

Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical
Engineering

Department of Physics
Programme: Mathematical physics



**Diracovy operátory s bariérami:
rozptyl a Kleinův paradox**

**Dirac operators with barriers:
scattering and the Klein paradox**

MASTER'S THESIS

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ZADÁNÍ DIPLOMOVÉ PRÁCE

Akademický rok: 2022/2023



Student: Bc. Lukáš Vácha

Studijní program: Matematická fyzika

Název práce: Diracovy operátory s bariérami: rozptyl a Kleinův paradox
(česky)

Název práce: Dirac operators with barriers: scattering and the Klein paradox
(anglicky)

Jazyk práce: angličtina

Pokyny pro vypracování:

- 1) Vyřešit rozptyl pro Diracův operátor s obecnou (elektrostatickou, Lorentzovou skalární, "magnetickou") obdélníkovou bariérou.
- 2) Vyřešit stejný problém pro Diracův operátor s delta potenciálem.
- 3) Seznámit se s výsledky aproximací Diracových operátorů s delta potenciály pomocí Diracových operátorů se škálovanými regulárními potenciály. Je známo, že vazebná konstanta musí být v této limitě renormalizována.
- 4) Diskutovat detailně vztah mezi renormalizací a takzvaným Kleinovým paradoxem.

Doporučená literatura:

- [1] M. Tušek, Approximation of one-dimensional relativistic point interactions by regular potentials revised, Letters in Mathematical Physics 110 (2020).
- [2] V. Růžek, One-dimensional relativistic point interactions - approximations by regular potentials, application to models of the Dirac materials Master's Thesis, Czech Technical University in Prague, <https://dspace.cvut.cz/handle/10467/95493>, (2021).
- [3] P. Šeba, Klein's paradox and the relativistic point interaction, Letters in Mathematical Physics 18 (1989).
- [4] A. Calogeracos, N. Dombey, Klein tunnelling and the Klein paradox, International Journal of Modern Physics A 14 (1999).
- [5] B. Thaller, The Dirac Equation, Springer-Verlag, 1992.

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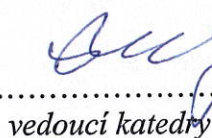
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V Praze dne 20.10.2022



DIPLOMA THESIS ASSIGNMENT

Academic year: 2022/2023

Student: Bc. Lukáš Vácha

Study programme: **Mathematical physics**

Thesis title: Diracovy operátory s bariérami: rozptyl a Kleinův paradox
(in Czech)

Thesis title: Dirac operators with barriers: scattering and the Klein paradox
(in English)

Language of the Thesis: English

Instructions:

- 1) Solve the scattering problem for Dirac operators with general (electrostatic, Lorentz scalar, “magnetic”) rectangular barriers.
- 2) Solve the same problem for Dirac operators with delta potentials.
- 3) Get familiar with results on approximations of Dirac operators with delta potentials by means of Dirac operators with scaled regular potentials. It is known that coupling constants have to be renormalized in the limit.
- 4) Discuss in detail the relation between this renormalization and the so-called Klein paradox.

Doporučená literatura:

- [1] M. Tušek, Approximation of one-dimensional relativistic point interactions by regular potentials revised, Letters in Mathematical Physics 110 (2020).
- [2] V. Růžek, One-dimensional relativistic point interactions - approximations by regular potentials, application to models of the Dirac materials Master's Thesis, Czech Technical University in Prague, <https://dspace.cvut.cz/handle/10467/95493>, (2021).
- [3] P. Šeba, Klein's paradox and the relativistic point interaction, Letters in Mathematical Physics 18 (1989).
- [4] A. Calogeracos, N. Dombey, Klein tunnelling and the Klein paradox, International Journal of Modern Physics A 14 (1999).
- [5] B. Thaller, The Dirac Equation, Springer-Verlag, 1992.

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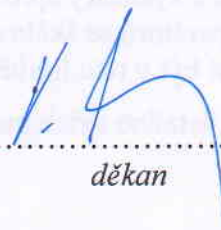
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V Praze dne 20.10.2022

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Diracovy operátory s bariérami: rozptyl a Kleinův paradox

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Bc. Lukáš Vácha

Název práce:

Diracovy operátory s bariérami: rozptyl a Kleinův paradox

Autor: Bc. Lukáš Vácha

Studijní program: Matematická fyzika

Druh práce: Diplomová práce

Vedoucí práce: doc. Ing. Matěj Tušek, Ph.D.
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Abstrakt: Diplomová práce se zabývá relativistickým kvantovým rozptylem pro Diracovu rovnici. Hledají se rozptylové koeficienty pro schodový, obdélníkový a delta potenciál. Dále se zkoumá nečekaná závislost koeficientů odrazu a průchodu na energii známá jako Kleinův paradox. V závěru práce se porovnává rozptyl na delta potenciálu s příslušnou aproximací potenciály tvaru obdélníku.

Klíčová slova: Diracova rovnice, Kvantové tunelování, Rozptyl, Kleinův paradox

Title:

Dirac operators with barriers: scattering and the Klein paradox

Author: Bc. Lukáš Vácha

Abstract: The thesis deals with the scattering problem for the Dirac equation. In particular, the reflection and transmission coefficients for the step-like, rectangular, and delta potentials are calculated. An unexpected dependence of these coefficients on energy, known as the Klein paradox, is discussed. Finally, we compare the scattering coefficients for the delta interaction and its approximation by scaled rectangular potentials.

Key words: Dirac Equation, Quantum tunneling, Scattering, Klein paradox

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Introduction

The scattering problem is broadly discussed in the non-relativistic quantum theory [1, Chapter 12]. It is a powerful tool used to study the interactions between particles or a particle and a field. It is used to determine the probability of a particle scattering off another particle or a set of particles. We assume that the other particles form an effective potential barrier, on which the examined particle is scattering. Usually, in the three-dimensional case, scattering angles are examined. In one dimension, that is what we focus on in this work, the probability of passing through the barrier is expressed using the transmission coefficient, and the probability of reflecting back is expressed by the reflection coefficient. In contrast to classical mechanics, even when the energy of the particle is lower than the height of the potential barrier the transmission coefficient can be positive. This is known as quantum tunneling. The probability of transmission typically decays exponentially with increasing barrier height and width. In other words, the larger and higher the barrier, the exponentially smaller is the probability that a particle will tunnel through it [2].

This exponential decay of the transmission coefficient is a fundamental aspect of the tunneling effect, and it underlies many of the practical applications of tunneling, such as in the design of tunnel diodes and other electronic devices. Overall, the exponential decay of the transmission coefficient is an important characteristic of the tunneling effect, and it explains how particles can pass through potential barriers that they would not be able to cross classically [3].

Even more surprisingly, in relativistic quantum mechanics, specifically for fermions, it is observed that this transmission amplitude does not decay exponentially and even may be equal to one for specific setting. This phenomenon is known as the Klein paradox. The paradox is observed as an unexpected, oscillating dependence of the scattering coefficients (transmission and reflection) on energy during the scattering of fermions (e.g. electrons) on the step-like or the rectangular electrostatic barrier even for energies less than the height of the barrier. Katsnelson et al. describe an experiment with this phenomenon in one of their papers as follows:

The term Klein paradox usually refers to a counterintuitive relativistic process in which an incoming electron starts penetrating through a potential barrier if its height V_0 exceeds twice the electron's rest energy mc^2 (where m is the electron mass and c the speed of light). In this case, the transmission probability T depends only weakly on the barrier height, approaching the perfect transparency for very high barriers, in stark contrast to the conventional, nonrelativistic tunneling where T exponentially decays with increasing V_0 . This relativistic effect can be attributed to the fact that a sufficiently strong potential, being repulsive for electrons, is attractive for positrons and results in positron states inside the barrier, which align

in energy with the electron continuum outside. (M. I. Katsnelson [4])

There is a suggestion on how to conduct an experiment on this phenomenon in this paper [4]. There is even outlined how it could possibly be used in FET transistors. Another experiment that leads to indirect evidence of the Klein paradox is described in [5].

Note that the phenomenon was theoretically examined for the first time by Oskar Benjamin Klein in 1928 [6]. It was later discussed in detail by Norman Dombey and Alex Calogeracosse in the articles [7, 8, 9]. Petr Šeba [10] described the point interaction for the Dirac equation mathematically rigorously and also mentioned a possible connection with the Klein paradox. The aim of this work is to better clarify the relation between the Klein paradox and the point interaction, its approximations and especially the re-normalization of the coupling constant. I hope this thesis will bring a straightforward overview of this topic. In the scattering on rectangular barriers, the occurrence of the paradox depends on the relation of coupling constants for the electrostatic and the Lorentz scalar potential together with the effective magnetic potential. As can be seen in Section 3.2, the electrostatic interaction promotes the paradox, while the other two inhibit it. Similarly, the same is true for the point interaction. Moreover, there is a direct connection with the re-normalization of the coupling constants. According to [11] formula (4.7) branches the same way as the decision, if the Klein paradox occurs, cf. (4.8).

In Chapters 1 and 2 we describe the needed explanation and properties of the differential operator in the Dirac equation, the operator one can call the Dirac Hamiltonian. Free Dirac Hamiltonian is described in Chapter 1 and one can find the operator with added potential in Chapter 2. Chapter 3 is dedicated to scattering on step-like and rectangular potentials. Finally, Chapter 4 illuminates the point interaction and its connection to the Klein paradox.

Chapter 1

Free Dirac Hamiltonian

In our three-dimensional world, the stationary Dirac equation is a differential equation on $L^2(\mathbb{R}^3, d^3x; \mathbb{C}^4)$. This thesis focuses only on the scattering in one dimension. In that case it is possible to represent the Dirac Hamiltonian in the Hilbert space $L^2(\mathbb{R}, dx; \mathbb{C}^2) \cong L^2(\mathbb{R}, dx) \otimes \mathbb{C}^2 = \mathcal{H}$. These spaces are isometric, we will not distinguish between them anymore and we will jointly denote them by \mathcal{H} [12, Theorem II.10 (b)]. We set the units to be $c = 1 = \hbar$ and we consider the mass m to be positive. We define a formal differential operator D , which appears in the Dirac equation as follows

$$D = -i \frac{d}{dx} \otimes \sigma^1 + m \otimes \sigma^3 = -i \frac{d}{dx} \sigma^1 + m \sigma^3, \quad (1.1)$$

where σ^i are the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and we add

$$\sigma^0 = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

So for our purposes, we consider a Hamiltonian, the operator denoted H_0 , with a domain $H^1(\mathbb{R}, dx; \mathbb{C}^2)$ which acts as the differential operator D (1.1). It will be proven later that H_0 is self-adjoint on the first Sobolev space, denoted $H^1(\mathbb{R}, dx; \mathbb{C}^2)$ or $W^{1,2}(\mathbb{R}, dx; \mathbb{C}^2)$, it consists of functions from \mathcal{H} , whose first weak derivative (in the sense of distributions) is also in \mathcal{H} , symbolically

$$H^1(\mathbb{R}, dx; \mathbb{C}^2) = \{f \in \mathcal{H} \mid f' \in \mathcal{H}\}.$$

To sum up, we can write the operator H_0 as follows

$$\begin{aligned} H_0 \psi &= D \psi, \\ \forall \psi \in \text{Dom}(H_0) &= H^1(\mathbb{R}, dx; \mathbb{C}^2). \end{aligned}$$

Let us start by describing the basic properties of this operator.

Proposition 1. [13, Theorem 1.1.] H_0 is self-adjoint.

Proof. The free Hamiltonian H_0 is, through the Fourier-Plancherel transform, unitarily equivalent to the multiplication operator \tilde{H}_0 (multiplying by matrix \tilde{H}_p).

$$(\mathcal{F}H_0\mathcal{F}^{-1}) = \tilde{H}_0, \quad (1.2)$$

$$\tilde{H}_p = \begin{pmatrix} m & p \\ p & -m \end{pmatrix},$$

where \mathcal{F} is the continuous extension of \mathfrak{F} from $L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ to $L^2(\mathbb{R})$ in each component and

$$\mathfrak{F}[\phi(x)](p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ipx} \phi(x) dx = \hat{\phi}(p).$$

The operator \tilde{H}_0 is self-adjoint on the maximal domain [14, Theorem XIII.85], which is

$$\text{Dom}(\tilde{H}_0) = \{\psi \in L^2(\mathbb{R}, dp; \mathbb{C}^2) \mid \tilde{H}_p \psi \in \mathcal{H}\}.$$

This means that the original operator H_0 is self-adjoint on the first Sobolev space

$$\text{Dom}(H_0) = \{\psi \in \mathcal{H} \mid \psi' \in \mathcal{H}\} = H^1(\mathbb{R}, dx; \mathbb{C}^2).$$

□

The variable p will be referred as momentum. We also need to know the spectrum of H_0 , as we know that possible energies of the quantum system are elements of $\sigma(H_0)$.

Proposition 2. [13, Theorem 1.1.]

$$\sigma(H_0) = (-\infty; -m] \cup [m; +\infty)$$

Proof. The same way as in the proof of the previous proposition, we study the spectrum of the operator \tilde{H}_0 (1.2). We calculate the spectrum of the matrix \tilde{H}_p for all p , which is

$$\det(\tilde{H}_p - \lambda \mathbb{I}) = -m^2 + \lambda^2 - p^2 = 0,$$

$$\lambda(p) = \pm \sqrt{m^2 + p^2}.$$

Spectrum of \tilde{H} is, from the unitary equivalence, equal to the spectrum of H_0 . We can write [15, Theorem 2.1.2.]

$$\sigma(\tilde{H}_0) = \sigma(H_0) = \overline{\text{Ran}(\lambda)} = \lambda(\mathbb{R}) = (-\infty; -m] \cup [m; +\infty).$$

□

Since H_0 is self-adjoint, the residual spectrum is empty. We will later see that the point spectrum is also empty. So we conclude that the spectrum is purely continuous, actually, the spectrum is purely absolutely continuous [16, Chapter 2.1]. Now we need to find the generalized eigenstates belonging to every energy E from the spectrum. To this purpose, we solve the differential equation

$$(D - E\mathbb{I})\Psi = 0, \quad (1.3)$$

with D from (1.1). For the components ψ_1 and ψ_2 of Ψ we have two ordinary linear differential equations

$$\begin{aligned} -i\psi_2' + (m - E)\psi_1 &= 0, \\ -i\psi_1' + (-m - E)\psi_2 &= 0. \end{aligned} \quad (1.4)$$

In order to solve the system (1.4), we take the derivative of one of them and substitute it in the other one. We arrive at only one ordinary differential equation of second order

$$\psi_1'' - (E^2 - m^2)\psi_1 = 0. \quad (1.5)$$

This is an equation for the linear harmonic oscillator (1.5). From [17], we know that the function ψ_1 will be smooth and we could have taken the derivative. By solving this equation and calculating the second function, we arrive at

$$\begin{aligned} \Psi_{+,E}(x) &= \left(\frac{1}{\sqrt{\frac{E-m}{E+m}}} \right) \exp\left(i \operatorname{sgn} E \sqrt{E^2 - m^2} x\right), \\ \Psi_{-,E}(x) &= \left(-\frac{1}{\sqrt{\frac{E-m}{E+m}}} \right) \exp\left(-i \operatorname{sgn} E \sqrt{E^2 - m^2} x\right). \end{aligned} \quad (1.6)$$

For the energies $E \in (-\infty; -m) \cup (m; +\infty)$, all linear combinations of functions (1.6) solve equation (1.3) and thus span the eigen(sub)space belonging to energy E . For the energies $E = \pm m$ the solution is a linear function in the form

$$\psi_1(x) = 2miK_1x + K_2, \quad \psi_2(x) = K_1,$$

respectively

$$\psi(x) = K_1, \quad \psi_2(x) = -2miK_1x + K_2.$$

for two arbitrary integration constants K_1 and K_2 . Since none of the solutions to (1.3) is in \mathcal{H} , the point spectrum of H_0 is empty.

Why have we chosen the pair of linear independent solutions (1.6)? Where did the signum function appear? According to the following interpretation based on the quantum electrodynamics (QED), the momentum of a particle is given by its energy and its pseudospin. The travel direction of the particle is determined by the sameness or difference in the sign of energy and pseudospin. In this manner Ψ_+ has a positive pseudospin and Ψ_- has a negative pseudospin, given in the the subscript. A typical example of the relativistic fermions in two dimensions are the electrons in graphene, as described in a paper from Katsnelson et al.

For the case of graphene, the latter symmetry is a consequence of its crystal symmetry because graphene's quasiparticles have to be described by two-component wavefunctions, which is needed to define relative contributions of sublattices A and B in quasiparticles' make-up. The two-component description for graphene is very similar to the one by spinor wavefunctions in QED but the 'spin' index for graphene indicates sublattices rather than the real spin of electrons and is usually referred to as pseudospin σ .

There are further analogies with QED. The conical spectrum of graphene is the result of intersection of the energy bands originating

from sublattices A and B and, accordingly, an electron with energy E propagating in the positive direction originates from the same branch of the electronic spectrum as the hole with energy $-E$ propagating in the opposite direction. This yields that electrons and holes belonging to the same branch have pseudospin σ pointing in the same direction, which is parallel to the momentum for electrons and antiparallel for holes. This allows one to introduce chirality, that is formally a projection of pseudospin on the direction of motion, which is positive and negative for electrons and holes, respectively. The term chirality is often used to refer to the additional built-in symmetry between electron and hole parts of graphene's spectrum and is analogous (although not completely identical) to the chirality in three-dimensional QED.

(M. I. Katsnelson, K. S. Novoselov, and A. K. Geim, [4])

According to this quotation, $p_0 = \text{sgn}(E)\sqrt{E^2 - m^2}$ is momentum in (1.6). For positive p , the wave $\exp(ipx)$ travels from left to the right and the wave $\exp(-ipx)$ aims to the left. Momentum p_0 of waves (1.6) has all the time the same sign as energy E . This all implies that particles traveling to the right are in some sense equivalent to antiparticles traveling to the left.

From now on we assume the variable E is from the spectrum of the relevant operator and sometimes we will change the notation a little bit and write the parameters E and m as the arguments of the function to be clear. For the scattering, we will need normalized eigenstates. We will find a proper normalization in the following section.

1.1 Formal normalization

It is a usual approach to normalize to a delta function. That means we are looking for a constant A such that

$$\langle A\Psi(E)|A\Psi(E')\rangle = \delta(E - E'). \quad (1.7)$$

We took Ψ in both arguments of $\langle \cdot | \cdot \rangle$ with the same sign in the subscript, both $+$ or both $-$. For the left-hand side, we get

$$\begin{aligned} \langle A\Psi(E)|A\Psi(E')\rangle &= |A|^2 \left(1 + \frac{\sqrt{E - m}\sqrt{E' - m}}{\sqrt{E + m}\sqrt{E' + m}} \right) \int_{\mathbb{R}} \exp(i(p - p')x) dx = \\ &= |A|^2 \left(1 + \frac{\sqrt{E - m}\sqrt{E' - m}}{\sqrt{E + m}\sqrt{E' + m}} \right) 2\pi\delta(p - p') = \\ &= |A|^2 \left(1 + \frac{\sqrt{E - m}\sqrt{E' - m}}{\sqrt{E + m}\sqrt{E' + m}} \right) \frac{\sqrt{E^2 - m^2}}{|E|} 2\pi\delta(E - E'), \end{aligned}$$

where $p = \sqrt{E^2 - m^2}$, $p' = \sqrt{E'^2 - m^2}$ and we used relation (sum runs over all zero points x_i of function g)

$$\delta(g(x)) = \sum \frac{\delta(x - x_i)}{|g'(x_i)|},$$

and thus

$$\delta(p - p') = \frac{\sqrt{E^2 - m^2}}{|E|} \delta(E - E').$$

Relation (1.7) is satisfied for the choice

$$A = \frac{1}{\sqrt{4\pi}} \left(\frac{E+m}{E-m} \right)^{\frac{1}{4}}.$$

Finally, the normalized solutions of (1.4) are [13, (4.77) and (4.78)]

$$\begin{aligned} \Psi_1(E, m, x) &= \left(\frac{\left(\frac{E+m}{E-m}\right)^{\frac{1}{4}}}{\left(\frac{E-m}{E+m}\right)^{\frac{1}{4}}} \right) \frac{1}{\sqrt{4\pi}} \exp\left(i \operatorname{sgn} E \sqrt{E^2 - m^2} x\right), \\ \Psi_2(E, m, x) &= \left(\frac{\left(\frac{E+m}{E-m}\right)^{\frac{1}{4}}}{-\left(\frac{E-m}{E+m}\right)^{\frac{1}{4}}} \right) \frac{1}{\sqrt{4\pi}} \exp\left(-i \operatorname{sgn} E \sqrt{E^2 - m^2} x\right). \end{aligned} \quad (1.8)$$

However, the above definition of $\langle \cdot | \cdot \rangle$ is clearly only formal, because the functions Ψ_1, Ψ_2 are not in fact in \mathcal{H} . In the next section we will describe the normalization procedure mathematically correctly.

1.2 Generalized eigenfunctions

In this section, we find rigorously the generalized eigenfunctions by constructing a Gelfand triple (also called Rigged Hilbert space).

Let's have a Hilbert space \mathcal{H} with the inner product $\langle \cdot | \cdot \rangle$ (linear in the second argument) and \mathcal{H}_+ its dense Banach subspace with the inclusion (embedding)

$$j : \mathcal{H}_+ \rightarrow \mathcal{H}.$$

Further, we assume that j is a continuous (bounded) mapping. We define \mathcal{H}_- as a set of all continuous anti-linear functionals on \mathcal{H}_+ . We denote the actions of the functional as the (angle) bracket, the same as the inner product, because it is in some sense an extension of the former inner product on \mathcal{H} . The triplet of spaces $\mathcal{H}_+, \mathcal{H}$ and \mathcal{H}_- with inclusions

$$\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-$$

constitutes the Gelfand triple.

Definition 1.2.1. System of generalized eigenfunctions [18, Supplement 1.2., Definition 2.4.]

Let M be a space with measure, suppose further that we are given a self-adjoint operator A and a vector-valued function $\Phi(m)$, $m \in M$, that is defined almost everywhere on M and takes values in the space \mathcal{H}_- of the rigging of a Hilbert space \mathcal{H} . A vector-valued function $\Phi(m)$ is called a system of generalized eigenvectors or eigenfunctions of the operator A if the following conditions are fulfilled:

1. For any $h_+ \in \mathcal{H}_+$ the function $m \mapsto (\Phi(m), h_+)$ on M belongs to $L^2(M)$;
2. the map $h_+ \mapsto (\Phi(\cdot), h_+)$ can be extended to a unitary operator $U : \mathcal{H} \rightarrow L^2(M)$;

In addition, if 3. is true, the system is complete.

3. there exists a real-valued function $a : M \rightarrow \mathbb{R}$ that is measurable and almost everywhere finite on M and is such that $A = U^{-1}\hat{a}U$, where \hat{a} is the multiplication operator by the function $a = a(m)$ in $L^2(M, dm)$, that is, U turns A into the multiplication operator by $a(m)$.

$\Phi(m)$ are functionals on space \mathcal{H} parameterized by elements of M .

Now we want to find the system of generalized eigenfunctions for our self-adjoint operator H_0 on the space

$$\mathcal{H} = \mathcal{H} = L^2(\mathbb{R}, dx) \otimes \mathbb{C}^2, \quad L^2(M) = L^2(\sigma(H), dE; \mathbb{C}^2).$$

We will choose \mathcal{H}_+ so that the functions $\exp(\pm ipx)$ are in its dual space. We will check if $\Psi \in \mathcal{H}_-$ from (1.8) fulfills condition 2. The candidate for the generalized eigenfunction Ψ depends on x and E variables, the action of the functional on a test function takes off x -dependency by integrating and the result remains only E -dependent. Later we will see that

$$\forall \varphi \in \mathcal{H}_+ : (\Psi(E, x), \varphi(x)) \in L^2(\sigma(H), dE; \mathbb{C}^2).$$

To find a complete system of generalized eigenfunctions, we start with the following unitary equivalence which transforms operator H_0 into a multiplication by a matrix,

$$\begin{aligned} \mathcal{F} \otimes \mathbb{I} : L^2(\mathbb{R}, dx; \mathbb{C}^2) &\rightarrow L^2(\mathbb{R}, dp; \mathbb{C}^2) \text{ is unitary,} \\ (\mathcal{F} \otimes \mathbb{I})H_0(\mathcal{F}^{-1} \otimes \mathbb{I}) &= \begin{pmatrix} m & p \\ p & -m \end{pmatrix}, \\ (\mathcal{F} \otimes \mathbb{I}) \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} &= \begin{pmatrix} \langle \hat{\Psi}(p, x) | \varphi_1(x) \rangle \\ \langle \hat{\Psi}(p, x) | \varphi_2(x) \rangle \end{pmatrix} = \begin{pmatrix} \hat{\varphi}_1 \\ \hat{\varphi}_2 \end{pmatrix}, \\ \hat{\Psi}(p, x) &= \frac{1}{\sqrt{2\pi}} e^{-ipx}. \end{aligned}$$

Here we interpret $\langle f | g \rangle$ as the integral $\int_{\mathbb{R}} \overline{f(x)} g(x) dx$ or its continuous extension for all f, g in $L^2(\mathbb{R}, dx)$. Due to the relation $p^2 = E^2 - m^2$ we need to change the kernel of the Fourier transform to

$$\tilde{\Psi}(E, x) = \frac{1}{\sqrt{2\pi}} K(E) e^{-i \operatorname{sgn} E \sqrt{E^2 - m^2} x}, \quad (1.9)$$

where $K(E)$ is a constant depending only on E , which we are looking for. We denote

$$\tilde{\varphi}_j = \langle \tilde{\Psi}(E, x) | \varphi_j(x) \rangle = K(E) \hat{\varphi}_j(\operatorname{sgn} E \sqrt{E^2 - m^2}).$$

We require $\varphi \mapsto \tilde{\varphi}$ to be unitary (and thus isometric) on $L^2(\mathbb{R}, dx; \mathbb{C}^2)$, that means for $j \in \hat{2}$ we need to satisfy the following

$$\begin{aligned} \|\varphi_j\|^2 = \|\hat{\varphi}_j\|^2 = \|\tilde{\varphi}_j\|^2 &= \int_{\sigma(H_0)} |K(E)|^2 |\hat{\varphi}_j(\operatorname{sgn} E \sqrt{E^2 - m^2})|^2 dE = \\ &= \int_{\mathbb{R}} |K(E)|^2 \frac{\sqrt{E^2 - m^2}}{|E|} |\hat{\varphi}_j(p)|^2 dp = \|\hat{\varphi}_j\|^2, \end{aligned}$$

where we used substitution $p = \operatorname{sgn} E \sqrt{E^2 - m^2}$, $dp = \frac{|E|}{\sqrt{E^2 - m^2}} dE$ in the integral. For the last equality, it is sufficient to opt for

$$K(E) = \sqrt[4]{\frac{E^2}{E^2 - m^2}} = \frac{\sqrt{E}}{\sqrt[4]{E - m} \sqrt[4]{E + m}}.$$

Without loss of generality, we chose $K(E)$ positive and we keep that the same in the following. Hence, we arrived at

$$\tilde{\Psi}(E, x) = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{E}}{\sqrt[4]{E-m}\sqrt[4]{E+m}} e^{-i \operatorname{sgn} E \sqrt{E^2 - m^2} x}.$$

We define G by the following

$$G : L^2(\mathbb{R}, dx) \rightarrow L^2(\sigma(H_0), dE),$$

$$G(\varphi_j) = \langle \tilde{\Psi}(E, x) | \varphi_j(x) \rangle.$$

We extend continuously the operator G to $L^2(\mathbb{R}, dx)$ similarly to the Fourier-Plancherel transform. We continue to diagonalize the Hamiltonian,

$$(G \otimes \mathbb{I})H_0((G^{-1} \otimes \mathbb{I})) = \begin{pmatrix} m & \operatorname{sgn} E \sqrt{E^2 - m^2} \\ \operatorname{sgn} E \sqrt{E^2 - m^2} & -m \end{pmatrix} =$$

$$= \begin{pmatrix} m & \sqrt{E-m}\sqrt{E+m} \\ \sqrt{E-m}\sqrt{E+m} & -m \end{pmatrix} = M(E).$$

The operator G is unitary, which follows from the above. Now we diagonalize the matrix $M(E)$ by real orthonormal vectors. Its eigenvalues are $\sigma(M(E)) = \{-E; E\}$ and the orthonormal eigenvectors are

$$a_+ = \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{E+m} \\ \sqrt{E-m} \end{pmatrix}, \quad a_- = \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{E-m} \\ -\sqrt{E+m} \end{pmatrix}.$$

So we can write the matrix $M(E)$ in the form

$$M(E) = A \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix} A^T,$$

$$A = \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{E+m} & \sqrt{E-m} \\ \sqrt{E-m} & -\sqrt{E+m} \end{pmatrix}.$$

Overall, the mapping $G \otimes A : L^2(\mathbb{R}, dx; \mathbb{C}^2) \rightarrow L^2(\sigma(H_0), dE; \mathbb{C}^2)$ is unitary. The generalized eigenfunctions of H_0 are

$$\Psi_1(E, m, x) = a_+ \tilde{\Psi}(E, x) = \frac{1}{\sqrt{4\pi}} \exp(i \operatorname{sgn} E \sqrt{E^2 - m^2} x) \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix}$$

$$\Psi_2(E, m, x) = a_- \tilde{\Psi}(E, x) = \frac{1}{\sqrt{4\pi}} \exp(-i \operatorname{sgn} E \sqrt{E^2 - m^2} x) \begin{pmatrix} \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \\ -\left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \end{pmatrix}.$$

However, the matrix formed out of these eigenvectors converts the Hamiltonian to a diagonal matrix $\operatorname{diag}(E; -E)$. For later use in the scattering part, we need both eigenvectors to correspond to the same eigenvalue. In order to do that, we just change E to $-E$ in the second eigenfunction. So the needed functions are

$$\Psi_{\rightarrow}(E, m, x) = \frac{1}{\sqrt{4\pi}} \exp(i \operatorname{sgn} E \sqrt{E^2 - m^2} x) \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix},$$

$$\Psi_{\leftarrow}(E, m, x) = \frac{1}{\sqrt{4\pi}} \exp(i \operatorname{sgn} E \sqrt{E^2 - m^2} x) \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ -\left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix}. \quad (1.10)$$

Chapter 2

Dirac Hamiltonian with potential

In this chapter, we add a potential term to free operator (1.1) and we have the Hamiltonian in the following form

$$H_{a_0, a_1, a_2, a_3} = -i \frac{d}{dx} \otimes \sigma^1 + m \otimes \sigma^3 + \sum_{\mu=0}^3 a_\mu V(x) \otimes \sigma^\mu, \quad (2.1)$$

where $a_0 \sigma^0$ is a scalar electrostatic potential, $a_1 \sigma^1$ can be gauged away by unitary transform as we will show in the next section, $a_2 \sigma^2$ effectively describes magnetic field (it is the remain of the magnetic field in the two-dimensional problem [19, 11]) and $a_3 \sigma^3$ is a Lorentz scalar interaction [20]. For all $\mu \in \{0, 1, 2, 3\}$, consider a_μ as arbitrary real coupling constants and let V be a bounded function. With these conditions, the Hamiltonian will remain self-adjoint on the same domain as the free Hamiltonian, i.e. first Sobolev space $H^1(\mathbb{R}, dx; \mathbb{C}^2)$. From now on we will use the Einstein summation rule over $\mu \in \{0; 1; 2; 3\}$ and omit the sum symbol.

2.1 Unitary equivalence

It is easy to see that unitarily equivalent operators to H_{a_0, a_1, a_2, a_3} give the same scattering coefficients. We will use this fact in Chapter 3.2. The first important equivalence is given by the following unitary operator

$$U_x = \exp\left(-i a_1 \sigma^0 \int V(x) dx\right).$$

The second needed equivalence is given by

$$U_\sigma = \exp\left(-i \frac{\pi}{4} \sigma^1\right) = \frac{\sqrt{2}}{2} (\mathbb{I} - i \sigma^1).$$

Let us see how $U^\dagger H_{a_0, a_1, a_2, a_3} U$ looks like in these two cases. In the first case notice that U_x commutes with all terms in H_{a_0, a_1, a_2, a_3} except the derivative term, where we have

$$-i \sigma^1 \frac{d}{dx} U_x = -a_1 V(x) \sigma^1 U_x - i \sigma^1 U_x \frac{d}{dx}.$$

This yields

$$U_x^\dagger H_{a_0, a_1, a_2, a_3} U_x = -i \sigma^1 \frac{d}{dx} + m \sigma^3 + a_3 V(x) \sigma^3 + a_0 V(x) \sigma^0 + a_2 V(x) \sigma^2 = H_{a_0, 0, a_2, a_3}, \quad (2.2)$$

where exactly term with σ^1 canceled out. This means, it is redundant to work with an operator with all four parameters and it is enough from now on to have just a_0, a_2, a_3 nonzero. In the transformation with U_σ , we have

$$\begin{aligned} U_\sigma^\dagger H_{a_0, a_1, a_2, a_3} U_\sigma &= -i\sigma^1 \frac{d}{dx} + a_0 V(x) \sigma^0 + a_1 V(x) \sigma^1 + m\sigma^2 + a_3 V(x) \sigma^2 - a_2 V(x) \sigma^3 \\ &= H_{a_0, a_1, m, -a_2} + m(\sigma^2 - \sigma^3) = H_{a_0, a_1, a_3, -a_2} + m(\sigma^2 - \sigma^3) \end{aligned} \quad (2.3)$$

by using the commutation relations of Pauli matrices. In this case, the parameters at σ^2 and σ^3 swapped up to the mass term and their signs. We can also use both of these at the same time and arrive at

$$U_\sigma^\dagger U_x^\dagger H_{a_0, a_1, a_2, a_3} U_x U_\sigma = H_{a_0, 0, a_3, -a_2} + m(\sigma^2 - \sigma^3).$$

2.2 Generalized eigenfunctions for Hamiltonian with a constant potential

We assume constant potential $V(x) = 1$ and we denote

$$\begin{aligned} \tilde{m} &= m + a_3, \\ \tilde{E} &= E - a_0. \end{aligned}$$

For a special case, when $a_2 = 0$, we have $H_{a_0, 0, 0, a_3} = H_0$ with mass \tilde{m} instead of m and eigenvalues \tilde{E} . Keep in mind that the action of H_0 is given by (1.1). In this case, let us start with a look at the spectrum of H_{a_0, a_1, a_2, a_3} . We want to solve

$$\begin{aligned} (H_{a_0, a_1, a_2, a_3} - E\mathbb{I})\psi &= 0, \\ \begin{pmatrix} \tilde{m} - \tilde{E} & -i\frac{d}{dx} + a_1 - ia_2 \\ -i\frac{d}{dx} + a_1 + ia_2 & -\tilde{m} - \tilde{E} \end{pmatrix} \psi &= 0. \end{aligned}$$

We pass to the Fourier image ($\tilde{H}_{a_0, a_1, a_2, a_3} = \mathcal{F}H_{a_0, a_1, a_2, a_3}\mathcal{F}^{-1}$), where

$$\begin{aligned} (\tilde{H}_{a_0, a_1, a_2, a_3} - E\mathbb{I})\psi &= 0, \\ \begin{pmatrix} \tilde{m} - \tilde{E} & p + a_1 - ia_2 \\ p + a_1 + ia_2 & -\tilde{m} - \tilde{E} \end{pmatrix} \psi &= 0. \end{aligned}$$

and we want to have $\det(\tilde{H}_{a_0, a_1, a_2, a_3} - E\mathbb{I}) = 0$. This is exactly

$$\begin{aligned} \tilde{E}^2 - \tilde{m}^2 - a_2^2 - (a_1 + p)^2 &= 0, \\ E(p) &= \pm \sqrt{\tilde{m}^2 + a_2^2 + (a_1 + p)^2} + a_0. \end{aligned}$$

We know that $\sigma(\tilde{H}_{a_0, a_1, a_2, a_3}) = \overline{\text{Ran}(E_+) \cup \text{Ran}(E_-)}$ [15, Theorem 2.1.2.]. The spectrum of H_{a_0, a_1, a_2, a_3} is therefore

$$\sigma(H_{a_0, a_1, a_2, a_3}) = \left(-\infty; a_0 - \sqrt{\tilde{m}^2 + a_2^2}\right] \cup \left[a_0 + \sqrt{\tilde{m}^2 + a_2^2}; +\infty\right).$$

We denote momentum $p_{a_0, a_1, a_2, a_3} = -a_1 + \text{sgn}(E)\sqrt{\tilde{E}^2 - \tilde{m}^2 - a_2^2}$. Eigenvectors are proportional to $\exp(\pm i p_{a_0, a_1, a_2, a_3} x)$. We normalize eigenvectors in the same way as in Section 1.2, but instead of (1.9) we take

$$\begin{aligned}\tilde{\Psi}(E, x) &= \frac{1}{\sqrt{2\pi}} K(E) \exp \left[-i \left(-a_1 + \text{sgn}(E)\sqrt{\tilde{E}^2 - \tilde{m}^2 - a_2^2} \right) x \right], \\ &= \frac{1}{\sqrt{2\pi}} K(E) \exp \left[-i p_{a_0, a_1, a_2, a_3}(E) x \right].\end{aligned}$$

If we use the same procedure and analogous substitution in the integral, we get

$$K(E) = \sqrt[4]{\frac{\tilde{E}^2}{\tilde{E}^2 - \tilde{m}^2 - a_2^2}}$$

and

$$\tilde{\Psi}(E, x) = \frac{1}{\sqrt{2\pi}} \sqrt[4]{\frac{\tilde{E}^2}{\tilde{E}^2 - \tilde{m}^2 - a_2^2}} \exp \left[-i \left(-a_1 \pm \sqrt{\tilde{E}^2 - \tilde{m}^2 - a_2^2} \right) x \right].$$

The matrix $M(E)$ is now

$$M(E) = \begin{pmatrix} \tilde{m} + a_0 & p_{a_0, a_1, a_2, a_3} + a_1 - ia_2 \\ p_{a_0, a_1, a_2, a_3} + a_1 + ia_2 & -\tilde{m} + a_0 \end{pmatrix}.$$

We denote $\tilde{p} = \text{sgn}(E)\sqrt{\tilde{E}^2 - \tilde{m}^2 - a_2^2}$. Eigenvectors of $M(E)$ are

$$\begin{aligned}a_+ &= \frac{1}{\sqrt{2\tilde{E}(\tilde{E} + \tilde{m})}} \begin{pmatrix} \tilde{p} - ia_2 \\ \tilde{E} + \tilde{m} \end{pmatrix}, \\ a_- &= \frac{1}{\sqrt{2\tilde{E}(\tilde{E} - \tilde{m})}} \begin{pmatrix} \tilde{p} + ia_2 \\ \tilde{E} - \tilde{m} \end{pmatrix}.\end{aligned}$$

Now it is easy to get the eigenvectors of $H_{a_0, 0, a_2, a_3}$,

$$\begin{aligned}\Psi_+(\tilde{E}, \tilde{m}, x) &= \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{\tilde{p}}\sqrt{\tilde{E} - \tilde{m}}} \begin{pmatrix} \tilde{p} - ia_2 \\ \tilde{E} + \tilde{m} \end{pmatrix} \exp[i(-a_1 + \tilde{p})x], \\ \Psi_-(\tilde{E}, \tilde{m}, x) &= \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{\tilde{p}}\sqrt{\tilde{E} - \tilde{m}}} \begin{pmatrix} \tilde{p} + ia_2 \\ -(\tilde{E} - \tilde{m}) \end{pmatrix} \exp[i(-a_1 - \tilde{p})x].\end{aligned}$$

We flip the sign at E in the second function for the same reason as in the previous chapter and arrive at

$$\begin{aligned}\Psi_{\rightarrow}(\tilde{E}, \tilde{m}, x) &= \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{\tilde{p}}\sqrt{\tilde{E} - \tilde{m}}} \begin{pmatrix} \tilde{p} - ia_2 \\ \tilde{E} + \tilde{m} \end{pmatrix} \exp[i(-a_1 + \tilde{p})x], \\ \Psi_{\leftarrow}(\tilde{E}, \tilde{m}, x) &= \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{\tilde{p}}\sqrt{-\tilde{E} - \tilde{m}}} \begin{pmatrix} \tilde{p} + ia_2 \\ \tilde{E} + \tilde{m} \end{pmatrix} \exp[i(-a_1 + \tilde{p})x].\end{aligned}$$

Chapter 3

Scattering

To start this chapter and to know how to work with the scattering, we introduce the Lippman-Schwinger equation [21]. We modify the form [22, (2.27)] to one dimension and arrive at

$$\phi_{\pm}(x, p_0, n) = \Psi_n(x, p_0) - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} R_{E \pm 0i}(x-s)V(s)a_{\mu}\sigma^{\mu}\phi_{\pm}(s, p_0, n)ds. \quad (3.1)$$

This is an equation for the generalized eigenfunctions of Hamiltonian with potential (2.1) [18]. Keep all the time in mind that $p_0 = \text{sgn } E\sqrt{E^2 - m^2}$. We have written the functions (1.8) in p -representation, i.e.

$$\begin{aligned} \Psi_{\rightarrow}(E, m, x) &= \frac{1}{\sqrt{4\pi}} \exp(ip_0x) \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix}, \\ \Psi_{\leftarrow}(E, m, x) &= \frac{1}{\sqrt{4\pi}} \exp(-ip_0x) \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ -\left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix}. \end{aligned}$$

Note that $n \in \{\rightarrow, \leftarrow\}$ and R is the resolvent kernel of the free Dirac Hamiltonian (1.1) according to [23, Section 3.1]

$$R_z(x-s) = \frac{i}{2} \left[Z(z) + \text{sgn}(x-s)\sigma^1 \right] \exp(ip_0|x-s|),$$

$$Z(z) = \begin{pmatrix} \zeta(z) & 0 \\ 0 & \zeta^{-1}(z) \end{pmatrix}, \quad \zeta(z) = \frac{z+m}{p_0}.$$

The particle is scattering on potential V . We will approximate the function $\phi_{\pm}(x, p_0, n)$ to the first order by taking $\Psi_n(x, p_0)$ as $\phi_{\pm}(x, p_0, n)$ on the right-side of the equation (3.1). We split the integration into intervals $(-\infty, x)$ and $(x, +\infty)$, the result then looks like the following

$$\begin{aligned} \phi_{\pm}(x, p_0, \rightarrow) &= e^{ip_0x} \mathbb{A} \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix} + e^{-ip_0x} \mathbb{B} \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix}, \\ \phi_{\pm}(x, p_0, \leftarrow) &= e^{ip_0x} \mathbb{A}\sigma^3 \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix} + e^{-ip_0x} \mathbb{B}\sigma^3 \begin{pmatrix} \left(\frac{E+m}{E-m}\right)^{\frac{1}{4}} \\ \left(\frac{E-m}{E+m}\right)^{\frac{1}{4}} \end{pmatrix} \end{aligned}$$

with

$$\mathbb{A} = \mathbb{I} + -\frac{i}{2\sqrt{2\pi}}\mathcal{V}_-(x) \begin{pmatrix} a_0\zeta(z) + a_1 + ia_2 + a_3\zeta(z) & a_0 + (a_1 - ia_2)\zeta(z) - a_3 \\ a_0 + (a_1 + ia_2)\zeta^{-1}(z) + a_3 & (a_0 - a_3)\zeta^{-1}(z) + a_1 - ia_2 \end{pmatrix},$$

$$\mathbb{B} = -\frac{i}{2\sqrt{2\pi}}\mathcal{V}_+(x) \begin{pmatrix} a_0\zeta(z) - a_1 - ia_2 + a_3\zeta(z) & -a_0 + (a_1 - ia_2)\zeta(z) + a_3 \\ -a_0 + (a_1 + ia_2)\zeta^{-1}(z) - a_3 & (a_0 - a_3)\zeta^{-1}(z) - a_1 + ia_2 \end{pmatrix},$$

$$\mathcal{V}_+(x) = \frac{1}{\sqrt{4\pi}} \int_x^{+\infty} V(s)ds,$$

$$\mathcal{V}_-(x) = \frac{1}{\sqrt{4\pi}} \int_{-\infty}^x V(s)ds$$

and

$$z = \lim_{\varepsilon \rightarrow 0} (E \pm \varepsilon i) = E \pm 0i.$$

From all this, we can find a linear combination $\Phi(x, p_0)$ of $\phi_{\pm}(x, p_0, \rightarrow)$ and $\phi_{\pm}(x, p_0, \leftarrow)$ such that

$$\Phi(x, p_0) = \begin{cases} \Psi_{\rightarrow}(E(p_0), m, x) + R\Psi_{\leftarrow}(E(p_0), m, x) & \text{if } x < -a, \\ T\Psi_{\rightarrow}(E(p_0), m, x) & \text{if } x > a. \end{cases} \quad (3.2)$$

This ansatz we will use later. In order to use this for the scattering, we have to assume that in the time $t \rightarrow -\infty$ we have an initial wave (eigenfunction of H_0) coming from $x \rightarrow -\infty$ and traveling to the right (with momentum $p_0 > 0$) then we let the potential act only in a bounded neighborhood around zero and finally we "measure" the reflected and the transmitted waves at the time $t \rightarrow +\infty$ [2].

3.1 Scattering on step-like potential

We want to scatter on the potential barrier of the Heaviside theta function in form

$$V(x) = \Theta(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x < 0. \end{cases}$$

In fact, this potential does not meet our assumptions and requirements from the previous paragraph such as the potential being nonzero only on a bounded neighborhood around zero. However, this example appears in literature like in [13] and thus we mention it here to show the complete picture. We stick to a non-magnetic potential, i.e. $a_2 = 0$, and also consider $a_1 = 0$ which is no restriction according to (2.2). So the Hamiltonian in this situation reads as follows

$$H_{\Theta} = \begin{cases} H_{a_0,0,0,a_3} = -i\sigma^1 \frac{d}{dx} + \tilde{m}\sigma^3 + a_0\sigma^0 & \text{if } x > 0, \\ H_0 = -i\sigma^1 \frac{d}{dx} + m\sigma^3 & \text{if } x < 0. \end{cases}$$

We take an initial wave (1.10) with \rightarrow subscript and let it come from $x \rightarrow -\infty$ near zero and scatter. That means we solve the Dirac equation on negative and positive real axes separately and then connect them such that in the $x < 0$ region we have

the initial and the reflected waves and in the $x > 0$ we have just the transmitted wave according to (3.2). Hence, the total wave u is of the form

$$u(x) = \begin{cases} \Psi_{\rightarrow}(E, m, x) + R_{\Theta}(E)\Psi_{\leftarrow}(E, m, x) & \text{if } x < 0, \\ T_{\Theta}(E)\Psi_{\rightarrow}(\tilde{E}, \tilde{m}, x) & \text{if } x > 0, \end{cases}$$

which we require to be continuous. The continuity condition turns into the following system of equations

$$(1 + R_{\Theta})\sqrt{\kappa} = T_{\Theta}, \quad (1 - R_{\Theta}) = T_{\Theta}\sqrt{\kappa},$$

where

$$\kappa = \sqrt{\frac{(E + m)(\tilde{E} - \tilde{m})}{(E - m)(\tilde{E} + \tilde{m})}}.$$

We separate R from the first equation and substitute it into the other one and get the results for the reflection coefficient R and the transmission coefficient T [24],

$$R_{\Theta} = \frac{1 - \kappa}{1 + \kappa}, \quad T_{\Theta} = \frac{2\sqrt{\kappa}}{1 + \kappa}.$$

It is reasonable only to consider

$$\begin{aligned} E &\in \sigma(H_{\Theta}) \cap \sigma(H_0), \\ E &\in ((-\infty; -m] \cup [m; +\infty)) \cap ((-\infty; a_0 - \tilde{m}] \cup [a_0 + \tilde{m}; +\infty)). \end{aligned}$$

For these energies κ remains real. Otherwise, if κ was purely imaginary (and $\kappa \neq 0$), the squares of transmission and reflection coefficients would not sum to one,

$$\begin{aligned} |R|_{\Theta}^2 &= \frac{|1 - \kappa|^2}{|1 + \kappa|^2} = \frac{1 + |\kappa|^2}{1 + |\kappa|^2} = 1, \\ |T|_{\Theta}^2 &= \frac{4|\sqrt{\kappa}|^2}{|1 + \kappa|^2} = \frac{4|\kappa|}{1 + |\kappa|^2} \neq 0. \end{aligned}$$

In the positive case, when $\kappa \in \mathbb{R}$, the square of the absolute value of T_{Θ} and R_{Θ} are according to [13, Section 4.5]

$$\begin{aligned} |R|_{\Theta}^2 &= \frac{(1 - \kappa)^2}{(1 + \kappa)^2}, \\ |T|_{\Theta}^2 &= \frac{4\kappa}{(1 + \kappa)^2}. \end{aligned}$$

Here, it is easy to check that $|T|_{\Theta}^2 + |R|_{\Theta}^2 = 1$,

$$\begin{aligned} |T|_{\Theta}^2 + |R|_{\Theta}^2 &= \frac{(1 - \kappa)^2 + 4\kappa}{(1 + \kappa)^2} = \frac{1 - 2\kappa + \kappa^2 + 4\kappa}{(1 + \kappa)^2} = \\ &= \frac{1 + 2\kappa + \kappa^2}{(1 + \kappa)^2} = \frac{(1 + \kappa)^2}{(1 + \kappa)^2} = 1. \end{aligned}$$

As you can see in Figure 3.1, even for energies below the height of the barrier,

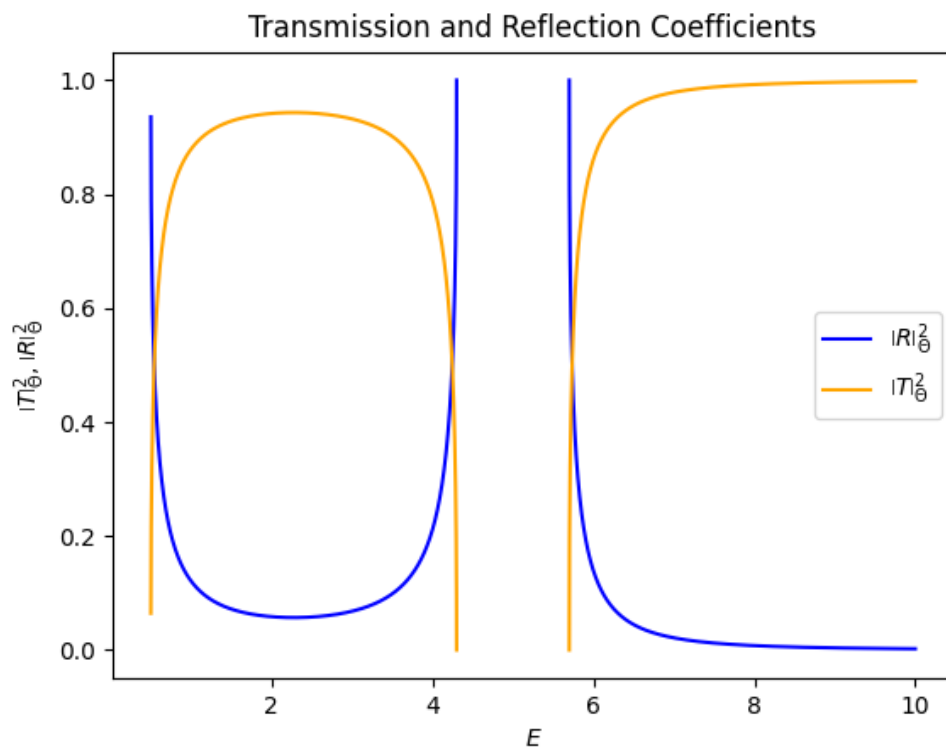


Figure 3.1: Dependence of $|T|_{\Theta}^2$ and $|R|_{\Theta}^2$ for the step-like potential on energy with $a_0 = 5$, $m = 0.5$ and $a_3 = 0.2$

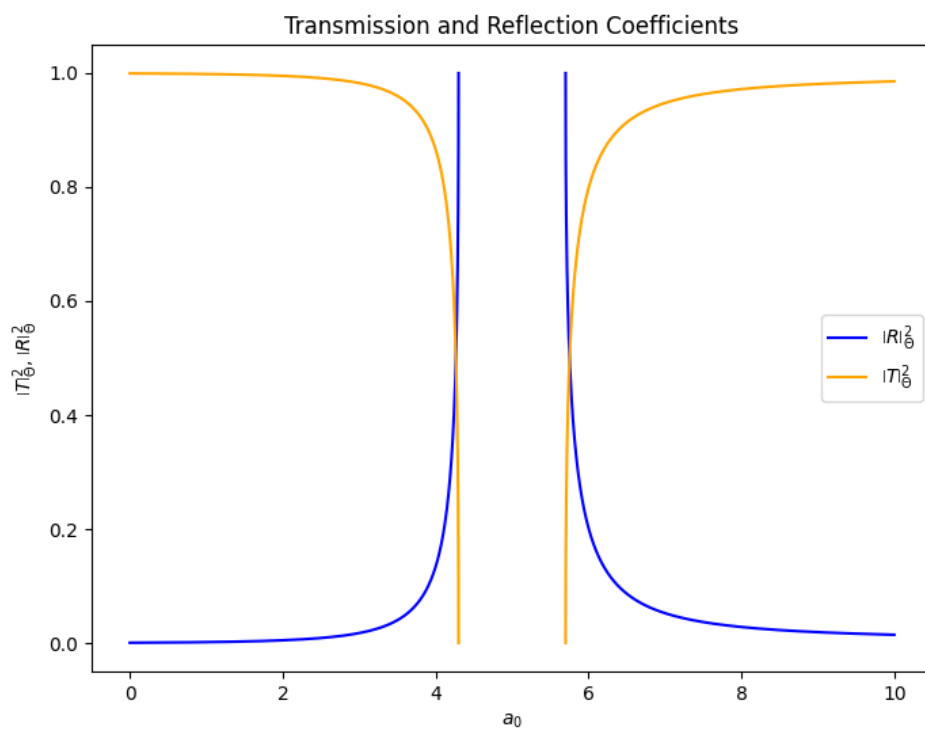


Figure 3.2: Dependence of $|T|_{\Theta}^2$ and $|R|_{\Theta}^2$ for the step-like potential on a_0 with $E = 5$, $m = 0.5$ and $a_3 = 0.2$

i.e. $E < a_0 = 5$, the probability of transmission through the barrier is close to 100 %. Note that there is a forbidden belt around a_0 , $E \notin (a_0 - m - a_3; a_0 + m + a_3)$, in Figure 3.1 $E \notin (4.3; 5.7)$. The effect of a high probability of passing through in region $E \in (m; a_0 - m - a_3)$ is known as the Klein paradox [6]. Particles have effectively negative energy in the potential region ($x > 0$) and we assume that particles transform into their corresponding antiparticles when arriving at the potential interface. Similarly, in Figure 3.2 you can see this paradox for $a_0 > E + m + a_3 = 5.7$, where we have plotted the height of the electrostatic barrier a_0 as a dependent variable.

3.2 Scattering on rectangular potential

In this section, we deal with the scattering on the barrier of the form

$$V(x) = \chi_{(-a;a)}(x) = \begin{cases} 1 & \text{if } |x| < a, \\ 0 & \text{if } |x| > a. \end{cases}$$

For now a is an arbitrary positive real constant, half the barrier width. Scattering on a well of this kind is discussed in [25]. As we already know from (2.2), we can set $a_1 = 0$. In order to simplify things a bit more, we will discuss two more specific cases. The case $a_3 = m = 0$ can be, by a unitary equivalence, transformed by (2.3) to a case $a_2 = 0$. Therefore, from now on, we assume $a_2 = 0$ and let us recall that the Hamiltonian under these assumptions is

$$H_\chi = \begin{cases} H_{a_0,0,0,a_3} = -i\sigma^1 \frac{d}{dx} + \tilde{m}\sigma^3 + a_0\sigma^0 & \text{if } |x| > a, \\ H_0 = -i\sigma^1 \frac{d}{dx} + m\sigma^3 & \text{if } |x| > a. \end{cases}$$

Now we need to solve the Dirac equation on the separate intervals $(-\infty; -a)$, $(-a; a)$ and $(a; +\infty)$. We will consider only simple scattering, i.e. we have an initial wave propagating from $x \rightarrow -\infty$, part of it reflects (R_l) on the left interface and part of it transmits (T_l) into the middle section and encounters the second interface. Here again, one part reflects (R_r) and the other transmits (T_r) to $x \rightarrow +\infty$, cf. Figure 3.3. After the use ansatz (3.2) on each interface, we arrive at the connection conditions

1. at point $-a$:

$$\Psi_\leftarrow(E, m, -a) + R_l \Psi_\rightarrow(E, m, -a) = T_l \Psi_\rightarrow(\tilde{E}, \tilde{m}, -a) + T_l R_r \Psi_\leftarrow(\tilde{E}, \tilde{m}, -a),$$

2. at point a :

$$T_l \Psi_\rightarrow(\tilde{E}, \tilde{m}, a) + T_l R_r \Psi_\leftarrow(\tilde{E}, \tilde{m}, a) = T_l T_r \Psi_\rightarrow(E, m, a).$$

The spinors Ψ_\rightarrow and Ψ_\leftarrow are 2-component, so we have four equations that are linear for variables $R_l, T_l, T_l R_r, T_l T_r$. We can rewrite the system in these variables as

$$\mathbb{P} \begin{pmatrix} R_l \\ T_l \\ T_l R_r \\ T_l T_r \end{pmatrix} = \begin{pmatrix} -\Psi_\rightarrow(E, m, -a) \\ 0 \end{pmatrix},$$

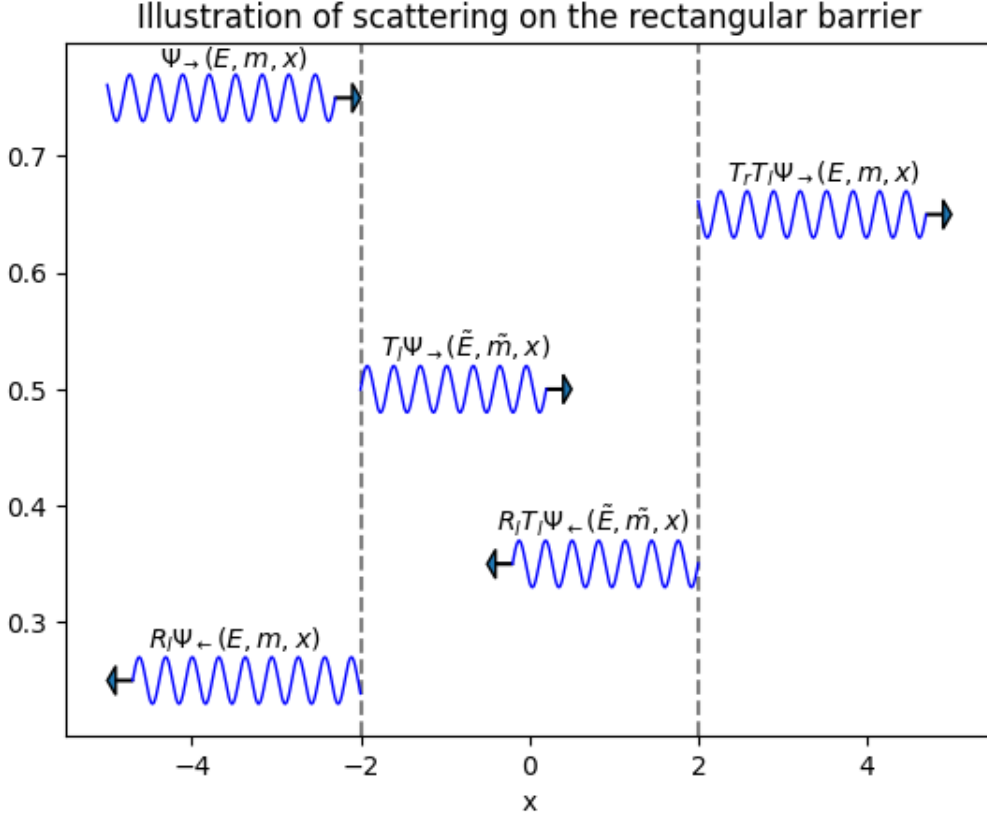


Figure 3.3: Illustration of the scattering on the rectangular barrier for $a = 2$

$$\mathbb{P} = \begin{pmatrix} \Psi_{\rightarrow}(E, m, -a) & -\Psi_{\rightarrow}(\tilde{E}, \tilde{m}, -a) & \Psi_{\leftarrow}(\tilde{E}, \tilde{m}, -a) & 0 \\ 0 & \Psi_{\rightarrow}(\tilde{E}, \tilde{m}, a) & \Psi_{\leftarrow}(\tilde{E}, \tilde{m}, a) & -\Psi_{\rightarrow}(E, m, a) \end{pmatrix}.$$

In order to solve this system of equations and denote

$$\begin{aligned} p_0 &= \sqrt{E^2 - m^2}, \\ p_{a_0,0,0,a_3} &= \sqrt{\tilde{E}^2 - \tilde{m}^2}, \\ \kappa &= \sqrt{\frac{(E+m)(\tilde{E}-\tilde{m})}{(E-m)(\tilde{E}+\tilde{m})}}. \end{aligned} \quad (3.3)$$

We calculate R_l, R_r, T_l, T_r from $R_l, T_l, T_l R_r, T_l T_r$ and then we can see the transmission coefficient $T = T_l T_r$ and the reflection coefficient $R = R_l$. Finally, we present the squares of the absolute values of T and R ,

$$\begin{aligned} |T|^2 &= \frac{4\kappa^2}{4\kappa^2 + (1 - \kappa^2)^2 \sin^2(2p_{a_0,0,0,a_3} a)}, \\ |R|^2 &= \frac{(1 - \kappa^2)^2 \sin^2(2p_{a_0,0,0,a_3} a)}{4\kappa^2 + (1 - \kappa^2)^2 \sin^2(2p_{a_0,0,0,a_3} a)}. \end{aligned} \quad (3.4)$$

It might be convenient to look at the transmission probability in the form

$$|T|^2 = \frac{1}{1 + \frac{(1-\kappa^2)^2}{4\kappa^2} \sin^2(2p_{a_0,0,0,a_3} a)}.$$

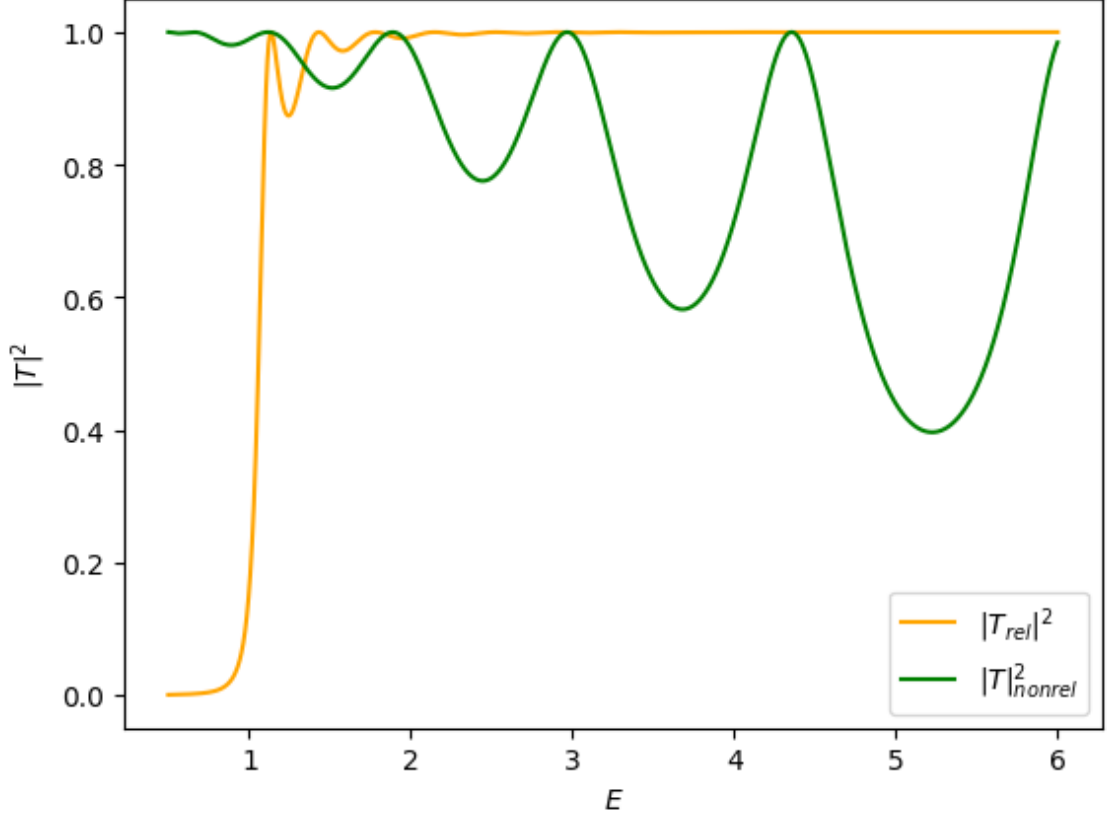


Figure 3.4: Dependence of $|T|^2$ relativistic and non-relativistic for the rectangular potential with $a_0 = 0.5$; $m = 0.5$; $a_3 = 0$; $a = 4$

This is consistent with literature such as [8, 26] and they add up to one as they should. It is important to emphasize that E is always from the spectrum $\sigma(H_{a_0,0,0,a_3}) = \sigma(H_0)$. The important quantity is $p_{a_0,0,0,a_3}$, it can be real or purely imaginary, we will discuss these specific cases separately.

1. $E = \pm \tilde{m}$,

$$|T|^2 = \frac{1}{1 + \frac{4\tilde{m}^2 a^2 (a_0 \pm a_3)}{a_0 \pm 2m \pm a_3}} = \frac{a_0 \pm 2m \pm a_3}{a_0 \pm 2m \pm a_3 + 4\tilde{m}^2 a^2 (a_0 \pm a_3)},$$

$$|R|^2 = \frac{1}{1 + \frac{a_0 \pm 2m \pm a_3}{4\tilde{m}^2 a^2 (a_0 \pm a_3)}} = \frac{4\tilde{m}^2 a^2 (a_0 \pm a_3)}{a_0 \pm 2m \pm a_3 + 4\tilde{m}^2 a^2 (a_0 \pm a_3)}.$$

2. $E \in (-\infty; a_0 - \tilde{m}) \cup (a_0 + \tilde{m}; +\infty)$, all quantities in (3.4) are real, especially κ and $p_{a_0,0,0,a_3}$ from (3.3) are real. If we plot both $|T|^2$ and $|R|^2$, we can see oscillations in the dependency on E or a_0 similarly to the non-relativistic case for large energies, see part $E > 1$ in Figure 3.4. The difference in the behavior for small energies will be described in the next section. The extremes, where $|T|^2 = 1$, are in the points

$$E_k = \pm \sqrt{\frac{k^2 \pi^2}{4a^2} + \tilde{m}^2} + a_0, \quad (3.5)$$

for all $k \in \mathbb{Z}$ arbitrary and when all the conditions above are met.

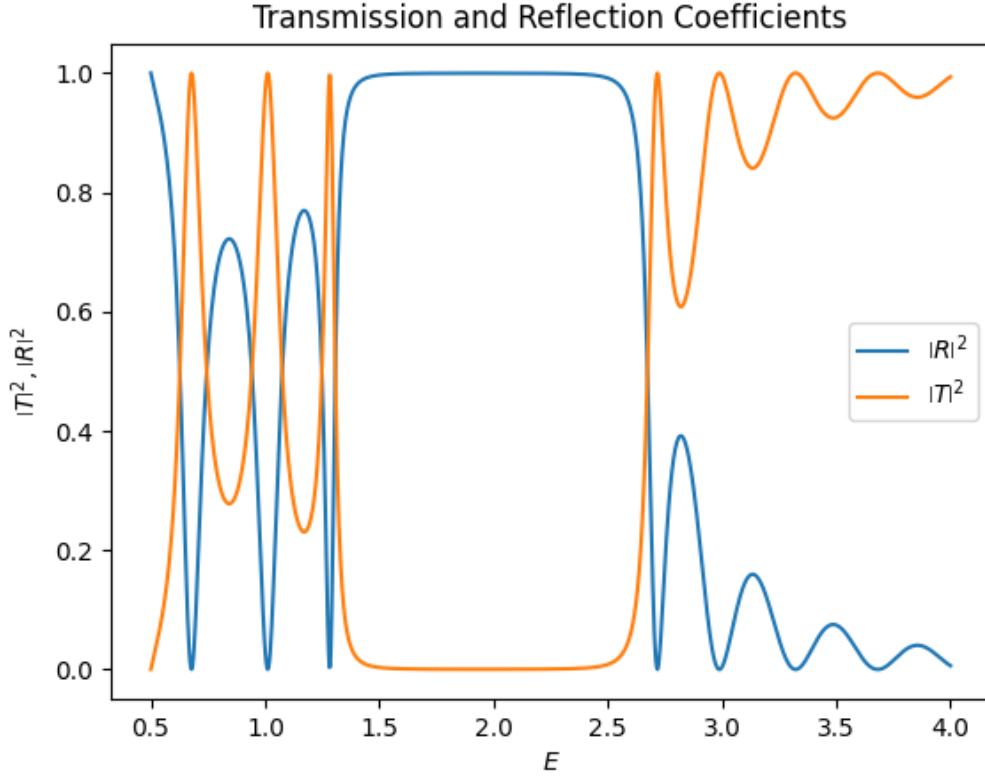


Figure 3.5: Dependence of $|T|^2$ and $|R|^2$ for the rectangular potential on energy with $a_0 = 2$; $m = 0.5$; $a_3 = 0.1$; $a = 4$

3. $E \in (a_0 - \tilde{m}; a_0 + \tilde{m})$, note that now both κ and $p_{a_0,0,0,a_3}$ from (3.3) are purely imaginary and $\kappa^2 < 0$. By using $\sin(2ip_{a_0,0,0,a_3}a) = \sin(2i|p_{a_0,0,0,a_3}|a) = i \sinh(2|p_{a_0,0,0,a_3}|a)$ we can write the relation (3.4) in the form

$$|T|^2 = \frac{1}{1 + \frac{(1-\kappa^2)^2}{-4\kappa^2} \sinh^2(2|p_{a_0,0,0,a_3}|a)}. \quad (3.6)$$

The behavior (3.6) is similar to non-relativistic case for $E \in (m; a_0)$. In Figure 3.5, you can see this exponential dumping between $E = a_0 - m - a_3 = 1.4$ and $E = a_0 + m + a_3 = 2.6$.

Let us recap the well-known non-relativistic case to compare both cases. Let us have an electrostatic barrier of height a_0 , a particle with mass m and energy E , for positive $(E - a_0)$ we have

$$|T|_{\text{nonrel}}^2 = \frac{1}{1 + \frac{a_0^2 \sin^2\left(2a\sqrt{2m(E-a_0)}\right)}{4E(E-a_0)}},$$

$$|R|_{\text{nonrel}}^2 = \frac{1}{1 + \frac{4E(E-a_0)}{a_0^2 \sin^2\left(2a\sqrt{2m(E-a_0)}\right)}}.$$

Otherwise, when $E < a_0$, we have

$$|T|_{\text{nonrel}}^2 = \frac{1}{1 - \frac{a_0^2 \sinh^2(2\sqrt{2m(E-a_0)}a)}{4E(E-a_0)}}.$$

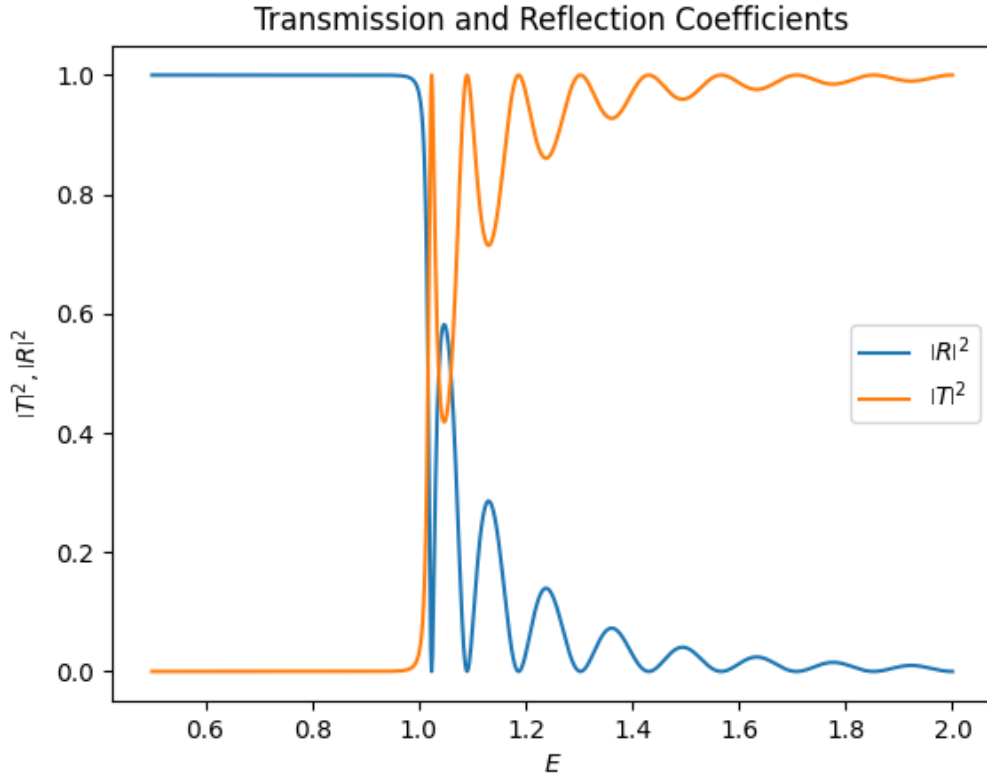


Figure 3.6: Dependence of $|T|^2$ and $|R|^2$ for the rectangular potential on energy with $a_0 = 0.5$; $m = 0.5$; $a_3 = 0$; $a = 10$

To compare the relativistic and non-relativistic transmission coefficients, see Figure 3.4. You can see the oscillation behavior in the $E > a_0$ region in both cases. You can see the difference, where in the relativistic case the amplitude of the oscillations decreases, while on the other hand, in the non-relativistic case it increases. In Figure 3.6, we have raised the width of the barrier ($a = 10$), you can see that the oscillations are denser according to (3.5).

3.3 The Klein paradox

The Klein paradox occurs when the height of the electrostatic barrier is greater than twice the mass of the particle, with correct units $2mc^2$, plus the Lorentz scalar potential, i.e. $a_0 > 2m + a_3 = 2mc^2 + a_3$. In this case, the intersection of the examined interval $(m; a_0)$, i.e. energies below the height of the electrostatic barrier, and the interval $(-\infty; a_0 - \tilde{m})$, where we see the oscillating behavior, is nonempty. In this region, we can see the paradox, which is visible in Figures 3.5 for $E \in (0.5; 1.4)$ and Figure 3.7 for $E \in (0.5; 1.5)$.

You can compare the relativistic and non-relativistic transmission coefficients in Figure 3.7. From zero to the height of the barrier, in this case between 0 and 2, the non-relativistic passage is exponential (in hyperbolic sinus relation), so soon very close to zero, while in the relativistic case even for energies below the electrostatic wall height, explicitly for the values of energy from formula (3.5), $|T|^2 = 1$. Another picture with different setting of parameters is shown in Figure 3.8. The usual explanation

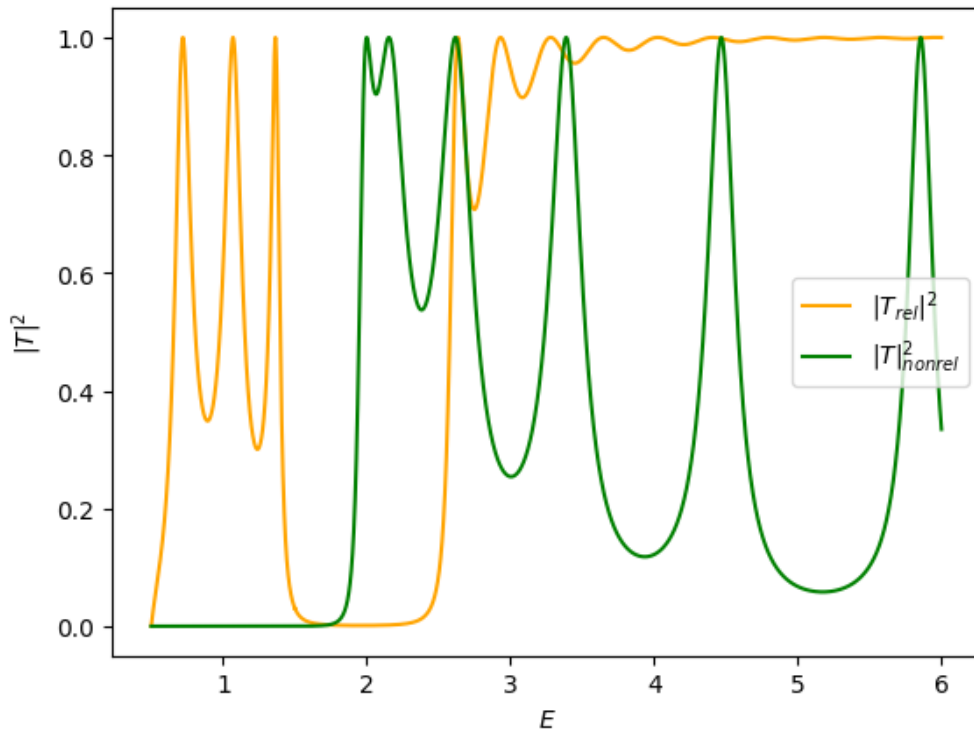


Figure 3.7: Dependence of $|T|^2$ relativistically and non-relativistically for the rectangular potential on energy, The Klein paradox, $a_0 = 2$; $m = 0.5$; $a_3 = 0$; $a = 4$

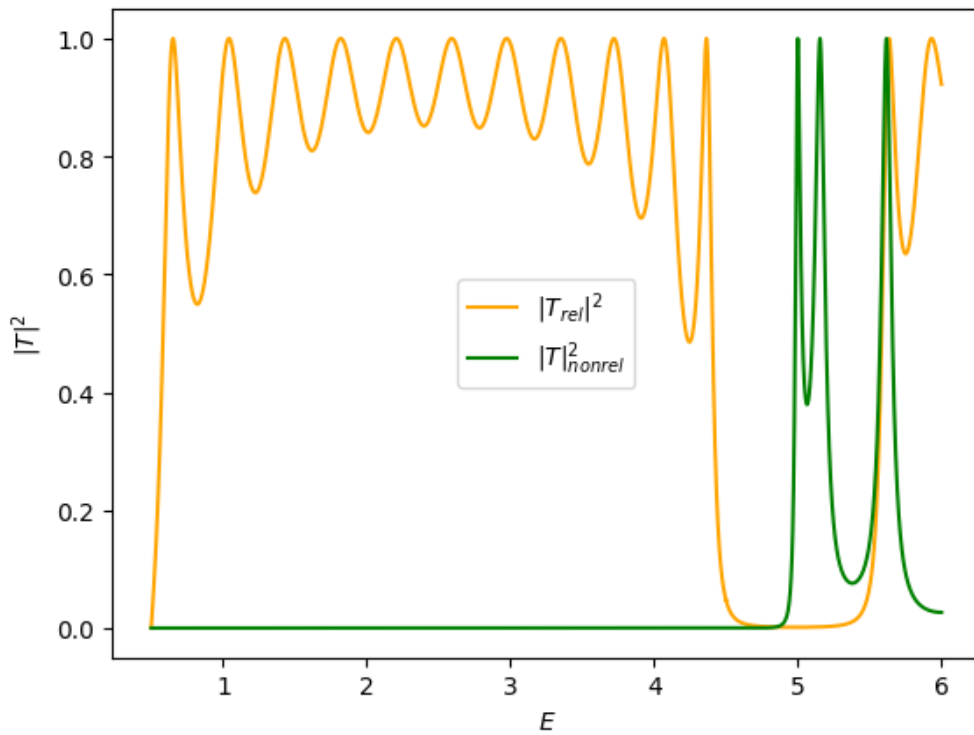


Figure 3.8: Dependence of $|T|^2$ relativistically and non-relativistically for the rectangular potential on energy, The Klein paradox, $a_0 = 5$; $m = 0.5$; $a_3 = 0$; $a = 4$

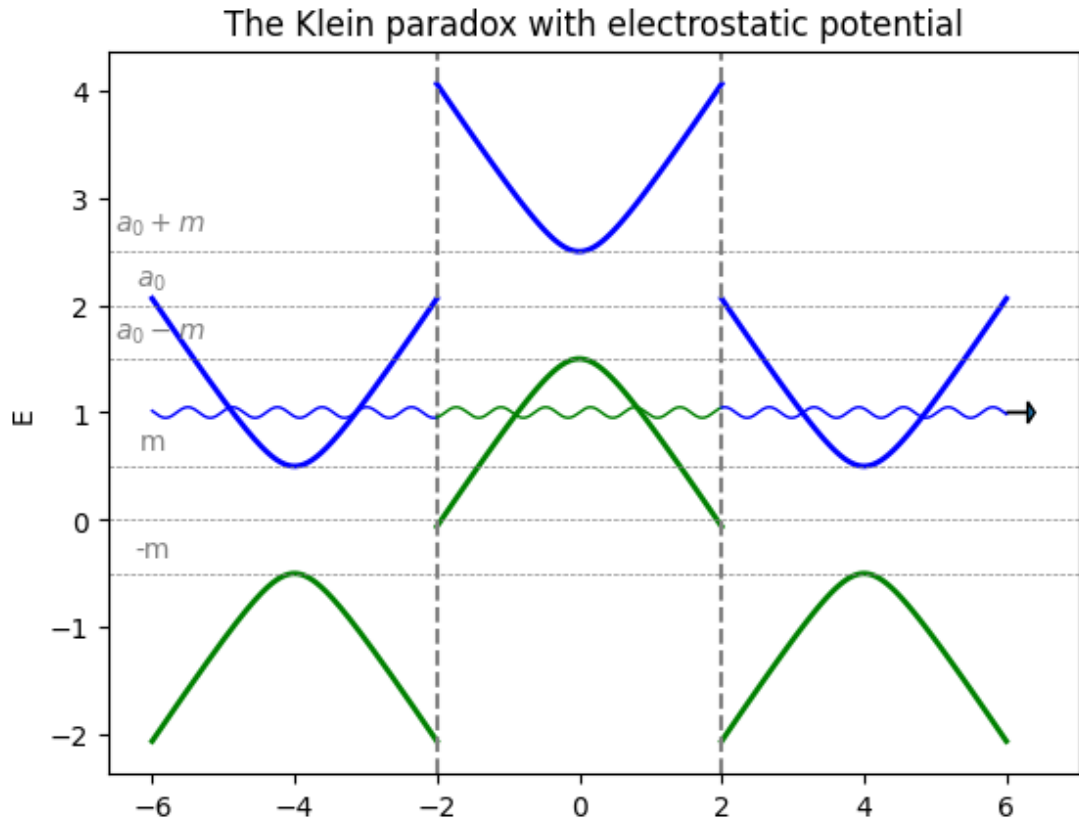


Figure 3.9: Illustration of the Klein paradox with the electrostatic potential

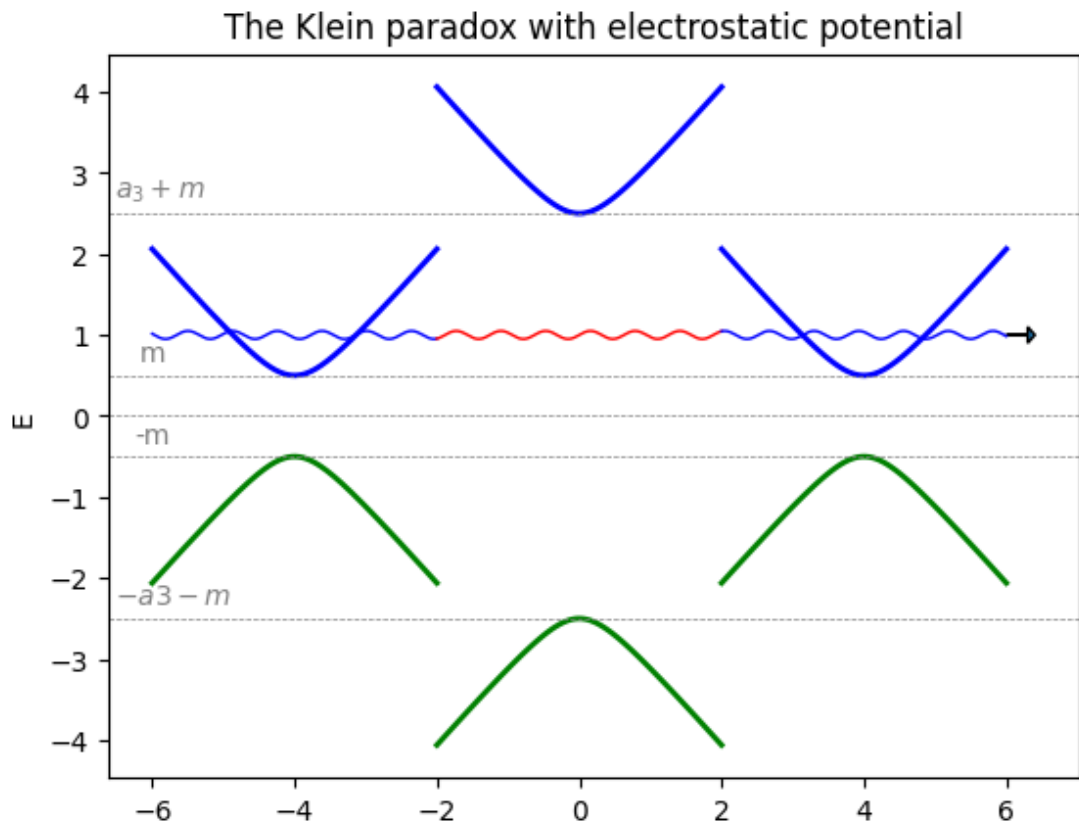


Figure 3.10: Illustration of the scattering on the Lorentz potential barrier

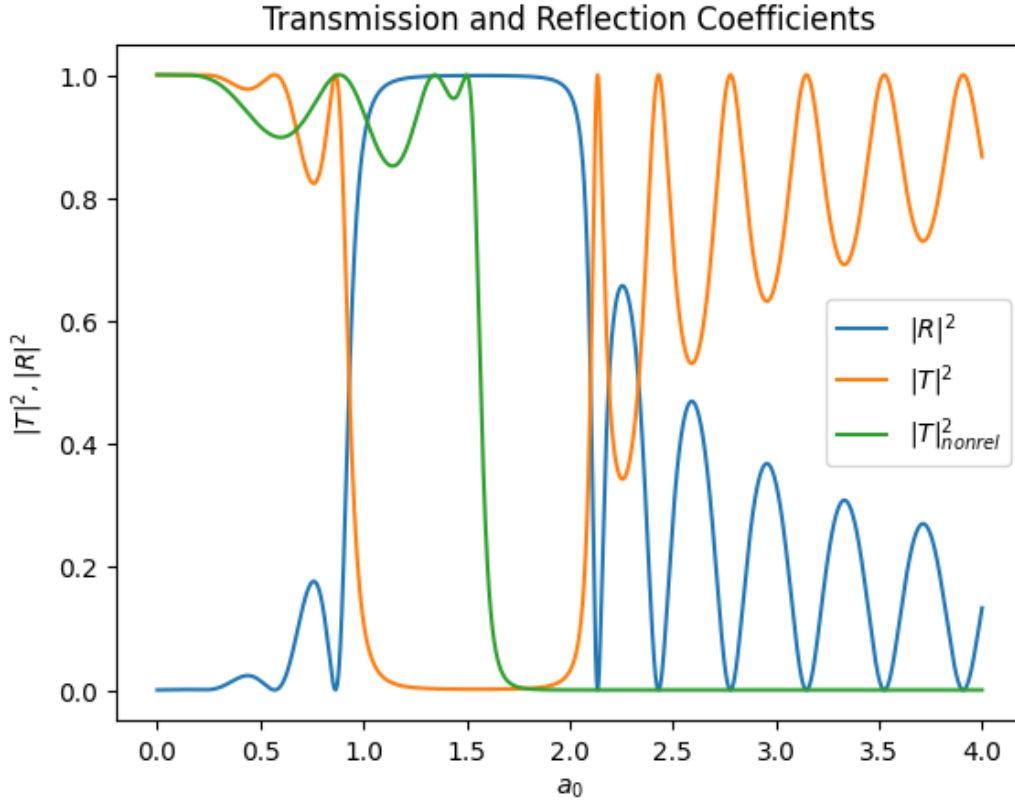


Figure 3.11: Dependence of $|T|^2$ and $|R|^2$ for the rectangular potential on the height of the electrostatic wall (non)-relativistically with $E = 1.5$; $m = 0.5$; $a_3 = 0$; $a = 4$

of the paradox is that the electron is traveling inside the barrier in the form of a positron. In Figure 3.9, you can see symbolically the spectrum of the Hamiltonian in separate intervals, an electron traveling from the left (blue wave) is traveling through $(-a; a)$ region in the form of a positron (green wave), its energy is in the bottom branch of the spectrum (bottom curve). It then transforms back into an electron in point a . However, from Figure 3.10 it is obvious that no paradox can happen. If we have an electron with energy between m and $a_3 + m$, there is no way to travel inside the barrier, in the interval $(-a; a)$. In Figure 3.12, you can see the oscillating behavior only for energies greater than $a_0 + m + a_3 = 1.5$. Otherwise, the transmission probability depends on energy in the hyperbolic sin relation, that is approximately exponential, and you can see that the probability is very close to zero, which is no big difference to the non-relativistic.

Up until now, we have looked at the scattering coefficients as functions of energy E with parameters a, a_0, a_3, m , but it is convenient to look at $|T|^2$ and $|R|^2$ as functions of the height of the electrostatic barrier or the Lorentz barrier, respectively. It will be especially important when comparing with the delta interaction. We will describe what this dependence looks like. As you can see in Figure 3.11 the curves are vertically reflected in comparison with the E dependence, so we can see the Klein paradox in the region $a_0 > E + m + a_3 = 2$. The non-relativistic transmission coefficient is very close to zero, while the relativistic one is often equal to the value of one. In the mentioned region, the probability of passing through the barrier is much greater than according to the non-relativistic Schrödinger models.

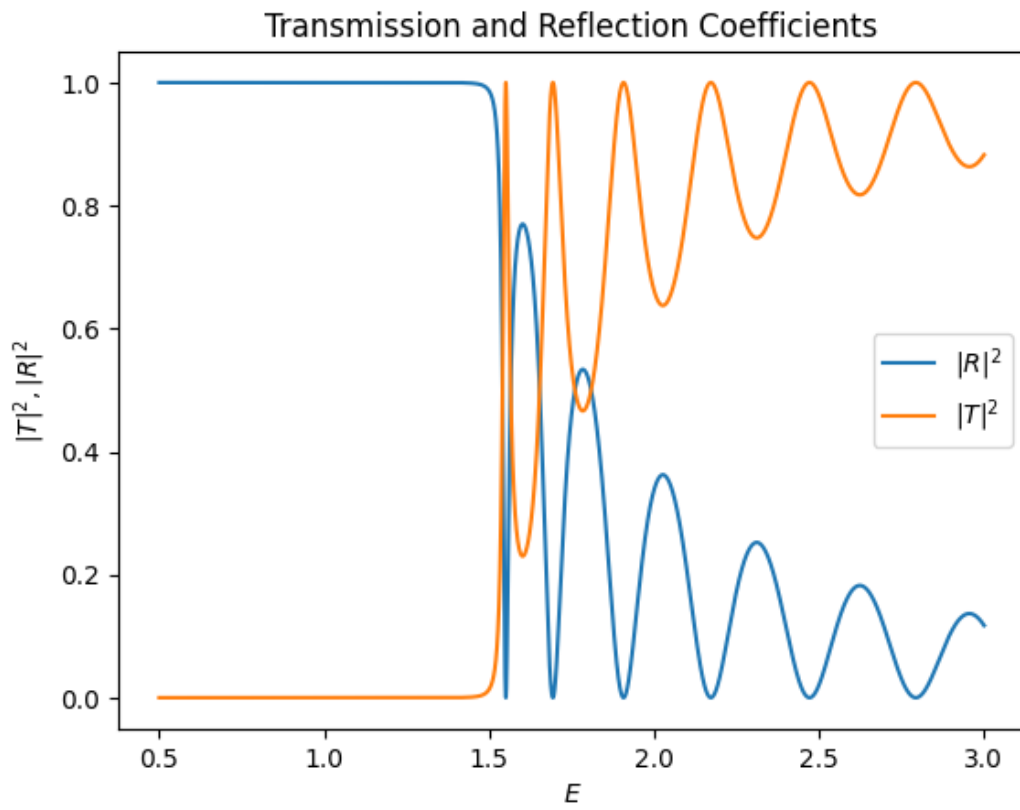


Figure 3.12: Dependence of $|T|^2$ and $|R|^2$ for the rectangular potential on energy on energy with $a_0 = 0$; $m = 0.5$; $a_3 = 1$; $a = 4$

Chapter 4

Point interaction

4.1 Approximation of the delta interaction by rectangles

Our aim now is to get to the point interaction. We know that the functions

$$V_\varepsilon(x) = \frac{1}{2\varepsilon} \chi_{(-\varepsilon;\varepsilon)}(x) \quad (4.1)$$

goes to the delta function as ε goes to zero in the space of distributions \mathcal{D}' . Because we want to study the delta interaction in the next section, it motivates us to try to take $a = \varepsilon$ into the model with rectangular potentials. After substituting this in (3.4), we arrive at

$$\begin{aligned} |T|^2 &= \frac{4\kappa^2}{4\kappa^2 + (1 - \kappa^2)^2 \sin^2 \left(2\varepsilon \sqrt{\left(E - \frac{a_0}{2\varepsilon}\right)^2 - \left(m + \frac{a_3}{2\varepsilon}\right)^2} \right)}, \\ |R|^2 &= \frac{(1 - \kappa^2)^2 \sin^2 \left(2\varepsilon \sqrt{\left(E - \frac{a_0}{2\varepsilon}\right)^2 - \left(m + \frac{a_3}{2\varepsilon}\right)^2} \right)}{4\kappa^2 + (1 - \kappa^2)^2 \sin^2 \left(2\varepsilon \sqrt{\left(E - \frac{a_0}{2\varepsilon}\right)^2 - \left(m + \frac{a_3}{2\varepsilon}\right)^2} \right)}. \end{aligned}$$

Now we want to take the limit as $\varepsilon \rightarrow 0^+$. We denote the argument of sin in (3.4) by ν after taking the limit. This quantity will play an important role in the next sections,

$$\lim_{\varepsilon \rightarrow 0^+} (2\varepsilon p_{a_0, 0, 0, a_3}) = \sqrt{a_0^2 - a_3^2} = \nu. \quad (4.2)$$

Finally, the scattering coefficients after taking the limit are

$$\begin{aligned} |T|_L^2 &= \lim_{\varepsilon \rightarrow 0} |T|^2 = \frac{4\kappa_L^2}{4\kappa_L^2 + (1 - \kappa_L^2)^2 \sin^2(\nu)} = \frac{1}{1 + \frac{(1 - \kappa_L^2)^2}{4\kappa_L^2} \sin^2 \nu}, \\ |R|_L^2 &= \lim_{\varepsilon \rightarrow 0} |R|^2 = \frac{(1 - \kappa_L^2)^2 \sin^2(\nu)}{4\kappa_L^2 + (1 - \kappa_L^2)^2 \sin^2(\nu)}. \end{aligned} \quad (4.3)$$

Note that κ changed to $\kappa_L = \sqrt{\frac{(E+m)(a_0+a_3)}{(E-m)(a_0-a_3)}}$. One can see this relation in Figure 4.1.

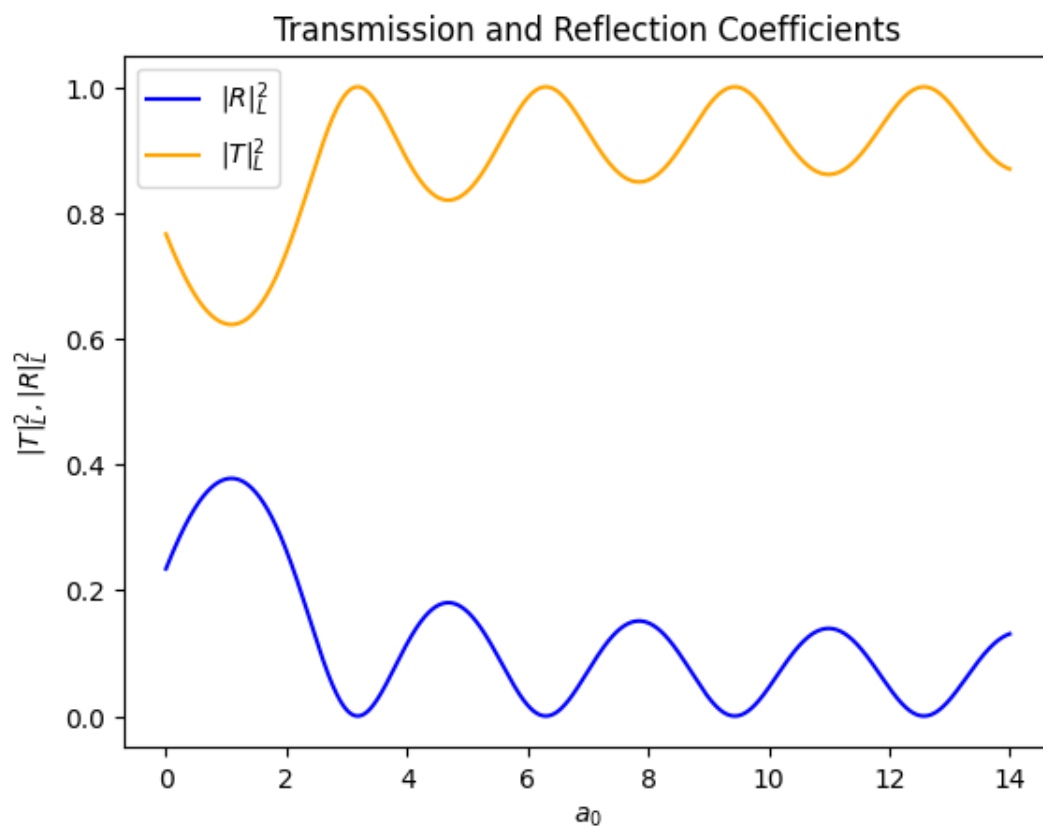


Figure 4.1: Dependence of $|T|^2$ and $|R|^2$ for the proper limit delta interaction on a_0 with $E = 1.5$; $m = 0.5$; $a_3 = 0.5$

4.2 Dirac Hamiltonian with point interaction

In this section, we will discuss the point interaction which is often formally prescribed as a delta potential. If we take the limit of operators with potentials (4.1) in the distributional sense, we will obtain a formal operator

$$H_{a_0, a_1, a_2, a_3}^\delta = -i\sigma^1 \frac{d}{dx} + \sigma^3 m + a_\mu \delta(x) \sigma^\mu. \quad (4.4)$$

However, we want to well define the operator in \mathcal{H} [27, 23]. To do that we need to see how δ acts also on the functions with a discontinuity at $x = 0$. It is reasonable to define the value of $\psi(0)$ as an arithmetic mean of limits from left and right, i.e.

$$\psi(0) = \frac{\psi(0_+) + \psi(0_-)}{2}.$$

We adopted the notation $\psi(0_\pm) = \lim_{x \rightarrow 0^\pm} \psi(x)$. With this, the operator acts on $\psi \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2) \subset \mathcal{H}$ as follows

$$\begin{aligned} H_{a_0, a_1, a_2, a_3}^\delta \psi(x) &= -i\sigma^1 \{\psi'(x)\} - i\sigma^1 (\psi(0_+) - \psi(0_-)) \delta(x) + \\ &+ \sigma^3 m \psi(x) + a_\mu \sigma^\mu \frac{\psi(0_+) + \psi(0_-)}{2} \delta(x). \end{aligned}$$

We require the result to be in \mathcal{H} . For that

$$\begin{aligned} \left[-i\sigma^1 (\psi(0_+) - \psi(0_-)) + a_\mu \sigma^\mu \frac{\psi(0_+) + \psi(0_-)}{2} \right] \delta(x) &= 0, \\ -2i\sigma^1 (\psi(0_+) - \psi(0_-)) + a_\mu \sigma^\mu (\psi(0_+) + \psi(0_-)) &= 0 \end{aligned}$$

need to be satisfied. It can also be written as

$$(2i\sigma^1 + a_\mu \sigma^\mu) \psi(0_-) = (2i\sigma^1 - a_\mu \sigma^\mu) \psi(0_+). \quad (4.5)$$

We arrive at the domain of the operator

$$\begin{aligned} \text{Dom}(H_{a_0, a_1, a_2, a_3}^\delta) &= \\ &= \{ \psi \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2) \mid (2i\sigma^1 + a_\mu \sigma^\mu) \psi(0_-) = (2i\sigma^1 - a_\mu \sigma^\mu) \psi(0_+) \}. \end{aligned}$$

And the operator acts the same as D from (1.1) [23]. If $(2i\sigma^1 - a_\mu \sigma^\mu)$ is invertible, (4.5) can be written in the form

$$\psi(0_+) = \Lambda_1 \psi(0_-),$$

where

$$\Lambda_1 = (2i\sigma^1 - a_\mu \sigma^\mu)^{-1} (2i\sigma^1 + a_\mu \sigma^\mu). \quad (4.6)$$

We obtain this operator by the limit in a distributional sense from the Hamiltonian with potential (4.1) [28]. However, if we take the limit of resolvents of the Hamiltonian with potential (4.1) (with $a_1 = 0$), we will get a different operator, specifically $H_{\hat{a}_0, 0, \hat{a}_2, \hat{a}_3}^\delta$, where for all $\mu \in \{0; 2; 3\}$,

$$\hat{a}_\mu = \begin{cases} 2 \frac{\text{tg}(\frac{\nu}{2})}{\nu} a_\mu & \text{if } \nu^2 > 0, \\ a_\mu & \text{if } \nu = 0, \\ 2 \frac{\text{tgh}(\frac{-i\nu}{2})}{-i\nu} a_\mu & \text{if } \nu^2 < 0, \end{cases} \quad (4.7)$$

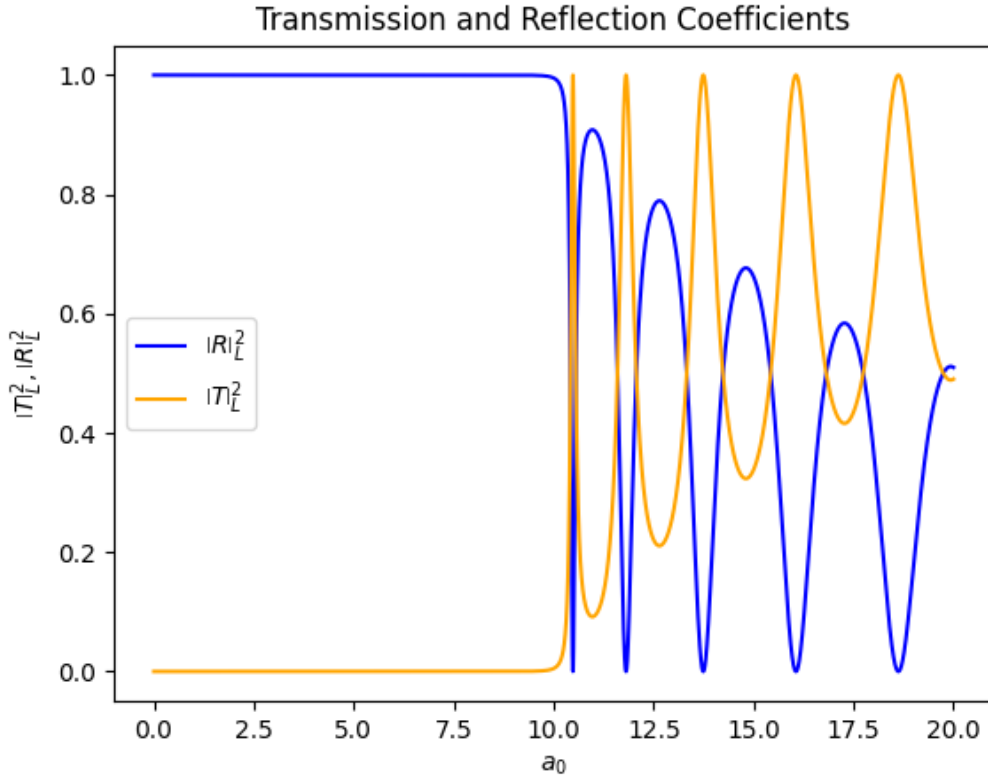


Figure 4.2: The Klein paradox for delta interaction, $a_3 = 10$; $m = 0.5$; $E = 1.5$

$\nu = \sqrt{a_0^2 - a_2^2 - a_3^2}$ and assuming $a_1 = 0$ [28]. This is often called the re-normalization of the coupling constant. We see that the options in (4.7) correspond exactly to the options in choosing the sign of p_{a_0, a_1, a_2, a_3}^2 in Section 3.2, because the sign of p_{a_0, a_1, a_2, a_3}^2 is the same as the sign of ν^2 from (4.2). We can similarly to (3.6) rewrite (4.3) and get

$$\begin{aligned}
 |T|_L^2 &= \frac{1}{1 + \frac{(1-\kappa_L^2)^2}{-4\kappa_L^2} \sinh^2 |\nu|} & \text{if } \nu^2 < 0, \\
 |T|_L^2 &= \frac{1}{1 + \frac{(1-\kappa_L^2)^2}{4\kappa_L^2} \sin^2 \nu} & \text{if } \nu^2 > 0.
 \end{aligned} \tag{4.8}$$

For completeness, we add the limit, when $a_3 \rightarrow a_0$ ($\nu \rightarrow 0$)

$$\lim_{a_3 \rightarrow a_0} |T|_L^2 = \frac{1}{1 + \frac{E+m}{E-m} a_0^2}.$$

In Figure 4.3, you see the threshold $a_0 = 10$, where re-normalization of \hat{a}_0 passes from hyperbolic tangent to tangent relation (purple) and from hyperbolic functions \sinh and \cosh to trigonometry functions \sin and \cos in the transmission coefficient (orange), cf. (4.8). This transition from hyperbolic to trigonometric function is also to be seen in Figure 4.2. In region $a_0 \in (0; 10)$ you can see this exponential (hyperbolic sin) dumping ($a_0 < a_3$) and for $a_0 > 10$ there is the Klein paradox present ($a_0 > a_3$). This is because functions tg and \sin are periodic, while tgh , \sinh and \cosh are not. We will describe the re-normalization influence on the Klein paradox illustratively on

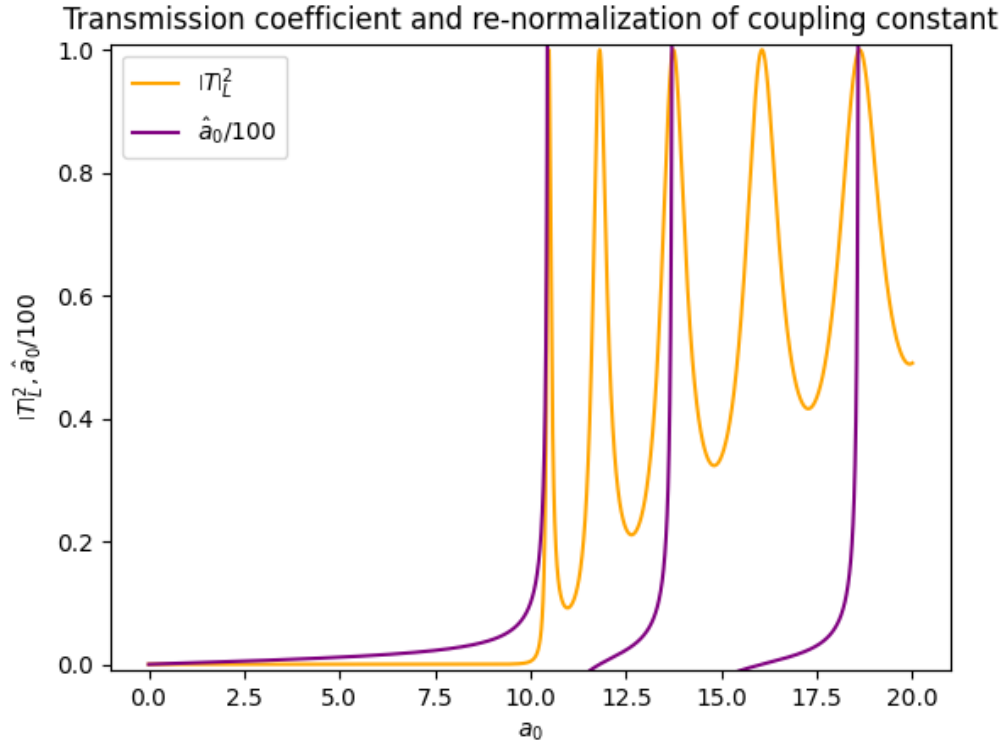


Figure 4.3: Transmission coefficient for delta interaction with $a_3 = 10$; $m = 0.5$; $E = 1.5$ and re-normalization of coupling constant a_0

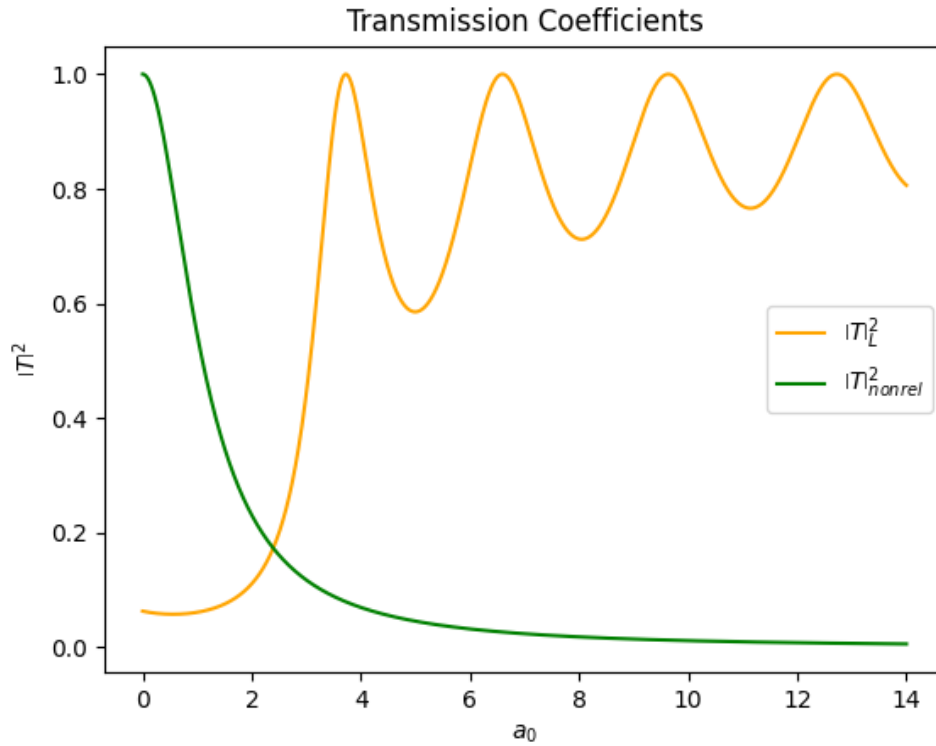


Figure 4.4: Transmission coefficient for (non)-relativistic delta interaction with $a_3 = 2$; $m = 0.5$; $E = 1.5$

two examples. Firstly, take $a_0 \neq 0$ and $a_1 = a_2 = a_3 = 0$. Relation (4.7) reduces to

$$\hat{a}_0 = 2 \operatorname{tg} \frac{a_0}{2},$$

because $\nu = a_0$. We see that the reason to the Klein paradox in exactly this form of the re-normalization of the coupling constant a_0 . The function tg is periodic, and therefore we see the oscillation behavior in the transmission coefficient. This means that for an arbitrary large electrostatic barrier the limit operator is the same as for a very weak barrier, we just subtract appropriate number of periods of tangent. So we have a full transparency even for very strong electrostatic barriers.

Second example is the pure Lorentz interaction, i.e. $a_3 \neq 0$ and $a_0 = a_1 = a_2 = 0$. Here, (4.7) reduces to

$$\hat{a}_3 = 2 \operatorname{tgh} \frac{a_3}{2},$$

which is monotonous function, thus the transmission amplitude is also monotonous function of $\nu = a_3$ and one sees no paradox.

We can conclude that the resolvent norm operator is the differential operator D (1.1) with domain

$$\begin{aligned} \operatorname{Dom}(H_{\hat{a}_0, \hat{a}_1, \hat{a}_2, \hat{a}_3}^\delta) = \\ = \{ \psi \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2) \mid (2i\sigma^1 + \hat{a}_\mu \sigma^\mu) \psi(0_-) = (2i\sigma^1 - \hat{a}_\mu \sigma^\mu) \psi(0_+) \}. \end{aligned}$$

In fact, for $a_1 = 0$ and if $(2i\sigma^1 - \hat{a}_\mu \sigma^\mu)^{-1}$ exists, this is the same as

$$\operatorname{Dom}(H_{\hat{a}_0, 0, \hat{a}_2, \hat{a}_3}^\delta) = \{ \psi \in H^1(\mathbb{R}_-; \mathbb{C}^2) \oplus H^1(\mathbb{R}_+; \mathbb{C}^2) \mid \psi(0_+) = \Lambda \psi(0_-) \}$$

with

$$\Lambda = \exp(-i\sigma^1 a_\mu \sigma^\mu),$$

cf. [28, 29]. This implies an interesting fact that

$$(2i\sigma^1 - \hat{a}_\mu \sigma^\mu)^{-1} (2i\sigma^1 + \hat{a}_\mu \sigma^\mu) = \exp(-i\sigma^1 a_\mu \sigma^\mu)$$

for $a_1 = 0$ and if $(2i\sigma^1 - \hat{a}_\mu \sigma^\mu)^{-1}$ exists.

$$\begin{array}{ccc} & D + a_\mu \sigma^\mu \delta \longrightarrow |T|_1^2 & \\ & \nearrow \mathcal{D}' & \\ |T|_L^2 \longleftarrow D + V_\varepsilon a_\mu \sigma^\mu & & \downarrow \text{re-normalization} \\ & \searrow \text{norm resolvent} & D + \hat{a}_\mu \sigma^\mu \delta \longrightarrow |T|_\delta^2 \\ & \text{=} & \end{array} \quad (4.9)$$

Let us repeat once more the different types of convergence at this point to clarify better the situation. If we take the operator with scaled potentials (4.1), we can take the limit in distributional sense and get (4.4) with coupling constants without hats. If we take this limit in the norm resolvent sense, we will get the operator with coupling constants re-normalized, the ones with hats. As to be seen in (4.9), it is very important to distinguish between these two types of convergence.

4.3 Scattering on delta barrier

We have computed the scattering coefficients for the scaling barriers in (4.3). For the scattering, taking in account the limit operators, we take an initial wave and a reflected wave on the negative real axis and a transmitted wave on the positive real axis, i.e.

$$\Lambda[\Psi_{\rightarrow}(E, m, 0_-) + R\Psi_{\leftarrow}(E, m, 0_-)] = T\Psi_{\rightarrow}(E, m, 0_+).$$

Let us start with a general matrix Λ ,

$$\Lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix}.$$

This means equations

$$\begin{aligned} \lambda_{11}(1 + R) + \lambda_{12}\kappa_{\delta}^{-1}(1 - R) &= T, \\ \lambda_{21}\kappa_{\delta}(1 + R) + \lambda_{22}(1 - R) &= T, \end{aligned}$$

where we adopt the notation

$$\begin{aligned} \kappa_{\delta} &= \sqrt{\frac{E + m}{E - m}}, \\ \nu &= \sqrt{a_0^2 - a_2^2 - a_3^2}. \end{aligned}$$

An easy solution to this pair of linear equations is

$$\begin{aligned} R &= \frac{\lambda_{11} - \lambda_{22} + \lambda_{12}\kappa_{\delta}^{-1} - \lambda_{21}\kappa_{\delta}}{\lambda_{12}\kappa_{\delta}^{-1} + \lambda_{21}\kappa_{\delta} - \lambda_{11} - \lambda_{22}}, \\ T &= 2 \frac{\lambda_{12}\lambda_{21} - \lambda_{11}\lambda_{22}}{\lambda_{12}\kappa_{\delta}^{-1} + \lambda_{21}\kappa_{\delta} - \lambda_{11} - \lambda_{22}}. \end{aligned}$$

4.3.1 Point limit case

We will see here what would have happened if we had not taken the re-normalization of coupling constants in account. As Λ we had taken Λ_1 (4.6), we would have got

$$\begin{aligned} |R|_1^2 &= \frac{4a_2^2 + 4 \left[(a_0 - a_3)\kappa_{\delta}^{-1} - (a_0 + a_3)\kappa_{\delta} \right]^2}{4 \left[(a_0 - a_3)\kappa_{\delta}^{-1} + (a_0 + a_3)\kappa_{\delta} \right] + (\nu^2 - 4 - a_2^2)^2}, \\ |T|_1^2 &= \frac{(\nu^2 - 4 - a_2^2)^2 - 4a_2 + 16a_0^2 - 16a_3^2}{4 \left[(a_0 - a_3)\kappa_{\delta}^{-1} + (a_0 + a_3)\kappa_{\delta} \right] + (\nu^2 - 4 - a_2^2)^2}. \end{aligned}$$

We can see that these coefficients do not match the once computed in the limit of scaling barriers, cf. (4.3), and therefore we need to take the norm resolvent limit which means re-normalizing the coupling constants.

4.3.2 Resolvent limit case

If we took the limit in a resolvent sense, that means the norm limit of resolvents of H with rectangular potentials (4.1), we would get an operator with a transition matrix [28, 29]

$$\Lambda = \exp(-i\sigma^1 a_{\mu} \sigma^{\mu}).$$

We can calculate the exponential of the matrix by formula [11, Appendix A],

$$\begin{aligned}\nu &= \sqrt{\det(-i\sigma^1 a_\mu \sigma^\mu) - \left(\frac{\text{Tr}(-i a_\mu \sigma^1 \sigma^\mu)}{2}\right)^2} = \sqrt{a_0^2 - a_2^2 - a_3^2}, \\ \Lambda &= \exp(-ia_1) \left[\cos \nu \sigma^0 + \frac{\sin \nu}{\nu} (-i a_\mu \sigma^1 \sigma^\mu + i a_1 \sigma^0) \right] = \\ &= e^{-ia_1} \begin{pmatrix} \cos \nu + \frac{\sin \nu}{\nu} a_2 & -i \frac{\sin \nu}{\nu} (a_0 - a_3) \\ -i \frac{\sin \nu}{\nu} (a_0 + a_3) & \cos \nu - \frac{\sin \nu}{\nu} a_2 \end{pmatrix}\end{aligned}$$

If we use this matrix for scattering, we get

$$\begin{aligned}R &= \frac{2a_2 - i \left[(a_0 - a_3) \kappa_\delta^{-1} - (a_0 + a_3) \kappa_\delta \right]}{-2\nu \cos \nu + i \sin \nu \left[(a_0 - a_3) \kappa_\delta^{-1} + (a_0 + a_3) \kappa_\delta \right]} e^{-ia_1} \sin \nu, \\ T &= \frac{-2\nu e^{-2ia_1}}{-2\nu \cos \nu + i \sin \nu \left[(a_0 - a_3) \kappa_\delta^{-1} + (a_0 + a_3) \kappa_\delta \right]}.\end{aligned}$$

Hence the amplitudes are

$$\begin{aligned}|R|_\delta^2 &= \frac{4\kappa_\delta^2 a_2^2 + \left[(a_0 - a_3) \kappa_\delta^{-1} - (a_0 + a_3) \kappa_\delta \right]^2}{4\nu^2 \cos^2 \nu + \left[(a_0 - a_3) \kappa_\delta^{-1} + (a_0 + a_3) \kappa_\delta \right]^2} \sin^2 \nu, \\ |T|_\delta^2 &= \frac{4\nu^2}{4\nu^2 \cos^2 \nu + \left[(a_0 - a_3) \kappa_\delta^{-1} + (a_0 + a_3) \kappa_\delta \right]^2} \sin^2 \nu.\end{aligned}\tag{4.10}$$

This is better to be written in form

$$|T|_\delta^2 = \frac{1}{1 + \frac{\left[(a_0 - a_3) \kappa_\delta^{-1} - (a_0 + a_3) \kappa_\delta \right]^2}{4\nu^2} \sin^2 \nu}.$$

In the case $a_2 = 0$ and with the right κ , (4.10) gives the same result as (4.3), where we approximated by rectangles. Note that the re-normalization of coupling constants is crucial to get consistent results.

For non-relativistic delta interaction the transmission coefficient is

$$|T|_{nonrel}^2 = \frac{1}{1 + \frac{\tilde{m} a_0^2}{2E}}.$$

You can see the comparison of relativistic and non-relativistic transmission coefficients in Figure 4.4. You can again see the Klein paradox for a high electrostatic barrier. For large values of a_0 , the probability of penetration is high in the relativistic case, while close to zero for the non-relativistic one.

Conclusion

In this work, we have presented a comprehensive study of the Hamiltonian in the Dirac equation, with and without a potential, respectively, and used some properties of these operators to develop a scattering theory. Specifically, we introduced the Lippman-Schwinger equation for scattering and utilized its results to analyze the transmission and reflection coefficients for a variety of potential types. We examined the scattering problem on step-like and rectangle potentials, and used rectangle potentials to approximate delta point interactions, studying different forms of this approximation and types of convergence within the context of functional analysis.

Our research has illuminated the relation between the re-normalization of coupling constant and the Klein paradox, as outlined by Petr Šeba in [10]. Specifically, in Chapter 4, we showed that the reason to the Klein paradox is the re-normalization of coupling constants according to (4.7). The oscillation behavior in the tg function in this relation effects the transmission coefficients (4.8) and causes the Klein paradox. This means that for an arbitrary large electrostatic barrier, the barrier is transparent. We can find a value of the coupling constant a_0 as big as we want and still have 100 % probability of passing through the barrier.

To provide a more complete picture of our findings, we calculated the reflection and transmission coefficients for all the potential barriers examined and visualized these coefficients on graphs for different parameter settings. Through our analysis, we have made significant contributions to the field of scattering theory and deepened our understanding of the behavior of Dirac particles in the presence of various potentials.

In conclusion, this work presents a thorough investigation into the scattering of Dirac particles on different potential types in one dimension, utilizing well-established methods and tools of functional analysis. Our findings shed new light on the relationship between re-normalization of coupling constants and the Klein paradox and provide valuable insights into the behavior of Dirac particles under a variety of conditions. We hope that our research will inspire further study and development in this important area of theoretical physics.

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