beta\sigma}\right) \times \left(\sqrt{54\beta}\, t^{1/4} + \sqrt{\frac{6}{5\pi}}\frac{\beta^{1/4}}{\alpha^{1/4}} + \frac{4\sqrt{\beta}}{\sqrt{\pi\alpha}} + \sqrt{E_{\beta,\sigma}\beta\sigma}\right), \quad (4.131)$$

$$\xi_{[A,\infty)}(t) := 2\beta e^{-2\beta R}\left(\tilde{c}_3 t^{-3} + \tilde{c}_4 t^{-4}\right) + e^{-\gamma t}. \quad (4.132)$$

Then,

$$\left| \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} \right| \le \xi_{(0,A)}(t)\mathbf{1}_{(0,A)} + \xi_{[A,\infty)}(t)\mathbf{1}_{[A,\infty)}. \quad (4.133)$$

Proof. We first prove the bound that we will use for $t \in (0, A)$. Observing that

$$6\left(\frac{1 + 20\sqrt{\beta/\alpha}}{1 + 10\sqrt{\beta/\alpha}}\right)^2 \beta \le 54\beta, \quad (4.134)$$

we get from Lemma 3.1 that for $t \ge 0$

$$\left\| e^{-iHt} f_R - e^{-ik_0^2 t} f_{R_2(t)} \right\|_2 \le \|f_R\|_2 \left(\sqrt{54\beta\sqrt{t} + \frac{6\sqrt{\beta}}{5\pi\sqrt{\alpha}}} + \frac{4\sqrt{\beta}}{\sqrt{\pi\alpha}} \right). \quad (4.135)$$

Using this together with Eq. (4.116) for $\|f_R\|_2^2$ and Eq. (4.122) for $\|g_R\|_2^2$

we get

$$\left|\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right| \tag{4.136}$$

$$= \frac{1}{\|f_R\|_2^2}\left(\|\mathbf{1}_R e^{-iHt}\psi\|_2 + \|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2\right)$$

$$\times\left|\|\mathbf{1}_R e^{-iHt}\psi\|_2 - \|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2\right| \tag{4.137}$$

$$\leq \frac{\|\psi\|_2 + \|f_R\|_2}{\|f_R\|_2^2}\left\|\mathbf{1}_R\left(e^{-iHt}\psi - e^{-ik_0^2 t} f_{R_2(t)}\right)\right\|_2 \tag{4.138}$$

$$\leq \frac{2\|f_R\|_2 + \|g_R\|_2}{\|f_R\|_2^2}\left\|e^{-iHt}\psi - e^{-ik_0^2 t} f_{R_2(t)}\right\|_2 \tag{4.139}$$

$$\leq \frac{2 + \sqrt{E_{\beta,\sigma}\beta\sigma}}{\|f_R\|_2}\left(\left\|e^{-iHt} f_R - e^{-ik_0^2 t} f_{R_2(t)}\right\|_2 + \left\|e^{-iHt} g_R\right\|_2\right) \tag{4.140}$$

$$\leq \left(2 + \sqrt{E_{\beta,\sigma}\beta\sigma}\right)\left(\sqrt{54\beta\sqrt{t} + \frac{6\sqrt{\beta}}{5\pi\sqrt{\alpha}}} + \frac{4\sqrt{\beta}}{\sqrt{\pi\alpha}} + \sqrt{E_{\beta,\sigma}\beta\sigma}\right). \tag{4.141}$$

For $X, Y \geq 0$,

$$X^2 + Y^2 \leq (X+Y)^2, \tag{4.142}$$

taking the square root, and choosing $X = \sqrt{x}$, $Y = \sqrt{y}$, with $x, y \geq 0$, we have

$$\sqrt{x+y} \leq \sqrt{x} + \sqrt{y}, \tag{4.143}$$

hence

$$\left|\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right| \leq \xi_{(0,A)}(t). \tag{4.144}$$

We now prove the bound used for $t \in [A, \infty)$. Using Corollary 4.1 and

Eq. (4.127) for $\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2$ we get that

$$\left|\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right| \tag{4.145}$$

$$\leq \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} + \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} \tag{4.146}$$

$$\leq \xi_{[A,\infty)}. \tag{4.147}$$

□

Having control over the difference between Π_T and Π_T^{o} we can now prove Lemma 4.3, which provides an estimate on the difference between $\operatorname{Var} T$ and $\operatorname{Var}_{\mathrm{o}} T$.

Proof (of Lemma 4.3). Consider at first the mean. Recalling Eq. (4.55) from Lemma 4.2 and Eq. (4.66), we have

$$|\langle t\rangle - \langle t\rangle_{\mathrm{o}}| \leq \int_0^\infty \left|\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right| dt. \tag{4.148}$$

Substituting Eq. (4.133) from Lemma 4.6 and performing the integral we immediately get Eq. (4.88).

Now consider the variance. Using Eqs. (4.56) and (4.67) for $\operatorname{Var} T$ and $\operatorname{Var}_{\mathrm{o}} T$ we get

$$|\operatorname{Var} T - \operatorname{Var}_{\mathrm{o}} T|$$
$$= \left|2\int_0^\infty t\left(\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}\right) dt + \langle t\rangle_{\mathrm{o}}^2 - \langle t\rangle^2\right| \tag{4.149}$$

From the error estimate on the mean given in Eq. (4.88) we have

$$\left|\langle t\rangle_{\mathrm{o}}^2 - \langle t\rangle^2\right| = \left|-(\langle t\rangle - \langle t\rangle_{\mathrm{o}})^2 + 2\langle t\rangle_{\mathrm{o}}\left(\langle t\rangle_{\mathrm{o}} - \langle t\rangle\right)\right| \leq \omega^2 + \frac{2}{\gamma}\omega, \tag{4.150}$$

therefore

$$
\begin{aligned}
&|\mathrm{Var}\, T - \mathrm{Var}_0\, T| \\
&\le 2\int_0^\infty t \left| \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - \frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} \right| dt + \omega^2 + \frac{2}{\gamma}\omega. \qquad (4.151)
\end{aligned}
$$

Using again the bound (4.133) for the non-escape probability and integrating we get Eq. (4.89). □

4.6 Proof of Theorem 4.1

4.6.1 Proof of Statement 1

First, we sketch the idea behind the proof. The approximate time variance $\mathrm{Var}_0\, T = 1/\gamma^2$ is independent of σ, while the energy variance (4.112) can be made very small by making σ very big. Therefore, the same is true for the approximate product $P_0 = \mathrm{Var}\, E/\gamma^2$; this suggests a possible violation of the uncertainty relation. On the other side, by increasing σ the error $\varepsilon_P = \varepsilon_T \mathrm{Var}\, E$ grows very fast and soon becomes too big to make statements on the validity of the uncertainty relation.

The statement of the Theorem in symbolical form is

$$[P_0 - \varepsilon_P \ge 1/4 \vee P_0 + \varepsilon_P < 1/4] \Rightarrow P_0 - \varepsilon_P \ge 1/4, \qquad (4.152)$$

that is equivalent to

$$P_0 + \varepsilon_P \ge 1/4. \qquad (4.153)$$

The quantities P_0 and ε_P are functions of the parameters α, β, and σ, therefore a sufficient condition for this inequality to be true is that the parameter regions corresponding to $P_0 < 1/4$ and to $\varepsilon_P < 1/4$ do not intersect. This sufficient condition stays sufficient if we make the regions bigger by using a $\tilde{P}_0 \le P_0$ and an $\tilde{\varepsilon}_P \le \varepsilon_P$ in place of P_0 and ε_P.

To find the approximations $\tilde{P}_0$ and $\tilde{\varepsilon}_P$ we will benefit from the fact that the expression (4.112) for $\operatorname{Var} E$ and the expression (4.87) for ε_T are sums of positive terms, therefore we can simply drop some terms from each sum.

We start considering P_0. From the energy variance Eq. (4.112) we get

$$P_0 = \frac{2\alpha^2\beta^2 E_{\beta,\sigma}^2 + \frac{\beta^2}{2\sigma^2}(1 + E_{\beta,\sigma}^2) + \frac{\beta}{2\sigma}\left(\beta^2 + 4\alpha^2 + \frac{3}{2\sigma^2}\right) E_{\beta,\sigma}}{16\alpha^2\beta^2\left(1 + \beta\sigma E_{\beta,\sigma}\right)^2} \tag{4.154}$$

$$= \frac{1}{8\left(\beta\sigma + E_{\beta,\sigma}^{-1}\right)^2}\left[1 + \frac{1 + E_{\beta,\sigma}^{-2}}{4\alpha^2\sigma^2} + \frac{E_{\beta,\sigma}^{-1}}{4\alpha^2\beta\sigma^3}\left(\beta^2\sigma^2 + 4\alpha^2\sigma^2 + \frac{3}{2}\right)\right]. \tag{4.155}$$

We can simplify this expression with the change of variables

$$\tilde{\alpha} := \alpha\sigma, \qquad \tilde{\beta} := \beta\sigma, \tag{4.156}$$

and with the definition

$$E_{\tilde{\beta}} := \sqrt{\pi} e^{\tilde{\beta}^2}(1 + \operatorname{Erf}(\tilde{\beta})) = E_{\beta,\sigma}, \tag{4.157}$$

getting

$$P_0 = \frac{1}{8\left(\tilde{\beta} + E_{\tilde{\beta}}^{-1}\right)^2}\left[1 + \frac{1 + E_{\tilde{\beta}}^{-2}}{4\tilde{\alpha}^2} + \frac{E_{\tilde{\beta}}^{-1}}{4\tilde{\alpha}^2\tilde{\beta}}\left(\tilde{\beta}^2 + 4\tilde{\alpha}^2 + \frac{3}{2}\right)\right]. \tag{4.158}$$

These variables are particularly convenient because they transform the parameters of the problem from (α, β, σ) to only $(\tilde{\alpha}, \tilde{\beta})$. Notice that

$$\frac{e^{-\tilde{\beta}^2}}{2\sqrt{\pi}} \leq E_{\tilde{\beta}}^{-1} \leq \frac{e^{-\tilde{\beta}^2}}{\sqrt{\pi}}, \tag{4.159}$$

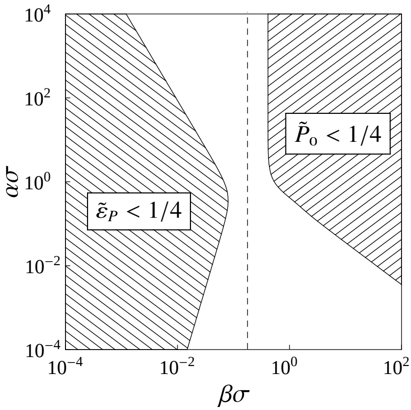


Figure 4.2: Regions where $\tilde{P}_o < 1/4$ and where $\tilde{\varepsilon}_P < 1/4$. The dashed line corresponds to $\beta\sigma = \tilde{\beta}_0 = 10^{-3/4}$.

therefore defining

$$\tilde{P}_o := \frac{\pi}{8\left(\sqrt{\pi}\tilde{\beta} + e^{-\tilde{\beta}^2}\right)^2}\left[1 + \frac{4\pi + e^{-2\tilde{\beta}^2}}{16\pi\tilde{\alpha}^2} + \frac{e^{-\tilde{\beta}^2}}{8\sqrt{\pi}\tilde{\alpha}^2\tilde{\beta}}\left(\tilde{\beta}^2 + 4\tilde{\alpha}^2 + \frac{3}{2}\right)\right], \tag{4.160}$$

we get

$$P_o \geq \tilde{P}_o. \tag{4.161}$$

We now need to characterize the region of the $(\tilde{\alpha}, \tilde{\beta})$-plane where $\tilde{P}_o < 1/4$. Figure 4.2 suggests that this region does not extend in $\tilde{\beta}$ further than the value $\tilde{\beta}_0 := 10^{-3/4}$. To verify this conjecture we consider the border of this region, that is characterized by the equation

$$\tilde{P}_o(\tilde{\alpha}, \tilde{\beta}) = 1/4. \tag{4.162}$$

We solve this equation for $\tilde{\alpha}$, considering $\tilde{\beta}$ a parameter. With the definitions

$$a_{\tilde{\beta}} := 1 + \frac{e^{-\tilde{\beta}^2}}{2\sqrt{\pi}\tilde{\beta}} - \frac{2}{\pi}\left(\sqrt{\pi}\tilde{\beta} + e^{-\tilde{\beta}^2}\right)^2, \tag{4.163}$$

$$b_{\tilde{\beta}} := \frac{4\pi + e^{-2\tilde{\beta}^2}}{16\pi} + \frac{e^{-\tilde{\beta}^2}}{8\sqrt{\pi}\tilde{\beta}}\left(\tilde{\beta}^2 + \frac{3}{2}\right), \tag{4.164}$$

we can rewrite Eq. (4.162) as

$$a_{\tilde{\beta}}\,\tilde{\alpha}^2 + b_{\tilde{\beta}} = 0. \tag{4.165}$$

Observing that $b_{\tilde{\beta}} > 0$, we have that this equations has no solutions in case $a_{\tilde{\beta}} > 0$. For $\tilde{\beta} \le \tilde{\beta}_0$, by direct calculation we verify that

$$a_{\tilde{\beta}} \ge 1 + \frac{e^{-\tilde{\beta}_0^2}}{2\sqrt{\pi}\tilde{\beta}_0} - \frac{2}{\pi}\left(\sqrt{\pi}\tilde{\beta}_0 + 1\right)^2 > 0, \tag{4.166}$$

therefore in the region $\tilde{\beta} \le \tilde{\beta}_0$ there is no $\tilde{\alpha}$ that solves Eq. (4.162), and $\tilde{P}_0$ is always greater than $1/4$ there.

We now turn to analyze the error on the product ε_P. From Eq. (4.87) we have $\varepsilon_T \ge 2\zeta$, therefore

$$\varepsilon_P = \varepsilon_T \operatorname{Var} E = \gamma^2 P_0 \varepsilon_T \ge \gamma^2 \tilde{P}_0 \varepsilon_T \tag{4.167}$$

$$\ge \frac{\pi\gamma^2\varepsilon_T}{16\left(\pi\tilde{\beta}^2 + 1\right)}\left(1 + \frac{1}{4\tilde{\alpha}^2}\right) \ge \frac{\pi\gamma^2\zeta}{8\left(\pi\tilde{\beta}^2 + 1\right)}\left(1 + \frac{1}{4\tilde{\alpha}^2}\right). \tag{4.168}$$

Now for $A \ge 0$ let

$$\tilde{\zeta}_A := \frac{\sqrt{\pi}}{2} e^{\beta^2\sigma^2}\beta\sigma A^2 + 2\beta e^{-2\beta R}\tilde{c}_3 A^{-1}, \tag{4.169}$$

then Lemma 4.3 gives

$$\zeta \ge \tilde{\zeta}_A. \tag{4.170}$$

In particular, the last inequality is true for the A that minimizes $\tilde{\zeta}_A$, that is such that

$$\frac{d\tilde{\zeta}_A}{dA} = \sqrt{\pi}e^{\beta^2\sigma^2}\beta\sigma A - 2\beta e^{-2\beta R}\tilde{c}_3 A^{-2} = 0, \tag{4.171}$$

that implies

$$A = \left(\frac{2e^{-2\beta R}\tilde{c}_3}{\sqrt{\pi}e^{\beta^2\sigma^2}\sigma}\right)^{1/3} = \left(\frac{2\tilde{c}_3}{\sqrt{\pi}\sigma}\right)^{1/3} e^{-\frac{2}{3}\beta R - \frac{1}{3}\beta^2\sigma^2}. \tag{4.172}$$

Substituting that into $\tilde{\zeta}_A$ we get

$$\frac{3\pi^{1/6}}{2^{1/3}}\beta\sigma^{1/3}\tilde{c}_3^{2/3}e^{\frac{1}{3}\beta^2\sigma^2 - \frac{4}{3}\beta R} =: \tilde{\zeta}. \tag{4.173}$$

From the definition of $\tilde{c}_3$, Eq. (4.74), we see that

$$\tilde{c}_3 \geq 27\frac{2^2}{\alpha}M_{K,\infty}^2(2)\, z_{ac,K}^2(0). \tag{4.174}$$

From Definition 5.3 and Eq. (5.44) we get

$$z_{ac,K}(0) \geq 2, \tag{4.175}$$

while Definition 4.1 implies

$$M_{K,\infty}(2) \geq e^{\beta R}\frac{\sigma^3}{\sqrt{2}}E_{\beta,\sigma/\sqrt{2}} \geq \frac{\sigma^3}{\sqrt{2}}e^{\beta R + \frac{1}{2}\beta^2\sigma^2}, \tag{4.176}$$

therefore

$$\tilde{c}_3 \geq 27\frac{8}{\alpha}\sigma^6 e^{2\beta R + \beta^2\sigma^2}. \tag{4.177}$$

Substituting that into $\tilde{\zeta}$ we get

$$\tilde{\zeta} \geq \frac{54\cdot 2^{2/3}\pi^{1/6}}{\alpha^{2/3}}\beta\sigma^{13/3}e^{\beta^2\sigma^2} = \frac{54\cdot 2^{2/3}\pi^{1/6}}{\tilde{\alpha}^{2/3}}\tilde{\beta}\sigma^{12/3}e^{\tilde{\beta}^2}. \tag{4.178}$$

Using this and setting

$$\tilde{\varepsilon}_P(\tilde{\alpha},\tilde{\beta}) := \left(27 \cdot 2^{2/3}\pi^{1/6}\frac{\pi\tilde{\beta}^2}{\pi\tilde{\beta}^2+1}\tilde{\beta}e^{\tilde{\beta}^2}\right)\left(4\tilde{\alpha}^2+1\right)\tilde{\alpha}^{-2/3} \tag{4.179}$$

then Eq. (4.168) gives

$$\varepsilon_P \geq \tilde{\varepsilon}_P. \tag{4.180}$$

We now study the region where $\tilde{\varepsilon}_P \leq 1/4$. Figure 4.2 suggests that this region is completely on the left of $\tilde{\beta}_0$. For $\tilde{\beta} = \tilde{\beta}_0$ we get by direct calculation

$$\tilde{\varepsilon}_P(\tilde{\alpha},\tilde{\beta}_0) \geq \frac{4}{5}\left(4\tilde{\alpha}^2+1\right)\tilde{\alpha}^{-2/3}. \tag{4.181}$$

The function $\left(4\tilde{\alpha}^2+1\right)\tilde{\alpha}^{-2/3}$ is greater than $4\tilde{\alpha}^{4/3}$, but also than $\tilde{\alpha}^{-2/3}$, and these two bounds cross at $\tilde{\alpha} = 1/2$, therefore

$$\tilde{\varepsilon}_P(\tilde{\alpha},\tilde{\beta}_0) \geq \frac{2^{11/3}}{5} > \frac{1}{4}. \tag{4.182}$$

for all values of $\tilde{\alpha}$. Observing that $\tilde{\varepsilon}_P$ grows with growing $\tilde{\beta}$, we can conclude that

$$\varepsilon_P \geq \tilde{\varepsilon}_P(\tilde{\alpha},\tilde{\beta}) > \frac{1}{4} \qquad \forall\tilde{\alpha} \geq 0, \forall\tilde{\beta} \geq \tilde{\beta}_0. \tag{4.183}$$

Hence, we have that the region where ε_P is less than $1/4$ and that where P_o is less than $1/4$ do not overlap.

4.6.2 Proof of Statement 2

To prove Statement 2 in Theorem 4.1 we need to know how P_o and ε_P behave as β goes to 0. This implies that we need to know this behavior for $\mathrm{Var}\,E$, $\mathrm{Var}_o\,T$, and ε_T, and therefore also for $\tilde{c}_3$ and $\tilde{c}_4$ (recall Lemma 4.3). This information will be determined in the next Lemmas, to prove which we will make use of the following auxiliary result.

Lemma 4.7. *Let the one-parameter family of potentials* $\{V_b\}_{b\in[0,\infty)}$ *be in the set* C_V. *Then,*

$$\exists B > 0, \varepsilon > 0 : \|V_b\|_1 > \varepsilon, \ \forall b > B. \tag{4.184}$$

Proof. Let us assume that the statement of the Lemma is false. Then,

$$\forall B > 0, \varepsilon > 0, \ \exists b_\varepsilon > B : \|V_{b_\varepsilon}\|_1 < \varepsilon. \tag{4.185}$$

Form Property 3 of Definition 4.3 we have that $\lim_{b\to\infty} \beta(b) = 0$, i.e.

$$\forall \varepsilon_\beta > 0, \ \exists B_\beta > 0 : \beta(b) < \varepsilon_\beta, \ \forall b > B_\beta. \tag{4.186}$$

Given ε, we choose $\varepsilon_\beta = \varepsilon$, to which a certain B_β corresponds; then, we choose $B = B_\beta$. All together this gives

$$\forall \varepsilon > 0, \ \exists b_\varepsilon > 0 : \|V_{b_\varepsilon}\|_1 < \varepsilon, \ \beta(b_\varepsilon) < \varepsilon. \tag{4.187}$$

Then,

$$\|rV_{b_\varepsilon}\|_1 \leq R_V \|V_{b_\varepsilon}\|_1 < R_V \varepsilon. \tag{4.188}$$

Consider now the integral equation (5.131) for the Jost function F_b, that is

$$F_b(k) = 1 + \int_0^{R_V} e^{ikr} V_b(r) \varphi_b(k,r)\, dr, \qquad \forall k \in \mathbb{C} \tag{4.189}$$

and the bound for the generalized eigenfunctions φ_b given in Eq. (5.123), i.e.

$$|\varphi_b(k,r)| \leq 4e^{4\|r'V_b(r')\|_1} \frac{r}{1+|k|r} e^{|\operatorname{Im} k|r}, \qquad \forall k \in \mathbb{C}, \ r \geq 0. \tag{4.190}$$

For $b = b_\varepsilon$ we can write

$$|\varphi_{b_\varepsilon}(k,r)| \leq 4re^{4R_V\varepsilon + |\operatorname{Im} k|r}, \tag{4.191}$$

and

$$|F_{b_\varepsilon}(k)| \geq \left|1 - \left|\int_0^{R_V} e^{ikr} V_{b_\varepsilon}(r)\varphi_{b_\varepsilon}(k,r)\,dr\right|\right| \tag{4.192}$$

$$\geq 1 - \left|\int_0^{R_V} e^{ikr} V_{b_\varepsilon}(r)\varphi_{b_\varepsilon}(k,r)\,dr\right| \tag{4.193}$$

$$\geq 1 - \int_0^{R_V} e^{|\operatorname{Im} k|r} |V_{b_\varepsilon}(r)||\varphi_{b_\varepsilon}(k,r)|\,dr \tag{4.194}$$

$$\geq 1 - 4R_V e^{2(|\operatorname{Im} k|+2\varepsilon)R_V}\varepsilon. \tag{4.195}$$

In particular, for $k = k_0(b_\varepsilon)$ we get

$$|F_{b_\varepsilon}(k_0(b_\varepsilon))| \geq 1 - 4R_V e^{2(\beta(b_\varepsilon)+2\varepsilon)R_V}\varepsilon \geq 1 - 4R_V e^{6\varepsilon R_V}\varepsilon, \tag{4.196}$$

therefore for ε small enough we can make the right hand side of Eq. (4.196) as close to one as wanted, therefore we have that

$$\exists b > 0 : |F_b(k_0(b))| \geq 1/2. \tag{4.197}$$

On the other side, by definition of resonance,

$$|F_b(k_0(b))| = 0,\ \forall b \geq 0, \tag{4.198}$$

hence a contradiction. □

Lemma 4.8. *Let $\sigma = \beta$, the assumptions of Corollary 4.1 and Hypothesis 4.1 be satisfied, then as $\beta \to 0$*

$$\tilde{c}_3 = O(1), \tag{4.199}$$

$$\tilde{c}_4 = O\left(\frac{1}{\beta^5}\left[\log\left(\frac{1}{\beta}\right)\right]^{12}\right). \tag{4.200}$$

Proof. The quantities $\tilde{c}_3$ and $\tilde{c}_4$ depend on $z_{ac}(n)$, $z_{ac,K}(n)$, $M_{K,\infty}(n)$, and $M_1(n)$, which in turn are combinations of r_0, s_K, s, $C_{n,K}$, C_n, and $q = \frac{1}{2\|V\|_1} + 6R_V$ (see Definitions 5.2 and 5.3, and the definitions given in

Theorems 5.1 and 5.2), so we first determine how the latter quantities behave as $\beta \to 0$. Wherever we use the order-notation in this proof we always refer to the limit $\beta \to 0$.

First, $s_K = 1$ because of Eq. (4.76), and $r_0 = O(1)$ because of Property 4 of Definition 4.3. Moreover, Lemma 4.7 implies that $1/\|V\|_1$ is bounded from above, therefore $q = O(1)$. Under the assumptions on the potential stated in Section 4.2.2, Definition 5.2 for s becomes

$$\frac{1}{s} = \sum_{n=0}^{\nu_{\tilde{K}}-1} \frac{1}{\beta_n}, \tag{4.201}$$

hence

$$s \leq \beta, \tag{4.202}$$

$$\frac{1}{s} \leq \frac{\nu_{\tilde{K}}}{\beta} = O\left(\beta^{-1} (\log \beta)^2\right), \tag{4.203}$$

having used Property 5 of Definition 4.3. Using these results in the definition of the constants $C_{n,K}$ given in Theorem 5.1 and of the constants C_n given in Theorem 5.2 we get

$$C_{n,K} = O(1), \qquad C_n = O(1), \qquad n = 1, 2, 3. \tag{4.204}$$

Similarly, from Definition 5.3 we get

$$z_{ac,K}(n) = O(1), \qquad z_{ac}(n) = O(1), \qquad n = 1, 2, 3. \tag{4.205}$$

We now turn to the constants $M_{K,\infty}(n)$ and $M_1(n)$ given in Definition 4.1. Recalling that $\sigma = \beta$, the only quantity that needs to be determined is

$$E_{\beta,\sigma/\sqrt{2}} = E_{\beta,\beta/\sqrt{2}} = \sqrt{\pi} e^{\beta^4/2} \left[1 + \mathrm{Erf}\left(\frac{\beta^2}{\sqrt{2}}\right)\right] = O(1). \tag{4.206}$$

Then, we have

$$M_{K,\infty}(n) = O(1), \qquad M_1(n) = O\left(\beta^{-n}(\log\beta)^{2n+1}\right), \qquad n = 0, 1, 2. \tag{4.207}$$

Substituting these results into the definitions of $\tilde{c}_3$ and $\tilde{c}_4$ given in Definition 4.1, we get the statement of the Lemma. □

Lemma 4.9. *Let $\sigma = \beta$, the assumptions of Corollary 4.1 and Hypothesis 4.1 be satisfied, then for the wave function ψ we have*

$$\operatorname{Var} E = O\left(\beta^{-2}\right), \tag{4.208}$$

$$\operatorname{Var}_0 T = O\left(\beta^{-2}\right), \tag{4.209}$$

$$\varepsilon_T = O\left(\beta^{-2+2/17}(\log\beta)^{12}\right), \qquad \textit{as } \beta \to 0. \tag{4.210}$$

Proof. From Eq. (4.112) for $\operatorname{Var} E$, using Eq. (4.206), we get immediately

$$\operatorname{Var} E = O\left(\beta^{-2}\right), \quad \text{as } \beta \to 0. \tag{4.211}$$

Recalling that $\operatorname{Var}_0 T = 1/\gamma^2 = 1/(4\alpha\beta)^2$, we have also that

$$\operatorname{Var}_0 T = O\left(\beta^{-2}\right), \quad \text{as } \beta \to 0. \tag{4.212}$$

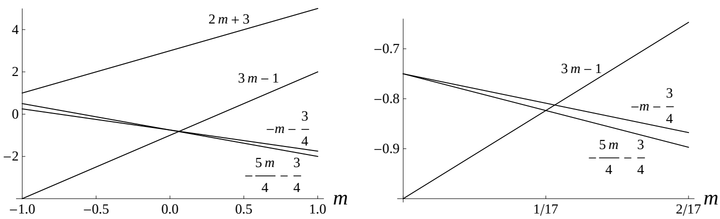
We now turn to the β-order of the error ε_T. Substituting the formulas (4.199) and (4.200) for the β-order of the constants $\tilde{c}_3$ and $\tilde{c}_4$ into Lemma 4.3 we get

$$\omega_{(0,A)} = O\left(\beta^{1/2}A^{5/4}\right) + O\left(\beta^{1/4}A\right), \tag{4.213}$$

$$\omega_{[A,\infty)} = O\left(\beta A^{-2}\right) + O\left(\beta^{-4}(\log\beta)^{12}A^{-3}\right), \tag{4.214}$$

$$\zeta_{(0,A)} = O\left(\beta^{1/2}A^{9/4}\right) + O\left(\beta^{1/4}A^{2}\right), \tag{4.215}$$

$$\zeta_{[A,\infty)} = O\left(\beta A^{-1}\right) + O\left(\beta^{-4}(\log\beta)^{12}A^{-2}\right), \qquad \text{as } \beta \to 0; \tag{4.216}$$



(a) (b)

Figure 4.3: (a) Plot of the β-order of ω given by Eq. (4.220) as a function of m; (b) Close up view of the optimal region.

therefore,

$$\omega = O\left(\beta^{-4}(\log\beta)^{12}A^{-3}\right) + O\left(\beta A^{-2}\right) + O\left(\beta^{1/4}A\right) + O\left(\beta^{1/2}A^{5/4}\right), \tag{4.217}$$

$$\zeta = O\left(\beta^{-4}(\log\beta)^{12}A^{-2}\right) + O\left(\beta A^{-1}\right) + O\left(\beta^{1/4}A^{2}\right) + O\left(\beta^{1/2}A^{9/4}\right), \tag{4.218}$$

$$\text{as } \beta \to 0. \tag{4.219}$$

For every $A > 0$ we can write $A = \beta^{-1-m}$ with $m \in \mathbb{R}$, hence

$$\omega = O\left(\beta^{-1+3m}(\log\beta)^{12}\right) + O\left(\beta^{3+2m}\right) + O\left(\beta^{-3/4-m}\right) + O\left(\beta^{-3/4-5/4m}\right), \tag{4.220}$$

$$\zeta = O\left(\beta^{-2+2m}(\log\beta)^{12}\right) + O\left(\beta^{2+m}\right) + O\left(\beta^{-7/4-2m}\right) + O\left(\beta^{-7/4-9/4m}\right), \tag{4.221}$$

$$\text{as } \beta \to 0. \tag{4.222}$$

Plotting the exponents of every term as functions of m (Fig. 4.3), it is easy to see that the choice that minimizes ω is such that

$$-1 + 3m = -\frac{3}{4} - \frac{5}{4}m, \tag{4.223}$$

i.e. $m = 1/17$. Then, the value for the parameter A that minimizes in terms of β-orders the error ω on the mean is

$$A = \beta^{-18/17}. \tag{4.224}$$

In the same way one sees that this value minimizes ζ too. Substituting we get

$$\omega = O\left(\beta^{-14/17}(\log\beta)^{12}\right), \tag{4.225}$$

$$\zeta = O\left(\beta^{-32/17}(\log\beta)^{12}\right), \qquad \text{as } \beta \to 0, \tag{4.226}$$

and recalling that $\gamma = 4\alpha\beta$,

$$\varepsilon_T = 2\zeta + \omega^2 + \frac{2}{\gamma}\omega = O\left(\beta^{-32/17}(\log\beta)^{12}\right), \qquad \text{as } \beta \to 0. \tag{4.227}$$

□

We are now ready to prove Statement 2 in Theorem 4.1.

Proof (of Statement 2 in Theorem 4.1). From Lemma 4.9 we can calculate the β-order of the approximate product P_0 and of its error ε_P, indeed

$$P_0 = \operatorname{Var} E \operatorname{Var}_0 T = O\left(\beta^{-4}\right), \tag{4.228}$$

$$\varepsilon_P = \varepsilon_T \operatorname{Var} E = O\left(\beta^{-4+2/17}(\log\beta)^{12}\right), \qquad \text{as } \beta \to 0. \tag{4.229}$$

Then,

$$P_0 - \varepsilon_P = O\left(\beta^{-4}\right)\left[1 - O\left(\beta^{2/17}(\log\beta)^{12}\right)\right] = O\left(\beta^{-4}\right), \qquad \text{as } \beta \to 0, \tag{4.230}$$

and the statement of the Theorem follows immediately. □

4.7 Proof of Theorem 4.2

To prove Theorem 4.2 we will use Lemma 4.9, but we also need estimates of Γ and τ, for which we need pointwise bounds on $\mathbb{P}(T \le t)$ and Π_E.

Lemma 4.10. *Let $\sigma = \beta$, the assumptions of Corollary 4.1 and Hypothesis 4.1 be satisfied, then for the lifetime τ of the wave function ψ we have*

$$\tau = \frac{1}{\gamma}\left[1 + O\left(\beta^{4/17}(\log\beta)^{12}\right)\right], \qquad as\, \beta \to 0. \tag{4.231}$$

Proof. At first, notice that from Eq. (4.54) we have

$$\mathbb{P}(T \le t) = \int_0^t \Pi_T(t')dt' = 1 - \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2}, \tag{4.232}$$

therefore the lifetime τ is such that

$$\frac{\|\mathbf{1}_R e^{-iH\tau}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} = \frac{1}{e}. \tag{4.233}$$

Moreover, from Eq. (4.127) we have

$$\frac{\|\mathbf{1}_R e^{-ik_0^2 t} f_{R_2(t)}\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} = e^{-\gamma t}, \tag{4.234}$$

and using Lemma 4.6 we get that for any $A > 0$

$$\left|\frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - e^{-\gamma t}\right| \le \xi_{(0,A)}(t)\mathbf{1}_{(0,A)} + \xi_{[A,\infty)}(t)\mathbf{1}_{[A,\infty)}. \tag{4.235}$$

We use the fact that

$$\begin{aligned} \xi_{(0,A)}(t) &\le \xi_{(0,A)}(A), &\quad \text{for } t \in (0, A), \\ \xi_{[A,\infty)}(t) &\le \xi_{[A,\infty)}(A), &\quad \text{for } t \in [A, \infty), \end{aligned}$$

and define

$$\xi := \xi_{(0,A)}(A) + \xi_{[A,\infty)}(A), \tag{4.236}$$

getting

$$\left| \frac{\|\mathbf{1}_R e^{-iHt}\psi\|_2^2}{\|\mathbf{1}_R\psi\|_2^2} - e^{-\gamma t} \right| \leq \xi. \tag{4.237}$$

It is convenient to consider the equation

$$e^{-\gamma t} = \frac{1}{e}, \tag{4.238}$$

whose solution is $1/\gamma$. Then, the lifetime τ can not be greater than the solution of the equation

$$e^{-\gamma t} + \xi = \frac{1}{e}, \tag{4.239}$$

nor less than the solution of the equation

$$e^{-\gamma t} - \xi = \frac{1}{e}, \tag{4.240}$$

which are

$$\frac{1}{\gamma}\left(1 + \log \frac{1}{1 - e\xi}\right), \tag{4.241}$$

$$\frac{1}{\gamma}\left[1 - \log\left(1 + e\xi\right)\right] \tag{4.242}$$

respectively. Using the bounds

$$\log \frac{1}{1-x} = \int_0^x \frac{1}{1-x'} dx' \leq 2x, \qquad \text{for } 0 < x \leq \frac{1}{2}, \tag{4.243}$$

$$\log(1+x) \leq x \leq 2x, \qquad \text{for } x > 0, \tag{4.244}$$

we get

$$1 - 2e\xi \leq \gamma\tau \leq 1 + 2e\xi, \tag{4.245}$$

that implies

$$\tau = \frac{1}{4\alpha\beta}(1 + O(\xi)), \qquad \text{as } \beta \to 0. \tag{4.246}$$

To determine the behavior of ξ as β goes to zero we substitute in Lemma 4.6 the formulas (4.199) and (4.200) for the β-order of the constants $\tilde{c}_3$ and $\tilde{c}_4$ and set $\sigma = \beta$, getting

$$\xi_{(0,A)}(t) = O\left(\beta^{1/2}\right) t^{1/4} + O\left(\beta^{1/4}\right), \tag{4.247}$$

$$\xi_{[A,\infty)}(t) = O(\beta)\, t^{-3} + O\left(\beta^{-4} (\log\beta)^{12}\right) t^{-4}, \qquad \text{as } \beta \to 0. \tag{4.248}$$

As suggested by Eq. (4.224), we set

$$A = \beta^{-18/17}, \tag{4.249}$$

therefore

$$\xi = O\left(\beta^{4/17} (\log\beta)^{12}\right), \qquad \text{as } \beta \to 0. \tag{4.250}$$

Recalling Eq. (4.237), we see that the arrival time cumulative distribution function pointwise converges to $1 - e^{-\gamma t}$. Moreover, using Eq. (4.245) we get the proposition. □

Lemma 4.11. *Let $\sigma = \beta$ and let Γ denote the linewidth of the wave function ψ. Then,*

$$\Gamma = \gamma + O(\beta^2), \qquad \text{as } \beta \to 0. \tag{4.251}$$

Proof. Note that $E = k^2$ implies

$$\frac{|\hat{\psi}(k)|^2}{\|\psi\|_2^2}\, dk = \frac{|\hat{\psi}(E^{1/2})|^2}{\|\psi\|_2^2} \frac{1}{2\sqrt{E}} dE, \tag{4.252}$$

so that the probability density for energy reads

$$\Pi_E(E) = \frac{|\hat{\psi}(E^{1/2})|^2}{\|\psi\|_2^2} \frac{1}{2\sqrt{E}}. \tag{4.253}$$

Let $K = \alpha/4$. We now look at Π_E on $[0, K^2)$ and $[K^2, \infty)$ separately and show that for β small enough it attains its maximum on the latter interval.

Corollary 4.1 shows that $\hat{\psi}^{(n)} \in L^\infty_{loc} \cap L^1_w$ for $n = 0, 1, 2$ so that Lemma 5.22 applies to it; using the assumption that the Hamiltonian has no zero-resonance we then get for $E \in [0, K^2)$

$$\Pi_E(E) = \frac{|\hat{\psi}(E^{1/2})|^2}{\|\psi\|_2^2} \frac{1}{2\sqrt{E}} \leq \frac{\|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2}{2\|\psi\|_2^2} K. \tag{4.254}$$

Plugging $\sigma = \beta$ into Eq. (4.123) for $\|\psi\|_2^2$ and into the bound on $\|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty$ given by Eq. (4.77) with $n = 1$ and using Property 2 of Definition 4.3, we see that for $E \in [0, K^2)$

$$\Pi_E(E) = O(\beta), \qquad \text{as } \beta \to 0. \tag{4.255}$$

Let us now look at the probability density for energies in $[K^2, \infty)$. From Eq. (4.8) for $\hat{f}_R$ and setting

$$\rho(k) = -\frac{1}{2} \frac{e^{i(k_0 - k)R}}{k - k_0} \bar{S}(k) \tag{4.256}$$

we obtain

$$\hat{\psi}(k) = \hat{f}_R(k) + \hat{g}_R(k) = \rho(k) - \frac{1}{2} \frac{e^{i(k_0 + k)R}}{k + k_0} + \hat{g}_R(k). \tag{4.257}$$

We will see that $\rho(k)$ gives the main contribution to $\hat{\psi}(k)$, and therefore to $\Pi_E(E)$. To this end, consider

$$\begin{aligned} &\left| \frac{1}{\sqrt{E}} |\hat{\psi}(E^{1/2})|^2 - \frac{1}{\alpha} |\rho(E^{1/2})|^2 \right| \\ &\quad = \left| k^{-\frac{1}{2}} |\hat{\psi}(k)| - \alpha^{-\frac{1}{2}} |\rho(k)| \right| \left| k^{-\frac{1}{2}} |\hat{\psi}(k)| + \alpha^{-\frac{1}{2}} |\rho(k)| \right|. \end{aligned} \tag{4.258}$$

We start bounding the factor with the sum, just by bounding the summands separately. Since $\hat{\psi}$ contains $\hat{g}_R$, we need a bound on it. From

Eqs. (5.31), (5.35) and (5.29) we see that for $r \geq R_V$

$$f(k_0, r) = e^{ik_0 r}, \tag{4.259}$$

$$\bar{\psi}^+(k, r) = \frac{1}{2i}(e^{ikr} - S(-k)e^{-ikr}) \tag{4.260}$$

and hence

$$|\hat{g}_R(k)| = \left| \int_R^\infty f(k_0, R) \exp\left(-\frac{(r-R)^2}{2\sigma^2} \right) \bar{\psi}^+(k, r)\, dr \right| \tag{4.261}$$

$$\leq \int_R^\infty \exp\left(\beta r - \frac{(r-R)^2}{2\sigma^2} \right) dr \tag{4.262}$$

$$= e^{\beta R} \frac{\sigma}{\sqrt{2}} E_{\beta, \sigma/\sqrt{2}}. \tag{4.263}$$

Using this, the fact that $|S| = 1$, and Eq. (4.206) we find that

$$k^{-\frac{1}{2}} |\hat{\psi}(k)| \leq \frac{1}{\sqrt{k}} \left[\frac{e^{\beta R}}{|k - k_0|} + \frac{\beta e^{\beta R}}{\sqrt{2}} E_{\beta, \beta/\sqrt{2}} \right] \tag{4.264}$$

$$\leq \frac{e^{\beta R}}{\sqrt{K}} \left[\frac{1}{\beta} + \frac{\beta}{\sqrt{2}} E_{\beta, \beta/\sqrt{2}} \right] = O(\beta^{-1}), \tag{4.265}$$

$$|\rho(k)| \leq \frac{e^{\beta R}}{2\beta} = O(\beta^{-1}), \quad \text{as } \beta \to 0. \tag{4.266}$$

Let us now estimate the factor with the difference in Eq. (4.258). Consider

$$
\begin{aligned}
&\left| k^{-\frac{1}{2}} |\hat{\psi}(k)| - \alpha^{-\frac{1}{2}} |\rho(k)| \right| \\
&\leq \left| k^{-\frac{1}{2}} \hat{\psi}(k) - \alpha^{-\frac{1}{2}} \rho(k) \right| \\
&\leq \left| \left(k^{-\frac{1}{2}} - \alpha^{-\frac{1}{2}} \right) \rho(k) + k^{-\frac{1}{2}} \frac{1}{2} \frac{e^{i(k_0+k)R}}{k+k_0} + k^{-\frac{1}{2}} \hat{g}_R(k) \right| \\
&\leq \left| k^{-\frac{1}{2}} \alpha^{-\frac{1}{2}} \frac{\alpha - k}{k^{\frac{1}{2}} + \alpha^{\frac{1}{2}}} \rho(k) + k^{-\frac{1}{2}} \frac{1}{2} \frac{e^{i(k_0+k)R}}{k+k_0} + k^{-\frac{1}{2}} \hat{g}_R(k) \right| \\
&\leq \frac{K^{-\frac{1}{2}} \alpha^{-\frac{1}{2}}}{K^{\frac{1}{2}} + \alpha^{\frac{1}{2}}} \frac{e^{\beta R}}{2} \frac{|k-\alpha|}{\sqrt{(k-\alpha)^2 + \beta^2}} + \frac{e^{\beta R}}{2\sqrt{K}(K+\alpha)} + \frac{\beta e^{\beta R}}{\sqrt{2K}} E_{\beta, \beta/\sqrt{2}} \\
&\leq \frac{K^{-\frac{1}{2}} \alpha^{-\frac{1}{2}}}{K^{\frac{1}{2}} + \alpha^{\frac{1}{2}}} \frac{e^{\beta R}}{2} + \frac{e^{\beta R}}{2\sqrt{K}(K+\alpha)} + \frac{\beta e^{\beta R}}{\sqrt{2K}} E_{\beta, \beta/\sqrt{2}} \\
&= O(1), \quad \text{as } \beta \to 0.
\end{aligned} \tag{4.267}
$$

Plugging these inequalities into Eq. (4.258) and letting

$$
\begin{aligned}
\delta := \frac{e^{\beta R}}{2\|\psi\|_2^2} &\left(\frac{1}{2} \frac{K^{-\frac{1}{2}} \alpha^{-\frac{1}{2}}}{K^{\frac{1}{2}} + \alpha^{\frac{1}{2}}} + \frac{1}{2\sqrt{K}(K+\alpha)} + \frac{\beta}{\sqrt{2K}} E_{\beta, \beta/\sqrt{2}} \right) \\
&\times \left(\frac{1}{\sqrt{K}} \left[\frac{1}{\beta} + \frac{\beta}{\sqrt{2}} E_{\beta, \beta/\sqrt{2}} \right] + \frac{1}{2\alpha^{\frac{1}{2}} \beta} \right)
\end{aligned} \tag{4.268}
$$

we obtain that

$$
\left| \Pi_E(E) - \frac{1}{2\alpha} \frac{|\rho(E^{1/2})|^2}{\|\psi\|_2^2} \right| \leq \delta. \tag{4.269}
$$

From Eq. (4.123) for $\|\psi\|_2^2$, we see that

$$
\|\psi\|_2^{-2} = 2\beta e^{-2\beta R} \left[1 + \sqrt{\pi} \beta^2 e^{\beta^4} (1 + \mathrm{Erf}(\beta^2)) \right]^{-1} = O(\beta), \quad \text{as } \beta \to 0, \tag{4.270}
$$

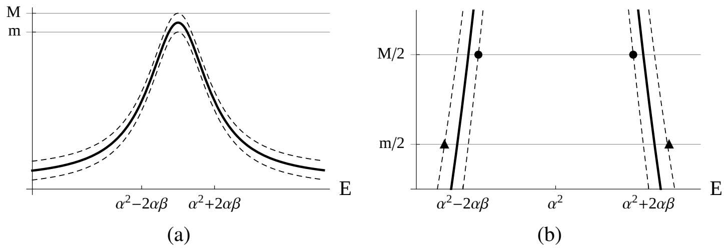


Figure 4.4: (a) The thick line is a plot of $|\rho(E^{1/2})|^2/2\alpha||\psi||_2^2$ and the dashed lines are a plot of $|\rho(E^{1/2})|^2/2\alpha||\psi||_2^2 \pm \delta$. According to Eq. (4.269), the function Π_E lies between the dashed lines. The constant M is therefore the largest possible maximum of Π_E and m is the smallest possible maximum. (b) A closeup of Fig. 4.4a is plotted to show that the distance between the two ● gives a lower bound on the linewidth Γ of ψ and the distance between the two ▲ gives an upper bound.

which together with Eq. (4.267) implies that

$$\delta = O(1), \quad \text{as}\, \beta \to 0. \tag{4.271}$$

Evaluating ρ in α we see that there constants $B, C > 0$ such that

$$\frac{1}{2\alpha}\frac{|\rho(\alpha)|^2}{||\psi||_2^2} = \frac{1}{4\alpha\beta\left[1 + \sqrt{\pi}\beta^2 e^{\beta^4}(1 + \mathrm{Erf}(\beta^2))\right]} \geq \frac{C}{\beta}, \quad \forall \beta < B, \tag{4.272}$$

which together with Eqs. (4.269) and (4.271) shows that

$$\Pi_E(\alpha^2) \geq \frac{C}{\beta}, \quad \forall \beta < B. \tag{4.273}$$

Considering Eq. (4.255) and the fact that $\alpha^2 \in [K^2, \infty)$, we can conclude that the probability density Π_E attains its maximum in $[K^2, \infty)$ for β small enough.

We now determine the linewidth of Π_E. The basic idea is that for small enough β the linewidth of $\Pi_E(E)$ is approximately the linewidth of $|\rho(E^{1/2})|^2/2\alpha\|\psi\|_2^2$, because the difference (4.269) between these two functions is small compared to the maximum of Π_E, which according to Eq. (4.273) approximately β^{-1} for β small enough. According to Eq. (4.269) the function Π_E lies between the two functions

$$\frac{|\rho(E^{1/2})|^2}{2\alpha\|\psi\|_2^2} \pm \delta \tag{4.274}$$

(cf. Fig. 4.4a). These functions attain their maximum for $E^{1/2} = \alpha$. Now let

$$m := \frac{|\rho(\alpha)|^2}{2\alpha\|\psi\|_2^2} - \delta = \frac{e^{2\beta R}}{8\alpha\beta^2\|\psi\|_2^2} - \delta, \tag{4.275}$$

$$M := \frac{|\rho(\alpha)|^2}{2\alpha\|\psi\|_2^2} + \delta = \frac{e^{2\beta R}}{8\alpha\beta^2\|\psi\|_2^2} + \delta. \tag{4.276}$$

The linewidth of Π_E is therefore bounded from above by the distance between the two solutions of (cf. Fig. 4.4b)

$$\frac{|\rho(E^{1/2})|^2}{2\alpha\|\psi\|_2^2} + \delta = \frac{m}{2}, \tag{4.277}$$

and bounded from below by the distance between the two solutions of

$$\frac{|\rho(E^{1/2})|^2}{2\alpha\|\psi\|_2^2} - \delta = \frac{M}{2}. \tag{4.278}$$

First, let us look at Eq. (4.277). Using Eq. (4.256) for ρ it is straightfoward to see that the two solutions of Eq. (4.277) are

$$E_U^{\pm} = \left(\alpha \pm \left[\frac{e^{2\beta R}}{8\alpha\|\psi\|_2^2}\frac{1}{m/2-\delta} - \beta^2\right]^{1/2}\right)^2, \tag{4.279}$$

so that the upper bound on the linewidth reads

$$
\begin{aligned}
E_U^+ - E_U^- &= 4\alpha\beta \left[\frac{e^{2\beta R}}{8\alpha\beta^2 \|\psi\|_2^2} \frac{1}{m/2 - \delta} - 1 \right]^{1/2} \\
&= 4\alpha\beta \left[\frac{e^{2\beta R}}{8\alpha\beta^2 \|\psi\|_2^2} \left(\frac{e^{2\beta R}}{16\alpha\beta^2 \|\psi\|_2^2} - \frac{3}{2}\delta \right)^{-1} - 1 \right]^{1/2} \\
&= 4\alpha\beta \left[\frac{1}{1 - 24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta} + \frac{24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta}{1 - 24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta} \right]^{1/2} .
\end{aligned}
\tag{4.280}
$$

Similarly to Eq. (4.270), we get $\|\psi\|_2^2 = O(\beta^{-1})$ as $\beta \to 0$, that together with Eq. (4.271) for δ gives

$$
24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta = O(\beta), \quad \text{as } \beta \to 0, \tag{4.281}
$$

and hence

$$
\Gamma \leq E_U^+ - E_U^- = 4\alpha\beta(1 + O(\beta)), \quad \text{as } \beta \to 0. \tag{4.282}
$$

Let us now consider Eq. (4.278). In the same way as before we see that its two solutions are

$$
E_L^{\pm} = \left(\alpha \pm \left[\frac{e^{2\beta R}}{8\alpha \|\psi\|_2^2} \frac{1}{M/2 + \delta} - \beta^2 \right]^{1/2} \right)^2 , \tag{4.283}
$$

so that the lower bound on the linewidth satisfies

$$
\begin{aligned}
E_L^+ - E_L^- &= 4\alpha\beta \left[\frac{e^{2\beta R}}{8\alpha\beta^2 \|\psi\|_2^2} \frac{1}{M/2 + \delta} - 1 \right]^{1/2} \\
&= 4\alpha\beta \left[\frac{1}{1 + 24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta} - \frac{24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta}{1 + 24\alpha\beta^2 \|\psi\|_2^2 e^{-2\beta R}\delta} \right]^{1/2} \\
&= 4\alpha\beta(1 - O(\beta)), \qquad \text{as } \beta \to 0.
\end{aligned}
\tag{4.284}
$$

Collecting Eqs. (4.282) and (4.284) we get the assertion of the Lemma.

□

We can finally prove Theorem 4.2.

Proof (of Theorem 4.2). Lemma 4.10 and Lemma 4.11 together give that

$$\Gamma\tau = 1 + O\Big(\beta^{4/17}\,(\log\beta)^{12}\Big) \to 1, \qquad \text{as } \beta \to 0, \tag{4.285}$$

while the fact that

$$\operatorname{Var} E \operatorname{Var} T \geq P_0 - \varepsilon_P, \tag{4.286}$$

together with Statement 2 of Theorem 4.1, gives

$$\lim_{\beta\to 0} \operatorname{Var} E \operatorname{Var} T = \infty. \tag{4.287}$$

□

4.8 Appendix: Proof of Corollary 4.1

By Definition 5.2 we immediately have Eq. (4.76). To prove the estimates on the norms of $\hat{\psi}^{(n)}$ observe that

$$\|\mathbf{1}_K \hat{\psi}^{(n)}\|_\infty \le \|\mathbf{1}_K \hat{f}_R^{(n)}\|_\infty + \|\mathbf{1}_K \hat{g}_R^{(n)}\|_\infty \tag{4.288}$$

Since $\|\mathbf{1}_K \hat{f}_R^{(n)}\|_\infty$ has been determined in Lemma 5.3, we are left with calculating $\|\mathbf{1}_K \hat{g}_R^{(n)}\|_\infty$. We use for $\hat{g}_R$ the bound given in Eq. (4.263); similarly,

$$\begin{aligned}
&|\dot{\hat{g}}_R(k)| \\
&= \left| \int_R^\infty \exp\left(ik_0 r - \frac{(r-R)^2}{2\sigma^2} \right) \frac{1}{2i} \left(ir(e^{ikr} + S(-k)e^{-ikr}) + \dot{S}(-k)e^{-ikr} \right) dr \right| \qquad (4.289) \\
&\le \int_R^\infty \exp\left(\beta r - \frac{(r-R)^2}{2\sigma^2} \right) \left(r + \frac{|\dot{S}(-k)|}{2} \right) dr \qquad (4.290) \\
&\le e^{\beta R} \left[\sigma^2 + \left(R + \beta\sigma^2 + \frac{|\dot{S}(-k)|}{2} \right) \frac{\sigma}{\sqrt{2}} E_{\beta, \sigma/\sqrt{2}} \right] \qquad (4.291)
\end{aligned}$$

and

$$\begin{aligned}
&|\ddot{\hat{g}}_R(k)| \\
&= \bigg| \int_R^\infty \exp\left(ik_0 r - \frac{(r-R)^2}{2\sigma^2} \right) \frac{1}{2i} \Big[-r^2(e^{ikr} - S(-k)e^{-ikr}) \\
&\qquad - 2ir\dot{S}(-k)e^{-ikr} - \ddot{S}(-k)e^{-ikr} \Big] dr \bigg| \qquad (4.292) \\
&\le e^{\beta R} \Big[\sigma^2 \left(2R + |\dot{S}(-k)| + \beta\sigma^2 \right) \\
&\qquad + \left(\frac{|\ddot{S}(-k)|}{2} + |\dot{S}(-k)|(R + \beta\sigma^2) + \sigma^2 + (R + \beta\sigma^2)^2 \right) \frac{\sigma}{\sqrt{2}} E_{\beta, \sigma/\sqrt{2}} \Big]. \qquad (4.293)
\end{aligned}$$

From these inequalities, using the bounds on $\|\mathbf{1}_K S^{(n)}\|_\infty$ from Theorem 5.1, we obtain

$$\|\mathbf{1}_K \hat{g}_R\|_\infty \leq e^{\beta R} \frac{\sigma}{\sqrt{2}} E_{\beta,\sigma/\sqrt{2}}, \tag{4.294}$$

$$\|\mathbf{1}_K \dot{\hat{g}}_R\|_\infty \leq e^{\beta R} \left[\sigma^2 + \left(R + \beta\sigma^2 + \frac{C_{1,K}}{2}\right) \frac{\sigma}{\sqrt{2}} E_{\beta,\sigma/\sqrt{2}}\right], \tag{4.295}$$

$$\begin{aligned}\|\mathbf{1}_K \ddot{\hat{g}}_R\|_\infty \leq e^{\beta R}\Bigg[&\sigma^2 \left(2R + C_{1,K} + \beta\sigma^2\right) + \Bigg(\frac{C_{2,K}}{2} \\ &+ C_{1,K}(R + \beta\sigma^2) + \sigma^2 + (R + \beta\sigma^2)^2\Bigg) \frac{\sigma}{\sqrt{2}} E_{\beta,\sigma/\sqrt{2}}\Bigg].\end{aligned} \tag{4.296}$$

These bounds together with the bounds on $\|\mathbf{1}_K \hat{f}_R^{(n)}\|_\infty$ given in Lemma 5.3 imply Eq. (4.77).

We will now prove Eq. (4.78). Note that

$$\|\hat{\psi}^{(n)} w\|_1 \leq \|\hat{f}_R^{(n)} w\|_1 + \|\hat{g}_R^{(n)}\|_\infty \|w\|_1 \tag{4.297}$$

$$= \|\hat{f}_R^{(n)} w\|_1 + \|\hat{g}_R^{(n)}\|_\infty \int_0^\infty \frac{1}{1 + r^2}\, dr \tag{4.298}$$

$$= \|\hat{f}_R^{(n)} w\|_1 + \frac{\pi}{2} \|\hat{g}_R^{(n)}\|_\infty. \tag{4.299}$$

From the inequalities (4.263)-(4.293), using the bounds on $\|S^{(n)}\|_\infty$ from Theorem 5.2, we obtain

$$\|\hat{g}_R w\|_1 \leq \frac{\pi}{2} \|\hat{g}_R\|_\infty \leq e^{\beta R} \frac{\pi\sigma}{2^{3/2}} E_{\beta,\sigma/\sqrt{2}}, \tag{4.300}$$

$$\|\dot{\hat{g}}_R w\|_1 \leq \frac{\pi}{2} \|\dot{\hat{g}}_R\|_\infty \leq e^{\beta R} \left[\frac{\pi\sigma^2}{2} + \left(R + \beta\sigma^2 + \frac{C_1}{2s}\right) \frac{\pi\sigma}{2^{3/2}} E_{\beta,\sigma/\sqrt{2}}\right], \tag{4.301}$$

$$
\begin{aligned}
\|\ddot{\hat{g}}_R w\|_1 &\le \frac{\pi}{2}\|\ddot{\hat{g}}_R\|_\infty \\
&\le e^{\beta R}\Bigg[\frac{\pi\sigma^2}{2}\left(2R + \frac{C_1}{s} + \beta\sigma^2\right) \\
&\qquad + \left(\frac{C_2}{2s^2} + \frac{C_1}{s}(R+\beta\sigma^2) + \sigma^2 + (R+\beta\sigma^2)^2\right)\frac{\pi\sigma}{2^{3/2}}E_{\beta,\sigma/\sqrt{2}}\Bigg].
\end{aligned}
\tag{4.302}
$$

These bounds together with the bounds on $\|\hat{f}_R^{(n)} w\|_1$ given in Lemma 5.3 imply Eq. (4.78).

Equation (4.79) is then an immediate consequence of Theorem 5.3. □

Chapter 5

On Quantitative Scattering Estimates

5.1 Introduction

A quantum mechanical particle with wave function Ψ scattering off a rotationally symmetric, compactly supported potential V in three dimensions is described by the Schrödinger equation

$$i\partial_t \Psi = H\Psi = (-\Delta + V)\Psi, \tag{5.1}$$

where H is the Hamiltonian, with domain $\mathcal{D}(H)$. A common way to study the scattering behavior of this equation is via dispersive estimates [23, 24, 43, 53]. If P_{ac} denotes the projector on the absolutely continuous spectral subspace of the Hamiltonian H, $R > 0$ and $\mathbf{1}_R := \mathbf{1}_{[0,R]}$, then it is well known that these dispersive estimates can be brought in the form[1]

$$\|\mathbf{1}_R e^{-iHt} P_{ac} \Psi\|_2^2 \le C t^{-3}, \tag{5.2}$$

but little is known quantitatively about the constant C. The main result of this Chapter (Theorems 5.3 and 5.4) are quantitative bounds on the constant C, depending on the initial wave function Ψ, the potential V and spectral properties of H.

To achieve this we use the well known method of stationary phase applied to the expansion of $e^{-iHt} P_{ac} \Psi$ in generalized eigenfunctions, in combination with a detailed analysis of the S-matrix in the complex momentum

Note: The results in this Chapter were developed in collaboration with Nicola Vona. Nicola Vona and I contributed equally to the work that led to the present Chapter.

[1] Note that this holds only if H does not have a zero resonance (see Definition 5.1), while if it has it then t^{-3} must be replaced by t^{-1}.

plane. Such an analysis is of interest in its own right, and our main result in this regard are Theorems 5.1 and 5.2, which provide quantitative bounds on the S-matrix and its derivatives. To obtain the needed detailed knowledge about the analytic properties of the S-matrix, we restrict to rotationally symmetric, compactly supported potentials. This allows us to employ the scattering theory of Res Jost (see [38, Chapter 12] for a textbook exposition), which in particular expresses the S-matrix in terms of one analytic function, the so-called Jost function. Expressing the Jost function in terms of its zeros via the Hadamard factorization, and using the fact that the zeros of the Jost function coincide with bound states, virtual states and resonances of H (see Section 5.8 for a detailed discussion), we are then able to relate our scattering bounds explicitly to the spectral properties of H.

A discussion of analytic properties of the S-matrix and in particular of the Hadamard factorization of the Jost function is also found in [47, 38]. Regge's paper [47] contains most ideas needed for arriving at the Hadamard factorization, but they are not worked out rigorously. Newton, on the other hand, gives more details in [38, Chapter 12] yet he does not provide a full-fledged proof either. His discussion is our starting point. We work out all details needed for proving the Hadamard factorization of the Jost function in full rigor. In particular, we show that although the genus of the zeros of the Jost function is one, it is possible to write its Hadamard factorization as if the genus was zero. The convergence of the genus-zero factorization of the Jost function is not granted by the general theory of entire functions, and the justification for using it is missing in Regge and Newton. This was recognized by Boas [2]. Moreover, we also explicitly show some well known properties of the Jost function of which we have not been able to find proofs, as for instance the fact that it is an analytic function of exponential type.

As a side result to our study of the Jost function, we also obtain an explicit quantitative bound on the number $n(r)$ of zeros of the Jost function within a ball of radius r (Lemma 5.2). Bounds in any dimension have been given by Zworski [63, 64], who proved that $n(r) \leq C_n(r+1)^n$, where n denotes the dimension, but without explicit control over the constant C_n.

Quantitative dispersive estimates are especially relevant for applications in physics, e.g. radioactive decay [13], the study of which motivated this work. The key feature of radioactive elements is their exponential decay (see [56] for a rigorous proof of this phenomenon), but it is well understood that for large times the exponential decay breaks down and polynomial decay takes over [55, 41]. Recently, this has even be verified experimentally [52]. A detailed understanding of this polynomial time regime in radioactive decay is needed for a precise study of the decay process, for example to calculate its variance in time. Even though the exact treatment of time distributions in quantum mechanics is a debated topic [36], it is clear that any possible distribution will depend on $e^{-iHt}\Psi$ and exact knowledge of it is needed for all times $t \in [0, \infty)$.

5.2 Statement of main result

To state our main result (Theorems 5.3 and 5.4) rigorously, we first need to introduce the setting in which we work and the notation that we use.

5.2.1 Assumptions on the potential and Definitions

For two functions $f, g : \mathbb{R} \to \mathbb{C}$ we will use the notation

$$f(x) \sim g(x) \qquad \text{as } x \to x_0 \tag{5.3}$$

to mean that the following limit exists and

$$\lim_{x \to x_0} \frac{f(x)}{g(x)} = 1. \tag{5.4}$$

Throughout this Chapter we consider a non-zero, three-dimensional, rotationally symmetric potential $V = V(r)$, that is real, with support contained in $[0, R_V]$, such that $\sup(\operatorname{supp} V) = R_V$, and $\|V\|_1 < \infty$. We also assume that the potential admits the asymptotic expansion

$$V(r) \sim \sum_{n=0}^{M} d_n (R_V - r)^{\delta_n}, \qquad \text{as } r \to R_V^-, \tag{5.5}$$

with $0 \leq M < \infty$, $-1 < \delta_0 < \cdots < \delta_N$, $d_n \in \mathbb{R}$, and d_n not all zero.

We will only be concerned with the case of zero angular momentum, to avoid the angular momentum barrier potential, which would not have compact support. In this case the three-dimensional Schrödinger Equation (5.1) is equivalent to the one dimensional problem

$$i\partial_t \psi = (-\partial_r^2 + V)\psi \quad \text{with} \quad \Psi(r, \theta, \phi) = \frac{\psi(r)}{r}. \tag{5.6}$$

The self-adjointness of $(-\partial_r^2 + V)$ is ensured by the next

Lemma 5.1. *Let the potential V satisfy $\|V\|_1 < \infty$ and let*

$$H_0 = -\frac{d^2}{dr^2} \tag{5.7}$$

denote the self-adjoint free Schrödinger operator that acts on $\{\phi \in L^2(\mathbb{R}^+) \,|\, \phi(0) = 0\}$. Then, V is infinitesimally form-bounded with respect to H_0, $H = H_0 + V$ can be constructed by the standard quadratic form technique, and its form domain $Q(H)$ is equal to the form domain $Q(H_0)$ of the free operator.

Proof. For ease of notation introduce $\psi'(r) := \frac{d}{dr}\psi(r)$. Then, the form corresponding to H_0 and its form domain read

$$h_0(\phi, \psi) = \langle \phi', \psi' \rangle, \tag{5.8}$$

$$Q(H_0) = \{\psi \in L^2(\mathbb{R}^+) | \psi' \in L^2(\mathbb{R}^+), \psi(0) = 0\}. \tag{5.9}$$

It is well known that h_0 is closed on $Q(H_0)$ under the norm

$$\|\psi\|_{+1} = \sqrt{h_0(\psi, \psi) + \|\psi\|_2^2} = \sqrt{\|\psi'\|_2^2 + \|\psi\|_2^2}. \tag{5.10}$$

So in order to see that V is infinitesimally form-bounded with respect to H_0, we need to show that for all $\varepsilon > 0$ and $\psi \in Q(H_0)$ there is $c_\varepsilon \in \mathbb{R}$ such that

$$|\langle \psi, V\psi \rangle| \leq \varepsilon h_0(\psi, \psi) + c_\varepsilon \|\psi\|_2^2. \tag{5.11}$$

Now, assume that $\|\psi\|_\infty^2 \leq 2\|\psi\|_2\|\psi'\|_2$ for all $\psi \in Q(H_0)$, then using the fact that for arbitrary $a, b > 0$ and all $\varepsilon > 0$ there is a $c_\varepsilon > 0$ such that $ab = a^2\sqrt{b^2/a^2} \leq \varepsilon b^2 + c_\varepsilon a^2$, we get

$$\|\psi\|_\infty^2 \leq \varepsilon \|\psi'\|_2^2 + c_\varepsilon \|\psi\|_2^2. \tag{5.12}$$

This implies for all $\psi \in Q(H_0)$ that

$$|\langle \psi, V\psi \rangle| \leq \|V\|_1 \|\psi\|_\infty^2 \leq \varepsilon \|\psi'\|_2^2 + c_\varepsilon \|\psi\|_2^2 = \varepsilon h_0(\psi, \psi) + c_\varepsilon \|\psi\|_2^2, \tag{5.13}$$

thereby proving the infinitesimally form-boundedness of V with respect to H_0. The rest of the Lemma then follows directly from the KLMN Theorem [44, Theorem X.17].

It remains to prove that $\|\psi\|_\infty^2 \leq 2\|\psi\|_2\|\psi'\|_2$ for all $\psi \in Q(H_0)$, which will follow from a standard argument given in the proof of Theorem 8.5 in [31]. Due to Theorem 7.6 in [31], $C_0^\infty := \{f \in C^\infty(\mathbb{R}^+) | f(0) = 0\}$ is dense in $Q(H_0)$ with respect to the norm $\|\cdot\|_{+1}$. Hence, there exists a sequence $\psi_m \in C_0^\infty \cap Q(H_0)$ that converges to $\psi \in Q(H_0)$. For this sequence we have

$$\psi_m^2(r) = 2\int_0^r \psi_m(r')\psi_m'(r')\, dr'. \tag{5.14}$$

The convergence $\psi_m \to \psi$ in the norm $\|\cdot\|_{+1}$ implies that $\psi_m \to \psi$ and

$\psi'_m \to \psi'$ in the norm $\|\cdot\|_2$, and thereby we have

$$\left|\int_0^r (\psi(r')\psi'(r') - \psi_m(r')\psi'_m(r'))\,dr'\right| \tag{5.15}$$
$$\leq \int_0^r \left|\psi(\psi' - \psi'_m) + \psi'_m(\psi - \psi_m)\right|\,dr' \tag{5.16}$$
$$\leq \langle|\psi|, |\psi' - \psi'_m|\rangle + \langle|\psi'_m|, |\psi - \psi_m|\rangle \tag{5.17}$$
$$\leq \|\psi\|_2\|\psi' - \psi'_m\|_2 + \|\psi'\|_2\|\psi - \psi_m\|_2 \tag{5.18}$$
$$\to 0 \quad \text{as } m \to \infty, \tag{5.19}$$

so that the right hand side of Eq. (5.14) converges pointwise to

$$2\int_0^r \psi(r')\psi'(r')\,dr' \tag{5.20}$$

Moreover, via Theorem 2.7 in [31] we can ensure that the left hand side of Eq. (5.14) converges pointwise almost everywhere to $\psi^2(r)$ by passing to a subsequence. Thus, we have proven that for all $\psi \in Q(H_0)$

$$\psi^2(r) = 2\int_0^r \psi(r')\psi'(r')\,dr' \tag{5.21}$$

and thereby

$$\|\psi\|_\infty^2 = 2\sup_{r\in\mathbb{R}^+}\left|\int_0^r \psi(r')\psi'(r')\,dr'\right| \tag{5.22}$$
$$\leq 2\sup_{r\in\mathbb{R}^+}\int_0^r |\psi(r')|\,|\psi'(r')|\,dr' \tag{5.23}$$
$$\leq 2\langle|\psi|, |\psi'|\rangle \tag{5.24}$$
$$\leq 2\|\psi\|_2\|\psi'\|_2. \tag{5.25}$$

□

To study the scattering behavior induced by the Schrödinger Eq. (5.6), we use generalized eigenfunctions, which solve the time-independent

Schrödinger equation

$$(-\partial_r^2 + V(r))\phi(k,r) = k^2\phi(k,r). \tag{5.26}$$

To keep notation short, we write

$$\phi'(k,r) := \partial_r\phi(k,r) \quad \text{and} \quad \dot{\phi}(k,r) := \partial_k\phi(k,r). \tag{5.27}$$

The following definitions and equations can all be found in Chapter 12 of Newton's book [38]. Following his exposition, we define the regular eigenfunctions $\varphi(k,r)$ as the solutions of Schrödinger's Eq. (5.26) that satisfy the boundary conditions

$$\varphi(k,0) = 0 \quad \text{as well as} \quad \varphi'(k,0) = 1 \tag{5.28}$$

and we define the irregular eigenfunctions $f(k,r)$ as the solutions of Schrödinger's Eq. (5.26) that satisfy the boundary condition

$$f(k,r) = e^{ikr} \quad \text{for} \quad r \geq R_V. \tag{5.29}$$

Note that this boundary condition as it is formulated hinges on the assumption that the potential V has compact support. Later we will use this property of $f(k,r)$ in an essential way. The Jost function F is defined as the Wronskian of f and φ, i.e.

$$F(k) = W(f(k,r),\varphi(k,r)) := f(k,r)\varphi'(k,r) - f'(k,r)\varphi(k,r). \tag{5.30}$$

We define

$$\psi^+(k,r) := \frac{k\varphi(k,r)}{F(k)}, \tag{5.31}$$

and P_{ac} and P_e to be the projections on the subspace of absolute continuity of H and on the span of all eigenvectors of H, respectively. Then the generalized eigenfunction expansion of a function $\psi \in L^2(\mathbb{R}^+)$ reads

$$P_{ac}\psi(r) = \int_0^\infty \hat{\psi}(k)\psi^+(k,r)\,dk \quad \text{with} \tag{5.32}$$

$$\hat{\psi}(k) := \mathcal{F}\psi(k) := \int_0^\infty \psi(r)\bar{\psi}^+(k,r)\,dr. \tag{5.33}$$

We also need the relation

$$\varphi(k,r) = \frac{1}{2ik}(F(-k)f(k,r) - F(k)f(-k,r)), \tag{5.34}$$

which is an immediate consequence of the Jost function's definition in Eq. (5.30) and of the fact that $f(k,r)$ and $f(-k,r)$ span the solution space of Schrödinger's Eq. (5.26). In particular, Eq. (5.34) evaluated for $r \geq R_V$ reads

$$\varphi(k,r) = \frac{1}{2ik}(F(-k)e^{ikr} - F(k)e^{-ikr}), \qquad r \geq R_V. \tag{5.35}$$

The S-matrix element for zero angular momentum can now be expressed (see [38, Chapter 12] for details) as

$$S(k) = \frac{F(-k)}{F(k)}. \tag{5.36}$$

In [38, Chapter 12] it is also shown that the functions $f(k,r), \varphi(k,r)$ and $F(k)$ admit analytic extensions to the whole complex k-plane. Therefore, we can make

Definition 5.1. *A resonance is a zero of the Jost function $F(k)$ in $\{k \in \mathbb{C} | \operatorname{Im} k < 0, \operatorname{Re} k \neq 0\}$. We say that the potential has a zero resonance, if and only if $F(0) = 0$. A virtual state is defined to be a zero of $F(k)$ in $\{k \in \mathbb{C} | \operatorname{Im} k < 0, \operatorname{Re} k = 0\}$.*

Moreover, bound states of the potential correspond to the zeros of $F(k)$ in $\{k \in \mathbb{C} | \operatorname{Im} k > 0, \operatorname{Re} k = 0\}$. The resonances appear in couples symmetric about the imaginary axis and are infinitely many, while there are just finitely many virtual and bound states [38, 47, 51]. For further discussion about the zeros of the Jost function and their physical meaning see Section 5.8.

We will also use the symmetry relations [38, pages 339, 340]

$$F(k) = \bar{F}(-\bar{k}), \tag{5.37}$$

$$f(k, r) = \bar{f}(-\bar{k}, r). \tag{5.38}$$

Finally, we introduce the weight function

$$w(x) := \frac{1}{1 + x^2} \tag{5.39}$$

and say $\psi \in L^1_w$ if and only if $\|\psi w\|_1 < \infty$. Moreover, we call L^∞_{loc} the space of functions ψ such that $\|\mathbf{1}_R \psi\|_\infty$ is finite for every $R > 0$.

5.2.2 Main result

The main result (Theorems 5.3 and 5.4) rests upon bounds on the derivatives of the S-matrix given in Theorems 5.1 and 5.2. To state these bounds, we need

Definition 5.2. *Let α_n, β_n, η_m, $\kappa_l > 0$. We number the zeros of the Jost function other than $k = 0$ with increasing modulus; among them, we denote the bound states by $i\eta_m$, the virtual states by $-i\kappa_l$, and the resonances by $k_n = \alpha_n - i\beta_n$ and $-\bar{k}_n$. Let $N < \infty$ be the number of the bound states and $N' < \infty$ that of the virtual states, then we define*

$$\frac{1}{\eta} := \sum_{m=0}^{N-1} \frac{1}{\eta_m}, \qquad \frac{1}{\kappa} := \sum_{l=0}^{N'-1} \frac{1}{\kappa_l} \tag{5.40}$$

and for given $K > 0$, let ν_K be the smallest non-negative integer such that

$\alpha_n \geq 2K$ for all $n \geq \nu_K$. Then

$$\frac{1}{s_K} := \frac{1}{\eta} + \frac{1}{\kappa} + \sum_{n=0}^{\nu_K - 1} \frac{1}{\beta_n} \tag{5.41}$$

in case the right hand side is not zero, and $s_K := 1$ otherwise. Let $\tilde{K} := 6\|V\|_1$ and

$$\frac{1}{s} := \frac{1}{s_{\tilde{K}}}. \tag{5.42}$$

Theorem 5.1. *Let $\alpha := \min_{n\in\mathbb{N}^0} \alpha_n$, $K > 0$ and*

$$r_0 := \sum_{n=0}^{\infty} \frac{5\beta_n}{\alpha_n^2 + \beta_n^2}. \tag{5.43}$$

Then

$$\|\mathbf{1}_K \dot{S}\|_\infty \leq \frac{2}{s_K}\left[1 + s_K(R_V + r_0)\right] =: \frac{C_{1,K}}{s_K}, \tag{5.44}$$

$$\|\mathbf{1}_K \ddot{S}\|_\infty \leq \frac{4}{s_K^2}\left\{3 + 2s_K^2\left[\frac{r_0}{\alpha} + (R_V + r_0)^2\right]\right\} =: \frac{C_{2,K}}{s_K^2}, \tag{5.45}$$

$$\begin{aligned}\|\mathbf{1}_K \dddot{S}\|_\infty \leq \frac{4}{s_K^3}\Bigg\{&15 + 6s_K(R_V + r_0) + 12s_K^2\frac{r_0}{\alpha} \\ &+ s_K^3\left[\frac{7r_0}{\alpha} + \frac{12r_0}{\alpha}(R_V + r_0) + 8(R_V + r_0)^3\right]\Bigg\} =: \frac{C_{3,K}}{s_K^3}.\end{aligned} \tag{5.46}$$

Note that $r_0 < \infty$ as shown in Lemma 5.10. The bounds in Theorem 5.1 are valid for any K, but for big values of K, the bounds given in Theorem 5.2 are more convenient.

Theorem 5.2. *Let*

$$q := \frac{1}{2\|V\|_1} + 6R_V, \quad r_0 := \sum_{n=0}^{\infty} \frac{5\beta_n}{\alpha_n^2 + \beta_n^2} \quad \text{and} \quad \alpha := \min_{n\in\mathbb{N}^0} \alpha_n. \tag{5.47}$$

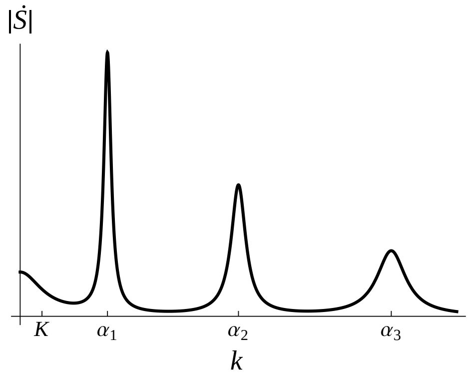


Figure 5.1: Schematic plot of $|\dot{S}(k)|$, where resonances are dominant.

Then

$$\|\dot{S}\|_\infty \le \frac{2}{s}\left[1 + s(3R_V + r_0)\right] =: \frac{C_1}{s}, \tag{5.48}$$

$$\|\ddot{S}\|_\infty \le \frac{4}{s^2}\left\{3 + 2s^2\left[\frac{r_0}{\alpha} + (3R_V + r_0)^2 + R_V q\right]\right\} =: \frac{C_2}{s^2}, \tag{5.49}$$

$$\begin{aligned}\|\dddot{S}\|_\infty \le \frac{4}{s^3}\bigg\{15 + 6s(R_V + r_0) + 12s^2\frac{r_0}{\alpha} + s^3\bigg[\frac{7r_0}{\alpha} + \frac{12r_0}{\alpha}(R_V + r_0)\\ + 8(3R_V + r_0)^3 + 18R_V q^2\bigg]\bigg\} =: \frac{C_3}{s^3}.\end{aligned} \tag{5.50}$$

Remark 5.1. Let us explain, why we look at bounds for $k \in [0, K)$ and $k \in [0, \infty)$ rather than only for $k \in [0, \infty)$ or for $k \in [0, K)$ and $k \in [K, \infty)$. In the proof of Theorem 5.3 we will find that one gets much tighter bounds treating the region around $k = 0$ more carefully. For this reason, bounds for $k \in [0, K)$ and $k \in [K, \infty)$ would be most useful. However, physically interesting situations are mainly those in which resonances dominate the scattering behavior and in such a situation the bounds for $k \in [0, \infty)$ are as good as bounds for $k \in [K, \infty)$, just easier to prove. Let us briefly explain why they are equally good in case resonances are dominant. The absolute value of the derivatives of the S-matrix have peaks centered around the real part of every resonance and around $k = 0$ due to the bound and virtual states (see Lemma 5.13 and Fig. 5.1). If the resonances are dominant, then the peak at $k = 0$ is smaller than some of the resonance peaks. This circumstance is discussed in Section 5.3, where we also explain that in this case a good choice for K is $\alpha_0/4$, hence $\|\mathbf{1}_{[K,\infty)}S^{(n)}\|_\infty = \|S^{(n)}\|_\infty$. In contrast, if bound and virtual states are dominant, then bounds for $k \in [K, \infty)$ rather than for $k \in [0, \infty)$ may be advantageous.

To keep the statement of our main result as concise as possible we define auxiliary constants. These constants contain the radius R that appear in our estimate 5.2. The first number in their argument is the order of the derivative of the S-matrix in which they are used, the second one being just an index.

Definition 5.3. *Let $R > 0$. Using the constants introduced in Theorems 5.1 and 5.2, define*

$$z_{ac,K}(0,0) := \frac{1}{2}\left(2Rs_K + C_{1,K}\right), \tag{5.51}$$

$$z_{ac,K}(0,1) := 1, \tag{5.52}$$

$$z_{ac,K}(1,0) := \frac{1}{4}\left(2R^2 s_K^2 + 2RC_{1,K}s_K + C_{2,K}\right), \tag{5.53}$$

$$z_{ac,K}(1,1) := \frac{1}{2}\left(2Rs_K + C_{1,K}\right), \tag{5.54}$$

$$z_{ac,K}(1,2) := 1, \tag{5.55}$$

$$z_{ac,K}(2,0) := \frac{1}{6}(2R^3 s_K^3 + 3R^2 s_K^2 C_{1,K} + 3Rs_K C_{2,K} + C_{3,K}), \tag{5.56}$$

$$z_{ac,K}(2,1) := \frac{1}{2}(2R^2 s_K^2 + 2Rs_K C_{1,K} + C_{2,K}), \tag{5.57}$$

$$z_{ac,K}(2,2) := 2Rs_K + C_{1,K}, \tag{5.58}$$

$$z_{ac,K}(2,3) := 2, \tag{5.59}$$

$$z_{ac,K}(n) := \sum_{m=0}^{n+1} z_{ac,K}(n,m), \tag{5.60}$$

and

$$z_{e,K}(0) := \sqrt{2}, \tag{5.61}$$

$$z_{e,K}(1) := \frac{1}{\sqrt{2}}\Big[2s_K + (2Rs_K + C_{1,K})\eta_0\Big], \tag{5.62}$$

$$z_{e,K}(2) := \frac{1}{\sqrt{2}}\left(C_{2,K}\eta_0^2 + 2\eta_0 s_K\,(C_{1,K} + Rs_K)\,(R\eta_0 + 1) + 4s_K^2\right). \tag{5.63}$$

Define $z_{ac}(n,m)$, $z_{ac}(n)$, and $z_e(n)$ in exactly the same way, but with index K omitted everywhere.

Recalling Definition 5.2, we now state the main result in Theorems 5.3 and 5.4.

Theorem 5.3. *Let $t > 0$, $R \geq R_V$, $K > s$, and*

$$\lambda := \begin{cases} 0, & \text{if } F(0) \neq 0 \\ 1, & \text{if } F(0) = 0. \end{cases} \tag{5.64}$$

Then there are constants c_n, such that

$$\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \leq \lambda(c_1 t^{-1} + c_2 t^{-2}) + c_3 t^{-3} + c_4 t^{-4} \tag{5.65}$$

for all ψ with $\hat{\psi}^{(m)} \in L^\infty_{loc} \cap L^1_w$ where $m = 0, 1, 2$. If $s, s_K, K \leq 1$, the constants satisfy

$$c_1 \leq \frac{81\pi^2}{K}\frac{|\hat{\psi}(0)|^2}{s_K^2} z_{ac,K}^2(0), \tag{5.66}$$

$$c_2 \leq \frac{53\pi^2}{K^3}\frac{|\hat{\psi}(0)|^2}{s_K^4} z_{ac,K}^2(1) + \frac{53\pi^2}{K}\frac{\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2}{s_K^2} z_{ac,K}^2(0), \tag{5.67}$$

$$c_3 \leq \frac{27}{K^5}\frac{\|\mathbf{1}_K\hat{\psi}\|_\infty^2}{s_K^6} z_{ac,K}^2(2) + \frac{23\pi^2}{K^3}\frac{\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2}{s_K^4} z_{ac,K}^2(1) + \frac{27}{K}\frac{\|\mathbf{1}_K\ddot{\hat{\psi}}\|_\infty^2}{s_K^2} z_{ac,K}^2(0), \tag{5.68}$$

$$\begin{aligned} c_4 \leq{}& 276\frac{\|\hat{\psi}w\|_1^2}{s^5}\left(1+\frac{1}{K^2}\right)^4\left(z_{ac}^2(2)+s^2z_{ac}^2(1)+s^4z_{ac}^2(0)\right) \\ &+304\frac{\|\dot{\hat{\psi}}w\|_1^2}{s^3}\left(1+\frac{1}{K^2}\right)^3\left(z_{ac}^2(1)+s^2z_{ac}^2(0)\right) \\ &+14\frac{\|\ddot{\hat{\psi}}w\|_1^2}{s}\left(1+\frac{1}{K^2}\right)^2 z_{ac}^2(0). \end{aligned} \tag{5.69}$$

Bounds on the constants c_n without the assumption $s, s_K, K \leq 1$ are given in Eqs. (5.438)-(5.441).

Remark 5.2. For $t > T$, Eq. (5.65) implies

$$\|P_{ac}\mathbf{1}_R e^{-iHt}P_{ac}\psi\|_2^2 \leq \lambda\left(c_1+\frac{c_2}{T}\right)t^{-1}+(1-\lambda)\left(c_3+\frac{c_4}{T}\right)t^{-3}, \tag{5.70}$$

which is of the form of Eq. (5.2). However, the bound (5.65) is preferable because it allows a higher degree of accuracy on intermediate time scales, for example if $c_3 \ll c_4$.

Remark 5.3. The restriction $K > s$ in Theorem 5.3 is set to avoid unessential complications in the proof, where we divide the integration region of several integrals according to Fig. 5.7. This division is easier if $K > \delta$ and since we fix $\delta = s$ in the course of the proof, we end up with the condition $K > s$. Besides this restriction the value of K can be chosen freely, and it influences the size of the constants in Theorem 5.3. A choice for K meaningful for many potentials that respects the condition $K > s$ is presented in Section 5.3, however for some potentials a value of $K < s$ might lead to better results. In this case, the restriction $K > s$ can be removed with slight but cumbersome changes in the proof.

Remark 5.4. It is worth observing that $\hat{\psi}$ depends not only on the initial state, but also on the potential through the generalized eigenfunctions. So in general $\|\mathbf{1}_K\hat{\psi}^{(n)}\|_\infty$ and $\|\hat{\psi}^{(n)}w\|_1$ will depend on s_K and s, too (see Lemma 5.3 for an example).

Theorem 5.4. *Let $t, K > 0$, $R \geq R_V$, and*

$$\lambda := \begin{cases} 0, & \text{if } F(0) \neq 0 \\ 1, & \text{if } F(0) = 0. \end{cases} \tag{5.71}$$

Then there are constants $c_n > 0$, such that

$$\|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \leq \lambda(c_1 t^{-1} + c_2 t^{-2}) + c_3 t^{-3} + c_4 t^{-4} \tag{5.72}$$

for all ψ with $\hat{\psi}^{(m)} \in L^\infty_{loc} \cap L^1_w$ and $m = 0, 1, 2$. The constants satisfy

$$c_1 \leq \frac{81\pi^2}{2} \frac{|\hat{\psi}(0)|^2}{\eta_0} z_{e,K}^2(0) N, \tag{5.73}$$

$$c_2 \leq \frac{105\pi^2}{4} \left[\frac{|\hat{\psi}(0)|^2}{\eta_0^3 s_K^2} z_{e,K}^2(1) + \frac{\|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2}{\eta_0} z_{e,K}^2(0) \right] N, \tag{5.74}$$

$$c_3 \leq \left[9 \frac{\|\mathbf{1}_K \hat{\psi}\|_\infty^2}{\eta_0^5 s_K^4} z_{e,K}^2(2) + 166 \frac{\|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2}{\eta_0^3 s_K^2} z_{e,K}^2(1) + 9 \|\mathbf{1}_K \ddot{\hat{\psi}}\|_\infty^2 \frac{z_{e,K}^2(0)}{\eta_0} \right] N, \tag{5.75}$$

$$\begin{aligned} c_4 \leq \Bigg[& \frac{27}{2} \frac{\|\hat{\psi} w\|_1^2}{\eta_0^5 s^4} \left(1 + \frac{1}{K^2}\right)^4 \left(z_e^2(2) + \eta_0^2 s^2 z_e^2(1) + \eta_0^4 s^4 z_e^2(0) \right) \\ & + 12 \frac{\|\dot{\hat{\psi}} w\|_1^2}{\eta_0^3 s^2} \left(1 + \frac{1}{K^2}\right)^3 \left(z_e^2(1) + \eta_0^2 s^2 z_e^2(0) \right) \\ & + \frac{9}{8} \frac{\|\ddot{\hat{\psi}} w\|_1^2}{\eta_0} \left(1 + \frac{1}{K^2}\right)^2 z_e^2(0) \Bigg] N. \end{aligned} \tag{5.76}$$

Together, Theorems 5.3 and 5.4 yield the desired bound on the probability $\|\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2$ to find the particle inside a ball of radius R, because

$$\|\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 = \|P_{ac} \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 + \|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2. \tag{5.77}$$

Remark 5.5. Note that the bounds in our Theorems depend on r_0 that contains the location of all resonances, and seems therefore difficult to access. Nevertheless, we will now see that is connected to the scattering length (see [45, page 136])

$$a = \frac{\dot{S}(0)}{2iS(0)}, \tag{5.78}$$

that is experimentally measurable. From Eq. (5.215) of Lemma 5.13, choosing $k = 0$, one immediately gets (see also [27])

$$a = -R_V - \sum_{m=0}^{N-1} \frac{1}{\eta_m} + \sum_{l=0}^{N'-1} \frac{1}{\kappa_l} + \sum_{n=0}^{\infty} \frac{2\beta_n}{\alpha_n^2 + \beta_n^2}, \tag{5.79}$$

which implies

$$r_0 \leq \frac{5}{2}|a| + \frac{5}{2}\left|R_V + \sum_{m=0}^{N-1} \frac{1}{\eta_m} - \sum_{l=0}^{N'-1} \frac{1}{\kappa_l}\right|. \tag{5.80}$$

Note also that, although the scattering length is physically measured from the scattering cross section at zero energy, it actually depends on all resonances, not only on the first few.

As mentioned in the introduction, we also give a quantitative bound on the number of zeros of the Jost function inside a ball of radius $|k|$. It is a direct consequence of Lemma 5.4. A related result can be found in [63, 64] where the inequality $n(r) \leq C_n(r+1)^n$ was proven, with n denoting the dimension, but without explicit control over the constant C_n.

Lemma 5.2. *Let $n(|k|)$ be the number of zeros of the Jost function with modulus not greater than $|k|$. Then,*

$$n(|k|) \leq \frac{1}{\log 2}\left[4R_V|k| + \log\left(4\|rV(r)\|_1 e^{4\|rV(r)\|_1} + 1\right)\right]. \tag{5.81}$$

5.3 Application of the main result to meta-stable states

We consider as example the alpha-decay of long-lived elements treated by Skibsted in [56]. There the meta-stable state is modeled via the truncated Gamow function $f_R := \mathbf{1}_R f(k_0, \cdot)$ associated to the first resonance $k_0 = \alpha_0 - i\beta_0$, with $\alpha_0, \beta_0 > 0$ and f defined by Eq. (5.29). Skibsted showed in [56] that the velocity with which the alpha-particle escapes the nucleus is $2\alpha_0$, while the lifetime of the meta-stable state is $(4\alpha_0\beta_0)^{-1}$. Comparison with empirical data shows that $\alpha_0 \approx 1$, while the lifetime is very large and therefore $\beta_0 \ll 1$.

Let us determine the norms $\|\hat{f}_R^{(n)} w\|_1$ and $\|\mathbf{1}_K \hat{f}_R^{(n)}\|_\infty$ that appear in Theorems 5.3 and 5.4.

Lemma 5.3. *Let $R \geq R_V$, $K \in [0, \frac{\alpha_0}{2})$, then the truncated Gamow function $f_R := \mathbf{1}_R f(k_0, \cdot)$ satisfies*

$$\|\mathbf{1}_K \hat{f}_R\|_\infty \leq e^{\beta_0 R} \frac{2}{\alpha_0}, \tag{5.82}$$

$$\|\mathbf{1}_K \dot{\hat{f}}_R\|_\infty \leq e^{\beta_0 R} \left[\frac{2^2}{\alpha_0^2} + \frac{1}{\alpha_0} \left(2R + \frac{C_{1,K}}{s_K} \right) \right], \tag{5.83}$$

$$\|\mathbf{1}_K \ddot{\hat{f}}_R\|_\infty \leq e^{\beta_0 R} \left[\frac{2^4}{\alpha_0^3} + \left(2R + \frac{C_{1,K}}{s_K} \right) \frac{2^2}{\alpha_0^2} + \left(R^2 + R\frac{C_{1,K}}{s_K} + \frac{C_{2,K}}{2s_K^2} \right) \frac{2}{\alpha_0} \right], \tag{5.84}$$

and

$$\|\hat{f}_R w\|_1 \leq e^{\beta_0 R} \left[2 \log\left(\frac{2}{\beta_0} \right) + \frac{\pi}{2} \right], \tag{5.85}$$

$$\|\dot{\hat{f}}_R w\|_1 \leq e^{\beta_0 R} \left[\left(2 \log\left(\frac{2}{\beta_0} \right) + \frac{\pi}{2} \right) \left(R + \frac{C_1}{2s} \right) + \frac{\pi}{\beta_0} \right], \tag{5.86}$$

$$\|\ddot{\hat{f}}_R w\|_1 \leq e^{\beta_0 R}\Bigg[\left(2\log\left(\frac{2}{\beta_0}\right)+\frac{\pi}{2}\right)\left(R^2+\frac{C_1}{s}R+\frac{C_2}{2s^2}\right) + \frac{\pi}{\beta_0}\left(2R+\frac{C_1}{s}\right)+\frac{4}{\beta_0^2}\Bigg]. \tag{5.87}$$

Moreover, if there is a zero resonance, we have

$$|\hat{f}_R(0)| = \frac{e^{\beta_0 R}}{\sqrt{\alpha_0^2+\beta_0^2}}. \tag{5.88}$$

Proof. Lemma 3.2 in [56] shows that

$$\hat{f}_R(k) = -\frac{1}{2}\left[\frac{e^{i(k_0-k)R}}{k-k_0}\bar{S}(k)+\frac{e^{i(k_0+k)R}}{k+k_0}\right] \tag{5.89}$$

with $k_0 = \alpha_0 - i\beta_0$. From this we can already conclude that for $k \in [0, K]$

$$|\hat{f}_R| \leq \frac{e^{\beta_0 R}}{2}\left[\frac{1}{|k-k_0|}+\frac{1}{|k+k_0|}\right] \leq e^{\beta_0 R}\frac{1}{|k-k_0|} \leq e^{\beta_0 R}\frac{2}{\alpha_0}, \tag{5.90}$$

which proves Eq. (5.82). Moreover, we immediately obtain

$$\dot{\hat{f}}_R(k) = \frac{1}{2}\frac{e^{i(k_0-k)R}}{(k-k_0)^2}\left[(1+iR(k-k_0))\bar{S}(k)-(k-k_0)\dot{\bar{S}}(k)\right] + \frac{1}{2}\frac{e^{i(k_0+k)R}}{(k+k_0)^2}(1-iR(k+k_0)), \tag{5.91}$$

$$\begin{aligned}\ddot{\hat{f}}_R(k) = &-\frac{1}{2}\frac{e^{i(k_0-k)R}}{(k-k_0)^3}\Bigg[\left(1+iR(k-k_0)-\frac{R^2}{2}(k-k_0)^2\right)\bar{S}(k)\\ &-(1+iR(k-k_0))\dot{\bar{S}}(k)(k-k_0)+\frac{1}{2}\ddot{\bar{S}}(k)(k-k_0)^2\Bigg]\\ &-\frac{1}{2}\frac{e^{i(k_0+k)R}}{(k+k_0)^3}\left(1-iR(k+k_0)-\frac{R^2}{2}(k+k_0)^2\right),\end{aligned} \tag{5.92}$$

and this implies, along the same lines as before, Eqs. (5.83) and (5.84).

Now, let us consider

$$\|\hat{f}_R w\|_1 \leq e^{\beta_0 R} \int_0^\infty \frac{1}{|k-k_0|} w(k)\, dk. \tag{5.93}$$

The weight function w is needed for the integral to converge, while it is unessential in the region around $k = \alpha_0$, where $|k-k_0|^{-1}$ is biggest. Hence, we split the integral in a region where $|k-k_0|^{-1} \geq 1$, i.e. the interval $[\alpha_0 - (1-\beta_0^2)^{1/2}, \alpha_0 + (1-\beta_0^2)^{1/2}]$, and the rest. If we call the rest B, we have

$$\|\hat{f}_R w\|_1 \leq e^{\beta_0 R} \int_{\alpha_0 - \sqrt{1-\beta_0^2}}^{\alpha_0 + \sqrt{1-\beta_0^2}} \frac{1}{|k-k_0|} w(k)\, dk + e^{\beta_0 R} \int_B \frac{1}{|k-k_0|} w(k)\, dk \tag{5.94}$$

$$\leq e^{\beta_0 R} \int_{\alpha_0 - \sqrt{1-\beta_0^2}}^{\alpha_0 + \sqrt{1-\beta_0^2}} \frac{1}{|k-k_0|}\, dk + e^{\beta_0 R} \int_0^\infty w(k)\, dk \tag{5.95}$$

$$= e^{\beta_0 R} \left[2 \log\left(\frac{1}{\beta_0} + \frac{1}{\beta_0} \sqrt{1-\beta_0^2} \right) + \frac{\pi}{2} \right] \tag{5.96}$$

$$\leq e^{\beta_0 R} \left[2 \log\left(\frac{2}{\beta_0} \right) + \frac{\pi}{2} \right] \tag{5.97}$$

confirming Eq. (5.85). Similarly, we get

$$\|\dot{\hat{f}}_R w\|_1 \leq \frac{e^{\beta_0 R}}{2} \left[\int_0^\infty \frac{2}{|k-k_0|^2} w(k)\, dk + \int_0^\infty \frac{2R + |\dot{S}(k)|}{|k-k_0|} w(k)\, dk \right]. \tag{5.98}$$

The second integral can be estimated in the same way as $\|\hat{f}_R w\|_1$ by using Theorem 5.2 on the S-Matrix. The first integral satisfies

$$\int_0^\infty \frac{2}{|k-k_0|^2} w(k)\, dk \leq \int_{-\infty}^\infty \frac{2}{|k-k_0|^2}\, dk = \frac{2\pi}{\beta_0}. \tag{5.99}$$

Hence, Eq. (5.86) and analogously Eq. (5.87).

To derive Eq. (5.88), we only need to evaluate Eq. (5.89) at $k = 0$ and use the fact that $S(0) = -1$ in the presence of a zero resonance, which has been shown in [38, page 356]. □

5.3.1 Uranium 238

For concreteness we consider now the alpha decay of Uranium 238, which we model using simple barrier potential shown in Fig. 3.1. As parameter values we choose $r_1 = 1$, $r_2 = R_V = 3$ and $V_0 = 480$, because in natural units they correspond to the nuclear radius of Uranium, three times the nuclear radius and approximately the strength of the Coulomb repulsion $V_{\text{Coulomb}} = 36\,\text{MeV}$ experienced by an alpha particle sitting at $r = r_1$ (in SI-units we have $V_0 = 48\,\text{MeV}$, $r_1 = 7.2\,\text{fm}$, and $r_2 = 21.6\,\text{fm}$). The parameter V_0 was chosen, so that the decay rate $4\alpha_0\beta_0$ of the first resonance is in good agreement with the empirically measured decay rate, as is discussed later.

It is clear that the potential does not have any bound states, therefore we have to consider only Theorem 5.3, with $P_{ac} = \mathbf{1}$. This Theorem provides an estimate on the survival probability once the radius R is understood as the radius of a detector waiting for the alpha particle to hit it. Therefore, we use the value $R = 1.4 \times 10^{14}$, that corresponds to 1 m. It should be noted that to have a probability it is necessary to divide both sides of Eq. (5.65) by the L^2-norm of the initial wave function.

Due to the simplicity of the potential that we consider, we can determine the Jost function explicitly; it reads

$$\begin{aligned} F(k) =& e^{ikr_2}\Big[e^{-ikr_1}\cos((r_2-r_1)\sqrt{k^2-V_0}) \\ & - i\frac{k}{\sqrt{k^2-V_0}}\cos(kr_1)\sin((r_2-r_1)\sqrt{k^2-V_0}) \\ & - \frac{\sqrt{k^2-V_0}}{k}\sin(kr_1)\sin((r_2-r_1)\sqrt{k^2-V_0})\Big], \end{aligned} \tag{5.100}$$

and from this all parameters that appear in the bounds of Theorem 5.3 can be determined.

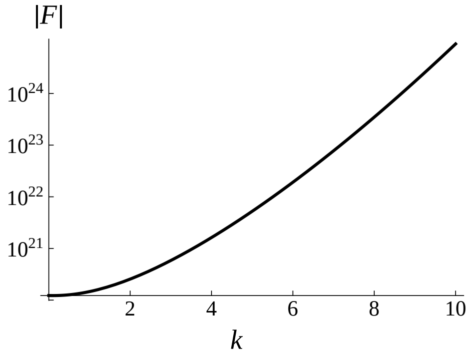


Figure 5.2: Plot of $|F(-ik)|$ for $k \geq 0$, showing that the model potential for Uranium 238 does neither have virtual states nor a zero resonance.

The first resonance numerically calculates to

$$k_0 = 3.0040 - i\,1.4068 \times 10^{-39}. \tag{5.101}$$

The decay rate $4\alpha_0\beta_0$ in SI-units is then $2.5682 \times 10^{-18}\,\mathrm{s}^{-1}$, which is in good agreement with the experimental value $4.9160 \times 10^{-18}\,\mathrm{s}^{-1}$ and thereby justifies our choice of parameters.

We need to know whether the potential has any virtual states or a zero resonance. For this purpose we plot $|F(-ik)|$ for $k \geq 0$. From Fig. 5.2 it can be seen that the Jost function $F(k)$ does not have zeros on the negative imaginary axis, so that the potential has neither virtual states nor a zero resonance.

Letting ν_K be the smallest integer such that $\alpha_n \geq 2K$ for all $n \geq \nu_K$, the parameter s_K that appears in Theorem 5.3 is in our case

$$\frac{1}{s_K} = \begin{cases} 1, & \text{if } \nu_K = 0, \\ \displaystyle\sum_{n=0}^{\nu_K - 1} \frac{1}{\beta_n}, & \text{otherwise.} \end{cases} \tag{5.102}$$

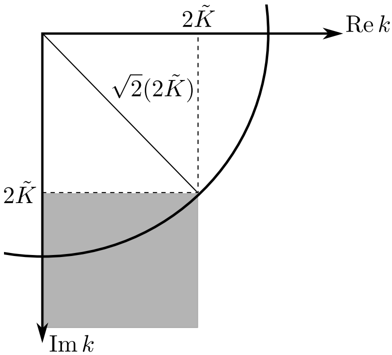


Figure 5.3: Plot of the complex k-plane, to illustrate how the number of zeros $n(\sqrt{2}(2\tilde{K}))$ in the ball of radius $\sqrt{2}(2\tilde{K})$ can be used to estimate $\nu_{\tilde{K}}$.

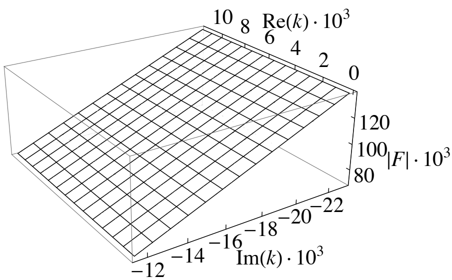


Figure 5.4: Plot of $|F(k)|$ in the shaded region shown in Fig. 5.3.

To minimize $1/s_K$ we therefore choose $K = \alpha_0/4$, so $\nu_K = 0$ and $1/s_K = 1$. Similarly, with $\nu_{\tilde{K}}$ being the smallest integer such that $\alpha_n \geq 2\tilde{K} = 12\|V\|_1$ for all $n \geq \nu_{\tilde{K}}$, we have

$$\frac{1}{s} = \sum_{n=0}^{\nu_{\tilde{K}}-1} \frac{1}{\beta_n} \leq \frac{\nu_{\tilde{K}}}{\beta_0}, \tag{5.103}$$

under the assumption that $\beta_0 \leq \beta_n$ for all $0 < n < \nu_{\tilde{K}}$. Therefore, we need a handle on $\nu_{\tilde{K}}$. Lemma 5.2 is of help here because it gives a bound on the number of zeros $n(r)$ in the ball of radius r. Since $\nu_{\tilde{K}}$ is the number of zeros in $\{z | \operatorname{Re} z \leq 2\tilde{K}, \operatorname{Im} z \leq 0\}$, we need to ensure that there are no zeros in the shaded region shown in Fig. 5.3 below the ball of the radius $\sqrt{2}(2\tilde{K})$. As can be seen from Fig. 5.4, $|F(k)| > 0$ in this region, so that

$$\begin{aligned} \nu_{\tilde{K}} \leq n(2^{\frac{3}{2}}\tilde{K}) &\leq \frac{1}{\log 2}\left[4R_V 2^{\frac{3}{2}}\tilde{K} + \log\left(4\|rV(r)\|_1 e^{4\|rV(r)\|_1} + 1\right)\right] \\ &= 2.9314 \times 10^5, \end{aligned} \tag{5.104}$$

and

$$\frac{1}{s} \leq 2.0837 \times 10^{44}. \tag{5.105}$$

To calculate r_0, consider Eqs. (5.215) and (5.178), from which we get

$$r_0 = \frac{5}{2}\left(R_V - \operatorname{Im}\frac{\dot{F}(0)}{F(0)}\right) = 0.1141. \tag{5.106}$$

Together with $\|V\|_1 = V_0(r_2 - r_1) = 960$ we now have everything that is needed to calculate the constants appearing in Theorems 5.1 and 5.2. They are given by

$$C_{1,K} = 8.2282 \qquad C_{2,K} = 89.8853 \qquad C_{3,K} = 1109.6900 \tag{5.107}$$

$$C_1 = 2.0000 \qquad C_2 = 12.0000 \qquad C_3 = 60.0000, \tag{5.108}$$

where we have assumed that $\alpha_0 = \min_{n>0}\{\alpha_n\}_n$. Using these values,

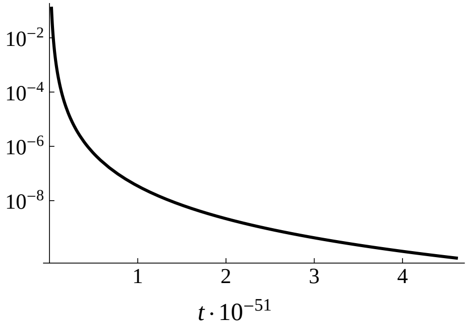


Figure 5.5: Plot of $\frac{1}{\|f_R\|_2^2}(c_3 t^{-3} + c_4 t^{-4})$ for $\frac{1}{10}(4\alpha_0\beta_0)^{-4/3} < t < 20(4\alpha_0\beta_0)^{-4/3}$.

Definition 5.3, and Lemma 5.3 we can finally calculate

$$c_3 = 3.3519 \times 10^{89}, \tag{5.109}$$

$$c_4 = 1.2293 \times 10^{235}. \tag{5.110}$$

From Theorem 5.3 we then have the bound on the survival probability

$$\frac{\|\mathbf{1}_R e^{-iHt} f_R\|_2^2}{\|f_R\|_2^2} \leq \frac{c_3}{\|f_R\|_2^2} t^{-3} + \frac{c_4}{\|f_R\|_2^2} t^{-4}, \tag{5.111}$$

with [56, Lemma 3.1]

$$\|f_R\|_2^2 = \frac{e^{2\beta_0 R}}{2\beta_0} = 3.5541 \times 10^{38}. \tag{5.112}$$

Figure 5.5 shows that the bound (5.111) becomes useful for $t > (4\alpha_0\beta_0)^{-4/3}$ with $(4\alpha_0\beta_0)^{-1}$ being one lifetime.

Note that, in contrast to the fact that $1/s \gg 1$, we find that

$$z_{ac}(0) = 1 + \frac{1}{2}(2Rs + 2(1 + 2sR_V + sr_0)) = 5.1141, \tag{5.113}$$

and similarly all other parameters $z_{ac,K}(m)$, $z_{ac}(m)$ and $z_e(m)$ are much smaller than $1/s$. Therefore, the bounds on the constants c_3 and c_4 are dominated by $1/s$, while the parameters $z_{ac,K}(m)$, $z_{ac}(m)$ and $z_e(m)$ play a minor role.

5.4 Proof of Theorem 5.1

For $K > 0$, s_K defined in Eq. (5.41), and $n \in \{1, 2, 3\}$, we want to establish the bounds

$$\|\mathbf{1}_K S^{(n)}\|_\infty \leq C_{n,K} s_K^{-n}. \tag{5.114}$$

Our starting point is the expression of the S-matrix in terms of the Jost function F

$$S(k) = \frac{F(-k)}{F(k)}. \tag{5.115}$$

We will exploit the fact that F is an entire function, which implies that it is possible to write it as a product of factors that depend only on the location of the zeros. Such a representation is called Hadamard factorization, and it is the main tool we will use to prove Theorem 5.1.

In order to write the Hadamard factorization of the Jost function, we need to determine some important parameters: the *order*, the *type* [3, page 8], the *convergence exponent of its zeros*, and the *genus of its zeros* [3, page 14]. We recall their definitions here. For an entire function f, let

$$M(|k|) := \sup_{\theta\in[0,2\pi]} |f(|k|e^{i\theta})|. \tag{5.116}$$

The function f is order ρ ($0 \leq \rho \leq \infty$) if and only if for every positive ε, but for no negative ε

$$M(|k|) = O\left(e^{|k|^{\rho+\varepsilon}}\right), \qquad \text{as } |k| \to \infty. \tag{5.117}$$

If the order of f is finite and not zero, then f is of finite type τ ($0 \leq \tau \leq \infty$)

if and only if for every positive ε, but for no negative ε

$$M(|k|) = O\left(e^{(\tau+\varepsilon)|k|^{\rho}}\right), \qquad \text{as } |k| \to \infty. \tag{5.118}$$

For example, the function e^k is of order one and type one. An entire function f of order one and finite type or of order less than one is said to be of *exponential type*. Let z_n be the zeros of the entire function f not lying on the origin. Their convergence exponent is defined as the infimum of the positive numbers α such that

$$\sum_{n=0}^{\infty} \frac{1}{|z_n|^{\alpha}} < \infty, \tag{5.119}$$

while their genus is the smallest integer $p \geq 0$ such that Eq. (5.119) is verified for $\alpha = p + 1$. Given the zeros of f, consider the products

$$\pi_0(k) := \prod_{n=0}^{\infty} \left(1 - \frac{k}{z_n}\right), \tag{5.120}$$

$$\pi_p(k) := \prod_{n=0}^{\infty} \left(1 - \frac{k}{z_n}\right) \exp\left(\frac{k}{z_n} + \frac{k^2}{2z_n^2} + \cdots + \frac{k^p}{p z_n^p}\right), \quad p \geq 1. \tag{5.121}$$

If the zeros of f are of genus p, then the product π_p is called *canonical product of the zeros of* f [3, page 18].

With these definitions, we can write the Hadamard factorization of f. Let f be of order ρ, its zeros of genus p, Q a polynomial of degree not greater than ρ, and let f have an m-fold zero in the origin. Then f can be written in the form [3, 2.7.2, page 22; see also page 18]

$$f(k) = k^m e^{Q(k)} \pi_p(k). \tag{5.122}$$

We will write such a representation for the Jost function F. Moreover, we will show that F is of exponential type (Lemma 5.6); as a consequence, we will be able to determine the coefficients of Q using a Theorem due to Pfluger (see Lemma 5.9). To arrive at the Hadamard factorization of F we need several intermediate Lemmas, whose structure is depicted in

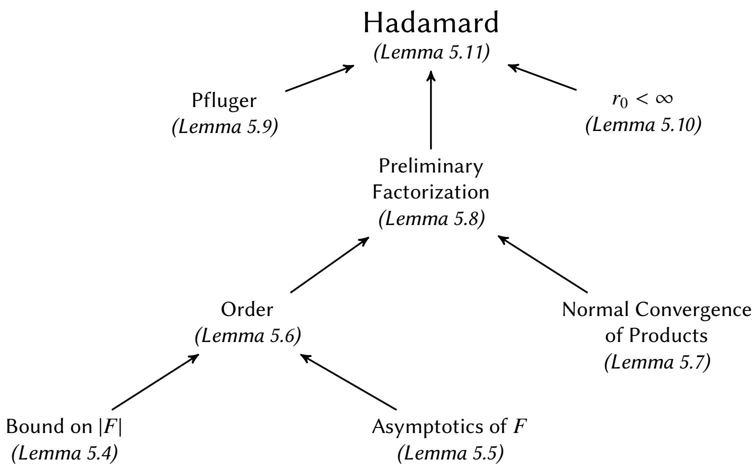


Figure 5.6: Overview of the Lemmas needed to write the Jost function in Hadamard's form.

Fig. 5.6.

5.4.1 Hadamard factorization of the Jost function

To determine the order and type of the Jost function the following two Lemmas are crucial. They elaborate some results presented in [38].

Lemma 5.4. *Let $\nu = \operatorname{Im} k$. Then, the Jost function F and the regular eigenfunctions φ satisfy the bounds*

$$|\varphi(k,r)| \le 4e^{4\|r'V(r')\|_1}\frac{r}{1+|k|r}e^{|\nu|r}, \tag{5.123}$$

$$|F(k)| \le \left(4\|rV(r)\|_1 e^{4\|rV(r)\|_1}+1\right)e^{2R_V|k|}. \tag{5.124}$$

Proof. For $r \in \mathbb{R}^+$ and $k \in \mathbb{C}$, the eigenfunctions φ are solutions of the

Lippmann-Schwinger equation [38, Eq. 12.4, page 330]

$$\varphi(k,r) = \frac{\sin kr}{k} + \int_0^r \frac{\sin k(r-r')}{k} V(r')\varphi(k,r')\,dr'. \tag{5.125}$$

Writing the solution of this equation as a Born series, it is possible to prove the bound [38, Eq. 12.8, page 332]

$$|\varphi(k,r)| \leq e^{q_k(r)} \frac{Cr}{1+|k|r} e^{|\nu|r}, \tag{5.126}$$

where

$$q_k(r) := \int_0^r \frac{Cr'}{1+|k|r'} |V(r')|\,dr', \tag{5.127}$$

and the constant C is such that [see 38, Eq. 12.6, page 331]

$$\left|\frac{\sin kr}{k}\right| \leq \frac{Cr}{1+|k|r} e^{|\nu|r}, \qquad r \geq 0. \tag{5.128}$$

From the bound [45, page 139]

$$\left|\frac{\sin k(y-x)}{k}\right| \leq \frac{4y}{1+|k|y} e^{|\nu|y+\nu x}, \qquad y \geq x \geq 0, \tag{5.129}$$

setting $x = 0$ and $y = r \geq 0$, we get

$$\left|\frac{\sin kr}{k}\right| \leq \frac{4r}{1+|k|r} e^{|\nu|r}. \tag{5.130}$$

As a consequence, we can choose $C = 4$. Observing that $q_k(r) \leq 4\|r'V(r')\|_1$, from (5.126) we get (5.123).

The integral equation (5.125), together with the relation between φ and F, Eq. (5.35), gives the integral equation for F [38, Eq. 12.36, page 341]

$$F(k) = 1 + \int_0^{R_V} e^{ikr} V(r)\varphi(k,r)\,dr. \tag{5.131}$$

Using this and the bound (5.123) we get

$$|F(k)| \leq 1 + 4e^{4\|r'V(r')\|_1} \int_0^{R_V} \frac{r}{1+|k|r} e^{2|\nu|r} |V(r)|\, dr \tag{5.132}$$

$$\leq 1 + 4\|rV(r)\|_1 e^{4\|rV(r)\|_1} e^{2|\nu|R_V} \tag{5.133}$$

$$\leq \left(4\|rV(r)\|_1 e^{4\|rV(r)\|_1} + 1\right) e^{2R_V|k|}. \tag{5.134}$$

□

Before giving the next Lemma, we use the results so far obtained to prove Lemma 5.2.

Proof (of Lemma 5.2). The bound (5.81) is a direct consequence of the bound (5.124), together with Eq. (2.5.11) of [3], that says

$$n(|k|)\log 2 \leq \log \max_{\theta\in[0,2\pi)} |F(2|k|e^{i\theta})|. \tag{5.135}$$

□

Lemma 5.5. *As $|k| \to \infty$, the Jost function F satisfies the asymptotic formulas*

$$\log |F(-i|k|)| \sim 2R_V|k|, \tag{5.136}$$

$$\log |F(i|k|)| \sim \frac{1}{2|k|} \int_0^{R_V} V(r)\, dr, \tag{5.137}$$

and the limit

$$\lim_{|k|\to\infty} \log |F(\pm|k|)| = 0. \tag{5.138}$$

Proof. We follow the presentation of [38, page 361].

Let $\nu = \operatorname{Im} k$, then Eqs. (5.125) and (5.123) imply that [38, Eq. 12.12]

$$\varphi(k, r) = \frac{\sin kr}{k} + o\left(\frac{e^{|\nu|r}}{|k|}\right), \qquad \text{as } |k| \to \infty. \tag{5.139}$$

Substituting this in (5.131), and considering only the direction $k = -i|k|$ gives

$$F(-i|k|) \sim \int_0^{R_V} \frac{e^{2|k|r}}{2|k|} V(r)\, dr \qquad \text{as } |k| \to \infty. \tag{5.140}$$

For $|k| \to \infty$ the integral is dominated by $r = R_V$, therefore it is convenient to write

$$F(-i|k|) \sim e^{2R_V|k|} \int_0^{R_V} \frac{e^{-2|k|(R_V-r)}}{2|k|} V(r)\, dr, \qquad \text{as } |k| \to \infty, \tag{5.141}$$

which implies

$$\log|F(-i|k|)| \sim 2R_V|k| + \log\left(\int_0^{R_V} \frac{e^{-2|k|(R_V-r)}}{2|k|} V(r)\, dr\right), \qquad \text{as } |k| \to \infty. \tag{5.142}$$

This gives (5.136), provided that the integral does not go to zero as $e^{-2R_V|k|}$ or faster. This is shown using Watson's Lemma (see e.g. [26, Lemma 11.1, page 283]) and Assumption (5.5), that give

$$\int_0^{R_V} e^{-2|k|(R_V-r)} V(r)\, dr \sim \sum_{n=0}^{M} \frac{\Gamma(\delta_n + 1) d_n}{|k|^{1+\delta_n}}, \qquad \text{as } |k| \to \infty. \tag{5.143}$$

Similarly, for the direction $k = i|k|$ we get

$$F(i|k|) = 1 + \frac{1}{2|k|} \int_0^{R_V} V(r)\, dr, \qquad \text{as } |k| \to \infty, \tag{5.144}$$

that, using Taylor's expansion, gives (5.137).

For (5.138) it is enough to use the fact that $\lim_{|k|\to\infty} F(|k|) = 1$ [45, Th. XI.58e, page 140] and the symmetry property of F [38, 12.32a, page 340]

$$\bar{F}(\bar{k}) = F(-k). \tag{5.145}$$

□

From the previous Lemmas we get

Lemma 5.6. *The Jost function has order one and type $2R_V$, and is therefore of exponential type. Moreover, the convergence exponent of its zeros is one.*

Proof. From the bound (5.124) we see that the Jost function has order not greater than one, while from the asymptotic formula (5.136) we get that the order can not be less than one, therefore it must be $\rho = 1$. The same reasoning gives $\tau = 2R_V$.

Let z_n denote the zeros of the Jost function F other than $k = 0$. Consider the function

$$g(k^2) := F(k)F(-k), \tag{5.146}$$

that is an entire function of k^2, whose zeros are $\{z_n^2\}_n$. Following the proof of the order of F, Eqs. (5.124), (5.136), and (5.137) imply that g is of order $1/2$. For a function of fractional order the convergence exponent of the zeros is equal to the order [3, 2.8.2, page 24], therefore

$$\sum_{n=0}^{\infty} \frac{1}{|z_n^2|^\alpha} \begin{cases} < \infty, & \alpha > 1/2, \\ = \infty, & \alpha < 1/2, \end{cases} \tag{5.147}$$

that shows that the convergence exponent of the zeros of F is one. □

The only parameter missing to write the Hadamard factorization of the Jost function F is the genus of its zeros, that will be determined in Lemma 5.11. However, we will write a product form for F already in Lemma 5.8. To that end, we will need to combine different infinite products, for which we will use the following notion of convergence. A product of continuous functions $\prod_n f_n$ is called *normally convergent* if $\sum_n (f_n - 1)$ is normally convergent, i.e. if every point $k \in \mathbb{C}$ has a neighborhood U_k such that $\sum_n \sup_{k' \in U_k} |f_n(k') - 1| < \infty$ (see [49, 1.2.1, page 7], and [48, 3.3.1, page 104]). We apply this notion to our case in the next Lemma.

Lemma 5.7. *Let $k_n = \alpha_n - i\beta_n$, with $\alpha_n, \beta_n > 0$, be the resonance zeros of the Jost function F. If the quantity*

$$r_0 \coloneqq \sum_{n=0}^{\infty} \frac{5\beta_n}{\alpha_n^2 + \beta_n^2} \tag{5.148}$$

is finite, then the products

$$\prod_{n=0}^{\infty} \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right), \tag{5.149}$$

$$\prod_{n=0}^{\infty} e^{2i\beta_n k/|k_n|^2}, \tag{5.150}$$

$$\prod_{n=0}^{\infty} \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right) e^{2i\beta_n k/|k_n|^2}, \tag{5.151}$$

are normally convergent. Moreover,

$$\prod_{n=0}^{\infty} \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right) e^{2i\beta_n k/|k_n|^2} = \exp\left(\frac{2}{5} i r_0 k\right) \prod_{n=0}^{\infty} \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right). \tag{5.152}$$

Proof. Let $k = \mu + i\nu$ and $\gamma_{0,k}$ the straight line connecting the origin to k, then we have the bounds:

$$\begin{aligned} \left| \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right) - 1 \right| &= \left| \frac{k^2 + 2i\beta_n k}{|k_n|^2} \right| \\ &\le \frac{|k|^2 + 2\beta_n |k|}{|k_n|^2} \sim \frac{2\beta_n |k|}{|k_n|^2}, \quad \text{as } n \to \infty, \end{aligned} \tag{5.153}$$

$$\begin{aligned}\left|e^{2i\beta_n k/|k_n|^2}-1\right| &= \left|\int_{\gamma_{0,k}} \frac{d}{dk'}\left(e^{2i\beta_n k'/|k_n|^2}\right) dk'\right| \\ &\leq \frac{2\beta_n|k|}{|k_n|^2} e^{2\beta_n|\nu|/|k_n|^2} \sim \frac{2\beta_n|k|}{|k_n|^2}, \quad \text{as } n\to\infty, \end{aligned} \tag{5.154}$$

$$\begin{aligned} p_n(k) &:= \left|\left(1-\frac{k}{k_n}\right)\left(1+\frac{k}{\bar{k}_n}\right)e^{2i\beta_n k/|k_n|^2}-1\right| \\ &= \left|\left(1-\frac{k^2+2i\beta_n k}{|k_n|^2}\right)e^{2i\beta_n k/|k_n|^2}-1\right| \\ &\leq \left|e^{2i\beta_n k/|k_n|^2}-1\right| + \left|\frac{k^2+2\beta_n k}{|k_n|^2}e^{2i\beta_n k/|k_n|^2}\right| \\ &\leq \frac{|k|^2+4\beta_n|k|}{|k_n|^2}e^{2\beta_n|\nu|/|k_n|^2} \sim \frac{4\beta_n|k|}{|k_n|^2}, \quad \text{as } n\to\infty. \end{aligned} \tag{5.155}$$

For every compact $K\subset\mathbb{C}$ let $h := \sup_{k\in K}|k|$, then there is a $n_K\in\mathbb{N}$ and a constant C_K such that

$$\sup_{k\in K} p_n(k) < C_K\frac{\beta_n h}{|k_n|^2}, \quad \forall n\geq n_K, \tag{5.156}$$

hence,

$$\sum_{n=n_K}^{\infty}\sup_{k\in K} p_n(k) < \sum_{n=n_K}^{\infty} C_K\frac{\beta_n h}{|k_n|^2} \leq \frac{C_K}{5}r_0 < \infty. \tag{5.157}$$

Similarly for the other products.

The continuity of the exponential allows us to write

$$\exp\left(\sum_{n=0}^{\infty}\frac{2i\beta_n k}{|k_n|^2}\right) = \exp\left(\frac{2}{5}ir_0k\right) = \prod_{n=0}^{\infty}\exp\left(\frac{2i\beta_n k}{|k_n|^2}\right), \tag{5.158}$$

indeed we can exchange it with the limit of the series. Moreover, the products (5.149) and (5.150) are normally convergent and therefore also compactly convergent [49, page 8] and we can multiply them factor by factor [49, page 6] getting (5.152). □

Although we do not know yet the genus of the Jost function, we can already write its Hadamard factorization. Indeed, the genus p and the convergence exponent ρ_1 of the zeros of F satisfy the relation $\rho_1 - 1 \leq p \leq \rho_1$ (see [3, page 17]), and Lemma 5.6 tells us that ρ_1 is one, hence the genus p must be either one or zero. In the next Lemma we will show that if the genus is zero, one can still write the Jost function in the same factorization form as if it had genus one. Analogously, in Lemma 5.11 we will prove that if the genus is one, we can write the Jost function in the same form as if it had genus zero. Moreover, in Lemma 5.11 we will be able to determine all constants that appear in the Hadamard factorization of the Jost function.

Lemma 5.8. *Let $a_1, b_1 \in \mathbb{R}$, $C \in \mathbb{C}$,*

$$\lambda := \begin{cases} 0, & \text{if } F(0) \neq 0 \\ 1, & \text{if } F(0) = 0, \end{cases} \tag{5.159}$$

$$B(k) := \prod_{m=0}^{N-1} \left(1 - \frac{k}{i\eta_m}\right) \prod_{l=0}^{N'-1} \left(1 + \frac{k}{i\kappa_l}\right), \tag{5.160}$$

$$P_1(k) := \prod_{n=0}^{\infty} \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right) e^{2i\beta_n k/|k_n|^2}, \tag{5.161}$$

then for the Jost function F the following representation holds

$$F(k) = (F(0) + \lambda C k)\, e^{(a_1 + ib_1)k} B(k) P_1(k). \tag{5.162}$$

Moreover, the product P_1 is an entire function of exponential type.

Proof. To write the Hadamard factorization given in Eq. (5.122) for F we need to know its genus. The genus p and the convergence exponent ρ_1 of the zeros of F satisfy the relation $\rho_1 - 1 \leq p \leq \rho_1$ (see [3, page 17]), hence by Lemma 5.6, p must be either one or zero. We at first assume that p is one. Using the fact that the Jost function can eventually have only a simple zero in $k = 0$, and that the number of bound states and virtual states is finite, the Hadamard factorization given in Eq. (5.122) yields directly Eq. (5.162). In this case, P_1 is the canonical product of the zeros $\{k_n\}_{n\in\mathbb{N}^0}$, therefore it is an entire function of order one thanks to Theorem 2.6.5 of [3, page 19].

Suppose now that p is zero. Let $a_0, b_0 \in \mathbb{R}$, and

$$P_0(k) := \prod_{n=0}^{\infty}\left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right), \tag{5.163}$$

then Eq. (5.122) gives

$$F(k) = (F(0) + \lambda C k)\, e^{(a_0+ib_0)k} B(k) P_0(k). \tag{5.164}$$

If the genus of the zeros of the Jost function is zero, then

$$\sum_{n=0}^{\infty} \frac{1}{|k_n|} < \infty, \tag{5.165}$$

and therefore

$$r_0 := \sum_{n=0}^{\infty} \frac{5\beta_n}{\alpha_n^2 + \beta_n^2} = \sum_{n=0}^{\infty} \frac{5}{|k_n|} \frac{\beta_n}{\sqrt{\alpha_n^2 + \beta_n^2}} \leq \sum_{n=0}^{\infty} \frac{5}{|k_n|} < \infty. \tag{5.166}$$

We can then use Eq. (5.152) of Lemma 5.7, that gives

$$P_0(k) = e^{-\frac{2}{5} i r_0 k} P_1(k). \tag{5.167}$$

Hence, Eq. (5.164) reduces to Eq. (5.162) once we set

$$\begin{cases} b_1 := b_0 - \frac{2}{5} r_0, \\ a_1 := a_0. \end{cases} \tag{5.168}$$

In this case the canonical product of the zeros $\{k_n\}_{n\in\mathbb{N}^0}$ is P_0, that is then an entire function of order one again thanks to Theorem 2.6.5 of [3, page 19]. Moreover, $r_0 < \infty$ therefore $e^{-\frac{2}{5} i r_0 k}$ is also an entire function of order one, and so P_1 is.

We have now only to show that P_1 is of finite type. The Jost function is of order one and of finite type, moreover the function

$$(F(0) + \lambda C k)\, e^{(a_1+ib_1)k} B(k) \tag{5.169}$$

that multiplies P_1 in Eq. (5.162) is clearly an entire function of order not greater than one and of finite type, therefore P_1 can only be of finite type, otherwise F could not be so. □

To determine the coefficients of the polynomial Q appearing in the Hadamard factorization of F, Eq. 5.122, i.e. to determine the constants a_1 and b_1 in Eq. (5.162), we will use a result by Pfluger [42, Th. 6B, page 15; see also Th. 5, page 11] (see also [3, 8.4.20, page 147] and [38, page 363]). We recall here the part of the theorem of interest to us.

Lemma 5.9 (Pfluger). *Let $z, z_n \in \mathbb{C}\ \forall n \in \mathbb{N}^0$,*

$$f(z) := \prod_{n=0}^{\infty} \left(1 - \frac{z}{z_n}\right)\left(1 + \frac{z}{\bar{z}_n}\right) e^{2i\beta_n z/|z_n|^2} \tag{5.170}$$

be an entire function of exponential type such that

$$\lim_{r\to\infty} \int_{-r}^{r} \frac{\log|f(x)|}{x^2}\, dx < \infty, \tag{5.171}$$

and whose zeros have density D, let $z = |z|e^{i\theta}$, and

$$\varsigma := \sum_{n=0}^{\infty} z_n^{-1}. \tag{5.172}$$

If the density of the zeros of f with positive real part is the same as the density of the zeros with negative real part, then

$$\frac{\log|f(z)|}{|z|} = \operatorname{Re}\varsigma\cos\theta - \operatorname{Im}\varsigma\sin\theta + \frac{\pi}{2}D|\sin\theta| + \epsilon(z), \tag{5.173}$$

where ϵ is a function of z such that

$$\limsup_{|z|\to\infty} \epsilon(z) = 0. \tag{5.174}$$

In order to apply this Lemma to the product

$$P_1(k) := \prod_{n=0}^{\infty}\left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right) e^{2i\beta_n k/|k_n|^2} \tag{5.175}$$

introduced in Lemma 5.8, we need to prove the following Lemma, which is therefore of technical nature. Nevertheless, the quantity r_0 will appear in the bounds of Theorems 5.1 and 5.2.

Lemma 5.10. *Let $n(|k|)$ be the number of zeros of the Jost function F within a ball of radius $|k|$, and let $k_n = \alpha_n - i\beta_n$, with $\alpha_n, \beta_n > 0$, be the resonance zeros of F. The limits*

$$\lim_{r\to\infty} \int_{-r}^{r} \frac{\log|P_1(\mu)|}{\mu^2}\, d\mu, \tag{5.176}$$

and

$$\lim_{|k|\to\infty} \frac{n(|k|)}{|k|} \tag{5.177}$$

exist and are finite. Moreover,

$$r_0 := \sum_{n=0}^{\infty} \frac{5\beta_n}{\alpha_n^2 + \beta_n^2} < \infty. \tag{5.178}$$

Proof. We use again the function g defined in Eq. (5.146). For $k \geq 0$, then $k = |k|$ and the symmetry property $F(-k) = \bar{F}(\bar{k})$ [38, 12.32a, page 340] implies

$$g(|k|^2) = F(|k|)F(-|k|) = F(|k|)\bar{F}(|k|) = |F(|k|)|^2. \tag{5.179}$$

Substituting (5.139) in (5.131) we get

$$F(|k|) \sim 1 - \frac{1}{|k|} \int_0^{R_V} V(r)\, dr, \qquad \text{as } |k| \to \infty, \tag{5.180}$$

that for g implies

$$g(|k|^2) = |F(|k|)|^2 \sim 1 - \frac{2}{|k|} \int_0^{R_V} V(r)\, dr. \qquad \text{as } |k| \to \infty, \tag{5.181}$$

Therefore $\log g(|k|^2) \to 0$ as $|k| \to \infty$, and

$$\int_1^{\infty} \frac{\log g(\mu^2)}{\mu^2}\, d\mu < \infty. \tag{5.182}$$

Consider now the function $g_1(k^2) := P_1(k)P_1(-k)$, which is the analogue of the function g for P_1. Note that for real argument g_1 is real-valued and positive (cf. Eq. (5.179)). From Eq. (5.162) we see that

$$\log g(k^2) = \log g_1(k^2) + O(\log k), \qquad \text{as } k \to \infty, \tag{5.183}$$

therefore Eq. (5.182) implies that

$$\int_1^{\infty} \frac{\log g_1(\mu^2)}{\mu^2}\, d\mu < \infty. \tag{5.184}$$

We have $g_1(0) = 1$, hence for $\mu \in \mathbb{R}$ it exists an $a_\mu \in \mathbb{R}$ such that

$$\log g_1(\mu^2) = \log g_1(0) + \int_0^{\mu^2} \frac{d}{dt} (\log g_1(t))\, dt = a_\mu \mu^2, \tag{5.185}$$

with

$$|a_\mu| \leq \sup_{0 \leq t \leq \mu^2} \frac{d}{dt} (\log g_1(t)) < \infty \tag{5.186}$$

because the function g_1 is entire and has no zeros on the real axis. As a consequence,

$$\int_{-1}^{1} \frac{\log g_1(\mu^2)}{\mu^2}\, d\mu < \infty \tag{5.187}$$

(for a general argument, see footnote 12 on page 5 of [42] and the comment after Eq. 8.2.2 in [3, page 136]). This, together with Eq. (5.184) and the fact that $\log g_1(|k|^2) = 2\log|P_1(|k|)|$, gives

$$\lim_{r\to\infty} \int_{-r}^{r} \frac{\log|P_1(\mu)|}{\mu^2}\, d\mu < \infty. \tag{5.188}$$

The convergence of the latter integral is equivalent to the convergence of the sum r_0 and to the existence and finiteness of the limit (5.177) because of Theorem 5 of [42] (see also Theorem 8.4.1 in [3, page 143] and the discussion on pages 133-135 of [3]), together with the fact that the set of the zeros of P_1 is equal to that of the zeros of F, except for finitely many elements. □

We remind the reader that the genus of the zeros z_n of an entire function f is the smallest integer $p \geq 0$ such that [3, 2.5.4, page 14]

$$\sum_{n=0}^{\infty} \frac{1}{|z_n|^{p+1}} < \infty. \tag{5.189}$$

In the next Lemma, we finally write the Hadamard factorization of the Jost function, with all the constants explicitly determined.

Lemma 5.11. *Let*

$$B(k) := \prod_{m=0}^{N-1} \left(1 - \frac{k}{i\eta_m}\right) \prod_{l=0}^{N'-1} \left(1 + \frac{k}{i\kappa_l}\right), \tag{5.190}$$

$$P_0(k) := \prod_{n=0}^{\infty} \left(1 - \frac{k}{k_n}\right)\left(1 + \frac{k}{\bar{k}_n}\right), \tag{5.191}$$

$$\lambda := \begin{cases} 0, & \text{if } F(0) \neq 0 \\ 1, & \text{if } F(0) = 0, \end{cases} \tag{5.192}$$

then for the Jost function F the following decomposition holds

$$F(k) = \left(F(0) + \lambda \dot{F}(0)k\right) e^{iR_V k} B(k) P_0(k). \tag{5.193}$$

Moreover, the genus of the zeros of F is one and their density is (cf. Lemma 5.10)

$$D := \lim_{|k|\to\infty} \frac{n(|k|)}{|k|} = \frac{2}{\pi} R_V. \tag{5.194}$$

Proof. We already proved in Lemma 5.8 that

$$F(k) = (F(0) + \lambda C k)\, e^{(a_1 + ib_1)k} B(k) P_1(k). \tag{5.195}$$

We at first notice that Eq. (5.152) of Lemma 5.7 together with Lemma 5.10 gives

$$P_0(k) = e^{-\frac{2}{5} i r_0 k} P_1(k). \tag{5.196}$$

We can now determine the constants a_1 and b_1 applying Lemma 5.9 to the function P_1. We can use it because P_1 is an entire function (Lemma 5.8), the integral condition (5.171) holds because of Lemma 5.10, and for every zero of P_1 with positive real part k_n there is exactly one zero with negative real part $-\bar{k}_n$. The quantity ς of Eq. (5.172) is in this case

$$\varsigma = \sum_{n=0}^{\infty} \left(\frac{1}{k_n} - \frac{1}{\bar{k}_n} \right) = \sum_{n=0}^{\infty} \frac{2i\beta_n}{|k_n|^2} = \frac{2}{5} i r_0. \tag{5.197}$$

Note that the density of the zeros of P_1 is equal to the density D of all of the zeros of F (cf. Lemma 5.10). Equation (5.173) then gives

$$\limsup_{|k|\to\infty} \frac{\log |P_1(k)|}{|k|} = -\frac{2}{5} r_0 \sin\theta + \frac{\pi}{2} D |\sin\theta|. \tag{5.198}$$

We will specialize this statement for the directions $\theta = \pm\pi/2, \pi$. From

Lemma 5.5 we have

$$\limsup_{|k|\to\infty} \frac{\log|F(i|k|)|}{|k|} = 0,$$
$$\limsup_{|k|\to\infty} \frac{\log|F(-|k|)|}{|k|} = 0,$$
$$\limsup_{|k|\to\infty} \frac{\log|F(-i|k|)|}{|k|} = 2R_V. \tag{5.199}$$

The factorization (5.195) implies

$$\begin{aligned}\frac{\log|P_1(k)|}{|k|} &= \frac{1}{|k|}\log\left|\frac{e^{-(a_1+ib_1)k}F(k)}{(F(0)+\lambda Ck)\,B(k)}\right| \\ &= b_1\sin\theta - a_1\cos\theta + \frac{\log|F(k)|}{|k|} - \frac{\log|(F(0)+\lambda Ck)\,B(k)|}{|k|} \\ &\sim b_1\sin\theta - a_1\cos\theta + \frac{\log|F(k)|}{|k|}, \quad \text{as } |k|\to\infty.\end{aligned} \tag{5.200}$$

Therefore, Eq. (5.198) gives

$$\begin{aligned}\limsup_{|k|\to\infty} \frac{\log|P_1(i|k|)|}{|k|} &= b_1 = -\frac{2}{5}r_0 + \frac{\pi}{2}D, \\ \limsup_{|k|\to\infty} \frac{\log|P_1(-|k|)|}{|k|} &= a_1 = 0, \\ \limsup_{|k|\to\infty} \frac{\log|P_1(-i|k|)|}{|k|} &= -b_1 + 2R_V = \frac{2}{5}r_0 + \frac{\pi}{2}D.\end{aligned} \tag{5.201}$$

Summing and subtracting the first and last lines

$$\begin{cases} b_1 = R_V - \frac{2}{5}r_0 \\ a_1 = 0 \\ D = \frac{2}{\pi}R_V. \end{cases} \tag{5.202}$$

To determine the constant C in Eq. (5.195), we calculate the logarithmic derivative of F. The infinite product P_1 appearing in Eq. (5.195) is normally convergent (Lemma 5.7 together with Lemma 5.10), therefore its logarithmic derivative can be calculated as if it were a finite product [49, page 10]. This gives

$$\frac{\dot{F}(k)}{F(k)} = \frac{\lambda}{k} + iR_V + \frac{\dot{B}(k)}{B(k)} + \sum_{n=0}^{\infty}\left(\frac{1}{k-k_n} + \frac{1}{k+\bar{k}_n}\right), \tag{5.203}$$

with

$$\frac{\dot{B}(k)}{B(k)} = \sum_{m=0}^{N-1}\frac{1}{k-i\eta_m} + \sum_{l=0}^{N'-1}\frac{1}{k+i\kappa_l}, \tag{5.204}$$

from which we can calculate $\dot{F}(k)$ for every k such that $F(k) \neq 0$. Moreover, we can calculate $\dot{F}$ at the zeros of F as limit of this result. In particular, if $F(0) = 0$, from Eq. (5.195) we have for $k > 0$

$$\dot{F}(k) = \left[\frac{1}{k} + iR_V + \frac{\dot{B}(k)}{B(k)} + \sum_{n=0}^{\infty}\left(\frac{1}{k-k_n} + \frac{1}{k+\bar{k}_n}\right)\right] Cke^{(a_1+ib_1)k}P_1(k)B(k). \tag{5.205}$$

In the limit $k \to 0$ we then have

$$C = \dot{F}(0). \tag{5.206}$$

Substituting this and Eq. (5.202) into Eq. (5.195) and using (5.196) we get (5.193).

We now determine the genus of F. The density is nonzero and finite if and only if $|k_n| \sim 2n/D$ as $n \to \infty$ (the two is due to the symmetry of the resonances with respect to the imaginary axis), but that implies

$$\sum_{n=0}^{\infty}\frac{1}{|k_n|} = \infty. \tag{5.207}$$

If the genus p of the zeros of F was zero, then the sum in Eq. (5.207) would be finite, therefore p must be one. □

5.4.2 Bounds

As a consequence of the product decomposition of the Jost function, we have the following Lemma about the differentiability of the S-matrix.

Lemma 5.12. *The S-matrix $S(k)$ is infinitely often differentiable for $k \geq 0$.*

Proof. Using the Jost function F, we introduce the auxiliary function

$$F_0(k) := \frac{F(k)}{F(0) + \lambda \dot{F}(0) k}. \tag{5.208}$$

From the product representation (5.193) of F we get a product decomposition for F_0, from which we have that F_0 is entire [3, Theorem 2.6.5, page 19], is such that $F_0(0) = 1$, and has no zero on the real axis.

For the S-matrix we can write

$$S(k) = \frac{F(-k)}{F(k)} = (1 - 2\lambda) \frac{F_0(-k)}{F_0(k)}. \tag{5.209}$$

Since F_0 is entire, it is infinitely often differentiable for any $k \geq 0$. Moreover, $F_0(k)$ is never zero for $k \geq 0$, therefore $F_0(-k)/F_0(k)$ is analytic for $k \geq 0$ and infinitely many derivatives of $S(k)$ exist for $k \geq 0$. □

Taking derivatives of the formula

$$S(k) = \frac{F(-k)}{F(k)}, \tag{5.210}$$

and using the definition

$$L(k) := \operatorname{Im} \frac{\dot{F}(k)}{F(k)}, \tag{5.211}$$

one gets

$$\dot{S} = -2iSL \tag{5.212}$$

$$\ddot{S} = -2iS\dot{L} - 4SL^2 \tag{5.213}$$

$$\dddot{S} = -2iS\ddot{L} - 12SL\dot{L} + 8iSL^3. \tag{5.214}$$

Therefore, we need to bound L and its derivatives. For this purpose we use the Hadamard factorization of F.

Lemma 5.13. *If $q \in \mathbb{N}$ then*

$$\operatorname{Im}\frac{\dot{F}(k)}{F(k)} = R_V + \operatorname{Im}\frac{\dot{B}(k)}{B(k)} - \sum_{n=0}^{\infty}\left(\frac{\beta_n}{|k-k_n|^2} + \frac{\beta_n}{|k+k_n|^2}\right), \tag{5.215}$$

$$\frac{d^q}{dk^q}\left(\frac{\dot{F}(k)}{F(k)}\right) = (-1)^q q!\left[\frac{\lambda}{k^{q+1}} + \sum_{n=0}^{\infty}\left(\frac{1}{(k-k_n)^{q+1}} + \frac{1}{(k+\bar{k}_n)^{q+1}}\right)\right] + \frac{d^q}{dk^q}\left(\frac{\dot{B}(k)}{B(k)}\right), \tag{5.216}$$

and

$$\frac{\dot{B}(k)}{B(k)} = \sum_{m=0}^{N-1}\frac{1}{k-i\eta_m} + \sum_{l=0}^{N'-1}\frac{1}{k+i\kappa_l}, \tag{5.217}$$

$$\operatorname{Im}\frac{\dot{B}(k)}{B(k)} = \sum_{m=0}^{N-1}\frac{\eta_m}{k^2+\eta_m^2} - \sum_{l=0}^{N'-1}\frac{\kappa_l}{k^2+\kappa_l^2} \tag{5.218}$$

$$\frac{d^q}{dk^q}\left(\frac{\dot{B}(k)}{B(k)}\right) = (-1)^q q!\left(\sum_{m=0}^{N-1}\frac{1}{(k-i\eta_m)^{q+1}} + \sum_{l=0}^{N'-1}\frac{1}{(k+i\kappa_l)^{q+1}}\right). \tag{5.219}$$

Proof. Equation (5.215) is achieved simply taking the imaginary part of Eq. (5.203); Eq. (5.216) is a direct application of Lemma 3.1 of [8, page 287] to the auxiliary function $F(k)/(F(0) + \lambda\dot{F}(0)k)$, that is of order one because of Lemma 5.6. □

Lemma 5.14. *Let*

$$L(k) := \operatorname{Im} \frac{\dot{F}(k)}{F(k)}. \tag{5.220}$$

For $K > 0$ the following bounds hold:

$$\sup_{k<K} |L(k)| \leq \frac{1}{s_K} \left[1 + s_K(R_V + r_0)\right], \tag{5.221}$$

$$\sup_{k<K} |\dot{L}(k)| \leq \frac{2}{s_K^2} \left(1 + s_K^2 \frac{2r_0}{\alpha}\right), \tag{5.222}$$

$$\sup_{k<K} |\ddot{L}(k)| \leq \frac{2}{s_K^3} \left(1 + s_K^3 \frac{7r_0}{\alpha}\right). \tag{5.223}$$

Proof. Consider the smallest non-negative integer ν_K such that $\alpha_n \geq 2K$ for all $n \geq \nu_K$, that implies $(\alpha_n - K)^2 \geq \alpha_n^2/4$. Then, from the expansion (5.215) for L, follows

$$\begin{aligned}
\sup_{k<K} |L(k)| &\leq R_V + \frac{1}{\eta} + \frac{1}{\kappa} + \sum_{n=0}^{\nu_K - 1} \frac{1}{\beta_n} + \sum_{n=\nu_K}^{\infty} \frac{\beta_n}{(\alpha_n - K)^2 + \beta_n^2} + \sum_{n=0}^{\infty} \frac{\beta_n}{|k_n|^2} \\
&\leq R_V + \frac{1}{s_K} + \sum_{n=\nu_K}^{\infty} \frac{4\beta_n}{\alpha_n^2 + \beta_n^2} + \sum_{n=0}^{\infty} \frac{\beta_n}{|k_n|^2} \\
&\leq R_V + \frac{1}{s_K} + \sum_{n=0}^{\infty} \frac{5\beta_n}{\alpha_n^2 + \beta_n^2} \\
&= \frac{1}{s_K} \left[1 + s_K(R_V + r_0)\right].
\end{aligned} \tag{5.224}$$

Analogously, for $\dot{L}$ the expansion given in Lemma 5.13 implies

$$\begin{aligned}
\dot{L}(k) = &\sum_{m=0}^{N-1} \frac{2\eta_m k}{(k^2 + \eta_m^2)^2} - \sum_{l=0}^{N'-1} \frac{2\kappa_l k}{(k^2 + \kappa_l^2)^2} \\
&- \sum_{n=0}^{\infty} \left[\frac{2\beta_n (k - \alpha_n)}{|k - k_n|^4} + \frac{2\beta_n (k + \alpha_n)}{|k + k_n|^4} \right].
\end{aligned} \tag{5.225}$$

Observe that, for $A, B \geq 0$,

$$\frac{2AB}{(A^2+B^2)^2} \leq \frac{A^2+B^2}{(A^2+B^2)^2} = \frac{1}{A^2+B^2} \leq \frac{1}{B^2}; \tag{5.226}$$

furthermore,

$$\frac{2\beta_n|k \pm \alpha_n|}{|k \pm k_n|^4} \leq \frac{2\beta_n|k \pm \alpha_n|}{|k \pm k_n|^3|k \pm \alpha_n|} = \frac{2\beta_n}{|k \pm k_n|^3}, \tag{5.227}$$

therefore

$$|\dot{L}(k)| \leq \sum_{m=0}^{N-1} \frac{1}{\eta_m^2} + \sum_{l=0}^{N'-1} \frac{1}{\kappa_l^2} + \sum_{n=0}^{\infty} \frac{2\beta_n}{|k-k_n|^3} + \sum_{n=0}^{\infty} \frac{2\beta_n}{|k+k_n|^3}, \tag{5.228}$$

and

$$\begin{aligned}
\sup_{k<K} |\dot{L}(k)| &\leq \frac{1}{\eta^2} + \frac{1}{\kappa^2} + \sum_{n=0}^{\nu_K-1} \frac{2}{\beta_n^2} + \sum_{n=\nu_K}^{\infty} \frac{2\beta_n}{[(\alpha_n-K)^2+\beta_n^2]^{3/2}} + \sum_{n=0}^{\infty} \frac{2\beta_n}{|k_n|^3} \\
&\leq \frac{1}{\eta^2} + \frac{1}{\kappa^2} + 2\left(\sum_{n=0}^{\nu_K-1} \frac{1}{\beta_n}\right)^2 + \sum_{n=\nu_K}^{\infty} \frac{16\beta_n}{[\alpha_n^2+\beta_n^2]^{3/2}} + \sum_{n=0}^{\infty} \frac{2\beta_n}{|k_n|^3} \\
&\leq \frac{1}{\eta^2} + \frac{1}{\kappa^2} + 2\left(\sum_{n=0}^{\nu_K-1} \frac{1}{\beta_n}\right)^2 + \sum_{n=0}^{\infty} \frac{18\beta_n}{|k_n|^3} \\
&\leq \frac{2}{s_K^2} + \frac{18}{5\alpha} \sum_{n=0}^{\infty} \frac{5\beta_n}{|k_n|^2} \\
&\leq \frac{2}{s_K^2}\left(1 + s_K^2 \frac{2r_0}{\alpha}\right).
\end{aligned} \tag{5.229}$$

Moreover, for $\ddot{L}$ again from the expansion given in Lemma 5.13 we get

$$\ddot{L}(k) = -2\sum_{m=0}^{N-1} \frac{\eta_m^3 - \eta_m k^2}{(k^2+\eta_m^2)^3} + 2\sum_{l=0}^{N'-1} \frac{\kappa_l^3 - \kappa_l k^2}{(k^2+\kappa_l^2)^3}$$
$$+ 2\sum_{n=0}^{\infty} \left[\frac{\beta_n^3 - \beta_n(k-\alpha_n)^2}{|k-k_n|^6} + \frac{\beta_n^3 - \beta_n(k+\alpha_n)^2}{|k+k_n|^6} \right]. \tag{5.230}$$

For $A, B \geq 0$,

$$\frac{B^3 - A^2 B}{(A^2+B^2)^3} = \frac{B(B^2-A^2)}{(A^2+B^2)^3} \leq \frac{B(B^2+A^2)}{(A^2+B^2)^3} = \frac{B}{(A^2+B^2)^2} \leq \frac{1}{B^3}. \tag{5.231}$$

Furthermore,

$$\frac{|\beta_n^3 - \beta_n(k \pm \alpha_n)^2|}{|k \pm k_n|^6} \leq \frac{\beta_n}{|k \pm k_n|^2} \frac{\beta_n^2 + (k \pm \alpha_n)^2}{|k \pm k_n|^4} = \frac{\beta_n}{|k \pm k_n|^4} \tag{5.232}$$

therefore

$$|\ddot{L}(k)| \leq \frac{2}{\eta^3} + \frac{2}{\kappa^3} + 2\sum_{n=0}^{\infty} \frac{\beta_n}{|k-k_n|^4} + \frac{2}{\alpha^2}\sum_{n=0}^{\infty} \frac{\beta_n}{|k_n|^2} \tag{5.233}$$

and

$$\sup_{k<K} |\ddot{L}(k)| \leq \frac{2}{\eta^3} + \frac{2}{\kappa^3} + \sum_{n=0}^{\nu_K - 1} \frac{2}{\beta_n^3} + 2\sum_{n=\nu_K}^{\infty} \frac{16\beta_n}{|k_n|^4} + \frac{2r_0}{5\alpha^2}$$
$$\leq \frac{2}{s_K^3}\left(1 + s_K^3 \frac{7r_0}{\alpha}\right). \tag{5.234}$$

□

We can now finally prove Theorem 5.1.

Proof (of Theorem 5.1). From Eqs. (5.212)-(5.214) we get the bounds

$$|\dot{S}| \leq 2|L|, \tag{5.235}$$

$$|\ddot{S}| \leq 2|\dot{L}| + 4|L|^2, \tag{5.236}$$

$$|\dddot{S}| \leq 2|\ddot{L}| + 12|L|\,|\dot{L}| + 8|L|^3. \tag{5.237}$$

Then, Lemma 5.14 implies the result. □

5.5 Proof of Theorem 5.2

For s given in Definition 5.2, and $n \in \{1, 2, 3\}$, we want to prove that

$$\|S^{(n)}\|_\infty \leq C_n s^{-n}, \tag{5.238}$$

We can not simply take the limit $K \to \infty$ in Theorem 5.1, indeed $s_K^{-1} \to \infty$ in this limit. To see this, consider

$$\lim_{K\to\infty} s_K^{-1} = \frac{1}{\eta} + \frac{1}{\kappa} + \sum_{n=0}^{\infty} \frac{1}{\beta_n}, \tag{5.239}$$

which does not converge due to the fact that $\beta_n = o(n)$ as $n \to \infty$, as shown in the next Lemma (see also [38, page 362]). As a consequence, we can use Theorem 5.1 only up to a certain value $\tilde{K}$, while for $k > \tilde{K}$ we will devise a different strategy.

Lemma 5.15. *Let $k_n = \alpha_n - i\beta_n$ be the zeros of the Jost function F such that $\alpha_n, \beta_n > 0$. Then* $\lim_{n\to\infty} |k_n|/n$ *and* $\lim_{n\to\infty} \alpha_n/n$ *exist and are such that*

$$0 < \lim_{n\to\infty} \frac{|k_n|}{n} < \infty, \qquad 0 < \lim_{n\to\infty} \frac{\alpha_n}{n} < \infty; \tag{5.240}$$

moreover,

$$\beta_n = o(n), \qquad \text{as } n \to \infty. \tag{5.241}$$

Proof. Let $n(|k|)$ be the number of zeros of F within a ball of radius $|k|$, and let $\tilde{n}(|k|)$ the number of resonances in the same ball. From Lemmas 5.10 and 5.11 we know that the following limit exists and that

$$0 < \lim_{|k|\to\infty} \frac{n(|k|)}{|k|} < \infty. \tag{5.242}$$

Clearly,

$$\lim_{|k|\to\infty} \frac{\tilde{n}(|k|)}{|k|} = \lim_{|k|\to\infty} \frac{n(|k|)}{|k|}, \tag{5.243}$$

therefore for every sequence $\{\lambda_n\}_{n\in\mathbb{N}^0}$ such that $\lambda_n > 0$ and $\lambda_n \to \infty$ as $n \to \infty$,

$$0 < \lim_{n\to\infty} \frac{\tilde{n}(\lambda_n)}{\lambda_n} = \lim_{|k|\to\infty} \frac{\tilde{n}(|k|)}{|k|} < \infty. \tag{5.244}$$

In particular, for $\lambda_n = |k_n|$, we get $\tilde{n}(|k_n|) = 2n$ (the 2 is due to the symmetry of the resonances), that implies that the limit

$$\lim_{n\to\infty} \frac{|k_n|}{n} \tag{5.245}$$

exists and satisfies Eq. (5.240). As a consequence, there is a constant $c \in \mathbb{R}^+$ such that

$$|k_n|^2 = \alpha_n^2 + \beta_n^2 \sim cn^2, \quad \text{as } n \to \infty, \tag{5.246}$$

therefore

$$\frac{\beta_n}{\alpha_n^2 + \beta_n^2} \sim \frac{\beta_n}{cn^2}, \quad \text{as } n \to \infty. \tag{5.247}$$

Together with Eq. (5.178) of Lemma 5.10, that implies

$$\frac{\beta_n}{\alpha_n^2 + \beta_n^2} = o(n^{-1}), \quad \text{as } n \to \infty, \tag{5.248}$$

and we get $\beta_n = o(n)$. Equation (5.246) then implies $\alpha_n \sim \sqrt{c}\,n$ as $n \to \infty$. □

For big values of k the product form of the Jost function F is not of help, and we instead use the relation $F(k) = f(k, 0)$, where f are the irregular eigenfunctions defined by Eq. (5.29). The eigenfunctions f satisfy the following well known bound (see [45, Theorem XI.57]; note that in this reference $\eta(r,-k)$ is equal to our $f(k,r)$, cf. [45, Theorem XI.57, page 138]).

Lemma 5.16. *Let $k \in [0,\infty)$ and*

$$Q_k(r) := \int_r^\infty \frac{2r'}{1+kr'} |V(r')|\, dr', \tag{5.249}$$

then

$$|f(k,r)| \le e^{Q_k(r)}. \tag{5.250}$$

We need to handle up to the third derivative of the Jost function. Therefore, we will extend Lemma 5.16 to $\partial_k^n f(k,r)$ with $n \le 3$, using a similar proof as that of Theorem XI.57 in [45]. Starting point is the Lippmann-Schwinger equation

$$f(k,r) = e^{ikr} - \int_r^\infty \frac{1}{k} \sin(k(r-r'))V(r')f(k,r')\, dr'. \tag{5.251}$$

We want to expand $\partial_k^n f(k,r)$ in a Born series, so that once we have a global bound in r for every summand, we get a global bound in r for $\partial_k^n f(k,r)$ (assuming the series converges). But this will not work because the first summand of the Born series for $\dot{f}$ is ire^{ikr} for which there is no global bound in r. We can solve the problem by looking at

$$y(k,r) := e^{-ikr} f(k,r) \tag{5.252}$$

rather than $f(k,r)$.

Lemma 5.17. *Let $k \in [0,\infty)$ and $q_k := e^{Q_k(0)} \|rV(r)\|_1$, then*

$$|\dot{y}(k,r)| \le 3\frac{e^{Q_k(r)}}{k} q_k. \tag{5.253}$$

Proof. From Eq. (5.251) we see that y satisfies

$$y(k,r) = 1 - \int_r^\infty e^{-ik(r-r')}\frac{1}{k}\sin(k(r-r'))V(r')y(k,r')\,dr' \tag{5.254}$$

$$=: 1 - \int_r^\infty g(k,r,r')V(r')y(k,r')\,dr', \tag{5.255}$$

so that

$$\dot{y}(k,r) = -\int_r^\infty \dot{g}(k,r,r')V(r')y(k,r')\,dr' - \int_r^\infty g(k,r,r')V(r')\dot{y}(k,r')\,dr' \tag{5.256}$$

$$=: x(k,r) - \int_r^\infty g(k,r,r')V(r')\dot{y}(k,r')\,dr'. \tag{5.257}$$

We want to use the inequality

$$\left|\frac{1}{k}\sin\left(k(r-r')\right)\right| \le \frac{2r'}{1+kr'}, \tag{5.258}$$

to prove which consider the following. Observe that for $x > 0$

$$\left|\frac{\sin x}{x}\right| \le \frac{2}{1+x}, \tag{5.259}$$

indeed

$$\left|\frac{\sin x}{x}\right|(1+x) = \left|\frac{\sin x}{x}\right| + |\sin x| \le 2. \tag{5.260}$$

Choosing $x = k(r'-r)$, with $r' > r$, we get

$$\left|\frac{1}{k}\sin\left(k(r-r')\right)\right| \le \frac{2(r'-r)}{1+k(r'-r)}, \tag{5.261}$$

that implies (5.258) because the function $2X/(1+kX)$ is monotonically increasing with $X > 0$ for all k. From Eq. (5.258) it is then easy to verify

$$|\dot{g}(k,r,r')| \le \frac{3r'}{k}. \tag{5.262}$$

Together with Lemma 5.16 and $|y| = |f|$ we thereby obtain

$$|x(k,r)| \le \frac{3}{k} e^{Q_k(0)} \|r' V(r')\|_1. \tag{5.263}$$

Now, we expand $\dot{y}$ in a Born series $\dot{y} = \sum_{n=0}^{\infty} \dot{y}_n$ with

$$\dot{y}_0 = x(k,r) \tag{5.264}$$

$$\dot{y}_{n+1} = -\int_r^{\infty} g(k,r,r') V(r') \dot{y}_n(k,r')\, dr' \tag{5.265}$$

and prove by induction that

$$|\dot{y}_n(k,r)| \le \frac{3}{k} e^{Q_k(0)} \|r' V(r')\|_1 \frac{Q_k^n(r)}{n!}. \tag{5.266}$$

Due to Eq. (5.263) the induction start is immediately evident. For the induction step assume that Eq. (5.266) holds, then

$$|\dot{y}_{n+1}(k,r)| \le \int_r^{\infty} |g(k,r,r') V(r')| |\dot{y}_n(k,r)|\, dr' \tag{5.267}$$

$$\le \frac{3}{k} e^{Q_k(0)} \|r'' V(r'')\|_1 \int_r^{\infty} \frac{2r'}{1+kr'} |V(r')| \frac{Q_k^n(r')}{n!}\, dr', \tag{5.268}$$

where we have used Eq. (5.258). From the definition of $Q_k(r)$ given in Lemma 5.16 it is evident that

$$\frac{d}{dr'} \frac{Q_k^{n+1}(r')}{(n+1)!} = \frac{2r'}{1+kr'} |V(r')| \frac{Q_k^n(r')}{n!}, \tag{5.269}$$

so that

$$|\dot{y}_{n+1}(k,r)| \le \frac{3}{k} e^{Q_k(0)} \|r'' V(r'')\|_1 \int_r^{\infty} \frac{d}{dr'} \frac{Q_k^{n+1}(r')}{(n+1)!}\, dr' \tag{5.270}$$

$$= \frac{3}{k} e^{Q_k(0)} \|r' V(r')\|_1 \frac{Q_k^{n+1}(r)}{(n+1)!}. \tag{5.271}$$

Hence, Eq. (5.266) is proven. Plugging this bound into

$$|\dot{y}(k,r)| \le \sum_{n=0}^{\infty} |\dot{y}_n(k,r)|, \tag{5.272}$$

we obtain the assertion of the Lemma. □

Lemma 5.18. *Let* $k \in [0,\infty)$ *and* $q_k := e^{Q_k(0)}\|rV(r)\|_1$*, then*

$$|\ddot{y}(k,r)| \le 6\frac{e^{Q_k(r)}}{k}\left[\frac{1}{k}(1+3q_k)+R_V\right]q_k. \tag{5.273}$$

Proof. We proceed in the same way as in the proof of Lemma 5.17. From Eq. (5.254) we get

$$\begin{aligned}\ddot{y}(k,r) = &-\int_r^\infty \ddot{g}(k,r,r')V(r')y(k,r')\,dr' \\ &-2\int_r^\infty \dot{g}(k,r,r')V(r')\dot{y}(k,r')\,dr' \\ &-\int_r^\infty g(k,r,r')V(r')\ddot{y}(k,r')\,dr' \end{aligned} \tag{5.274}$$

$$=: x(k,r) - \int_r^\infty g(k,r,r')V(r')\ddot{y}(k,r')\,dr' \tag{5.275}$$

Using Eq. (5.258) and Eq. (5.262) it is straightforward to check that

$$|\ddot{g}(k,r,r')| \le \frac{6r'}{k^2}(1+kr'). \tag{5.276}$$

Using this, inequality (5.262) for $\dot{g}$, and the bound on y obtained from

Lemma 5.16, we get

$$|x(k,r)| \leq \frac{6}{k}\left(\frac{3}{k}e^{2Q_k(0)}\|r'V(r')\|_1^2 + \frac{1}{k}e^{Q_k(0)}\|r'V(r')\|_1 + e^{Q_k(0)}\|r'^2V(r')\|_1\right) \tag{5.277}$$

$$\leq \frac{6}{k}\left(\frac{3}{k}q_k + \frac{1}{k} + R_V\right)q_k, \tag{5.278}$$

where we have used that $\|r^2V(r)\|_1 \geq R_V\|rV(r)\|_1$. Now, we can proceed in exactly the same way as in the proof of Lemma 5.17 to arrive at the assertion. □

Lemma 5.19. *Let $k \in [0,\infty)$ and $q_k := e^{Q_k(0)}\|rV(r)\|_1$, then*

$$|\dddot{y}(k,r)| \leq 18\frac{e^{Q_k(r)}}{k}\left[\frac{3}{k}(1+3q_k) + R_V\right]^2 q_k. \tag{5.279}$$

We omit the proof of this Lemma because it runs along the same lines as the proof of Lemma 5.18.

We can now prove some bounds on the imaginary part of the logarithmic derivative of the Jost function F. Note that the bounds that we got for $|y^{(n)}|$ all depend on powers of $e^{Q_k(0)} \leq e^{2\|V(r)\|_1/k}$ (cf. the definition of $Q_k(r)$ in Lemma 5.16), therefore they will be useful only for $k \approx \|V\|_1$ or bigger.

Lemma 5.20. *Let*

$$\tilde{K} := 6\|V\|_1, \quad L(k) := \operatorname{Im}\frac{\dot{F}(k)}{F(k)}, \quad \textit{and} \quad q := \frac{1}{2\|V\|_1} + 6R_V. \tag{5.280}$$

Then, for $k \geq \tilde{K}$,

$$|L(k)| \leq 2R_V\frac{\tilde{K}}{k}, \tag{5.281}$$

$$|\dot{L}(k)| \leq 4R_V\frac{\tilde{K}}{k}q, \tag{5.282}$$

$$|\ddot{L}(k)| \le 12 R_V \frac{\tilde{K}}{k} q^2, \tag{5.283}$$

and

$$|\dot{S}| \le 4 R_V \frac{\tilde{K}}{k}, \tag{5.284}$$

$$|\ddot{S}| \le 8 R_V \frac{\tilde{K}}{k} q + 16 R_V^2 \frac{\tilde{K}^2}{k^2}, \tag{5.285}$$

$$|\dddot{S}| \le 24 R_V \frac{\tilde{K}}{k} q^2 + 96 R_V^2 \frac{\tilde{K}^2}{k^2} q + 64 R_V^3 \frac{\tilde{K}^3}{k^3}. \tag{5.286}$$

Proof. Since $|L| \le |\dot{F}|/|F|$, we need an upper bound on $|\dot{F}|$ and a lower bound on $|F|$. For the upper bound we observe that $\dot{F}(k) = \dot{f}(k,0) = \dot{y}(k,0)$ and hence due to Lemma 5.17

$$|\dot{F}(k)| \le 3 \frac{e^{Q_k(0)}}{k} q_k = 3 \frac{e^{2Q_k(0)}}{k} \|rV(r)\|_1. \tag{5.287}$$

Upon using

$$Q_k(0) = \int_0^\infty \frac{2r'}{1+kr'} |V(r')|\, dr' \le \frac{2}{k} \|V\|_1 \le \frac{2}{\tilde{K}} \|V\|_1 = \frac{1}{3}, \tag{5.288}$$

$\|rV(r)\|_1 \le R_V \|V\|_1$ and $e^{2/3} < 2$, we obtain

$$|\dot{F}(k)| \le 3 \frac{e^{\frac{2}{3}}}{k} R_V \|V\|_1 \le 6 R_V \frac{\|V\|_1}{k}. \tag{5.289}$$

We derive the lower bound for $|F(k)|$ from the Lippmann-Schwinger equation (5.251). For $F(k) = f(k,0)$ it reads

$$F(k) = 1 + \int_0^\infty \frac{1}{k} \sin(kr') V(r') f(k,r'). \tag{5.290}$$

With the help of the bound on $f(k,r)$ from Lemma 5.16 and the bound on the sinus term in Eq. (5.258) we obtain for the integral

$$\left|\int_0^\infty \frac{1}{k}\sin(kr')V(r')f(k,r')\right| \leq e^{Q_k(0)} \int_0^\infty |V(r')| \frac{2r'}{1+kr'}\,dr' \tag{5.291}$$

$$\leq e^{2\frac{\|V\|_1}{k}} 2\frac{\|V\|_1}{k}. \tag{5.292}$$

Hence, for $k \geq \tilde{K}$ we have

$$|F(k)| \geq \left|1 - \left|\int_0^\infty \frac{1}{k}\sin(kr')V(r')f(k,r')\right|\right| \geq 1 - e^{\frac{1}{3}}\frac{1}{3} \geq \frac{1}{2}. \tag{5.293}$$

This and the upper bound on $|\dot{F}|$ imply the bound on L in Eq. (5.281).

To obtain the bound for $|\dot{L}|$ in Eq. (5.282), observe that with the help of the bounds for $|\dot{F}|$ in Eq. (5.289) and for $|F|$ in Eq. (5.293) we have

$$|\dot{L}| \leq \frac{|\ddot{F}|}{|F|} + \frac{|\dot{F}|^2}{|F|^2} \leq 2|\ddot{F}| + 12^2 R_V^2 \frac{\|V\|_1^2}{k^2}. \tag{5.294}$$

We get an upper bound for $|\ddot{F}|$ by using Lemma 5.18, Eq. (5.288) and $\|rV(r)\|_1 \leq R_V\|V\|_1$ as follows

$$|\ddot{F}(k)| = |\ddot{y}(k,0)| \leq 6\frac{e^{Q_k(0)}}{k}\|rV(r)\|_1 \left[\frac{1}{k}(1 + 3e^{Q_k(0)}\|rV(r)\|_1) + R_V\right] \tag{5.295}$$

$$\leq 12R_V\frac{\|V\|_1}{k}\left[\frac{1}{k}(1 + 6R_V\|V\|_1) + R_V\right] \tag{5.296}$$

$$\leq 12R_V\frac{\|V\|_1}{k}\left[\frac{1}{6\|V\|_1} + 2R_V\right]. \tag{5.297}$$

Plugging this into Eq. (5.294) yields

$$|\dot{L}| \leq 24R_V\frac{\|V\|_1}{k}\left[\frac{1}{6\|V\|_1} + 2R_V + 6R_V\frac{\|V\|_1}{k}\right]. \tag{5.298}$$

For $k \geq \tilde{K} = 6\|V\|_1$, we get

$$|\dot{L}| \leq 24R_V \frac{\|V\|_1}{k}\left[\frac{1}{6\|V\|_1} + 3R_V\right], \tag{5.299}$$

therefore Eq. (5.282) is verified.

We now prove Eq. (5.283). Using the bounds for $|\ddot{F}|$ in Eq. (5.297), for $|\dot{F}|$ in Eq. (5.289) and for $|F|$ in Eq. (5.293), we get

$$|\ddot{L}| \leq 2|\dddot{F}| + 6\cdot 12^2 R_V^2 \frac{\|V\|_1^2}{k^2}\left[\frac{1}{6\|V\|_1} + 2R_V\right] + 2\cdot 12^3 R_V^3 \frac{\|V\|_1^3}{k^3}. \tag{5.300}$$

Lemma 5.19, Eq. (5.288) and $\|rV(r)\|_1 \leq R_V\|V\|_1$ yield

$$|\dddot{F}(k)| = |\dddot{y}(k,0)| \leq 18\frac{e^{2Q_k(0)}}{k}\|rV(r)\|_1\left[\frac{3}{k}(1 + 3e^{Q_k(0)}\|rV(r)\|_1) + R_V\right]^2 \tag{5.301}$$

$$\leq 3\cdot 12R_V\frac{\|V\|_1}{k}\left[\frac{1}{2\|V\|_1} + 4R_V\right]^2 \tag{5.302}$$

along the same lines as before. Plugging this into Eq. (5.300) we obtain

$$|\ddot{L}| \leq 24R_V\frac{\|V\|_1}{k}\Bigg[3\left[\frac{1}{2\|V\|_1} + 4R_V\right]^2 + 36R_V\frac{\|V\|_1}{k}\left[\frac{1}{6\|V\|_1} + 2R_V\right] + 12^2R_V^2\frac{\|V\|_1^2}{k^2}\Bigg] \tag{5.303}$$

$$\leq 24R_V\frac{\|V\|_1}{k}\left[3\left[\frac{1}{2\|V\|_1} + 4R_V\right]^2 + 6R_V\left[\frac{1}{2\|V\|_1} + 4R_V\right] + 4R_V^2\right] \tag{5.304}$$

$$\leq 72R_V\frac{\|V\|_1}{k}\left[\frac{1}{2\|V\|_1} + 6R_V\right]^2, \tag{5.305}$$

which finishes the proof of Eq. (5.283).

From the bounds on L and on its derivatives we get the analogous bounds on the derivatives of the S-matrix, by using the inequalities (5.235), (5.236), and (5.237), that we repeat here:

$$|\dot{S}| \leq 2|L|, \tag{5.306}$$

$$|\ddot{S}| \leq 2|\dot{L}| + 4|L|^2, \tag{5.307}$$

$$|\dddot{S}| \leq 2|\ddot{L}| + 12|L|\,|\dot{L}| + 8|L|^3. \tag{5.308}$$

Substitution of the bounds (5.281)-(5.283) completes the proof. □

We now combine the bounds that we got for $k \geq \tilde{K}$ with those from Theorem 5.1, that we will use for $k \leq \tilde{K}$, to prove Theorem 5.2.

Proof (of Theorem 5.2). At first, we substitute $k = \tilde{K}$ in the bounds of Lemma 5.20, getting that, for $k \geq \tilde{K}$,

$$|\dot{S}| \leq 4R_V, \tag{5.309}$$

$$|\ddot{S}| \leq 8R_V q + 16R_V^2, \tag{5.310}$$

$$\begin{aligned} |\dddot{S}| &\leq 24R_V q^2 + 96R_V^2 q + 64R_V^3 \\ &\leq 8R_V(9q^2 + 14R_V^2). \end{aligned} \tag{5.311}$$

To get inequalities valid for any $k \geq 0$ we sum the latter bounds and those from theorem 5.1, choosing there $K = \tilde{K}$. In this way we have

$$\|\dot{S}\|_\infty \leq \frac{2}{s}\left[1 + s(3R_V + r_0)\right] \tag{5.312}$$

$$\|\ddot{S}\|_\infty \leq \frac{4}{s^2}\left\{3 + 2s^2\left[\frac{r_0}{\alpha} + (3R_V + r_0)^2 + R_V q\right]\right\} \tag{5.313}$$

$$\|\dddot{S}\|_\infty \leq \frac{4}{s^3}\Bigg\{15 + 6s(R_V + r_0) + 12s^2\frac{r_0}{\alpha} \\ + s^3\left[\frac{7r_0}{\alpha} + \frac{12r_0}{\alpha}(R_V + r_0) + 8(3R_V + r_0)^3 + 18R_V q^2\right]\Bigg\}, \tag{5.314}$$

that is Theorem 5.2. □

5.6 Proof of Theorem 5.3

We want to find an upper bound for

$$\|\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 = \|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 + \|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2. \tag{5.315}$$

Consider $\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2$ first. Using the expansion in generalized eigenfunctions, we get

$$e^{-iHt} P_{ac}\psi(r) = \int_0^\infty \hat{\psi}(k)\psi^+(k,r)e^{-ik^2 t}\, dk. \tag{5.316}$$

Due to Eq. (5.29), ψ^+ is known for $r \geq R_V$, but not for $r < R_V$, hence this expression can not be used directly. However, in the following Lemma we obtain an expression for $\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2$ that does not need explicit knowledge of how the generalized eigenfunctions behave for $r < R_V$. It is inspired by [56].

Lemma 5.21. *Let $\psi \in \mathcal{D}(H)$, $R \geq R_V$ and*

$$Z_{ac}(k,k') := \frac{W(\bar{\psi}^+(k',R), \psi^+(k,R))}{k'^2 - k^2}. \tag{5.317}$$

Then

$$\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 = \left\| \int_0^\infty Z_{ac}(k,\cdot)\hat{\psi}(k)e^{-ik^2 t} dk \right\|_2^2 \tag{5.318}$$

and

$$Z_{ac}(k,k') = \frac{i}{4}\Bigg[\frac{e^{i(k+k')R}S(k) - e^{-i(k+k')R}\bar{S}(k')}{k+k'} - \frac{e^{i(k-k')R}\bar{S}(k')S(k) - e^{-i(k-k')R}}{k-k'}\Bigg]. \tag{5.319}$$

Proof. Recall that the generalized Fourier transform is

$$\mathcal{F}\psi(k) = \int_0^\infty \psi(r)\bar{\psi}^+(k,r)\,dr, \tag{5.320}$$

and that it is a unitary operator on the subspace of absolute continuity of the Hamiltonian. Moreover, $P_{ac} = \mathcal{F}^{-1}\mathcal{F}$ (see (5.33)). Therefore we can write

$$\begin{aligned}\|P_{ac}\mathbf{1}_R e^{-iHt}P_{ac}\psi\|_2 = \|P_{ac}\mathbf{1}_R P_{ac}e^{-iHt}\psi\|_2 &= \|\mathcal{F}P_{ac}\mathbf{1}_R P_{ac}e^{-iHt}\psi\|_2\\ &= \|\mathcal{F}\mathbf{1}_R\mathcal{F}^{-1}\mathcal{F}e^{-iHt}\psi\|_2.\end{aligned} \tag{5.321}$$

Now,

$$\begin{aligned}&\left(\mathcal{F}\mathbf{1}_R\mathcal{F}^{-1}\mathcal{F}e^{-iHt}\psi\right)(k')\\ &= \int_0^\infty dr\,\bar{\psi}^+(k',r)\mathbf{1}_R(r)\int_0^\infty dk\,e^{-ik^2t}\hat{\psi}(k)\psi^+(k,r) \qquad (5.322)\\ &= \int_0^\infty dk\,e^{-ik^2t}\hat{\psi}(k)\int_0^\infty dr\,\mathbf{1}_R(r)\psi^+(k,r)\bar{\psi}^+(k',r), \qquad (5.323)\end{aligned}$$

so that, the integral kernel of $\mathcal{F}\mathbf{1}_R\mathcal{F}^{-1}$ reads

$$\int_0^\infty dr\,\mathbf{1}_R(r)\psi^+(k,r)\bar{\psi}^+(k',r). \tag{5.324}$$

This integral kernel can be expressed in terms of $\psi^+(k',R)$ with $R \geq R_V$.

Observing

$$\frac{d}{dr} W(\bar{\psi}^+(k', r), \psi^+(k, r)) = (k'^2 - k^2)\psi^+(k, r)\bar{\psi}^+(k', r) \tag{5.325}$$

and using $\psi^+(k, 0) = 0$, we get upon integration

$$\int_0^\infty dr\, \mathbf{1}_R(r)\psi^+(k, r)\bar{\psi}^+(k', r) = \frac{W(\bar{\psi}^+(k', R), \psi^+(k, R))}{k'^2 - k^2} = Z_{ac}(k, k') \tag{5.326}$$

and therefore

$$\left(\mathcal{F}\mathbf{1}_R\mathcal{F}^{-1}\mathcal{F}e^{-iHt}\psi\right)(k') = \int_0^\infty dk\, e^{-ik^2t}\hat{\psi}(k)Z_{ac}(k, k'), \tag{5.327}$$

which when plugged into Eq. (5.321) proves Eq. (5.318).

To prove Eq. (5.319) we use $\psi^+(k, R) = \frac{1}{2i}(S(k)e^{ikR} - e^{-ikR})$, which is a direct consequence of Eqs. (5.31) and (5.35). With this we get

$$\begin{aligned} W(\bar{\psi}^+(k', R), \psi^+(k, R)) = \;& \frac{i}{4}(k + k')\left(\bar{S}(k')S(k)e^{i(k-k')R} - e^{-i(k-k')R}\right) \\ & - \frac{i}{4}(k - k')\left(S(k)e^{i(k+k')R} - \bar{S}(k')e^{-i(k+k')R}\right). \end{aligned} \tag{5.328}$$

Plugging this into Eq. (5.317) finishes the proof. □

To extract a time decaying factor from the k-integral in Eq. (5.318), we employ the method of stationary phase. We use two integrations by parts because one is not enough to obtain the well known t^{-3}-factor as leading order. Observe that

$$e^{-ik^2t} = -\frac{\partial_k^2 e^{-ik^2t}}{2t(2tk^2 + i)}, \tag{5.329}$$

which when plugged into Eq. (5.318) yields upon integration by parts

$$
\begin{aligned}
&\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \\
&= \int_0^\infty \left| \int_0^\infty Z_{ac}(k,k')\hat{\psi}(k) \frac{\partial_k^2 e^{-ik^2 t}}{2t(2tk^2+i)}\, dk \right|^2 dk' \qquad (5.330)\\
&= \int_0^\infty \left| \int_0^\infty \partial_k^2 \left[Z_{ac}(k,k') \frac{\hat{\psi}(k)}{2t(2tk^2+i)} \right] e^{-ik^2 t}\, dk \right|^2 dk'. \qquad (5.331)
\end{aligned}
$$

The boundary terms vanish because of Lemma 5.25, for the proof of which we need the auxiliary Lemmas 5.22-5.24. They provide more knowledge about $Z_{ac}(k,k')$ and $\hat{\psi}(k)$ as well as their derivatives, especially in the limits $k \to 0$ and $k \to \infty$.

Lemma 5.22. *Let $K > 0$ be finite, $k \in [0,K]$, ψ satisfy the assumptions of Theorem 5.3, and*

$$\lambda := \begin{cases} 0, & \text{if } F(0) \neq 0 \\ 1, & \text{if } F(0) = 0. \end{cases} \qquad (5.332)$$

Then $\hat{\psi}(0) = -i\lambda\langle f(0,\cdot),\psi\rangle$ and

$$|\hat{\psi}(k)| \leq \lambda|\hat{\psi}(0)| + \|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty k. \qquad (5.333)$$

Proof. Using the fact that $S(0) = -1$ if $\lambda = 1$ and $S(0) = 1$ if $\lambda = 0$ (see [38, page 356] for the proof) we get

$$\bar{\psi}^+(0,r) = -\frac{1}{2i}(\bar{S}(0)\bar{f}(0,r) - \bar{f}(0,r)) = -i\lambda\bar{f}(0,r), \qquad (5.334)$$

and thereby

$$\hat{\psi}(0) = \int_0^\infty \psi(r)\bar{\psi}^+(0,r)\, dr = -i\lambda\langle f(0,\cdot),\psi\rangle. \qquad (5.335)$$

Moreover, observe that

$$|\hat{\psi}(k)| = \left|\hat{\psi}(0) + \int_0^k \dot{\hat{\psi}}(\tau)\, d\tau\right| \leq |\hat{\psi}(0)| + \|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty k = \lambda |\hat{\psi}(0)| + \|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty k, \tag{5.336}$$

indeed $\lambda^2 = \lambda$. □

Lemma 5.23. *Let $K > 0$ and $R \geq R_V$ be finite and recall Definition 5.3 and the definitions given in Theorem 5.1 and 5.2. Then for $k' \in [0, \infty)$ and $k \in [0, K)$*

$$\left|Z_{ac}(k, k')\right| \leq \frac{1}{2s_K}\left(2Rs_K + C_{1,K}\right) = \frac{z_{ac,K}(0,0)}{s_K}, \tag{5.337}$$

$$\left|Z_{ac}(k, k')\right| \leq \frac{1}{|k-k'|} = \frac{z_{ac,K}(0,1)}{|k-k'|}, \tag{5.338}$$

$$\left|\dot{Z}_{ac}(k, k')\right| \leq \frac{1}{4s_K^2}\left(2R^2 s_K^2 + 2RC_{1,K}s_K + C_{2,K}\right) = \frac{z_{ac,K}(1,0)}{s_K^2}, \tag{5.339}$$

$$\left|\dot{Z}_{ac}(k, k')\right| \leq \frac{2Rs_K + C_{1,K}}{2s_K|k-k'|} + \frac{1}{|k-k'|^2} = \frac{z_{ac,K}(1,1)}{s_K|k-k'|} + \frac{z_{ac,K}(1,2)}{|k-k'|^2}, \tag{5.340}$$

$$\begin{aligned}\left|\ddot{Z}_{ac}(k, k')\right| &\leq \frac{1}{6s_K^3}(2R^3 s_K^3 + 3R^2 s_K^2 C_{1,K} + 3Rs_K C_{2,K} + C_{3,K}) \\ &= \frac{z_{ac,K}(2,0)}{s_K^3},\end{aligned} \tag{5.341}$$

$$\begin{aligned}\left|\ddot{Z}_{ac}(k, k')\right| &\leq \frac{2R^2 s_K^2 + 2Rs_K C_{1,K} + C_{2,K}}{2s_K^2|k-k'|} + \frac{2Rs_K + C_{1,K}}{s_K|k-k'|^2} + \frac{2}{|k-k'|^3} \\ &= \frac{z_{ac,K}(2,1)}{s_K^2|k-k'|} + \frac{z_{ac,K}(2,2)}{s_K|k-k'|^2} + \frac{z_{ac,K}(2,3)}{|k-k'|^3}.\end{aligned} \tag{5.342}$$

For $k \in [0, \infty)$ we have the same bounds with the index K omitted on the right hand side.

Proof. Let $k \in [0, K)$ and

$$Z_{ac}(k,k') = \frac{i}{4}\Bigg[\frac{e^{i(k+k')R}S(k) - e^{-i(k+k')R}\bar{S}(k')}{k+k'} - \frac{e^{i(k-k')R}\bar{S}(k')S(k) - e^{-i(k-k')R}}{k-k'}\Bigg] \tag{5.343}$$

$$=: \frac{i}{4}\left[\frac{h_1(k,k')}{k+k'} - \frac{h_2(k,k')}{k-k'}\right]. \tag{5.344}$$

Now, Eq. (5.338) follows from the fact that $|S| = 1$ and $|k+k'| \geq |k-k'|$. To prove Eq. (5.337), we use $\bar{S}(k') = S(-k')$ and observe that via Lipschitz and Theorem 5.1

$$\frac{S(k) - S(-k')}{k-(-k')} \leq \frac{C_{1,K}}{s_K}. \tag{5.345}$$

Using this and

$$h_1(k,k') = \left(e^{i(k+k')R} - e^{-i(k+k')R}\right)S(k) + e^{-i(k+k')R}\left(S(k) - \bar{S}(k')\right), \tag{5.346}$$

we get

$$\left|\frac{h_1(k,k')}{k+k'}\right| \leq \left|\frac{e^{i(k+k')R} - e^{-i(k+k')R}}{k+k'}\right| + \left|\frac{S(k) - S(-k')}{k-(-k')}\right| \tag{5.347}$$

$$\leq 2R\left|\frac{\sin((k+k')R)}{(k+k')R}\right| + \left|\frac{S(k) - S(-k')}{k-(-k')}\right| \leq 2R + \frac{C_{1,K}}{s_K}. \tag{5.348}$$

Together with the analogous bound for the second summand in Eq. (5.343) this yields (5.337). To prove Eq. (5.340) observe that

$$\dot{Z}_{ac}(k,k') = \frac{i}{4}\left[\frac{\dot{h}_1(k,k')}{k+k'} - \frac{\dot{h}_2(k,k')}{k-k'} - \frac{h_1(k,k')}{(k+k')^2} + \frac{h_2(k,k')}{(k-k')^2}\right]. \tag{5.349}$$

Using the bounds on the derivatives of the S-matrix given in Theorem 5.1

we find

$$|\dot{h}_1(k,k')| = |iR\left(e^{i(k+k')R}S(k) + e^{-i(k+k')R}\bar{S}(k')\right) + e^{i(k+k')R}\dot{S}(k)| \tag{5.350}$$

$$\leq 2R + \frac{C_{1,K}}{s_K} \tag{5.351}$$

$$|\dot{h}_2(k,k')| = |iR\left(e^{i(k-k')R}\bar{S}(k')S(k) + e^{-i(k-k')R}\right) + e^{i(k-k')R}\bar{S}(k')\dot{S}(k)| \tag{5.352}$$

$$\leq 2R + \frac{C_{1,K}}{s_K}. \tag{5.353}$$

This and Eq. (5.349) immediately yield Eq. (5.340). To prove Eq. (5.339) note that the Taylor expansion of $h_1(x,k')$ and $h_2(x,k')$ in x around k reads

$$h_{1,2}(x,k') = h_{1,2}(k,k') + \dot{h}_{1,2}(k,k')(x-k) + \int_k^x \ddot{h}_{1,2}(\tau,k')(x-\tau)\,d\tau. \tag{5.354}$$

If we evaluate this at $x = -k'$ for h_1 and at $x = k'$ for h_2 and observe that $h_1(-k',k') = 0 = h_2(k',k')$, we get

$$h_{1,2}(k,k') = \dot{h}_{1,2}(k,k')(k \pm k') + \int_k^{\mp k'} \ddot{h}_{1,2}(\tau,k')(\tau \pm k')\,d\tau. \tag{5.355}$$

Plugging this into Eq. (5.349) and employing the variable substitutions $\tau = k-(k+k')\tau'$ for the $\ddot{h}_1$-integral and $\tau = k-(k-k')\tau'$ for the $\ddot{h}_2$-integral, then yields

$$\dot{Z}_{ac}(k,k') = \frac{i}{4}\Big[-\int_k^{-k'} \ddot{h}_1(\tau,k')\frac{\tau+k'}{(k+k')^2}\,d\tau + \int_k^{k'} \ddot{h}_2(\tau,k')\frac{\tau-k'}{(k-k')^2}\,d\tau\Big] \tag{5.356}$$

$$\begin{aligned} &= \frac{i}{4}\Big[\int_0^1 \ddot{h}_1(k-(k+k')\tau',k')(1-\tau')\,d\tau' \\ &\quad - \int_0^1 \ddot{h}_2(k-(k-k')\tau',k')(1-\tau')\,d\tau'\Big]. \end{aligned} \tag{5.357}$$

Moreover, the bounds on derivatives of the S-matrix due to Theorem 5.1 imply

$$\begin{aligned}
|\ddot{h}_1(k,k')| &= |-R^2\left(e^{i(k+k')R}S(k) - e^{-i(k+k')R}\bar{S}(k')\right) + 2iRe^{i(k+k')R}\dot{S}(k) \\
&\quad + e^{i(k+k')R}\ddot{S}(k)| && (5.358) \\
&\leq 2R^2 + 2R\frac{C_{1,K}}{s_K} + \frac{C_{2,K}}{s_K^2} && (5.359) \\
|\ddot{h}_2(k,k')| &= |-R^2\left(e^{i(k-k')R}\bar{S}(k')S(k) - e^{-i(k-k')R}\right) + 2iRe^{i(k-k')R}\bar{S}(k')\dot{S}(k) \\
&\quad + e^{i(k-k')R}\bar{S}(k')\ddot{S}(k)| && (5.360) \\
&\leq 2R^2 + 2R\frac{C_{1,K}}{s_K} + \frac{C_{2,K}}{s_K^2}. && (5.361)
\end{aligned}$$

Using this and Eq. (5.357), we obtain Eq. (5.339). Analogously to the proof of Eqs. (5.339) and (5.340), we arrive at Eqs. (5.341) and (5.342).

For $k \in [0,\infty)$ the proof is the same, except that we use the S-matrix bounds provided by Theorem 5.2 rather than those of Theorem 5.1. In effect this amounts to omitting the index K everywhere. □

Lemma 5.24. *Let $R \geq R_V$, $K > 0$, $k \in [0,K]$, and*

$$\lambda := \begin{cases} 0, & \text{if } F(0) \neq 0 \\ 1, & \text{if } F(0) = 0. \end{cases} \tag{5.362}$$

Then

$$\left|Z_{ac}(k,k')\right| \leq \lambda\frac{z_{ac,K}(0,0)}{s_K} + \frac{z_{ac,K}(1,0)}{s_K^2}k \qquad \text{if } k' \in [0,2K], \tag{5.363}$$

$$\left|Z_{ac}(k,k')\right| \leq \lambda\frac{z_{ac,K}(0,1)}{k'} + \left[\frac{z_{ac,K}(1,1)}{s_K|k-k'|} + \frac{z_{ac,K}(1,2)}{|k-k'|^2}\right]k \quad \text{if } k' \in [2K,\infty). \tag{5.364}$$

Proof. Clearly,

$$|Z_{ac}(k,k')| = \left| Z_{ac}(0,k') + \int_0^k \dot{Z}_{ac}(\tau,k')\,d\tau \right|$$
$$\le |Z_{ac}(0,k')| + \int_0^k |\dot{Z}_{ac}(\tau,k')|\,d\tau. \tag{5.365}$$

First, we prove Eq. (5.364). Observing that

$$Z_{ac}(0,k') = \frac{i}{4k'}\left[e^{ik'R} + e^{-ik'R}\bar{S}(k')\right](S(0)-1) \tag{5.366}$$

and using the fact that $S(0) = \mp 1$ for $\lambda = 1$ and 0, respectively (see [38, page 356] for the proof), we obtain

$$|Z_{ac}(0,k')| \le \lambda \frac{1}{k'}. \tag{5.367}$$

If we plug this into Eq. (5.365) and employ the bound for $|\dot{Z}_{ac}(k,k')|$ provided by Eq. (5.340), we arrive at

$$\left|Z_{ac}(k,k')\right| \le \lambda \frac{z_{ac,K}(0,1)}{k'} + \int_0^k \left[\frac{z_{ac,K}(1,1)}{s_K|\tau-k'|} + \frac{z_{ac,K}(1,2)}{|\tau-k'|^2}\right] d\tau. \tag{5.368}$$

Since $k \in [0,K]$ and $k' \in [2K,\infty)$, we have $|\tau - k'| \ge |k-k'|$ and this implies

$$\left|Z_{ac}(k,k')\right| \le \lambda \frac{z_{ac,K}(0,1)}{k'} + \left[\frac{z_{ac,K}(1,1)}{s_K|k-k'|} + \frac{z_{ac,K}(1,2)}{|k-k'|^2}\right] k, \tag{5.369}$$

which finishes the proof of Eq. (5.364). As for Eq. (5.363), note that

$$Z_{ac}(0,k') = \frac{i}{4k'}\left[e^{ik'R}(\bar{S}(k')+1) - \bar{S}(k')(e^{ik'R} - e^{-ik'R})\right](S(0)-1). \tag{5.370}$$

Now, via Lipschitz and Theorem 5.1 we see that

$$\left|\frac{\bar{S}(k')+1}{k'}\right| = \left|\frac{\bar{S}(k')-\bar{S}(0)}{k'-0}\right| \leq \|1_K \dot{S}\|_\infty \leq \frac{C_{1,K}}{s_K}, \tag{5.371}$$

which together with

$$\left|\frac{e^{ik'R}-e^{-ik'R}}{k'}\right| = \left|\frac{e^{2ik'R}-e^{0}}{k'-0}\right| \leq 2R, \tag{5.372}$$

the fact that $S(0) = \mp 1$ for $\lambda = 1$ and 0, respectively, and Eq. (5.370) yields

$$|Z_{ac}(0,k')| \leq \lambda \frac{1}{2}\left[2R + \frac{C_{1,K}}{s_K}\right] = \lambda \frac{z_{ac,K}(0,0)}{s_K}. \tag{5.373}$$

Plugging this and the bound for $|\dot{Z}_{ac}(k,k')|$ provided by Eq. (5.339) into Eq. (5.365) we have

$$|Z_{ac}(k,k')| \leq \lambda \frac{z_{ac,K}(0,0)}{s_K} + \int_0^k \frac{z_{ac,K}(1,0)}{s_K^2}\, d\tau. \tag{5.374}$$

Performing the integration in τ completes the proof of Eq. (5.363). □

These Lemmas allow us to show that the boundary terms due to the integration by parts in Eq. (5.331) vanish.

Lemma 5.25. *Let ψ satisfy the assumptions of Theorem 5.3, then*

$$\int_0^\infty Z_{ac}(k,k')\hat{\psi}(k)\frac{\partial_k^2 e^{-ik^2 t}}{2tk^2+i}\, dk = \int_0^\infty \partial_k^2\left[Z_{ac}(k,k')\frac{\hat{\psi}(k)}{2tk^2+i}\right] e^{-ik^2 t}\, dk. \tag{5.375}$$

Proof. Clearly, integrating by parts twice yields

$$\int_0^\infty Z_{ac}(k,k')\hat{\psi}(k)\frac{\partial_k^2 e^{-ik^2 t}}{2tk^2+i}\,dk = \left[\frac{Z_{ac}(k,k')\hat{\psi}(k)}{2tk^2+i}\partial_k e^{-ik^2 t}\right]_0^\infty \tag{5.376}$$

$$-\left[\partial_k\left(\frac{Z_{ac}(k,k)\hat{\psi}(k)}{2tk^2+i}\right)e^{-ik^2 t}\right]_0^\infty \tag{5.377}$$

$$+\int_0^\infty \partial_k^2\left(\frac{Z_{ac}(k,k')\hat{\psi}(k)}{2tk^2+i}\right)e^{-ik^2 t}\,dk, \tag{5.378}$$

so we need to show that the boundary terms vanish. We begin with the term (5.376). At infinity it vanishes because $Z_{ac}(k,k')$ is globally bounded (Lemma 5.23), $\hat{\psi}(k)\to 0$ as $k\to\infty$ ($\hat{\psi}$ is square integrable) and the time dependent factors tend to zero, too. At zero the term (5.376) vanishes because $Z_{ac}(0,k')$ and $\hat{\psi}(0)$ are bounded (Lemmas 5.23 and 5.22), while the time dependent factors are zero for $k=0$.

Now, look at Eq. (5.377) and observe that

$$\partial_k\left(\frac{Z_{ac}(k,k')\hat{\psi}(k)}{2tk^2+i}\right) = \left(\dot{Z}_{ac}(k,k')\hat{\psi}(k)+Z_{ac}(k,k')\dot{\hat{\psi}}(k)\right)\frac{1}{2tk^2+i} \tag{5.379}$$

$$-Z_{ac}(k,k')\hat{\psi}(k)\frac{4tk}{(2tk^2+i)^2}. \tag{5.380}$$

The last summand vanishes as $k\to 0$ and $k\to\infty$ for the same reasons (5.376) vanished, so let us focus on (5.379). For $k\to\infty$ it vanishes because $Z_{ac}(k,k')$ as well as $\dot{Z}_{ac}(k,k')$ are bounded (Lemma 5.23), $\hat{\psi}(k)$ tends to zero ($\hat{\psi}$ is square integrable), and $\dot{\hat{\psi}}(k)$ can only diverge slower than k ($\|\dot{\hat{\psi}}w\|_1<\infty$ by assumption). In case there is no zero resonance ($\lambda=0$) the term (5.379) evaluates to zero at $k=0$ because $|Z_{ac}(0,k')|\le k\,z_{ac,K}(1,0)/s_K^2$ (Lemma 5.24), $\dot{\hat{\psi}}(k)$ can only diverge slower than $1/k$ as $k\to 0$ ($\|\dot{\hat{\psi}}w\|_1<\infty$ by assumption), $|\dot{Z}_{ac}(0,k')|$ is bounded (Lemma 5.23) and $\hat{\psi}(0)=0$ (Lemma 5.22). In case there is a zero resonance ($\lambda=1$), then $S(0) = -1$ (see [38, page 356] for the proof), hence

$$Z_{ac}(0,k') = -\frac{i}{2k'}(e^{ik'R} + e^{-ik'R}\bar{S}(k')). \tag{5.381}$$

Furthermore,

$$\begin{aligned}\dot{Z}_{ac}(k,k') = \frac{i}{4}\Big[&- \frac{e^{i(k+k')R}S(k) - e^{-i(k+k')R}\bar{S}(k')}{(k+k')^2} \\ &+ \frac{e^{i(k-k')R}\bar{S}(k')S(k) - e^{-i(k-k')R}}{(k-k')^2}\Big] \\ &+ \frac{1}{k+k'}\Big(iR(e^{i(k+k')R}S(k) + e^{-i(k+k')R}\bar{S}(k')) + e^{i(k+k')R}\dot{S}(k)\Big) \\ &- \frac{1}{k-k'}\Big(iR(e^{i(k-k')R}\bar{S}(k')S(k) + e^{-i(k-k')R}) \\ &+ e^{i(k-k')R}\bar{S}(k')\dot{S}(k)\Big)\Big],\end{aligned} \tag{5.382}$$

implies that

$$\dot{Z}_{ac}(0,k') = \frac{i}{4k'}(e^{ik'R} + e^{-ik'R}\bar{S}(k'))\dot{S}(0). \tag{5.383}$$

Moreover, from $\bar{f}(k,r) = f(-k,r)$ and $\bar{S}(k) = S(-k)$ we get

$$\hat{\psi}(k) = \int_0^\infty \psi(r)\bar{\psi}^+(k,r)\,dr \tag{5.384}$$

$$= -\frac{1}{2i}\int_0^\infty \psi(r)(S(-k)f(-k,r) - f(k,r))\,dr. \tag{5.385}$$

Employing $\hat{\psi}(0) = -i\int_0^\infty \psi(r)f(0,r)\,dr$ (Lemma 5.22) we then obtain

$$\dot{\hat{\psi}}(0) = -\frac{1}{2i}\int_0^\infty \psi(r)(-\dot{S}(0)f(k,r) - S(0)\dot{f}(0,r) - \dot{f}(0,r))\,dr \tag{5.386}$$

$$= \frac{1}{2}\dot{S}(0)\hat{\psi}(0) \tag{5.387}$$

and by plugging Eqs. (5.381), (5.383), (5.384), and (5.386) into the term (5.379), we see that (5.379) evaluates to zero at $k = 0$. This finishes the proof. □

We are now in the position to prove Theorem 5.3.

Proof (Theorem 5.3). Let $t > 0$. We start from Eq. (5.331), which reads

$$\begin{aligned}
&\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \\
&= \frac{1}{4t^2}\int_0^\infty \left| \int_0^\infty \partial_k^2 \left[Z_{ac}(k,k')\hat{\psi}(k)\frac{1}{2tk^2+i}\right] e^{-ik^2t}\, dk \right|^2 dk'. \qquad (5.388)
\end{aligned}$$

For $A, B, C \in \mathbb{R}$

$$(A+B+C)^2 \le 3(A^2+B^2+C^2), \qquad (5.389)$$

therefore with the shorthands

$$g_1(k,k') := \ddot{Z}_{ac}(k,k')\hat{\psi}(k) + 2\dot{Z}_{ac}(k,k')\dot{\hat{\psi}}(k) + Z_{ac}(k,k')\ddot{\hat{\psi}}(k), \qquad (5.390)$$

$$g_2(k,k') := \dot{Z}_{ac}(k,k')\hat{\psi}(k) + Z_{ac}(k,k')\dot{\hat{\psi}}(k), \qquad (5.391)$$

we get

$$\begin{aligned}
&\|P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \\
&\le \frac{3}{4t^2}\int_0^\infty \left| \int_0^\infty g_1(k,k')\frac{1}{2tk^2+i}e^{-ik^2t}\, dk\right|^2 dk' \qquad (5.392)\\
&\quad + \frac{3}{t^2}\int_0^\infty \left| \int_0^\infty g_2(k,k')\frac{4tk}{(2tk^2+i)^2}e^{-ik^2t}\, dk\right|^2 dk' \qquad (5.393)\\
&\quad + \frac{3}{4t^2}\int_0^\infty \left| \int_0^\infty Z_{ac}(k,k')\hat{\psi}(k)\frac{4t(i-6tk^2)}{(2tk^2+i)^3}e^{-ik^2t}\, dk\right|^2 dk'. \qquad (5.394)
\end{aligned}$$

Note that Eq. (5.389) as well as $(A+B)^2 \le 2(A^2+B^2)$ will be used repeatedly throughout the proof, sometimes without mention.

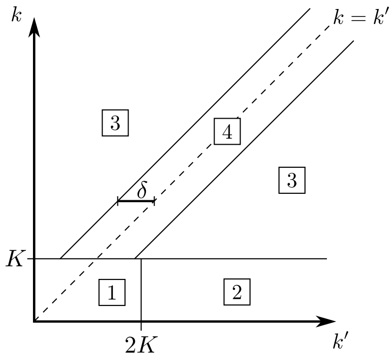


Figure 5.7: Division of the k-k'-plane used to estimate $||P_{ac}\mathbf{1}_R e^{-iHt} P_{ac}\psi||_2$.

Although we are not dealing with double integrals, it is useful to think of the k-k'-plane as it was the integration region, that we will divide as depicted in Fig. 5.7. Let us explain why. First, for a suitable $c_K > 0$, we can write by a change of variable

$$\left[\int_0^\infty \frac{1}{2t|2tk^2+i|}\,dk\right]^2 = \left[\frac{1}{2t^{3/2}}\int_0^\infty \frac{1}{|2k^2+i|}\,dk\right]^2 \le \frac{1}{2t^3}, \tag{5.395}$$

$$\left[\int_K^\infty \frac{1}{2t|2tk^2+i|}\,dk\right]^2 \le \frac{1}{t^4}\left[\int_K^\infty \frac{1}{2k^2}\,dk\right]^2 = \frac{c_K}{t^4}, \tag{5.396}$$

which suggests that the term (5.392) contains a t^{-3} contribution that comes from the part of the integration region where $k < K$, while the t^{-4} contribution comes from $k \ge K$. Second, $Z_{ac}(k,k')$ has an apparent singularity at $k = k'$ (see Eq. (5.319)). It is apparent in the sense that by performing the limit $k \to k'$ on the right hand side of Eq. (5.319) a finite quantity depending on derivatives of the S-matrix is obtained. Therefore, we will use a Taylor expansion in the stripe around $k = k'$, while we use a different strategy in the remaining regions.

Now, we split the integrals in Eqs. (5.392-5.394) according to Fig. 5.7. Let $h(k,k')$ be a placeholder for the integrands in Eqs. (5.392-5.394) and let the indicator functions $\mathbf{1}_{3,k'}(k)$ and $\mathbf{1}_{4,k'}(k)$ be one only on the regions 3 and 4, respectively. Then we obtain

$$
\begin{aligned}
&\int_0^\infty \left| \int_0^\infty h(k,k')\, dk \right|^2 dk' \\
&\leq 2 \int_0^{2K} \left[\int_0^K |h(k,k')|\, dk \right]^2 dk' && (5.397)\\
&\quad + 2 \int_{2K}^\infty \left[\int_0^K |h(k,k')|\, dk \right]^2 dk' && (5.398)\\
&\quad + 4 \int_0^\infty \left[\int_0^\infty \mathbf{1}_{3,k'} |h(k,k')|\, dk \right]^2 dk' && (5.399)\\
&\quad + 4 \int_0^\infty \left[\int_0^\infty \mathbf{1}_{4,k'} |h(k,k')|\, dk \right]^2 dk'. && (5.400)
\end{aligned}
$$

First, let us look at integral (5.392) in region 1. Using the bounds on $Z_{ac}(k,k')$ provided by Lemma 5.23 and

$$
\left[\int_0^K dk \frac{1}{\sqrt{4t^2k^4+1}} \right]^2 \leq \frac{1}{t} \left[\int_0^\infty dk \frac{1}{\sqrt{4k^4+1}} \right]^2 \leq \frac{2}{t}, \tag{5.401}
$$

obtained by change of variable, we get

$$
\begin{aligned}
&\frac{3}{2t^2} \int_0^{2K} dk' \left[\int_0^K dk |g_1(k,k')| \frac{1}{\sqrt{4t^2k^4+1}} \right]^2 && (5.402)\\
&\leq \frac{6K}{t^3} \left(\frac{z_{ac,K}(2,0)}{s_K^3} \|\mathbf{1}_K \hat{\psi}\|_\infty + 2 \frac{z_{ac,K}(1,0)}{s_K^2} \|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty + \frac{z_{ac,K}(0,0)}{s_K} \|\mathbf{1}_K \ddot{\hat{\psi}}\|_\infty \right)^2 && (5.403)\\
&\leq \frac{18K}{t^3 s_K^6} \Big(z_{ac,K}^2(2,0) \|\mathbf{1}_K \hat{\psi}\|_\infty^2 + 4 s_K^2 z_{ac,K}^2(1,0) \|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2 \\
&\qquad + s_K^4 z_{ac,K}^2(0,0) \|\mathbf{1}_K \ddot{\hat{\psi}}\|_\infty^2 \Big). && (5.404)
\end{aligned}
$$

In region 2 integral (5.392) takes the form

$$\frac{3}{2t^2}\int_{2K}^{\infty} dk' \left[\int_0^K dk |g_1(k,k')| \frac{1}{\sqrt{4t^2k^4+1}}\right]^2. \tag{5.405}$$

With the help of the bounds on $Z_{ac}(k,k')$ given in Lemma 5.23 and the fact that $|k'-k| \geq |k'-K|$ in region 2, we see that

$$\begin{aligned}
&|g_1(k,k')| \\
&\leq \frac{z_{ac,K}(2,1)\|\mathbf{1}_K\hat{\psi}\|_\infty + 2s_K z_{ac,K}(1,1)\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty + s_K^2 z_{ac,K}(0,1)\|\mathbf{1}_K\ddot{\hat{\psi}}\|_\infty}{s_K^2|k'-K|} \\
&\quad + \frac{z_{ac,K}(2,2)\|\mathbf{1}_K\hat{\psi}\|_\infty + 2s_K z_{ac,K}(1,2)\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty}{s_K|k'-K|^2} + \frac{z_{ac,K}(2,3)\|\mathbf{1}_K\hat{\psi}\|_\infty}{|k'-K|^3}.
\end{aligned} \tag{5.406}$$

Employing this in Eq. (5.405) together with the elementary inEq. (5.389) and Eq. (5.401), we obtain

$$\frac{3}{2t^2}\int_{2K}^{\infty} dk' \left[\int_0^K dk |g_1(k,k')| \frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.407}$$

$$\begin{aligned}
&\leq \frac{9}{t^3}\Bigg[\frac{3}{Ks_K^4}\Big(z_{ac,K}^2(2,1)\|\mathbf{1}_K\hat{\psi}\|_\infty^2 + 4s_K^2 z_{ac,K}^2(1,1)\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2 \\
&\quad + s_K^4 z_{ac,K}^2(0,1)\|\mathbf{1}_K\ddot{\hat{\psi}}\|_\infty^2\Big) \\
&\quad + \frac{2}{3K^3s_K^2}\Big(z_{ac,K}^2(2,2)\|\mathbf{1}_K\hat{\psi}\|_\infty^2 + 4s_K^2 z_{ac,K}^2(1,2)\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2\Big) \\
&\quad + \frac{z_{ac,K}^2(2,3)\|\mathbf{1}_K\hat{\psi}\|_\infty^2}{5K^5}\Bigg].
\end{aligned} \tag{5.408}$$

In region 3 the integral (5.392) reads (see Eq. (5.399))

$$\frac{3}{t^2}\int_0^{\infty} dk' \left[\int_0^{\infty} dk \mathbf{1}_{3,k'} |g_1(k,k')| \frac{1}{\sqrt{4t^2k^4+1}}\right]^2. \tag{5.409}$$

Now the k-integral ranges up to infinity and we could use $\|\hat{\psi}^{(n)}\|_\infty$ to handle the $\hat{\psi}$ dependency of g_1. However, the suprema can get big. In particular, as mentioned in Section 5.3, our bounds are most relevant for wave functions describing meta-stable systems. In this case, if $\alpha - i\beta$ is the resonance corresponding to the meta-stable state under consideration, then $\hat{\psi}$ will resemble a Breit Wigner function centered around $k = \alpha$, with width 2β and height $1/\sqrt{\beta}$. For small β, i.e. for long lifetime, the supremum of such a $\hat{\psi}$ is big, whereas the integral over $|\hat{\psi}|$ around $k = \alpha$ will be of order $\sqrt{\beta}$, which is small. Therefore, for states of physical interest, bounds depending on L^1-norms are more convenient than bounds involving suprema.

Since we are now in a region such that k can not be zero, we can pull the time dependency out of the integral via

$$\frac{1}{\sqrt{4t^2k^4+1}} \le \frac{1}{2tk^2} = \frac{1}{2t}\left(1+\frac{1}{k^2}\right)w(k) \le \frac{1}{2t}\left(1+\frac{1}{K^2}\right)w(k) \tag{5.410}$$

with $w(k) = (1+k^2)^{-1}$. It is useful to keep the weight function w as part of the integrand because $\hat{\psi}$ might not decay fast enough at infinity for $\|\hat{\psi}\|_1$ to be finite. Then

$$\frac{3}{t^2}\int_0^\infty dk' \left[\int_0^\infty dk \mathbf{1}_{3,k'} |g_1(k,k')| \frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.411}$$

$$\le \frac{3}{4t^4}\left(1+\frac{1}{K^2}\right)^2 \int_0^\infty dk' \left[\int_0^\infty dk \mathbf{1}_{3,k'} |g_1(k,k')| w(k)\right]^2 \tag{5.412}$$

$$\begin{aligned}
\le \frac{27}{4t^4}\left(1+\frac{1}{K^2}\right)^2 \int_0^\infty dk' \Bigg(&\left[\int_0^\infty dk \mathbf{1}_{3,k'} |\ddot{Z}_{ac}(k,k')\hat{\psi}(k)| w(k)\right]^2 \\
&+ \left[\int_0^\infty dk \mathbf{1}_{3,k'} |2\dot{Z}_{ac}(k,k')\dot{\hat{\psi}}(k)| w(k)\right]^2 \\
&+ \left[\int_0^\infty dk \mathbf{1}_{3,k'} |Z_{ac}(k,k')\ddot{\hat{\psi}}(k)| w(k)\right]^2 \Bigg),
\end{aligned} \tag{5.413}$$

where we have used the elementary inequality (5.389). At this point we employ Jensen's inequality to pull the square into the k-integrals, using

$|\hat{\psi}w|$, $|\dot{\hat{\psi}}w|$ and $|\ddot{\hat{\psi}}w|$, respectively, as measures. Hence,

$$\frac{3}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{3,k'}|g_1(k,k')|\frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.414}$$

$$\begin{aligned}
&\leq \frac{27}{4t^4}\left(1+\frac{1}{K^2}\right)^2 \\
&\quad\times\Big(\|\hat{\psi}w\|_1\int_0^\infty dk'\int_0^\infty dk\mathbf{1}_{3,k'}|\ddot{Z}_{ac}(k,k')|^2|\hat{\psi}(k)|w(k) \\
&\quad+4\|\dot{\hat{\psi}}w\|_1\int_0^\infty dk'\int_0^\infty dk\mathbf{1}_{3,k'}|\dot{Z}_{ac}(k,k')|^2|\dot{\hat{\psi}}(k)|w(k) \\
&\quad+\|\ddot{\hat{\psi}}w\|_1\int_0^\infty dk'\int_0^\infty dk\mathbf{1}_{3,k'}|Z_{ac}(k,k')|^2|\ddot{\hat{\psi}}(k)|w(k)\Big)
\end{aligned} \tag{5.415}$$

$$\begin{aligned}
&= \frac{27}{4t^4}\left(1+\frac{1}{K^2}\right)^2 \\
&\quad\times\int_K^\infty dk\left[\int_0^{k-\delta}dk'+\int_{k+\delta}^\infty dk'\right]\Big(\|\hat{\psi}w\|_1|\ddot{Z}_{ac}(k,k')|^2|\hat{\psi}(k)|w(k) \\
&\quad+4\|\dot{\hat{\psi}}w\|_1|\dot{Z}_{ac}(k,k')|^2|\dot{\hat{\psi}}(k)|w(k)+\|\ddot{\hat{\psi}}w\|_1|Z_{ac}(k,k')|^2|\ddot{\hat{\psi}}(k)|w(k)\Big),
\end{aligned} \tag{5.416}$$

where δ is defined in Fig. 5.7 and will be determined later. From the bounds on $Z_{ac}(k,k')$ in Lemma 5.23 we get

$$|\ddot{Z}_{ac}(k,k')|^2 \leq 3\left(\frac{z_{ac}^2(2,1)}{s^4(k'-k)^2}+\frac{z_{ac}^2(2,2)}{s^2(k'-k)^4}+\frac{z_{ac}^2(2,3)}{(k'-k)^6}\right), \tag{5.417}$$

$$|\dot{Z}_{ac}(k,k')|^2 \leq 2\left(\frac{z_{ac}^2(1,1)}{s^2(k'-k)^2}+\frac{z_{ac}^2(1,2)}{(k'-k)^4}\right), \tag{5.418}$$

$$|Z_{ac}(k,k')|^2 \leq \frac{z_{ac}^2(0,1)}{(k'-k)^2}, \tag{5.419}$$

which when plugged into Eq. (5.416) together with $\int_K^\infty dk|\hat{\psi}^{(n)}(k)|w(k) \leq$

$\|\hat{\psi}^{(n)}w\|_1$ yield

$$\frac{3}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{3,k'}|g_1(k,k')|\frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.420}$$

$$\leq \frac{27}{2t^4}\left(1+\frac{1}{K^2}\right)^2\left[3\|\hat{\psi}w\|_1^2\left(\frac{z_{ac}^2(2,1)}{s^4\delta}+\frac{z_{ac}^2(2,2)}{3s^2\delta^3}+\frac{z_{ac}^2(2,3)}{5\delta^5}\right)+\right.$$

$$\left.+\,8\|\dot{\hat{\psi}}w\|_1^2\left(\frac{z_{ac}^2(1,1)}{s^2\delta}+\frac{z_{ac}^2(1,2)}{3\delta^3}\right)+\|\ddot{\hat{\psi}}w\|_1^2\frac{z_{ac}^2(0,1)}{\delta}\right]. \tag{5.421}$$

In region 4 we employ Jensen's inequality in the same way as we did for region 3 and we use the bounds on $Z_{ac}(k,k')$ given in Lemma 5.23:

$$\frac{3}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{4,k'}|g_1(k,k')|\frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.422}$$

$$\leq \frac{27}{4t^4}\left(1+\frac{1}{K^2}\right)^2\int_K^\infty dk\int_{k-\delta}^{k+\delta}dk'\Big(\|\hat{\psi}w\|_1|\ddot{Z}_{ac}(k,k')|^2|\hat{\psi}(k)|w(k) \tag{5.423}$$

$$+\,4\|\dot{\hat{\psi}}w\|_1|\dot{Z}_{ac}(k,k')|^2|\dot{\hat{\psi}}(k)|w(k)+\|\ddot{\hat{\psi}}w\|_1|Z_{ac}(k,k')|^2|\ddot{\hat{\psi}}(k)|w(k)\Big)$$

$$\leq \frac{27}{2t^4}\left(1+\frac{1}{K^2}\right)^2\delta\left[\|\hat{\psi}w\|_1^2\frac{z_{ac}^2(2,0)}{s^6}+\|\dot{\hat{\psi}}w\|_1^2\frac{z_{ac}^2(1,0)}{s^4}+\|\ddot{\hat{\psi}}w\|_1^2\frac{z_{ac}^2(0,0)}{s^2}\right]. \tag{5.424}$$

Summing up Eqs. (5.404), (5.408), (5.421), and (5.424), we obtain the following bound for the integral (5.392)

$$\frac{3}{4t^2}\int_0^\infty\left|\int_0^\infty g_1(k,k')\frac{e^{-ik^2t}}{2tk^2+i}\,dk\right|^2dk'\leq t^{-3}C_1+t^{-4}C_2 \tag{5.425}$$

with

$$
\begin{aligned}
C_1 \leq & \Big(\frac{18K}{s_K^2} z_{ac,K}^2(0,0) + \frac{27}{K} z_{ac,K}^2(0,1)\Big) \|\mathbf{1}_K \ddot{\hat{\psi}}\|_\infty^2 \\
& + \Big(\frac{72K}{s_K^4} z_{ac,K}^2(1,0) + \frac{108}{K s_K^2} z_{ac,K}^2(1,1) + \frac{24}{K^3} z_{ac,K}^2(1,2)\Big) \|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2 \\
& + \Big(\frac{18K}{s_K^6} z_{ac,K}^2(2,0) + \frac{27}{K s_K^4} z_{ac,K}^2(2,1) + \frac{18}{3K^3 s_K^2} z_{ac,K}^2(2,2) \\
& \quad + \frac{9}{5K^5} z_{ac,K}^2(2,3)\Big) \|\mathbf{1}_K \hat{\psi}\|_\infty^2,
\end{aligned}
\tag{5.426}
$$

$$
\begin{aligned}
C_2 \leq & \frac{27}{2}\left(1 + \frac{1}{K^2}\right)^2 \Big(\delta \frac{z_{ac}^2(0,0)}{s^2} + \frac{z_{ac}^2(0,1)}{\delta}\Big) \|\ddot{\hat{\psi}} w\|_1^2 \\
& + \frac{27}{2}\left(1 + \frac{1}{K^2}\right)^2 \Big(\delta \frac{z_{ac}^2(1,0)}{s^4} + 8 \frac{z_{ac}^2(1,1)}{s^2 \delta} + 8 \frac{z_{ac}^2(1,2)}{3\delta^3}\Big) \|\dot{\hat{\psi}} w\|_1^2 \\
& + \frac{27}{2}\left(1 + \frac{1}{K^2}\right)^2 \Big(\delta \frac{z_{ac}^2(2,0)}{s^6} + 3 \frac{z_{ac}^2(2,1)}{s^4 \delta} + \frac{z_{ac}^2(2,2)}{s^2 \delta^3} \\
& \quad + 3 \frac{z_{ac}^2(2,3)}{5\delta^5}\Big) \|\hat{\psi} w\|_1^2.
\end{aligned}
\tag{5.427}
$$

Now, $\delta = s$ is seen to be the optimal choice in the sense that C_2 is, to leading order, proportional to s^{-5}, which is the best possible s dependence if $s \ll 1$.

The strategy we have followed to estimate integral (5.392) will be repeated for the remaining integrals. For better readability, we give the results now and the proofs later.

$$
\begin{aligned}
& \frac{3}{t^2} \int_0^\infty \left| \int_0^\infty g_2(k,k') \frac{4tk}{(2tk^2 + i)^2} e^{-ik^2 t}\, dk \right|^2 dk' \\
& \leq \lambda t^{-2} C_3 + t^{-3} C_4 + t^{-4} C_5
\end{aligned}
\tag{5.428}
$$

$$\frac{3}{4t^2}\int_0^\infty \left|\int_0^\infty Z_{ac}(k,k')\hat{\psi}(k)\frac{4t(i-6tk^2)}{(2tk^2+i)^3}e^{-ik^2t}\,dk\right|^2\,dk'$$
$$\leq \lambda(t^{-1}C_6+t^{-2}C_7)+t^{-3}C_8+t^{-4}C_9 \tag{5.429}$$

with

$$C_3 \leq \frac{12\pi^2}{s_K^4}\left(Kz^2_{ac,K}(1,0)+\frac{s_K^2}{K}z^2_{ac,K}(1,1)+\frac{s_K^4}{6K^3}z^2_{ac,K}(1,2)\right)|\hat{\psi}(0)|^2$$
$$+\frac{12\pi^2}{s_K^2}\left(Kz^2_{ac,K}(0,0)+\frac{s_K^2}{K}z^2_{ac,K}(0,1)\right)\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty, \tag{5.430}$$

$$C_4 \leq \frac{6\pi^2}{s_K^4}\left(Kz^2_{ac,K}(1,0)+\frac{s_K^2}{K}z^2_{ac,K}(1,1)+\frac{s_K^4}{3K^3}z^2_{ac,K}(1,2)\right)\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty \tag{5.431}$$

$$C_5 \leq 24\left(1+\frac{1}{K^2}\right)^3\left(\delta\frac{z^2_{ac}(1,0)}{s^4}+4\frac{z^2_{ac}(1,1)}{s^2\delta}+4\frac{z^2_{ac}(1,2)}{3\delta^3}\right)\|\hat{\psi}w\|^2_1$$
$$+24\left(1+\frac{1}{K^2}\right)^3\left(\delta\frac{z^2_{ac}(0,0)}{s^2}+2\frac{z^2_{ac}(0,1)}{\delta}\right)\|\dot{\hat{\psi}}w\|^2_1 \tag{5.432}$$

and

$$C_6 \leq \frac{81\pi^2}{s_K^2}\left(Kz^2_{ac,K}(0,0)+\frac{s_K^2}{2K}z^2_{ac,K}(0,1)\right)|\hat{\psi}(0)|^2 \tag{5.433}$$

$$C_7 \leq \frac{81\pi^2}{2s_K^4}\left(Kz^2_{ac,K}(1,0)+\frac{s_K^2}{K}z^2_{ac,K}(1,1)+\frac{s_K^4}{6K^3}z^2_{ac,K}(1,2)\right)|\hat{\psi}(0)|^2$$
$$+\frac{81\pi^2}{2s_K^2}\left(Kz^2_{ac,K}(0,0)+\frac{s_K^2}{K}z^2_{ac,K}(0,1)\right)\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty \tag{5.434}$$

$$C_8 \leq \frac{81\pi^2}{16s_K^4}\left(Kz^2_{ac,K}(1,0)+\frac{s_K^2}{K}z^2_{ac,K}(1,1)+\frac{s_K^4}{3K^3}z^2_{ac,K}(1,2)\right)\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty \tag{5.435}$$

$$C_9 \leq 54\left(1+\frac{1}{K^2}\right)^4\left(\delta\frac{z^2_{ac}(0,0)}{s^2}+\frac{z^2_{ac}(0,1)}{\delta}\right)\|\hat{\psi}w\|^2_1. \tag{5.436}$$

As before $\delta = s$ is seen to be the optimal choice in the sense C_5 and C_9 are, to leading order, proportional to s^{-3} and s^{-1}, respectively.

Summing up Eqs. (5.425), (5.428), and (5.429) we get

$$\|P_{ac}\mathbf{1}_R e^{-iHt}P_{ac}\psi\|_2^2 \\ \leq \lambda C_6 t^{-1} + \lambda(C_3 + C_7)t^{-2} + (C_1 + C_4 + C_8)\, t^{-3} + (C_2 + C_5 + C_9)\, t^{-4}. \tag{5.437}$$

Calculating the constants in front of the time factors we find

$$c_1 \leq 81\pi^2 \frac{|\hat{\psi}(0)|^2}{s_K^2}\left(K z_{ac,K}^2(0,0) + \frac{s_K^2}{2K} z_{ac,K}^2(0,1)\right), \tag{5.438}$$

$$c_2 \leq 53\pi^2 \frac{|\hat{\psi}(0)|^2}{s_K^4}\left(K z_{ac,K}^2(1,0) + \frac{s_K^2}{K} z_{ac,K}^2(1,1) + \frac{s_K^4}{6K^3} z_{ac,K}^2(1,2)\right) \\ + 53\pi^2 \frac{\|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2}{s_K^2}\left(K z_{ac,K}^2(0,0) + \frac{s_K^2}{K} z_{ac,K}^2(0,1)\right), \tag{5.439}$$

$$c_3 \leq 9 \frac{\|\mathbf{1}_K \ddot{\hat{\psi}}\|_\infty^2}{s_K^2}\left(2K z_{ac,K}^2(0,0) + \frac{3s_K^2}{K} z_{ac,K}^2(0,1)\right) \\ + 23\pi^2 \frac{\|\mathbf{1}_K \dot{\hat{\psi}}\|_\infty^2}{s_K^4}\left(K z_{ac,K}^2(1,0) + \frac{s_K^2}{K} z_{ac,K}^2(1,1) + \frac{s_K^4}{3K^3} z_{ac,K}^2(1,2)\right) \\ + 9 \frac{\|\mathbf{1}_K \hat{\psi}\|_\infty^2}{s_K^6}\left(2K z_{ac,K}^2(2,0) + \frac{3s_K^2}{K} z_{ac,K}^2(2,1) + \frac{2s_K^4}{3K^3} z_{ac,K}^2(2,2) + \frac{s_K^6}{5K^5} z_{ac,K}^2(2,3)\right), \tag{5.440}$$

$$\begin{aligned}
c_4 \le \frac{27}{2}\frac{\|\dddot{\hat{\psi}} w\|_1^2}{s}&\left(1+\frac{1}{K^2}\right)^2\left(z_{ac}^2(0,0)+z_{ac}^2(0,1)\right)\\
&+38\frac{\|\dot{\hat{\psi}} w\|_1^2}{s^3}\left(1+\frac{1}{K^2}\right)^3\Big[z_{ac}^2(1,0)+8z_{ac}^2(1,1)+\frac{8}{3}z_{ac}^2(1,2)\\
&\qquad+s^2(z_{ac}^2(0,0)+2z_{ac}^2(0,1))\Big]\\
&+92\frac{\|\hat{\psi} w\|_1^2}{s^5}\left(1+\frac{1}{K^2}\right)^4\Big[z_{ac}^2(2,0)+3z_{ac}^2(2,1)+z_{ac}^2(2,2)+\frac{3}{5}z_{ac}^2(2,3)\\
&\qquad+s^2\left(z_{ac}^2(1,0)+4z_{ac}^2(1,1)+\frac{4}{3}z_{ac}^2(1,2)\right)\\
&\qquad+s^4(z_{ac}^2(0,0)+z_{ac}^2(0,1))\Big].
\end{aligned}\tag{5.441}$$

Using the assumption $s, s_K, K \le 1$ and straightforward simplifications we obtain the proposition. □

Proof (of Eq. (5.428)). We will follow similar lines as for the proof of Eq. (5.425), with one notable difference, namely the time dependent factor in integral (5.428) is $4k/(2tk^2+i)^2$, whereas in integral (5.425) it was $t^{-1}(2tk^2+i)^{-1}$. This difference crucially influences the t-behavior coming from regions 1 and 2 because

$$\left[\int_0^\infty \left|\frac{4k}{(2tk^2+i)^2}\right| dk\right]^2 = \frac{1}{t^2}\left[\int_0^\infty \frac{4k}{4k^4+1}\, dk\right]^2 = \frac{\pi^2}{4t^2}. \tag{5.442}$$

The expected t^{-3} behavior can be recovered if $g_2(k,k') \sim ck$, $c \in \mathbb{C}$, as $k \to 0$ because

$$\left[\int_0^\infty k\left|\frac{4k}{(2tk^2+i)^2}\right| dk\right]^2 = \frac{1}{t^3}\left[\int_0^\infty \frac{4k^2}{4k^4+1}\, dk\right]^2 = \frac{\pi^2}{16t^3}. \tag{5.443}$$

The function g_2 consists only of $\hat{\psi}$, Z_{ac}, and their derivatives, whose behavior for $k \to 0$ was determined in Lemmas 5.23, 5.24 and 5.22.

These Lemmas show that in region 1

$$|g_2(k,k')| \\ \leq \lambda\left(\frac{z_{ac,K}(0,0)}{s_K}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty + \frac{z_{ac,K}(1,0)}{s_K^2}|\hat{\psi}(0)|\right) + 2\frac{z_{ac,K}(1,0)}{s_K^2}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty k, \tag{5.444}$$

while in region 2

$$|g_2(k,k')| \\ \leq \lambda\left(\frac{\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty z_{ac,K}(0,1)s_K + |\hat{\psi}(0)|z_{ac,K}(1,1)}{s_K|k-k'|} + \frac{|\hat{\psi}(0)|z_{ac,K}(1,2)}{|k-k'|^2}\right) \\ + 2\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty\left(\frac{z_{ac,K}(1,1)}{s_K|k-k'|} + \frac{z_{ac,K}(1,2)}{|k-k'|^2}\right)k. \tag{5.445}$$

We split the integral (5.393) following Eq. (5.397)-(5.400). Using Eqs. (5.442), (5.443), and (5.444), we see that the contribution to the integral (5.393) from region 1 satisfies

$$\frac{6}{t^2}\int_0^{2K} dk'\left[\int_0^K dk|g_2(k,k')|\frac{4tk}{4t^2k^4+1}\right]^2 \tag{5.446}$$

$$\leq \lambda\frac{12\pi^2K}{t^2}\left(\frac{z_{ac,K}^2(0,0)}{s_K^2}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2 + \frac{z_{ac,K}^2(1,0)}{s_K^4}|\hat{\psi}(0)|^2\right) \\ + \frac{6\pi^2K}{t^3}\frac{z_{ac,K}^2(1,0)}{s_K^4}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2. \tag{5.447}$$

In region 2 we use Eq. (5.445) and the fact that $k \leq K$ and $k' \geq 2K$, to get that

$$\frac{6}{t^2}\int_{2K}^{\infty} dk' \left[\int_0^K dk|g_2(k,k')|\frac{4tk}{4t^2k^4+1}\right]^2 \tag{5.448}$$

$$\le \lambda\frac{3\pi^2}{t^2}\int_{2K}^{\infty} dk'\Big(\frac{\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty z_{ac,K}(0,1)s_K + |\hat{\psi}(0)|z_{ac,K}(1,1)}{s_K|k'-K|}$$

$$+\frac{|\hat{\psi}(0)|z_{ac,K}(1,2)}{|k'-K|^2}\Big)^2$$

$$+\frac{3\pi^2}{t^3}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2\int_{2K}^{\infty} dk'\left(\frac{z_{ac,K}(1,1)}{s_K|k'-K|}+\frac{z_{ac,K}(1,2)}{|k'-K|^2}\right)^2 \tag{5.449}$$

$$= \lambda\frac{6\pi^2}{t^2}\Big(\frac{1}{Ks_K^2}\left(\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty z_{ac,K}(0,1)s_K + |\hat{\psi}(0)|z_{ac,K}(1,1)\right)^2$$

$$+\frac{|\hat{\psi}(0)|^2 z_{ac,K}^2(1,2)}{3K^3}\Big)$$

$$+\frac{6\pi^2}{t^3}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2\left(\frac{z_{ac,K}^2(1,1)}{Ks_K^2}+\frac{z_{ac,K}^2(1,2)}{3K^3}\right). \tag{5.450}$$

Now, we turn to region 3 and observe that for $k \ge K$

$$\frac{4tk}{4t^2k^4+1} \le \frac{1}{tk^3} \le \frac{1}{tK}\left(1+\frac{1}{k^2}\right)w(k) \le \frac{1}{tK}\left(1+\frac{1}{K^2}\right)w(k). \tag{5.451}$$

Hence, integral (5.393) in region 3 satisfies

$$\frac{12}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{3,k'}|g_2(k,k')|\frac{4tk}{4t^2k^4+1}\right]^2 \tag{5.452}$$

$$\leq \frac{12}{t^4}\frac{1}{K^2}\left(1+\frac{1}{K^2}\right)^2\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{3,k'}|g_2(k,k')|w(k)\right]^2 \tag{5.453}$$

$$\leq \frac{24}{t^4}\left(1+\frac{1}{K^2}\right)^3\int_0^\infty dk'\bigg(\left[\int_0^\infty dk\mathbf{1}_{3,k'}|\dot{Z}_{ac}(k,k')\hat{\psi}(k)|w(k)\right]^2$$

$$+\left[\int_0^\infty dk\mathbf{1}_{3,k'}Z_{ac}(k,k')\dot{\hat{\psi}}(k)|w(k)\right]^2\bigg). \tag{5.454}$$

Employing Jensen's inequality with $|\hat{\psi}w|$ and $|\dot{\hat{\psi}}w|$ as measures for the respective k-integrals, then yields

$$\frac{12}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{3,k'}|g_2(k,k')|\frac{4tk}{4t^2k^4+1}\right]^2 \tag{5.455}$$

$$\leq \frac{24}{t^4}\left(1+\frac{1}{K^2}\right)^3\int_K^\infty dk\left[\int_0^{k-\delta}dk'+\int_{k+\delta}^\infty dk'\right]$$

$$\times\left(\|\hat{\psi}w\|_1|\dot{Z}_{ac}(k,k')|^2|\hat{\psi}(k)|w(k)+\|\dot{\hat{\psi}}w\|_1|Z_{ac}(k,k')|^2|\dot{\hat{\psi}}(k)|w(k)\right). \tag{5.456}$$

Plugging in the bounds for $|Z_{ac}|^2$ and $|\dot{Z}_{ac}|^2$ provided by Eqs. (5.418), and (5.419), we obtain

$$\frac{12}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{3,k'}|g_2(k,k')|\frac{4tk}{4t^2k^4+1}\right]^2 \tag{5.457}$$

$$\leq \frac{24}{t^4}\left(1+\frac{1}{K^2}\right)^3\left[4\|\hat{\psi}w\|_1^2\left(\frac{z_{ac}^2(1,1)}{s^2\delta}+\frac{z_{ac}^2(1,2)}{3\delta^3}\right)+\|\dot{\hat{\psi}}w\|_1^2\frac{2z_{ac}^2(0,1)}{\delta}\right]. \tag{5.458}$$

In region 4, we can again use Jensen's inequality and and the bounds for

Z_{ac} given in Lemma 5.23. Thereby we see that integral (5.393) satisfies

$$\frac{12}{t^2}\int_0^\infty dk'\left[\int_0^\infty dk\mathbf{1}_{4,k'}|g_2(k,k')|\frac{4tk}{4t^2k^4+1}\right]^2 \tag{5.459}$$

$$\leq \frac{12}{t^4}\left(1+\frac{1}{K^2}\right)^3\int_K^\infty dk\int_{k-\delta}^{k+\delta} dk'$$
$$\times\left[\|\hat{\psi}w\|_1|\dot{Z}_{ac}(k,k')|^2|\hat{\psi}(k)|w(k)+\|\dot{\hat{\psi}}w\|_1|Z_{ac}(k,k')|^2|\dot{\hat{\psi}}(k)|w(k)\right] \tag{5.460}$$

$$\leq \frac{24}{t^4}\left(1+\frac{1}{K^2}\right)^3\delta\left[\|\hat{\psi}w\|_1^2\frac{z_{ac}^2(1,0)}{s^4}+\|\dot{\hat{\psi}}w\|_1^2\frac{z_{ac}^2(0,0)}{s^2}\right]. \tag{5.461}$$

Summing up the contributions for all regions, Eqs. (5.447), (5.450), (5.458), and (5.461), we obtain the desired result given in Eq. (5.428). □

Proof (of Eq. (5.429)). With the help of the elementary inequality

$$4\frac{|i-6tk^2|}{|2tk^2+i|^3}=\frac{4}{4t^2k^4+1}\frac{\sqrt{(6tk^2)^2+1}}{\sqrt{(2tk^2)+1}}\leq\frac{12}{4t^2k^4+1}, \tag{5.462}$$

we see that the time dependent factor in integral (5.394) satisfies

$$\left[\int_0^\infty 4\frac{|i-6tk^2|}{|2tk^2+i|^3}\,dk\right]^2\leq\left[\int_0^\infty\frac{12}{4t^2k^4+1}\,dk\right]^2$$
$$=\frac{1}{t}\left[\int_0^\infty\frac{12}{4k^4+1}\,dk\right]^2=\frac{9\pi^2}{t}, \tag{5.463}$$

$$\left[\int_0^\infty 4\frac{|i-6tk^2|}{|2tk^2+i|^3}k\,dk\right]^2\leq\left[\int_0^\infty\frac{12k}{4t^2k^4+1}\,dk\right]^2$$
$$=\frac{1}{t^2}\left[\int_0^\infty\frac{12k}{4k^4+1}\,dk\right]^2=\frac{9\pi^2}{4t^2}, \tag{5.464}$$

$$\left[\int_0^\infty 4\frac{|i-6tk^2|}{|2tk^2+i|^3}k^2\,dk\right]^2 \le \left[\int_0^\infty \frac{12k^2}{4t^2k^4+1}\,dk\right]^2$$
$$= \frac{1}{t^3}\left[\int_0^\infty \frac{12k^2}{4k^4+1}\,dk\right]^2 = \frac{9\pi^2}{16t^3}, \qquad (5.465)$$

therefore we need $Z_{ac}(k,k')\hat{\psi}(k) \sim ck^2$, $c \in \mathbb{C}$, as $k \to 0$ to obtain the expected t^{-3}-decay from integral (5.429) in regions 1 and 2. The behavior of Z_{ac} and $\hat{\psi}$ for $k \to 0$ was determined in Lemmas 5.24 and 5.22 and they imply that in region 1

$$\begin{aligned}&|Z_{ac}(k,k')\hat{\psi}(k)|\\ &\le \lambda\frac{z_{ac,K}(0,0)}{s_K}|\hat{\psi}(0)| + \lambda\left(\frac{z_{ac,K}(0,0)}{s_K}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty + \frac{z_{ac,K}(1,0)}{s_K^2}|\hat{\psi}(0)|\right)k\\ &\quad + \frac{z_{ac,K}(1,0)}{s_K^2}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty k^2 \qquad (5.466)\end{aligned}$$

and in region 2 we get the following bound by using the fact that $k' \le 2K$ whereas $k \ge K$

$$\begin{aligned}&|Z_{ac}(k,k')\hat{\psi}(k)|\\ &\le \lambda\frac{z_{ac,K}(0,1)}{|k'-K|}|\hat{\psi}(0)|\\ &\quad + \lambda\left(\frac{z_{ac,K}(0,1)s_K\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty + z_{ac,K}(1,1)|\hat{\psi}(0)|}{s_K|k'-K|} + \frac{z_{ac,K}(1,2)|\hat{\psi}(0)|}{|k'-K|^2}\right)k\\ &\quad + \left(\frac{z_{ac,K}(1,1)}{s_K|k'-K|} + \frac{z_{ac,K}(1,2)}{|k'-K|^2}\right)\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty k^2. \qquad (5.467)\end{aligned}$$

As before we will now follow the strategy used in the proof of Eq. (5.428). Using Eqs. (5.462)-(5.466), we see that in region 1 integral (5.394) satisfies

$$\frac{3}{2t^2}\int_0^{2K} dk' \left[\int_0^K dk |Z_{ac}(k,k')\hat{\psi}(k)| 4t \frac{|i-6tk^2|}{|2tk^2+i|^3}\right]^2 \tag{5.468}$$

$$\le \frac{81\pi^2 K}{t}\Big[\lambda \frac{z^2_{ac,K}(0,0)}{s_K^2}|\hat{\psi}(0)|^2 + \frac{\lambda}{2ts_K^4}(z^2_{ac,K}(0,0)s_K^2\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty + z^2_{ac,K}(1,0)|\hat{\psi}(0)|^2) + \frac{z^2_{ac,K}(1,0)\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty}{16t^2 s_K^4}\Big]. \tag{5.469}$$

Similarly, with the help of Eq. (5.467), we get for integral (5.394) in region 2 that

$$\frac{3}{2t^2}\int_{2K}^{\infty} dk' \left[\int_0^K dk |Z_{ac}(k,k')\hat{\psi}(k)| 4t \frac{|i-6tk^2|}{|2tk^2+i|^3}\right]^2 \tag{5.470}$$

$$\le \frac{81\pi^2}{2t}\int_{2K}^{\infty} dk' \Big[\lambda \frac{z^2_{ac,K}(0,1)}{|k'-K|^2}|\hat{\psi}(0)|^2 + \frac{\lambda}{4t}\left(\frac{z_{ac,K}(0,1)s_K\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty + z_{ac,K}(1,1)|\hat{\psi}(0)|}{s_K|k'-K|} + \frac{z_{ac,K}(1,2)|\hat{\psi}(0)|}{|k'-K|^2}\right)^2 + \frac{1}{16t^2}\left(\frac{z_{ac,K}(1,1)}{s_K|k'-K|} + \frac{z_{ac,K}(1,2)}{|k'-K|^2}\right)^2 \|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty\Big] \tag{5.471}$$

$$= \frac{81\pi^2}{2t}\Big[\lambda \frac{1}{K} z^2_{ac,K}(0,1)|\hat{\psi}(0)|^2 + \frac{\lambda}{2t}\Big(\frac{2}{Ks_K^2}(z^2_{ac,K}(0,1)s_K^2\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty + z^2_{ac,K}(1,1)|\hat{\psi}(0)|^2) + \frac{z^2_{ac,K}(1,2)|\hat{\psi}(0)|^2}{3K^3}\Big) + \frac{1}{8t^2}\left(\frac{z^2_{ac,K}(1,1)}{Ks_K^2} + \frac{z^2_{ac,K}(1,2)}{3K^3}\right)\|\mathbf{1}_K\dot{\hat{\psi}}\|^2_\infty\Big]. \tag{5.472}$$

Now, observe that due to Eq. (5.462) and (5.410)

$$4\frac{|i-6tk^2|}{|2tk^2+i|^3} \leq \frac{3}{t^2}\left(1+\frac{1}{K^2}\right)^2 w(k)^2 \leq \frac{3}{t^2}\left(1+\frac{1}{K^2}\right)^2 w(k). \tag{5.473}$$

Employing Eq. (5.473), Jensen's inequality with $|\hat{\psi}w|$ as measure and the bound for $|Z_{ac}|$ given in Eq. (5.419) we then see that in region 3

$$\frac{3}{t^2}\int_0^\infty dk' \left[\int_0^\infty dk \mathbf{1}_{3,k'}|Z_{ac}(k,k')\hat{\psi}(k)|4t\frac{|i-6tk^2|}{|2tk^2+i|^3}\right]^2 \tag{5.474}$$

$$\leq \frac{27}{t^4}\left(1+\frac{1}{K^2}\right)^4 \|\hat{\psi}w\|_1$$

$$\times \int_K^\infty dk \left[\int_0^{k-\delta} dk' + \int_{k+\delta}^\infty dk'\right] |Z_{ac}(k,k')|^2 |\hat{\psi}(k)| w(k) \tag{5.475}$$

$$\leq \frac{54}{\delta t^4}\left(1+\frac{1}{K^2}\right)^4 z_{ac}^2(0,1)\|\hat{\psi}w\|_1^2 \tag{5.476}$$

with δ to be determined later. Again using Jensen's inequality with $|\hat{\psi}w|$ as measure and the bounds for Z_{ac} provided by Lemma 5.23, it becomes clear that in region 4 integral (5.394) satisfies

$$\frac{3}{t^2}\int_0^\infty dk' \left[\int_0^\infty dk \mathbf{1}_{4,k'}|Z_{ac}(k,k')\hat{\psi}(k)|4t\frac{|i-6tk^2|}{|2tk^2+i|^3}\right]^2 \tag{5.477}$$

$$\leq \frac{27}{t^4}\left(1+\frac{1}{K^2}\right)^4 \|\hat{\psi}w\|_1 \int_K^\infty dk \int_{k-\delta}^{k+\delta} dk' |Z_{ac}(k,k')|^2 |\hat{\psi}(k)| w(k) \tag{5.478}$$

$$\leq \frac{54\delta}{t^4}\frac{z_{ac}^2(0,0)}{s^2}\left(1+\frac{1}{K^2}\right)^4 \|\hat{\psi}w\|_1^2. \tag{5.479}$$

Summing up the contributions from all regions, Eqs. (5.469), (5.472), (5.476), and (5.479), we obtain the desired result in Eq. (5.429). □

5.7 Proof of Theorem 5.4

We proceed in the same way as in the proof of Theorem 5.3, which was given in the previous Section. First we prove the analogue of Lemma 5.21.

Lemma 5.26. *Let $R \geq R_V$ and $\psi \in \mathcal{D}(H)$, then*

$$\|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \leq \sum_{n=0}^{N-1} \left| \int_0^\infty Z_e(k,n)\hat{\psi}(k) e^{-ik^2 t} dk \right|^2 \tag{5.480}$$

with

$$Z_e(k,n) := \sqrt{\frac{\eta_n}{2}} \left[S(k) \frac{e^{ikR}}{k + i\eta_n} + \frac{e^{-ikR}}{k - i\eta_n} \right]. \tag{5.481}$$

Proof. Let ϕ_n denote the bound states. Then

$$\begin{aligned} &\|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \\ &= \sum_{n=0}^{N-1} \frac{1}{\|\phi_n\|_2^2} \left\langle \mathbf{1}_R e^{-iHt} P_{ac}\psi, \phi_n \right\rangle \left\langle \phi_n, \mathbf{1}_R e^{-iHt} P_{ac}\psi \right\rangle \\ &= \sum_{n=0}^{N-1} \frac{1}{\|\phi_n\|_2^2} \left| \int_0^\infty dk\, e^{-ik^2 t} \hat{\psi}(k) \int_0^\infty dr \mathbf{1}_R \bar{\phi}_n(r) \psi^+(k,r) \right|^2. \end{aligned} \tag{5.482}$$

Observing

$$\frac{d}{dr} W(\bar{\phi}_n(r), \psi^+(k,r)) = ((i\eta_n)^2 - k^2) \bar{\phi}_n(r) \psi^+(k', r). \tag{5.483}$$

and using $\psi^+(k,0) = 0 = \phi_n(0)$, we get upon integration

$$\int_0^\infty dr\, \mathbf{1}_R(r) \bar{\phi}_n(r) \psi^+(k,r) = \frac{W(\bar{\phi}_n(R), \psi^+(k,R))}{(i\eta_n)^2 - k^2}. \tag{5.484}$$

This and the fact that $\|\phi_n\|_2 \geq \|\mathbf{1}_{[R,\infty)}\phi_n\|_2$ implies

$$\begin{aligned}&\|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \\ &\leq \sum_{n=0}^{N-1} \frac{1}{\|\mathbf{1}_{[R,\infty)}\phi_n\|_2^2} \left| \int_0^\infty dk\, e^{-ik^2 t} \hat{\psi}(k) \frac{W(\bar{\phi}_n(R), \psi^+(k,R))}{(i\eta_n)^2 - k^2} \right|^2, \end{aligned} \tag{5.485}$$

To calculate $\|\mathbf{1}_{[R,\infty)}\phi_n\|_2$ observe that $\phi_n(r) = e^{-\eta_n r}$ for $r \geq R_V$, which yields

$$\|\mathbf{1}_{[R,\infty)}\phi_n\|_2^2 = \int_R^\infty e^{-2\eta_n r}\, dr = \frac{e^{-2\eta_n R}}{2\eta_n}. \tag{5.486}$$

Using this, $\phi_n(R) = e^{-\eta_n R}$ and $\psi^+(k,R) = \frac{1}{2i}(S(k)e^{ikR} - e^{-ikR})$ we calculate

$$\begin{aligned}&\frac{1}{\|\mathbf{1}_{[R,\infty)}\phi_n\|_2} \frac{W(\bar{\phi}_n(R), \psi^+(k,R))}{(i\eta_n)^2 - k^2} \\ &= \sqrt{\frac{\eta_n}{2}} \frac{(k - i\eta_n)S(k)e^{ikR} + (k + i\eta_n)e^{-ikR}}{(i\eta_n)^2 - k^2} \qquad (5.487) \\ &= -\sqrt{\frac{\eta_n}{2}} \left[S(k) \frac{e^{ikR}}{k + i\eta_n} + \frac{e^{-ikR}}{k - i\eta_n} \right], \qquad (5.488)\end{aligned}$$

which when plugged into Eq. (5.485) yields Eq. (5.480). □

Next we want to show that the boundary terms due to partial integration in the stationary phase argument vanish, but for this we need more knowledge about how $Z_e(k,n)$ behaves for $k \to 0$ and $k \to \infty$. This is the purpose of the following Lemmas.

Lemma 5.27. *Let $K > 0$ and $R \geq R_V$. For $k \in [0, K)$,*

$$|Z_e(k,n)| \leq \sqrt{\frac{2}{\eta_0}} =: \frac{z_{e,K}(0)}{\eta_0^{1/2}}, \tag{5.489}$$

$$|\dot{Z}_e(k,n)| \leq \frac{1}{\sqrt{2} s_K \eta_0^{3/2}} \Big[2s_K + (2R s_K + C_{1,K})\eta_0 \Big] =: \frac{z_{e,K}(1)}{s_K \eta_0^{3/2}}, \tag{5.490}$$

$$
\begin{aligned}
|\ddot{Z}_e(k,n)| &\leq \frac{1}{\sqrt{2} s_K^2 \eta_0^{5/2}} \left(C_{2,K}\eta_0^2 + 2\eta_0 s_K \left(C_{1,K} + R s_K\right)(R\eta_0 + 2) + 4 s_K^2 \right) \\
&=: \frac{z_{e,K}(2)}{s_K^2 \eta_0^{5/2}}. \qquad (5.491)
\end{aligned}
$$

For $k \in [0, \infty)$ we have the same bounds with the index K omitted on the right hand side.

Proof. Let $k \in [0, K)$. Equation (5.481) for Z_e then immediately gives

$$
|Z_e(k,n)| \leq \sqrt{\frac{2}{\eta_n}}, \qquad (5.492)
$$

from which we obtain Eq. (5.489) by using the fact that $\eta_n \geq \eta_0$. Now, due to the bounds on the derivatives of S given in Theorem 5.1,

$$
\begin{aligned}
|\dot{Z}_e(k,n)| = &\sqrt{\frac{\eta_n}{2}} \bigg| (\dot{S}(k) + iRS(k)) \frac{e^{ikR}}{k + i\eta_n} - iR \frac{e^{-ikR}}{k - i\eta_n} \\
&- \frac{e^{-ikR}}{(k - i\eta_n)^2} - S(k) \frac{e^{ikR}}{(k + i\eta_n)^2} \bigg| \qquad (5.493) \\
\leq &\frac{1}{\sqrt{2} s_K} \left[\frac{2 s_K}{\eta_n^{3/2}} + (2R s_K + C_{1,K}) \frac{1}{\eta_n^{1/2}} \right], \qquad (5.494)
\end{aligned}
$$

and this implies Eq. (5.490) again using the fact that $\eta_n \geq \eta_0$. Similarly, we have due to Theorem 5.1

$$
\begin{aligned}
&|\ddot{Z}_e(k,n)| \\
&= \sqrt{\frac{\eta_n}{2}}\bigg| - R^2\Big(S(k)\frac{e^{ikR}}{k+i\eta_n} + \frac{e^{-ikR}}{k-i\eta_n}\Big) + 2iR\dot{S}(k)\frac{e^{ikR}}{k+i\eta_n} \\
&\quad - 2iRS(k)\frac{e^{ikR}}{(k+i\eta_n)^2} + 2iR\frac{e^{-ikR}}{(k-i\eta_n)^2} - 2\dot{S}(k)\frac{e^{ikR}}{(k+i\eta_n)^2} \\
&\quad + 2S(k)\frac{e^{ikR}}{(k+i\eta_n)^3} + 2\frac{e^{-ikR}}{(k-i\eta_n)^3} + \ddot{S}(k)\frac{e^{ikR}}{k+i\eta_n}\bigg| \qquad (5.495)\\
&\le \frac{1}{\sqrt{2}}\bigg[\frac{2R^2}{\eta_n^{\frac{1}{2}}} + 2R\frac{C_{1,K}}{s_K\eta_n^{\frac{1}{2}}} + 4R\frac{1}{\eta_n^{\frac{3}{2}}} + 2\frac{C_{1,K}}{s_K\eta_n^{\frac{3}{2}}} + \frac{4}{\eta_n^{\frac{5}{2}}} + \frac{C_{2,K}}{s_K^2\eta_n^{\frac{3}{2}}}\bigg], \qquad (5.496)
\end{aligned}
$$

from which we get Eq. (5.491) with the help of $\eta_n \ge \eta_0$.

Let $k \in [0,\infty)$. In this case the proof is exactly the same with the only difference that we use the S-matrix bounds provided by Theorem 5.2 rather than those in Theorem 5.1. In effect this amounts to omitting the index K in the bounds (5.489)-(5.491). □

Lemma 5.28. *Let $R \ge R_V$ and $K > 0$ be finite. Then for $k \in [0,K]$,*

$$|Z_e(k,n)| \le \lambda\frac{z_{e,K}(0)}{\eta_0^{1/2}} + \frac{z_{e,K}(1)}{s_K\eta_0^{3/2}}k. \qquad (5.497)$$

Proof. Clearly

$$
\begin{aligned}
|Z_e(k,n)| &= \left|Z_e(0,n) + \int_0^k \dot{Z}(k',n)\,dk'\right| \\
&\le |Z_e(0,n)| + \int_0^k |\dot{Z}(k',n)|\,dk'. \qquad (5.498)
\end{aligned}
$$

From Eq. (5.481) for Z_e and the fact that $S(0) = \mp 1$ for $\lambda = 1$ and 0 respectively (see [38, page 356] for the proof) we easily calculate

$$|Z_e(0,n)| = \frac{1}{\sqrt{2\eta_n}}|S(0) - 1| = \lambda\sqrt{\frac{2}{\eta_n}} \le \lambda\sqrt{\frac{2}{\eta_0}} = \lambda\frac{z_{e,K}(0)}{\eta_0^{1/2}}. \quad (5.499)$$

Plugging this and the bound for $|\dot{Z}_e|$ provided by Eq. (5.490) into Eq. (5.498) finishes the proof. □

Now, we are able to prove that the boundary terms due to partial integration in the stationary phase argument vanish.

Lemma 5.29. *Let ψ satisfy the assumptions stated in Theorem 5.4, then*

$$\int_0^\infty Z_e(k,n)\hat{\psi}(k)\frac{\partial_k^2 e^{-ik^2t}}{2tk^2+i}\,dk = \int_0^\infty \partial_k^2\left(\frac{Z_e(k,n)\hat{\psi}(k)}{2tk^2+i}\right)e^{-ik^2t}\,dk. \quad (5.500)$$

Proof. Clearly,

$$\begin{aligned}
&\int_0^\infty Z_e(k,n)\hat{\psi}(k)\frac{\partial_k^2 e^{-ik^2t}}{2tk^2+i}\,dk \\
&= \left[\frac{Z_e(k,n)\hat{\psi}(k)}{2tk^2+i}\partial_k e^{-ik^2t}\right]_0^\infty && (5.501)\\
&- \left[\partial_k\left(\frac{Z_e(k,n)\hat{\psi}(k)}{2tk^2+i}\right)e^{-ik^2t}\right]_0^\infty && (5.502)\\
&+ \int_0^\infty \partial_k^2\left(\frac{Z_e(k,n)\hat{\psi}(k)}{2tk^2+i}\right)e^{-ik^2t}\,dk && (5.503)
\end{aligned}$$

and

$$\begin{aligned}
\partial_k\left(\frac{Z_e(k,n)\hat{\psi}(k)}{2tk^2+i}\right) &= \left(\dot{Z}_e(k,n)\hat{\psi}(k) + Z_e(k,n)\dot{\hat{\psi}}(k)\right)\frac{1}{2t(2tk^2+i)} && (5.504)\\
&- Z_e(k,n)\hat{\psi}(k)\frac{4tk}{2t(2tk^2+i)^2}. && (5.505)
\end{aligned}$$

The same arguments given in the proof of Lemma 5.25 also apply to Eq. (5.501) and to Eq. (5.505), so we are left with handling Eq. (5.504). For $k \to \infty$ Eq. (5.504) tends to zero because the time dependent factor tends to zero like k^2, while $Z_e(k,n)$ and $\dot{Z}_e(k,n)$ are bounded for all k (see Lemma 5.27), $\hat{\psi}(k) \to 0$ as $k \to \infty$ ($\hat{\psi}$ is square integrable) and $\dot{\hat{\psi}}(k)$ can only diverge slower than k at infinity ($\|\dot{\hat{\psi}}w\|_1 < \infty$ by assumption). Let us now look at Eq. (5.504) for $k \to 0$. In case there is no zero resonance ($\lambda = 0$), Eq. (5.504) tends to zero for $k \to 0$ because $\hat{\psi}(0) = 0$ (Lemma 5.22), $|\dot{Z}_e(k,n)|$ is bounded (Lemma 5.27), $Z_e(k,n) \to 0$ at least like k (Lemma 5.28), and $\dot{\hat{\psi}}(k)$ can only diverge slower than $1/k$ ($\|\dot{\hat{\psi}}w\|_1 < \infty$ by assumption). In case there is a zero resonance ($\lambda = 1$), $S(0) = -1$ (see [38, page 356] for the proof). Hence,

$$Z_e(0,n) = -i\frac{1}{\sqrt{2\eta_n}}(S(0) - 1) = i\sqrt{\frac{2}{\eta_n}} \quad \text{and} \tag{5.506}$$

$$\dot{Z}_e(0,n) = \sqrt{\frac{\eta_n}{2}}\left[\left(\frac{R}{\eta_n} + \frac{1}{\eta_n^2}\right)(S(0) + 1) + \dot{S}(0)\frac{1}{i\eta_n}\right] = -i\frac{\dot{S}(0)}{\sqrt{2\eta_n}}. \tag{5.507}$$

On the other hand, we know from the proof of Lemma 5.25 that (Eq. (5.386))

$$\dot{\hat{\psi}}(0) = \frac{1}{2}\dot{S}(0)\hat{\psi}(0). \tag{5.508}$$

Plugging Eqs. (5.506), (5.507), and (5.508) into Eq. (5.504) evaluated at $k = 0$ shows that it vanishes also when a zero resonance is present. □

Finally we are in the position to prove Theorem 5.4.

Proof (of Theorem 5.4). Combining Lemma 5.26 with Lemma 5.29 and using

$$e^{-ik^2t} = -\frac{\partial_k^2 e^{-ik^2t}}{2t(2tk^2 + i)}, \tag{5.509}$$

we obtain

$$\|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2 \leq \sum_{n=0}^{N-1} \left| \int_0^\infty \partial_k^2 \left(Z_e(k,n)\hat{\psi}(k) \frac{1}{2t(2tk^2+i)} \right) e^{-ik^2 t}\, dk \right|^2 . \tag{5.510}$$

For $A, B, C \in \mathbb{R}$

$$(A+B+C)^2 \leq 3(A^2+B^2+C^2), \tag{5.511}$$

therefore with the shorthands

$$g_1(k,n) := \ddot{Z}_e(k,n)\hat{\psi}(k) + 2\dot{Z}_e(k,n)\dot{\hat{\psi}}(k) + Z_e(k,n)\ddot{\hat{\psi}}(k), \tag{5.512}$$

$$g_2(k,n) := \dot{Z}_e(k,n)\hat{\psi}(k) + Z_e(k,n)\dot{\hat{\psi}}(k), \tag{5.513}$$

we get

$$\|P_e \mathbf{1}_R e^{-iHt} P_{ac}\psi\|_2^2$$

$$\leq \frac{3}{4t^2} \sum_{n=0}^{N-1} \left[\int_0^\infty |g_1(k,n)| \frac{1}{\sqrt{4t^2k^4+1}}\, dk \right]^2 \tag{5.514}$$

$$+ \frac{3}{t^2} \sum_{n=0}^{N-1} \left[\int_0^\infty |g_2(k,n)| \frac{4tk}{4t^2k^4+1}\, dk \right]^2 \tag{5.515}$$

$$+ \frac{3}{4t^2} \sum_{n=0}^{N-1} \left[\int_0^\infty |Z_e(k,n)\hat{\psi}(k)| \frac{4t|i-6tk^2|}{|2tk^2+i|^3}\, dk \right]^2 . \tag{5.516}$$

Note that we will use Eq. (5.511) and $(A+B)^2 \leq 2A^2+2B^2$ throughout the proof often without mentioning it. Let $h(k,n)$ be a placeholder for the integrands in Eqs. (5.514)-(5.516), then the integration region of each of the above integrals will be divided as follows

$$\left| \int_0^\infty h(k,n)\, dk \right|^2 \leq 2 \left[\int_0^K |h(k,n)|\, dk \right]^2 + 2 \left[\int_K^\infty |h(k,n)|\, dk \right]^2 . \tag{5.517}$$

In contrast to the proof of Theorem 5.3 there is no need to handle the region around the diagonal separately because as one can see from Eq. (5.481) Z_e has no apparent singularity for $k \geq 0$. First consider Eq. (5.514). Using the bounds on Z_e and its derivatives given in Lemma 5.27 and

$$\left[\int_0^K dk \frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \leq \frac{1}{t}\left[\int_0^\infty dk \frac{1}{\sqrt{4k^4+1}}\right]^2 \leq \frac{2}{t}, \tag{5.518}$$

we find

$$\left[\int_0^K dk |g_1(k,n)| \frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.519}$$

$$\leq \frac{6}{t}\left[\frac{z_{e,K}^2(2)}{\eta_0^5 s_K^4}\|\mathbf{1}_K\hat{\psi}\|_\infty^2 + \frac{4z_{e,K}^2(1)}{\eta_0^3 s_K^2}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2 + \frac{z_{e,K}^2(0)}{\eta_0}\|\mathbf{1}_K\ddot{\hat{\psi}}\|_\infty^2\right]. \tag{5.520}$$

Equation (5.410) provides the bound

$$\frac{1}{\sqrt{4t^2k^4+1}} \leq \frac{1}{2t}\left(1+\frac{1}{K^2}\right)w(k), \tag{5.521}$$

that together with Lemma 5.27 implies

$$\left[\int_K^\infty dk|g_1(k,n)|\frac{1}{\sqrt{4t^2k^4+1}}\right]^2 \tag{5.522}$$

$$\leq \frac{1}{4t^2}\left(1+\frac{1}{K^2}\right)^2$$
$$\times\left[\int_0^\infty dk\left(\|\ddot{Z}_e(\cdot,n)\|_\infty|\hat{\psi}|+2\|\dot{Z}_e(\cdot,n)\|_\infty|\dot{\hat{\psi}}|+\|Z_e(\cdot,n)\|_\infty|\ddot{\hat{\psi}}|\right)w\right]^2 \tag{5.523}$$

$$\leq \frac{3}{4t^2}\left(1+\frac{1}{K^2}\right)^2$$
$$\times\left[\|\ddot{Z}_e(\cdot,n)\|_\infty^2\|\hat{\psi}w\|_1^2+4\|\dot{Z}_e(\cdot,n)\|_\infty^2\|\dot{\hat{\psi}}w\|_1^2+\|Z_e(\cdot,n)\|_\infty^2\|\ddot{\hat{\psi}}w\|_1^2\right] \tag{5.524}$$

$$\leq \frac{3}{4t^2}\left(1+\frac{1}{K^2}\right)^2\left[\frac{z_e^2(2)}{s^4\eta_0^5}\|\hat{\psi}w\|_1^2+4\frac{z_e^2(1)}{s^2\eta_0^3}\|\dot{\hat{\psi}}w\|_1^2+\frac{z_e^2(0)}{\eta_0}\|\ddot{\hat{\psi}}w\|_1^2\right]. \tag{5.525}$$

Now consider Eq. (5.515). We use Lemma 4 that gives a bound on $\hat{\psi}(k)$ for small k, Lemma 5.28 that gives a bound on $Z_e(k,n)$ for small k, the bound on $\dot{Z}_e$ provided by Lemma 5.27 and

$$\left[\int_0^\infty\left|\frac{4tk}{(2tk^2+i)^2}\right|dk\right]^2=\left[\int_0^\infty\frac{4k}{4k^4+1}\,dk\right]^2=\frac{\pi^2}{4}, \tag{5.526}$$

$$\left[\int_0^\infty k\left|\frac{4tk}{(2tk^2+i)^2}\right|dk\right]^2=\frac{1}{t}\left[\int_0^\infty\frac{4k^2}{4k^4+1}\,dk\right]^2=\frac{\pi^2}{16t} \tag{5.527}$$

to obtain

$$\left[\int_0^K |g_2(k,n)|\frac{4tk}{4t^2k^4+1}\,dk\right]^2 \tag{5.528}$$

$$\leq \Bigg[\int_0^\infty \Bigg(\lambda\Big(\frac{z_{e,K}(1)}{\eta_0^{3/2}s_K}|\hat{\psi}(0)| + \frac{z_{e,K}(0)}{\eta_0^{1/2}}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty\Big)$$

$$+ 2\frac{z_{e,K}(1)}{\eta_0^{3/2}s_K}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty k\Bigg)\frac{4tk}{4t^2k^4+1}\,dk\Bigg]^2 \tag{5.529}$$

$$\leq \frac{\pi^2}{2}\Bigg[2\lambda\Big(\frac{z_{e,K}^2(1)}{\eta_0^3 s_K^2}|\hat{\psi}(0)|^2 + \frac{z_{e,K}^2(0)}{\eta_0}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2\Big) + \frac{z_{e,K}^2(1)}{\eta_0^3 s_K^2 t}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2\Bigg]. \tag{5.530}$$

We also use the bound

$$\frac{4tk}{4t^2k^4+1} \leq \frac{1}{tK}\left(1+\frac{1}{K^2}\right)w(k), \tag{5.531}$$

provided by Eq. (5.451), which gives

$$\left[\int_K^\infty |g_2(k,n)|\frac{4tk}{4t^2k^4+1}\,dk\right]^2 \tag{5.532}$$

$$\leq \frac{1}{t^2}\left(1+\frac{1}{K^2}\right)^3\left[\int_K^\infty \left(|\hat{\psi}(k)|\frac{z_e(1)}{\eta_0^{3/2}s} + |\dot{\hat{\psi}}(k)|\frac{z_e(0)}{\eta_0^{1/2}}\right)w(k)\,dk\right]^2 \tag{5.533}$$

$$\leq \frac{2}{t^2}\left(1+\frac{1}{K^2}\right)^3\left[\|\hat{\psi}w\|_1^2\frac{z_e^2(1)}{\eta_0^3 s^2} + \|\dot{\hat{\psi}}w\|_1^2\frac{z_e^2(0)}{\eta_0}\right]. \tag{5.534}$$

Finally consider Eq. (5.516). In addition to the bounds on Z_e and $\hat{\psi}$ provided by Lemmas 5.28 and 5.22 respectively, that we have used to treat Eq. (5.515), we now need to use the bound

$$4\frac{|i-6tk^2|}{|2tk^2+i|^3} \leq \frac{12}{4t^2k^4+1}, \tag{5.535}$$

from Eq. (5.462), that gives

$$\left[\int_0^\infty 4t\frac{|i-6tk^2|}{|2tk^2+i|^3}\,dk\right]^2 \leq \left[\int_0^\infty \frac{12t}{4t^2k^4+1}\,dk\right]^2$$
$$= t\left[\int_0^\infty \frac{12}{4k^4+1}\,dk\right]^2 = 9\pi^2 t, \tag{5.536}$$
$$\left[\int_0^\infty 4t\frac{|i-6tk^2|}{|2tk^2+i|^3}k\,dk\right]^2 \leq \left[\int_0^\infty \frac{12tk}{4t^2k^4+1}\,dk\right]^2$$
$$= \left[\int_0^\infty \frac{12k}{4k^4+1}\,dk\right]^2 = \frac{9\pi^2}{4}, \tag{5.537}$$
$$\left[\int_0^\infty 4t\frac{|i-6tk^2|}{|2tk^2+i|^3}k^2\,dk\right]^2 \leq \left[\int_0^\infty \frac{12tk^2}{4t^2k^4+1}\,dk\right]^2$$
$$= \frac{1}{t}\left[\int_0^\infty \frac{12k^2}{4k^4+1}\,dk\right]^2 = \frac{9\pi^2}{16t}, \tag{5.538}$$

from which we obtain

$$\left[\int_0^K |Z_e(k,n)\hat{\psi}(k)|\frac{4t|i-6tk^2|}{|2tk^2+i|^3}\,dk\right]^2 \tag{5.539}$$
$$\leq \left[\int_0^\infty \left(\lambda|\hat{\psi}(0)|\frac{z_{e,K}(0)}{\eta_0^{1/2}} + \lambda\left(\frac{z_{e,K}(0)}{\eta_0^{1/2}}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty + \frac{z_{e,K}(1)}{\eta_0^{3/2}s_K}|\hat{\psi}(0)|\right)k\right.\right.$$
$$\left.\left. + \frac{z_{e,K}(1)}{\eta_0^{3/2}s_K}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty k^2\right)\frac{12t}{4t^2k^4+1}\,dk\right]^2 \tag{5.540}$$
$$\leq 27\pi^2 t\left[\lambda|\hat{\psi}(0)|^2\frac{z_{e,K}^2(0)}{\eta_0} + \frac{\lambda}{2t}\left(\frac{z_{e,K}^2(0)}{\eta_0}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2 + \frac{z_{e,K}^2(1)}{\eta_0^3 s_K^2}|\hat{\psi}(0)|^2\right)\right.$$
$$\left. + \frac{z_{e,K}^2(1)}{4t^2\eta_0^3 s_K^2}\|\mathbf{1}_K\dot{\hat{\psi}}\|_\infty^2\right]. \tag{5.541}$$

If we also use the bounds

$$4t\frac{|i-6tk^2|}{|2tk^2+i|^3} \le \frac{3}{t}\left(1+\frac{1}{K^2}\right)^2 w(k) \tag{5.542}$$

from Eq. (5.473), and those on Z_e given in Lemma 5.27, we get

$$\left[\int_K^{\infty} |Z_e(k,n)\hat{\psi}(k)|\frac{4t|i-6tk^2|}{|2tk^2+i|^3}\,dk\right]^2 \le \frac{9}{t^2}\left(1+\frac{1}{K^2}\right)^4 \frac{z_e^2(0)}{\eta_0}\|\hat{\psi}w\|_1^2. \tag{5.543}$$

Making use of Eq. (5.517), we plug Eq. (5.520) and Eq. (5.525) into Eq. (5.514), Eq. (5.530) and Eq. (5.534) into Eq. (5.515), Eq. (5.541) and Eq. (5.543) into Eq. (5.516) respectively. That completes the proof. □

5.8 Appendix: physical meaning of resonances, virtual states, and zero-resonance

The zeros of the Jost function have important physical meaning, that we will now briefly discuss (see also Fig. 5.8). In the following, we will use the symbols μ and ν to denote strictly positive real numbers.

Consider at first a zero of the form $i\nu$. It corresponds to a *bound state*, indeed the function $f(i\nu, r)$ (see Eq. (5.29)) is a solution of the Schrödinger equation (5.26) such that $f(i\nu, r) = e^{-\nu r}$ for $r \ge R_V$, therefore it is square integrable. In other words, $f(i\nu, r)$ is the eigenfunction corresponding to the eigenvalue $-\nu^2$. We assumed that the potential had compact support, therefore every state with positive energy can tunnel away, and there can be only bound states with negative energy. The zeros that correspond to bound states are simple [45, Th. XI.58d, page 140] and finitely many. The latter property can be easily established from Eq. (5.137), that implies that $|F(i\nu)| \to 1$ as $\nu \to \infty$, therefore the Jost function is non-zero from a certain value of ν on, and the zeros of a non-zero entire function can not have finite accumulation points (see also [38, page 361]). The exact

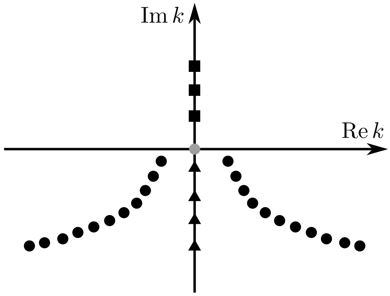


Figure 5.8: Location of the zeros of the Jost function $F(k)$, distinguished in bound states (■), virtual states (▲), resonances (●), and zero-resonance (●).

number of eigenstates is given by Levinson's Theorem [45, Theorem XI.59, page 142].

A zero of the form $\pm\mu + i\nu$ would correspond to a square integrable eigenfunction with eigenvalue $(\pm\mu + i\nu)^2 \in \mathbb{C}$, but this cannot be the case because the Hamiltonian is self-adjont and has therefore only real eigenvalues. As a consequence, the bound states are the only zeros in the positive imaginary half-plane.

The zeros in the negative imaginary half-plane correspond to functions f that increase exponentially in r as $r \to \infty$, and are therefore not square integrable. They are not physical states, but have nevertheless a dynamical meaning. Consider a zero of the form $\pm\mu - i\nu$; the property $\bar{F}(\bar{k}) = F(-k)$ [38, 12.32a, page 340] implies that these zeros come in couples symmetric with respect to the imaginary axis. The time evolution of the f corresponding to such a zero is given by the factor

$$e^{-i(\pm\mu - i\nu)^2 t} = e^{-i(\mu^2 - \nu^2)t} e^{\mp 2\mu\nu t}, \tag{5.544}$$

i.e. f exponentially increases and decreases in time for $-\mu$ and μ, respectively. Therefore, the f corresponding to a zero of the form $\mu - i\nu$ can be a good model for a meta-stable state: a normalizable state in some sense close to this f will have a time evolution similar to it, and can be used to describe a decaying system [16, 56]. These zeros are called *resonances*. Given a potential, the resonances can be found through a scattering experiment: when the projectile has energy μ^2 there is a chance that it forms the meta-stable state and is later released in a random direction, generating a peak in the cross section. The width of the peak can be shown to be related to ν (see for example [4]).

Besides the resonances, in the negative imaginary plane there can be zeros of the form $-i\nu$ too, that also correspond to functions f not square integrable. They are called *virtual states*. Their time evolution is expected to be given by a phase, therefore a physical state similar to a virtual state will evolve for some time almost only by a phase.[2] As a consequence, they can also be considered meta-stable [4, page 487]. In scattering experiments they manifest as a peak at zero energy. The virtual states are finitely many, and this can be proven in analogy with the bound states, using Eq. (5.136).

The only place on the real axis where there can be a zero is the origin [38, page 346]; such a zero is called *zero-resonance*, and it must be simple [37, pages 327, 328]. The corresponding f is not square integrable, and does not change at all in time. A zero-resonance is a meta-stable state, and leads to a peak at zero energy in the scattering cross section, but the presence of a zero in $k = 0$ has also a strong influence on the long-time behavior of *any* wave function [23]. This circumstance can be understood in terms of the stationary phase argument: long time corresponds to $k = 0$. It should be noted, that the presence of a zero-resonance is very untypical.

We observe that the resonances are infinitely many, indeed the function g defined in (5.146) is of fractional order, and has therefore infinitely many zeros (see [38, page 361]). Moreover, there are finitely many resonances below any half-line contained in the negative imaginary half-plane that goes through the origin, and inside any stripe in the negative imaginary half-plane [38, page 361]. That implies that, denoting the resonances by

[2] The time evolution of a physical state similar to a virtual state or to a resonance will after some time diverge from the multiplication by $e^{-ik^2 t}$ because of the accumulating error.

$\alpha_n - i\beta_n$ and ordering them with growing modulus, then as $n \to \infty$

$$\beta_n \to \infty, \qquad \alpha_n \to \infty, \qquad \frac{\beta_n}{\alpha_n} \to 0. \tag{5.545}$$

This implies also that the sets $\{\alpha_n\}_{n\in\mathbb{N}^0}$ and $\{\beta_n\}_{n\in\mathbb{N}^0}$ have a minimum.

Remark 5.6. If the potential has a shape like a single barrier, then we expect that $\min_n \beta_n = \beta_0$, indeed states with higher energy impinge more often on the barrier than states with lower energy, and therefore have more occasions to tunnel out. On the other side, if the potential has a more complicated shape this simple expectation could be wrong; for example if the potential has several barriers, then a state with higher energy after having passed the first barrier has more occasions to go back inside the first barrier than a state with lower energy.

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Eidesstattliche Versicherung

(Siehe Promotionsordnung vom 12.07.11, §8, Abs. 2 Pkt. 5)

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist. Kapitel 2, 3, 4 und 5 enthalten Resultate, die der Zusammenarbeit mit verschiedenen Koautoren entstammen (für Details siehe den Anfang des entsprechenden Kapitels).

München, den 12.02.2014 Robert Grummt