Multiple Reflections in One-Dimensional Quantum Scattering

Wolf Jung
Inst. Reine Angew. Math.
RWTH Aachen, D-52056 Aachen, Germany
http://www.iram.rwth-aachen.de/∼jung
jung@iram.rwth-aachen.de

February 13, 1998.

Abstract

Consider the one-dimensional scattering of an electron from two potentials with non-overlapping supports. The scattering amplitudes can be obtained from those of the single potentials with the Aktosun factorization formula, and these relations can be explained in terms of multiple reflections of partial waves in the region between the two potentials.

1 Introduction

The scattering of light by a parallel sheet of glass can be described in terms of the scattering by the front and back surfaces. We show that a similar description is possible for Schrödinger scattering with potentials $V_{1,2}$ of compact support, where $\operatorname{supp} V_1 \subset [a,\, b]$ is located left of $\operatorname{supp} V_2 \subset [c,\, d]$. Thus the scattering by $V = V_1 + V_2$ can be understood as a result of multiple reflections between the potentials V_1 and V_2. The scattering amplitudes for V are obtained from those of V_1 and V_2 according to

$$\tau_q^+ = \frac{\tau_{q,1}^+\, \tau_{q,2}^+}{1 - \varrho_{q,1}^-\, \varrho_{q,2}^+} \qquad \varrho_q^+ = \varrho_{q,1}^+ + \frac{\varrho_{q,2}^+\, \tau_{q,1}^+\, \tau_{q,1}^-}{1 - \varrho_{q,1}^-\, \varrho_{q,2}^+}\ .$$

These formulas have been obtained by Aktosun in [1], see also [2, 4, 5, 6]. There the focus is on partitioning of potentials. In [20], differential equations for the scattering amplitudes are obtained and the interpretation in terms of multiple reflections is given. P. Exner has informed me that a similar factorization is used in the theory of quantum wires, see [7] and the references therein. [23] contains an interpretation in terms of multiple reflections in that setting. For a recent application to random Schrödinger operators, see [14]. We discuss the interpretation and the application of the factorization formulas for V supported on two distinct intervals, and give a generalization to step potentials and to Dirac scattering.

The factorization formulas are exact, not an approximation for high energies, weak potentials ore large distances. But they can be used to obtain such approximations easily. This formalism may serve as an analogy for more involved three-dimensional scattering by multiple potentials, and it helps both to compute and to interpret standard examples of introductory courses in quantum mechanics.

This paper is organized as follows: In Section 2 we give a brief introduction to one-dimensional Schrödinger scattering. Formulas for transfer matrices are given in Section 3. The main results on multiple reflections are discussed in Section 4. The algebraic structure of the formulas is reviewed in Section 5. The results are generalized in Section 6, such that the amplitudes for the square-well potential can be calculated in terms of those of single-step potentials. Dirac scattering is discussed in Section 7, and Section 8 reviews the scattering of light.

2 The Scattering Amplitudes

In one-dimensional quantum mechanics, we have the Hilbert space $\mathcal{H} = L^2(\mathbb{R}, \mathbb{C})$, the position operator x and the momentum operator $p = -i\frac{d}{dx}$ (for Planck's constant $\hbar = 1$). The free Hamiltonian $H_0 = \frac{1}{2m}\,p^2 = -\frac{1}{2m}\,\frac{d^2}{dx^2}$ is the generator of the time evolution of a free particle, and a potential $V(x)$ is included by $H = H_0 + V$. The wave function ψ satisfies the Schrödinger equation $i\,\dot{\psi} = H\,\psi$. We assume that $m = 1/2$, thus $H_0 = p^2$. For $V \in L^1$, the wave operators $\Omega_\pm = \text{s}-\lim\limits_{t\to\pm\infty} \mathrm{e}^{iHt}\mathrm{e}^{-iH_0t}$ exist and the scattering operator $S = \Omega_+^*\,\Omega_-$ is unitary [19, Thm. XI.30]. In the stationary approach, one considers continuum eigenfunctions $\psi_q^\pm$, $q > 0$ of H which satisfy $H\,\psi_q^\pm = q^2\,\psi_q^\pm$ and $\psi_q^\pm = \Omega_-\,\mathrm{e}^{\pm iqx}$ in a suitable sense. The transmission amplitude $\tau_q^\pm$ and the reflection amplitude $\varrho_q^\pm$ are defined by the asymptotics of $\psi_q^\pm$ for $|x| \to \infty$. This works for $V \in L^1$, but we shall employ the stronger assumption that the (essential) support of V is compact: $V(x)$ shall vanish for $x < a$ and $x > b$.

Lemma 1
For $V \in L^1$ with $\operatorname{supp} V \subset [a,\, b]$ and $q > 0$ there are unique solutions $\psi_q^\pm$ of $-\psi'' + V(x)\,\psi = q^2\,\psi$ of the form

$$\psi_q^+(x) \;=\; \begin{cases} \mathrm{e}^{iqx} + \varrho_q^+\,\mathrm{e}^{-iqx} & \text{for} \quad x \le a \\[2ex] \tau_q^+\,\mathrm{e}^{iqx} & \text{for} \quad x \ge b \end{cases}$$

$$\psi_q^-(x) \;=\; \begin{cases} \tau_q^-\,\mathrm{e}^{-iqx} & \text{for} \quad x \le a \\[2ex] \mathrm{e}^{-iqx} + \varrho_q^-\,\mathrm{e}^{iqx} & \text{for} \quad x \ge b\;. \end{cases}$$

The scattering amplitudes $\tau_q^\pm$ and $\varrho_q^\pm$ satisfy the relations

$$|\tau_q^\pm|^2 + |\varrho_q^\pm|^2 = 1 \qquad \tau_q^- \;=\; \tau_q^+ \;\neq\; 0 \qquad \varrho_q^- \;=\; -\,\varrho_q^{+*}\,\frac{\tau_q^+}{\tau_q^{+*}}\;. \tag{1}$$

The scattering solution ψ_q^+ has the following interpretation: A plane wave e^{iqx} approaching a from the left is partially reflected by the potential V as $\varrho_q^+\,\mathrm{e}^{-iqx}$, partially transmitted as $\tau_q^+\,\mathrm{e}^{iqx}$. The current density $j(x) \;=\; \mathrm{Re}\,-i\psi_q^{+*}\psi_q^{+\prime}$ satisfies $j(x) \;=\; q\,(1-|\varrho_q^+|^2)$ for $x<a$ and $j(x) \;=\; q\,|\tau_q^+|^2$ for $x>b$. It is constant for a stationary state, thus we have $|\tau_q^+|^2 + |\varrho_q^+|^2 \;=\; 1$. The probability of transmission is given by $|\tau_q^+|^2$, and $|\varrho_q^+|^2$ is the probability of reflection. ψ_q^- is interpreted analogously, as a wave approaching from the right with momentum $-q$. The scattering operator has the representation $S\,\widehat{\psi}(\pm q) \;=\; \tau_q^\pm\,\widehat{\psi}(\pm q) \;+\; \varrho_q^\mp\,\widehat{\psi}(\mp q)$. See [17, p. 390], and for a discussion of the analogous statements in three dimensions, see [19, Sec. XI.6]. The mirror formulas (1) imply that S is unitary. If V is even, then we have $\psi_q^-(x) \;=\; \psi_q^+(-x)$, thus $\varrho_q^- \;=\; \varrho_q^+$ and ϱ_q^+/τ_q^+ is imaginary.

Proof of Lemma 1: The formulas (1) are proved in Section 3. To prove existence and uniqueness of ψ_q^+, observe that there is a unique solution of the form

$$\psi(x) \;=\; \begin{cases} \alpha\,\mathrm{e}^{iqx} + \beta\,\mathrm{e}^{-iqx} & \text{for} \quad x\le a \\ \mathrm{e}^{iqx} & \text{for} \quad x\ge b\;. \end{cases}$$

The current density $-\frac{i}{2}\left(\psi^*\,\psi' \;-\; \psi^{*\prime}\,\psi\right)$ is constant, which implies $|\alpha|^2 - |\beta|^2 = 1$. Thus we have $\alpha\neq 0$ and set $\psi_q^+ \;=1/\alpha\,\psi$. Note also that $\tau_q^+ \;=\; 1/\alpha \;\neq\; 0$, and that ψ_q^+ and ψ_q^- are linearly independent. ∎

Now we consider a translation of the potential V to the right by $z\in\mathbb{R}$. $\psi_q^\pm(x-z)$ satisfy $-\psi'' + V(x-z)\,\psi \;=\; q^2\,\psi$, and by observing the boundary conditions we obtain

Lemma 2
For the family of potentials $V_z(x) = V(x-z)$ we have

$$\psi_{q,z}^\pm(x) \;=\; \mathrm{e}^{\pm iqz}\,\psi_q^\pm(x-z) \qquad \tau_{q,z}^\pm \;=\; \tau_q^\pm \qquad \varrho_{q,z}^\pm \;=\; \mathrm{e}^{\pm i2qz}\,\varrho_q^\pm\;. \tag{2}$$

The formula $\varrho_{q,z}^+ \;=\; \mathrm{e}^{i2qz}\,\varrho_q^+$ has the following physical interpretation (for $z>0$): The electron travels to the right by z with momentum q, which yields a factor e^{iqz}. Then it is reflected (factor ϱ_q^+), and it travels back ($-z$) with momentum $-q$, which yields a factor e^{iqz} again.

By the Riemann-Lebesgue Lemma we have $S_z\,\widehat{\psi}(\pm q) \;\to\; \tau_q^\pm\,\widehat{\psi}(\pm q)$ weakly for $z\to\infty$. The weak limit of S_z is not unitary, thus the strong limit does not exist. This is different from the three-dimensional case, where we have the cluster property $\operatorname*{s-lim}_{z\to\infty} S_z \;=\; 1$, cf. [19, Thm. XI.33].

The high-energy asymptotics of the scattering amplitudes are given by the Born approximation

$$\tau_q^{\pm} = 1 - \frac{i}{2q}\int dx\, V(x) + \mathcal{O}(1/q^2) \qquad \varrho_q^{\pm} = -\frac{i}{2q}\int dx\, \mathrm{e}^{\pm i2q}\, V(x) + \mathcal{O}(1/q^2)\,. \tag{3}$$

If the potential V is piecewise absolutely continuous, then we have the estimate $\varrho_q^{\pm} = \mathcal{O}(1/q^2)$, and the eikonal approximation [12] for the transmission amplitude reads

$$\tau_q^{\pm} = \mathrm{e}^{i\int_a^b dx\,(\sqrt{q^2 - V(x)} - q)} + o(1/q^3)\,. \tag{4}$$

If V is piecewise AC^2, then $o(1/q^3)$ is strengthened to $\mathcal{O}(1/q^4)$.

3 The Transfer Matrix

To obtain the amplitudes, we have to find two linearly independent solutions of the Schrödinger equation on the interval $[a,\, b]$ and then solve a system of four linear equations, which expresses the fact that ψ_q^+ and $\psi_q^{+\prime}$ are continuous at a and b. This can be simplified by employing the transfer matrix of the differential equation. Take two linearly independent solutions $\psi_1(x)$ and $\psi_2(x)$ of $-\psi'' + V(x)\,\psi = q^2\,\psi$ and form the Wronski matrix

$$W_q(x) = \begin{pmatrix} \psi_1(x) & \psi_2(x) \\ \psi_1'(x) & \psi_2'(x) \end{pmatrix}\,. \tag{5}$$

Define the transfer matrix $M_q(x,\, y) := W_q(x)\, W_q^{-1}(y)$. It is real and has the determinant 1, since the Wronskian $\det W_q(x)$ is constant. For every $\psi(x)$ satisfying the differential equation we have

$$\begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = M_q(x,\, y) \begin{pmatrix} \psi(y) \\ \psi'(y) \end{pmatrix}\,. \tag{6}$$

Thus τ_q^+ and ϱ_q^+ are determined from the system of two linear equations

$$\begin{pmatrix} 1 \\ iq \end{pmatrix} \mathrm{e}^{iqa} + \begin{pmatrix} 1 \\ -iq \end{pmatrix} \varrho_q^+\, \mathrm{e}^{-iqa} = M_q(a,\, b) \begin{pmatrix} 1 \\ iq \end{pmatrix} \tau_q^+\, \mathrm{e}^{iqb}\,, \tag{7}$$

where $\operatorname{supp} V \subset [a,\, b]$. Conversely, the transfer matrix can be expressed in terms of τ_q^+ and ϱ_q^+. One could form the Wronski matrix with $\psi_q^{\pm}$ to achieve this, but the following calculation is much simpler and does not rely on the mirror formulas (1). Since M_q is real, we have

$$M_q(a,\, b)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathrm{Re}\; M_q(a,\, b)\begin{pmatrix} 1 \\ iq \end{pmatrix} \quad \text{and}$$

$$M_q(a,\, b)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{q}\,\mathrm{Im}\; M_q(a,\, b)\begin{pmatrix} 1 \\ iq \end{pmatrix}\,.$$

We apply this idea to (7) and find the following representation for $M_q(a,\, b)$:

$$\begin{pmatrix} \mathrm{Re}\, \dfrac{\mathrm{e}^{iq(a-b)} + \varrho_q^+\, \mathrm{e}^{-iq(a+b)}}{\tau_q^+} & \dfrac{1}{q}\, \mathrm{Im}\, \dfrac{\mathrm{e}^{iq(a-b)} + \varrho_q^+\, \mathrm{e}^{-iq(a+b)}}{\tau_q^+} \\ -q\, \mathrm{Im}\, \dfrac{\mathrm{e}^{iq(a-b)} - \varrho_q^+\, \mathrm{e}^{-iq(a+b)}}{\tau_q^+} & \mathrm{Re}\, \dfrac{\mathrm{e}^{iq(a-b)} - \varrho_q^+\, \mathrm{e}^{-iq(a+b)}}{\tau_q^+} \end{pmatrix} . \quad (8)$$

A very convenient way to obtain the scattering amplitudes from $M = M_q(a,\, b)$ is to solve the following equations for $\dfrac{1}{\tau_q^+}$ and $\dfrac{\varrho_q^+}{\tau_q^+}$:

$$\begin{aligned} \frac{\mathrm{e}^{iq(a-b)} + \varrho_q^+\, \mathrm{e}^{-iq(a+b)}}{\tau_q^+} &= M_{11} + iq\, M_{12} \\ \frac{\mathrm{e}^{iq(a-b)} - \varrho_q^+\, \mathrm{e}^{-iq(a+b)}}{\tau_q^+} &= M_{22} - \frac{i}{q}\, M_{21} \,. \end{aligned} \quad (9)$$

Now $1 = \det M_q(a,\, b) = \dfrac{1 - |\varrho_q^+|^2}{|\tau_q^+|^2}$ implies $|\tau_q^+|^2 + |\varrho_q^+|^2 = 1$, and we compute

$$\big(M_q(a,\, b)\big)^{-1} \begin{pmatrix} 1 \\ -iq \end{pmatrix} = \begin{pmatrix} 1 \\ -iq \end{pmatrix} \frac{1}{\tau_q^+}\, \mathrm{e}^{iq(a-b)} - \begin{pmatrix} 1 \\ iq \end{pmatrix} \frac{\varrho_q^{+*}}{\tau_q^{+*}}\, \mathrm{e}^{iq(a+b)} \,.$$

Comparing this with

$$\begin{pmatrix} 1 \\ -iq \end{pmatrix} \mathrm{e}^{-iqb} + \begin{pmatrix} 1 \\ iq \end{pmatrix} \varrho_q^-\, \mathrm{e}^{iqb} = M_q(b,\, a) \begin{pmatrix} 1 \\ -iq \end{pmatrix} \tau_q^-\, \mathrm{e}^{-iqb}$$

yields the mirror formulas (1) $\tau_q^- = \tau_q^+$ and $\varrho_q^- = -\, \varrho_q^{+*}\, \dfrac{\tau_q^+}{\tau_q^{+*}}$.

Examples

For $v \in \mathbb{R}$ and $b > 0$ consider $H_0 = p^2$ and $H = p^2 + V(x)$ with the square-well potential $V(x) = v$ for $|x| < b$, $V(x) = 0$ for $|x| > b$. For $q^2 > v$ we obtain

$$M_q(-b,\, b) = \begin{pmatrix} \cos 2rb & -\dfrac{1}{r} \sin 2rb \\ r \sin 2rb & \cos 2rb \end{pmatrix} \qquad \text{with} \quad r = \sqrt{q^2 - v}\,,$$

$$\tau_q^+ = \frac{2rq\, \mathrm{e}^{-i2qb}}{2rq\, \cos 2rb - i\,(r^2 + q^2)\, \sin 2rb} \qquad \varrho_q^+ = \frac{-iv \sin 2rb\, \mathrm{e}^{-i2qb}}{2rq\, \cos 2rb - i\,(r^2 + q^2)\, \sin 2rb} \,. \quad (10)$$

As a simple example, consider $H_0 + V$ with the point interaction $V(x) = -2\alpha\, \delta(x)$ [3]. By the KLMN Theorem [18, p. 167], this expression corresponds to a unique self-adjoint operator H with the same form domain as H_0. $\psi \in D_H$ satisfies $\psi'(0+) =$

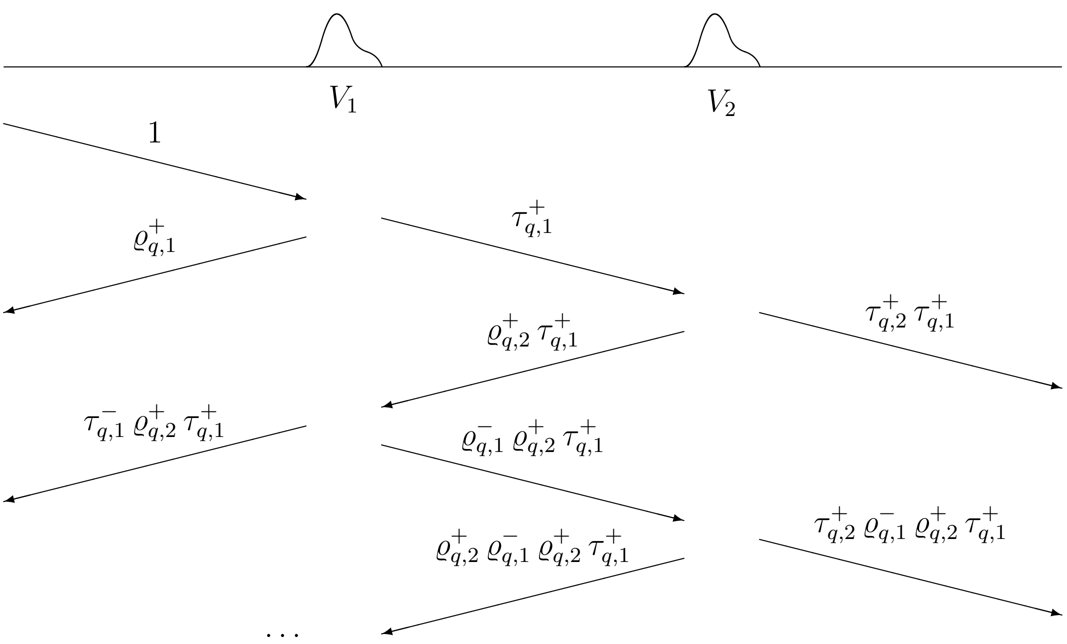
$\psi'(0-) - 2\alpha\,\psi(0)$. The formulas for the transfer matrix remain valid for this singular potential. We have

$$M_q(0-,\,0+) = \begin{pmatrix} 1 & 0 \\ 2\alpha & 1 \end{pmatrix}\,, \qquad \text{and from (9) we obtain}$$

$$\tau_q^+ \;=\; \frac{q}{q\,-\,i\alpha} \qquad\qquad \varrho_q^+ \;=\; \frac{i\alpha}{q\,-\,i\alpha}\;. \tag{11}$$

4 Multiple Reflections

In [8, p. 25–33], Feynman describes the reflection of light from a window as follows: A part of the beam is reflected at the front surface. The remaining part is transmitted and reaches the back surface. Again, some part is reflected and returns to the front surface . . . . Thus the total scattering by the parallel sheet of glass can be described in terms of the scattering by single surfaces. We want to show that a similar description is possible for Schrödinger scattering with potentials $V_{1,2}$ of compact support, where $\operatorname{supp} V_1 \subset [a,\,b]$ is located left of $\operatorname{supp} V_2 \subset [c,\,d]$.
Assume that a plane wave e^{iqx} is approaching V_1 from the left. Then a wave $\varrho^+_{q,1}\,\mathrm{e}^{-iqx}$ is reflected and $\tau^+_{q,1}\,\mathrm{e}^{iqx}$ is transmitted. The latter wave interacts with V_2, and $\varrho^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{-iqx}$ is reflected, $\tau^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{iqx}$ is transmitted. The reflected wave reaches V_1 from the right, $\tau^-_{q,1}\,\varrho^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{-iqx}$ is transmitted to the left, and $\varrho^-_{q,1}\,\varrho^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{iqx}$ is reflected back to V_2. The total wave reflected by $V_1 + V_2$ is given as a superposition $\varrho^+_{q,1}\,\mathrm{e}^{-iqx} + \tau^-_{q,1}\,\varrho^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{-iqx} + \ldots$, and the total transmitted wave is $\tau^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{iqx} + \tau^+_{q,2}\,\varrho^-_{q,1}\,\varrho^+_{q,2}\,\tau^+_{q,1}\,\mathrm{e}^{iqx} \;+\; \ldots$.



Thus we expect the relations (observe that $|\varrho^{\pm}_{q,i}| < 1$)

$$\tau^+_q \;=\; \tau^+_{q,2} \sum_{j=0}^{\infty} (\varrho^-_{q,1}\,\varrho^+_{q,2})^j\,\tau^+_{q,1} \;=\; \frac{\tau^+_{q,2}\,\tau^+_{q,1}}{1 \,-\, \varrho^-_{q,1}\,\varrho^+_{q,2}}$$

$$\varrho^+_q \;=\; \varrho^+_{q,1} \,+\, \tau^-_{q,1}\,\varrho^+_{q,2} \sum_{j=0}^{\infty} (\varrho^-_{q,1}\,\varrho^+_{q,2})^j\,\tau^+_{q,1} \;=\; \varrho^+_{q,1} \,+\, \frac{\tau^-_{q,1}\,\varrho^+_{q,2}\,\tau^+_{q,1}}{1 \,-\, \varrho^-_{q,1}\,\varrho^+_{q,2}}\;.$$

It is not obvious that this stationary description of a time-dependent intuition is appropriate, especially not for large wavelengths. But we shall see in the following theorem that these expectations are correct. Thus the scattering by $V_1 + V_2$ can be understood as a result of multiple reflections between the potentials V_1 and V_2. The formulas (12) are exact, not an approximation for high energies, weak potentials ore large distances. But they can be used to obtain such approximations easily, cf. (14). Another application of these formulas is to simplify the calculation of explicit examples.

Theorem 3
Consider $-\infty < a \le b \le c \le d < \infty$ *and potentials* $V_1,\, V_2 \in L^1$ *with* $\operatorname{supp} V_1 \subset [a,\, b]$ *and* $\operatorname{supp} V_2 \subset [c,\, d]$. *Define* $V = V_1 + V_2$. *Then for* $q > 0$ *the scattering amplitudes for* $p^2 + V$ *are obtained from those of* $p^2 + V_1$ *and* $p^2 + V_2$ *according to*

$$\tau^+_q = \frac{\tau^+_{q,1}\,\tau^+_{q,2}}{1 \,-\, \varrho^-_{q,1}\,\varrho^+_{q,2}} \qquad \varrho^+_q = \varrho^+_{q,1} \,+\, \frac{\varrho^+_{q,2}\,\tau^+_{q,1}\,\tau^-_{q,1}}{1 \,-\, \varrho^-_{q,1}\,\varrho^+_{q,2}}\;. \tag{12}$$

This can be interpreted as a result of multiple reflections between the potentials V_1 *and* V_2.

This is the Aktosun factorization formula [1]. We give a proof on p. 9.

Discussion

The formula for ϱ^+_q can also be written as

$$\varrho^+_q \;=\; \frac{\varrho^+_{q,1} \,+\, \varrho^+_{q,2}\,(\tau^+_{q,1}\,\tau^-_{q,1} \,-\, \varrho^+_{q,1}\,\varrho^-_{q,1})}{1 \,-\, \varrho^-_{q,1}\,\varrho^+_{q,2}} \;=\; \frac{\varrho^+_{q,1} \,+\, \varrho^+_{q,2}\,\dfrac{\tau^+_{q,1}}{\tau^{+\,*}_{q,1}}}{1 \,-\, \varrho^-_{q,1}\,\varrho^+_{q,2}}\;. \tag{13}$$

The latter form is most convenient to compute concrete examples. We have not employed the relations (1) to formulate the theorem, since the interpretation in terms of multiple reflections makes $\tau^-_{q,1}$ and $\varrho^-_{q,1}$ appear in (12) in a natural way. The case of $a = b$ or $c = d$ does not only mean a zero potential, but the theorem remains true for point interactions.

If τ^+_q and ϱ^+_q are defined by (12) and the amplitudes on the right hand sides of these equations satisfy the relations (1), then we have $|\tau^+_q|^2 + |\varrho^+_q|^2 = 1$ by Lemma 4. (If this was not the case, we would obtain additional restrictions on the possible values of the scattering amplitudes. This set must be closed under the composition defined by (12).)

If the potentials V_i are piecewise absolutely continuous, then we have $\varrho_{q,i}^{\pm} = \mathcal{O}(1/q^2)$ from the Born approximation (3), and (12) yields

$$\tau_q^+ \;=\; \tau_{q,1}^+\,\tau_{q,2}^+ \,+\, \mathcal{O}(1/q^4)\ , \tag{14}$$

thus $\tau_q^+ \;\approx\; \tau_{q,1}^+\,\tau_{q,2}^+$ is a good approximation at high energies. This can also be seen from the eikonal approximation (4) for V_i piecewise in AC^2. The proof of the Born approximation and of Theorem 3 is simpler than that of the eikonal approximation, but the latter shows that (14) breaks down, if the supports of V_1 and V_2 overlap. In [15], Kujawski checks the similar assumption of the additivity of phase shifts for an example, and remarks that this assumption is important for the Glauber multiple scattering formalism (in three dimensions). In [9, p. 85], Gasiorowicz suggests that scattering amplitudes shall be multiplied to obtain approximate solutions for potentials that are piecewise continuous, thus motivating the WKB method. The exact solution for these potentials can be obtained by multiplying the transfer matrices of square-well potentials [13], or by iterating (12) (where $b = c$ is allowed).

Note that $|\tau_q^+|$ may be larger than $|\tau_{q,1}^+\,\tau_{q,2}^+|$, even larger than $\max(|\tau_{q,1}^+|,\,|\tau_{q,2}^+|)$. This is due to interference, and it depends on the distance between the supports of V_1 and V_2. To illustrate this point, let us assume that V_2 is a translate of V_1: $V_2(x) = V_1(x-z)$ with $z \ge b-a$. From (2) we see that $\tau_{q,2}^+ = \tau_{q,1}^+$ and $\varrho_{q,2}^+ = \mathrm{e}^{i2qz}\,\varrho_{q,1}^+$. Thus

$$\tau_q^+ = \frac{(\tau_{q,1}^+)^2}{1 \,-\, \varrho_{q,1}^-\,\varrho_{q,1}^+\,\mathrm{e}^{i2qz}}\ ,$$

and if z is changed, $|\tau_q^+|$ varies between its minimum value $\frac{|\tau_{q,1}^+|^2}{1+|\varrho_{q,1}^+|^2}$ and its maximum value $\frac{|\tau_{q,1}^+|^2}{1-|\varrho_{q,1}^+|^2} = 1$: For suitable z we have complete transmission due to destructive interference between the partial reflected waves. This is known as resonance scattering.

The scattering amplitudes $\tau_q^{\pm}$ and $\varrho_q^{\pm}$ have meromorphic continuations to the upper q-halfplane and the bound-state energies $E = -s^2$, $s > 0$, correspond to simple poles at $q = is$. Thus the bound-state energies of $p^2 + V$ are determined from $\varrho_{is,1}^-\,\varrho_{is,2}^+ = 1$, since the poles for the single potentials will usually cancel out. For ϱ_q^+, this relies on (13) and the fact that the poles of $\tau_{q,1}^+\,\tau_{q,1}^- - \varrho_{q,1}^+\,\varrho_{q,1}^-$ corresponding to bound states of $p^2 + V_1$ are simple, since the leading terms of the Laurent series cancel out. (Note that the eigenfunction is proportional both to $\lim\limits_{q\to is}\frac{1}{\tau_{q,1}^+}\,\psi_{q,1}^+(x)$ and to $\lim\limits_{q\to is}\frac{1}{\tau_{q,1}^-}\,\psi_{q,1}^-(x)$.)

An Example

For $\alpha > 0$ and $z > 0$, consider two attracting delta potentials at distance z: $V_1(x) = -2\alpha\,\delta(x + z/2)$ and $V_2(x) = -2\alpha\,\delta(x - z/2)$. From (11) and (2) we get the scattering amplitudes

$$\tau^{\pm}_{q,1} \;=\; \frac{q}{q - i\alpha} \qquad\qquad \varrho^{\pm}_{q,1} \;=\; \frac{i\alpha}{q - i\alpha}\,\mathrm{e}^{\mp iqz}$$
$$\tau^{\pm}_{q,2} \;=\; \frac{q}{q - i\alpha} \qquad\qquad \varrho^{\pm}_{q,2} \;=\; \frac{i\alpha}{q - i\alpha}\,\mathrm{e}^{\pm iqz}\;.$$

For the singular potential $V(x) \;=\; V_1(x) \,+\, V_2(x) \;=\; -2\alpha\,\delta(|x| - z/2)$, Theorem 3 remains valid and yields

$$\tau^+_q \;=\; \frac{q^2}{(q - i\alpha)^2 \,+\, \alpha^2\,\mathrm{e}^{i2qz}} \qquad\qquad \varrho^+_q \;=\; i2\alpha\,\frac{q\,\cos qz \,-\, \alpha\,\sin qz}{(q - i\alpha)^2 \,+\, \alpha^2\,\mathrm{e}^{i2qz}}\;. \tag{15}$$

Observe that ϱ^+_q/τ^+_q is imaginary, since V is even, and that $\tau^+_0 = 0$, $\varrho^+_0 = -1$. The probabilities for transmission and reflection are given by

$$|\tau^+_q|^2 \;=\; \frac{q^4}{q^4 \,+\, 4\alpha^2\,(q\,\cos qz \,-\, \alpha\,\sin qz)^2} \qquad\qquad |\varrho^+_q|^2 \;=\; \frac{4\alpha^2\,(q\,\cos qz \,-\, \alpha\,\sin qz)^2}{q^4 \,+\, 4\alpha^2\,(q\,\cos qz \,-\, \alpha\,\sin qz)^2}\;.$$

This differs from the result in [16]. We have complete transmission at

$$qz \;=\; \arctan q/\alpha \,+\, n\pi\,,\ n \in \mathbb{N}_0\ : \qquad \tau^+_q \;=\; \frac{q + i\alpha}{q - i\alpha} \qquad \varrho^+_q \;=\; 0\;.$$

The bound-state energies are determined from the poles of (15) at $q = is$ with $s > 0$. This yields the equation

$$(s - \alpha)^2 \;=\; \alpha^2\,\mathrm{e}^{-2sz}\;, \qquad \text{or} \qquad |s - \alpha| \;=\; \alpha\,\mathrm{e}^{-sz}\;.$$

A graphical analysis shows that there is no solution with $s \geq 2\alpha$ and exactly one solution s_0 with $\alpha \,<\, s_0 \,<\, 2\alpha$. For $\alpha z \,>\, 1$ there is a second solution s_1 with $0 \,<\, s_1 \,<\, \alpha$. If z is increased, s_0 is decreased, and thus the ground-state energy $E_0 \;=\; -\,s_0^2$ is increased. This provides a well-known simple model for chemical bond [9, p. 93]: Suppose that we have two nuclei with positive charge at a distance z, and that the energy of an electron is given by $E_0(z)$. The nuclei are treated as classical particles. $-E_0'(z)$ is an attracting force between the nuclei, and their repulsion shall be described by a decreasing potential $W(z)$, which is infinite at $z = 0$ and tends to 0 sufficiently fast for $z \to \infty$. Then $W(z) + E_0(z)$ has a minimum at a finite distance $\widehat{z}$. If the nuclei are $\widehat{z}$ apart, the system of nuclei plus electron has a minimal total energy and forms a stable molecule ion. Note that $E_0 \,<\, -\alpha^2$, which is the bound-state energy of a single atom. A more involved model of a one-dimensional molecule could consist of two square-well potentials, and Theorem 3 simplifies the calculations for this example, too.

Proof of Theorem 3

We omit the subscript q to make the formulas more readable. $\psi^{\pm}_1$ satisfy the differential equation $-\psi'' + V_1\,\psi = q^2\,\psi$ with

$$\psi^+_1(x) \;=\; \begin{cases} \mathrm{e}^{iqx} \,+\, \varrho^+_1\,\mathrm{e}^{-iqx} & \text{for} \quad x \leq a \\ \tau^+_1\,\mathrm{e}^{iqx} & \text{for} \quad x \geq b \end{cases}$$

and for the wave traveling left

$$\psi_1^-(x) \;=\; \begin{cases} \tau_1^- \, \mathrm{e}^{-iqx} & \text{for} \quad x \le a \\ \mathrm{e}^{-iqx} \,+\, \varrho_1^- \, \mathrm{e}^{iqx} & \text{for} \quad x \ge b \;. \end{cases}$$

$\psi_2^\pm$ satisfy $-\psi'' + V_2\,\psi = q^2\,\psi$ with

$$\psi_2^+(x) \;=\; \begin{cases} \mathrm{e}^{iqx} \,+\, \varrho_2^+ \, \mathrm{e}^{-iqx} & \text{for} \quad x \le c \\ \tau_2^+ \, \mathrm{e}^{iqx} & \text{for} \quad x \ge d \;, \end{cases}$$

$$\psi_2^-(x) \;=\; \begin{cases} \tau_2^- \, \mathrm{e}^{-iqx} & \text{for} \quad x \le c \\ \mathrm{e}^{-iqx} \,+\, \varrho_2^- \, \mathrm{e}^{iqx} & \text{for} \quad x \ge d \;. \end{cases}$$

$\psi^\pm$ satisfy $-\psi'' + V\,\psi = q^2\,\psi$ with

$$\psi^+(x) \;=\; \begin{cases} \mathrm{e}^{iqx} \,+\, \varrho^+ \, \mathrm{e}^{-iqx} & \text{for} \quad x \le a \\ \tau^+ \, \mathrm{e}^{iqx} & \text{for} \quad x \ge d \;. \end{cases}$$

For $x < c$, ψ^+ satisfies $-\psi'' + V_1\,\psi = q^2\,\psi$, thus it is a linear combination of ψ_1^+ and ψ_1^-. The asymptotics for $x \to -\infty$ require the form $\psi^+(x) \;=\; \psi_1^+(x) + \xi\,\psi_1^-(x)$ for $x \le c$. Then we have $\varrho^+ \;=\; \varrho_1^+ \,+\, \xi\,\tau_1^-$. On the other hand, ψ^+ satisfies $-\psi'' + V_2\,\psi = q^2\,\psi$ for $x > b$. Thus it is a linear combination of ψ_2^+ and ψ_2^-, and the asymptotics for $x \to \infty$ yield the form $\psi^+(x) \;=\; \eta\,\psi_2^+(x)$ for $x \ge b$, thus $\tau^+ \;=\; \eta\,\tau_2^+$. The continuity of ψ^+ and $\psi^{+\prime}$ at $x = c$ implies

$$(\tau_1^+ + \xi\,\varrho_1^-) \begin{pmatrix} 1 \\ iq \end{pmatrix} \mathrm{e}^{iqc} + \xi \begin{pmatrix} 1 \\ -iq \end{pmatrix} \mathrm{e}^{-iqc} \;=\; \eta \begin{pmatrix} 1 \\ iq \end{pmatrix} \mathrm{e}^{iqc} + \eta\,\varrho_2^+ \begin{pmatrix} 1 \\ -iq \end{pmatrix} \mathrm{e}^{-iqc} \,, \tag{16}$$

which yields the system of linear equations for ξ and η

$$\tau_1^+ \,+\, \xi\,\varrho_1^- \;=\; \eta \qquad\qquad \xi \;=\; \eta\,\varrho_2^+ \;.$$

Observing that $|\varrho_1^-\,\varrho_2^+| \;<\; 1$ we find the unique solution

$$\eta = \frac{\tau_1^+}{1 \,-\, \varrho_1^-\,\varrho_2^+} \qquad \xi \;=\; \frac{\varrho_2^+\,\tau_1^+}{1 \,-\, \varrho_1^-\,\varrho_2^+} \;, \qquad \text{and thus}$$

$$\tau^+ \;=\; \frac{\tau_1^+\,\tau_2^+}{1 \,-\, \varrho_1^-\,\varrho_2^+} \qquad \varrho^+ \;=\; \varrho_1^+ \;+\; \frac{\varrho_2^+\,\tau_1^+\,\tau_1^-}{1 \,-\, \varrho_1^-\,\varrho_2^+}$$

is obtained. ∎

A different proof is as follows: Form the transfer matrix $M_q(a,\,c) = M_{q,1}(a,\,c)$ from $\tau_{q,1}^+$ and $\varrho_{q,1}^+$ and form $M_q(c,\,d) = M_{q,2}(c,\,d)$ from $\tau_{q,2}^+$ and $\varrho_{q,2}^+$ according to (8). Then τ_q^+ and ϱ_q^+ are obtained from $M_q(a,\,d) = M_q(a,\,c) \cdot M_q(c,\,d)$ according to (9). The lengthy calculations (similar to the proof of Lemma 4) are simplified by avoiding the matrix multiplication and evaluating the product $M_q(c,\,d) \cdot (1,\,iq)^T$ first. The mirror formulas (1) are used to express ${\tau_{q,1}^+}^*$ and ${\varrho_{q,1}^+}^*$ in terms of $\tau_{q,1}^\pm$ and $\varrho_{q,1}^\pm$.

5 A Lie Group

If we have V_1, V_2, V_3 with non-overlapping supports (ordered from left to right), we can apply Theorem 3 twice to obtain the scattering amplitudes for $V = V_1 + V_2 + V_3$. It does not matter if we consider $V_1 + (V_2 + V_3)$ or $(V_1 + V_2) + V_3$, thus (12) defines an associative composition. Lemma 4 shows that this is the multiplication of a Lie group. The second proof of Theorem 3 relies on the equality $M(a,\, d) = M_1(a,\, c) \cdot M_2(c,\, d)$, where the transfer matrices contain the scattering amplitudes, exponentials of iqa, iqb, iqc, iqd and factors $q^{\pm 1}$ according to (8). Setting $a = b = c = d = 0$ and $q = 1$ motivates the construction of the isomorphism φ:

Lemma 4
Consider the three-dimensional manifold
$\mathcal{S} = \{(\tau,\, \varrho) \in \mathbb{C}^2 \,|\, |\tau|^2 + |\varrho|^2 = 1,\, \tau \neq 0\}$. *The mapping*

$$\varphi \,:\, \mathcal{S} \to SL(2,\, \mathbb{R}), \quad (\tau,\, \varrho) \mapsto \begin{pmatrix} \mathrm{Re}\,\dfrac{1+\varrho}{\tau} & \mathrm{Im}\,\dfrac{1+\varrho}{\tau} \\ -\,\mathrm{Im}\,\dfrac{1-\varrho}{\tau} & \mathrm{Re}\,\dfrac{1-\varrho}{\tau} \end{pmatrix} \tag{17}$$

is a bijection, and the composition

$$* \,:\, \mathcal{S} \times \mathcal{S} \to \mathcal{S}, \quad (\tau_1,\, \varrho_1) * (\tau_2,\, \varrho_2) \;=\; \Big(\frac{\tau_1\, \tau_2}{1 - \varrho_1^-\, \varrho_2},\; \varrho_1 + \frac{\varrho_2\, \tau_1\, \tau_1^-}{1 - \varrho_1^-\, \varrho_2} \Big) \tag{18}$$

with $\tau_1^- = \tau_1$ *and* $\varrho_1^- = -\varrho_1^* \dfrac{\tau_1}{\tau_1^*}$ *is equivalent to the matrix multiplication in the Lie group* $SL(2,\, \mathbb{R}) = \{M \in \mathbb{R}^{2\times 2} \,|\, \det M = 1\}$. *Thus* φ *is an isomorphism:*
$(\mathcal{S},\, *) \;\to\; (SL(2,\, \mathbb{R}),\, \cdot)$.

The composition (18) is, of course, motivated by Theorem 3 and the mirror formulas (1). The homomorphism property is obvious from Aktosun's original formulation $\Lambda = \Lambda_1\, \Lambda_2$, and the statement on the range of φ is similar to the discussion in [14, p. 34]. Lemma 4 illustrates the algebraic structure of (12), proves the associativity for $V = V_1 + V_2 + V_3$, and shows that $|\tau_q^+|^2 + |\varrho_q^+|^2 = 1$ in (12). The physical interpretation of the group structure (beyond associativity) is limited however: If the τ_i and ϱ_i are the scattering amplitudes of potentials V_i and the compositions corresponding to "$V_1 + V_2$" and "$V_2 + V_1$" both make sense, the supports of V_1 and V_2 must reduce to a common point. Lemma 4 can also be formulated for the manifold $\widetilde{\mathcal{S}} = \{(\tau^+,\, \varrho^+,\, \tau^-,\, \varrho^-) \in \mathbb{C}^4 \,|\, |\tau^+|^2 + |\varrho^+|^2 = 1,\, \tau^+ \neq 0,\, \tau^- = \tau^+,\, \varrho^- = -\varrho^{+*} \frac{\tau^+}{\tau^{+*}}\}$.

Proof of Lemma 4

For $(\tau,\, \varrho) \in \mathcal{S}$, we have $\varphi(\tau,\, \varrho) \in \mathbb{R}^{2\times 2}$ and

$$\det \varphi(\tau,\, \varrho) \;=\; \mathrm{Re}\,\frac{1+\varrho}{\tau}\, \mathrm{Re}\,\frac{1-\varrho}{\tau} + \mathrm{Im}\,\frac{1+\varrho}{\tau}\, \mathrm{Im}\,\frac{1-\varrho}{\tau}$$

$$
\begin{aligned}
&= \operatorname{Re}\frac{1+\varrho}{\tau}\operatorname{Re}\frac{1-\varrho^*}{\tau^*} - \operatorname{Im}\frac{1+\varrho}{\tau}\operatorname{Im}\frac{1-\varrho^*}{\tau^*} \\
&= \operatorname{Re}\frac{1+\varrho}{\tau}\frac{1-\varrho^*}{\tau^*} = \operatorname{Re}\frac{1-\varrho\varrho^*+\varrho-\varrho^*}{\tau\tau^*} \\
&= \frac{1-|\varrho|^2}{|\tau|^2} = 1 ,
\end{aligned}
$$

thus φ maps $\mathcal{S}$ into $SL(2, \mathbb{R})$. To show that φ is bijective, we consider $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ with $\alpha\delta - \beta\gamma = 1$ and we have to find a unique $(\tau, \varrho) \in \mathcal{S}$ with $\varphi(\tau, \varrho) = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$. We obtain the equations

$$
\begin{aligned}
&\frac{1+\varrho}{\tau} = \alpha + i\beta && \frac{1-\varrho}{\tau} = \delta - i\gamma , \\
\text{or} \qquad &\frac{2}{\tau} = (\alpha+\delta) + i(\beta-\gamma) && \varrho = (\alpha+i\beta)\,\tau - 1 ,
\end{aligned}
$$

which have a unique solution with $\tau \neq 0$, since

$$
(\alpha+\delta)^2 + (\beta-\gamma)^2 = \alpha^2+\beta^2+\gamma^2+\delta^2 + 2(\alpha\delta-\beta\gamma) \geq 2 > 0 .
$$

A calculation of the determinant as above shows that $\dfrac{1-|\varrho|^2}{|\tau|^2} = \alpha\delta - \beta\gamma = 1$, thus $|\tau|^2 + |\varrho|^2 = 1$, which means $(\tau, \varrho) \in \mathcal{S}$, and φ is bijective.

Consider $(\tau_1, \varrho_1), (\tau_2, \varrho_2) \in \mathcal{S}$. Since $SL(2, \mathbb{R})$ is a group and φ is bijective, we can define a group structure on $\mathcal{S}$ by $\varphi(\tau, \varrho) = \varphi(\tau_1, \varrho_1) \cdot \varphi(\tau_2, \varrho_2)$ and φ becomes an isomorphism. We want to show that this composition satisfies (18). $\varphi(\tau, \varrho)$ is given by the matrix product

$$
\begin{pmatrix} \operatorname{Re}\dfrac{1+\varrho_1}{\tau_1} & \operatorname{Im}\dfrac{1+\varrho_1}{\tau_1} \\ -\operatorname{Im}\dfrac{1-\varrho_1}{\tau_1} & \operatorname{Re}\dfrac{1-\varrho_1}{\tau_1} \end{pmatrix} \cdot \begin{pmatrix} \operatorname{Re}\dfrac{1+\varrho_2}{\tau_2} & \operatorname{Im}\dfrac{1+\varrho_2}{\tau_2} \\ -\operatorname{Im}\dfrac{1-\varrho_2}{\tau_2} & \operatorname{Re}\dfrac{1-\varrho_2}{\tau_2} \end{pmatrix} .
$$

Thus we have

$$
\begin{aligned}
\operatorname{Re}\frac{1+\varrho}{\tau} &= \operatorname{Re}\frac{1+\varrho_1}{\tau_1}\operatorname{Re}\frac{1+\varrho_2}{\tau_2} - \operatorname{Im}\frac{1+\varrho_1}{\tau_1}\operatorname{Im}\frac{1-\varrho_2}{\tau_2} \\
&= \operatorname{Re}\frac{1+\varrho_1}{\tau_1}\operatorname{Re}\frac{1+\varrho_2}{\tau_2} - \operatorname{Im}\frac{1+\varrho_1}{\tau_1}\operatorname{Im}\frac{1+\varrho_2}{\tau_2} + 2\operatorname{Im}\frac{1+\varrho_1}{\tau_1}\operatorname{Im}\frac{\varrho_2}{\tau_2} \\
\operatorname{Im}\frac{1+\varrho}{\tau} &= \operatorname{Re}\frac{1+\varrho_1}{\tau_1}\operatorname{Im}\frac{1+\varrho_2}{\tau_2} + \operatorname{Im}\frac{1+\varrho_1}{\tau_1}\operatorname{Re}\frac{1-\varrho_2}{\tau_2} \\
&= \operatorname{Re}\frac{1+\varrho_1}{\tau_1}\operatorname{Im}\frac{1+\varrho_2}{\tau_2} + \operatorname{Im}\frac{1+\varrho_1}{\tau_1}\operatorname{Re}\frac{1+\varrho_2}{\tau_2} - 2\operatorname{Im}\frac{1+\varrho_1}{\tau_1}\operatorname{Re}\frac{\varrho_2}{\tau_2} ,
\end{aligned}
$$

which yields

$$
\frac{1+\varrho}{\tau} = \frac{1+\varrho_1}{\tau_1}\frac{1+\varrho_2}{\tau_2} - 2i\operatorname{Im}\Big(\frac{1+\varrho_1}{\tau_1}\Big)\frac{\varrho_2}{\tau_2}
$$

$$= \frac{1+\varrho_1}{\tau_1}\frac{1+\varrho_2}{\tau_2} - \frac{1+\varrho_1}{\tau_1}\frac{\varrho_2}{\tau_2} + \frac{1+\varrho_1^*}{\tau_1^*}\frac{\varrho_2}{\tau_2}$$

$$= \frac{1+\varrho_1}{\tau_1\tau_2} + \frac{1+\varrho_1^*}{\tau_1^*\tau_2}\,\varrho_2\ ,$$

and analogously $$\frac{1-\varrho}{\tau} = \frac{1-\varrho_1}{\tau_1\tau_2} - \frac{1-\varrho_1^*}{\tau_1^*\tau_2}\,\varrho_2\ .$$

Thus we obtain

$$\frac{1}{\tau} = \frac{1}{\tau_1\tau_2} + \frac{\varrho_1^*\varrho_2}{\tau_1^*\tau_2} = \frac{1-\varrho_1^-\varrho_2}{\tau_1\tau_2}$$

with $\varrho_1^- = -\varrho_1^*\frac{\tau_1}{\tau_1^*}$ (which is just an abbreviation in the context of Lemma 4). Finally we have

$$\frac{\varrho}{\tau} = \frac{\varrho_1}{\tau_1\tau_2} + \frac{\varrho_2}{\tau_1^*\tau_2}\ ,$$

$$\varrho = \frac{\varrho_1 + \frac{\tau_1}{\tau_1^*}\varrho_2}{1-\varrho_1^-\varrho_2} = \varrho_1 + \frac{\left(\frac{\tau_1}{\tau_1^*} + \varrho_1\varrho_1^-\right)\varrho_2}{1-\varrho_1^-\varrho_2}\ ,$$

and $\frac{\tau_1}{\tau_1^*} + \varrho_1\varrho_1^- = (\tau_1)^2 = \tau_1\tau_1^-$ completes the proof. ■

6 Generalization

We want to extend the formalism of scattering amplitudes to potentials $V \in L^1_{loc}$ with $V(x) = v_l$ for $x < a$ and $V(x) = v_r$ for $x > b$, where the constants v_l and v_r need not vanish. A single-step potentials can be treated in this way, and we will show that the square-well potential can be described by multiple reflections between two potential steps. We restrict ourselves to the case of $q > 0$ with $q^2 > v_l$ and $q^2 > v_r$ and set $l = \sqrt{q^2 - v_l}$ and $r = \sqrt{q^2 - v_r}$. (We use the parameter $q = \sqrt{E}$, since our main interest is in applications with $v_l = 0$ or $v_r = 0$.) The scattering solutions $\psi_q^\pm$ satisfy the differential equation $-\psi'' + V\,\psi = q^2\,\psi$ with

$$\psi_q^+(x) = \begin{cases} \mathrm{e}^{ilx} + \varrho_q^+\,\mathrm{e}^{-ilx} & \text{for} \quad x \le a \\ \sqrt{\frac{l}{r}}\,\tau_q^+\,\mathrm{e}^{irx} & \text{for} \quad x \ge b\ , \end{cases}$$

$$\psi_q^-(x) = \begin{cases} \sqrt{\frac{r}{l}}\,\tau_q^-\,\mathrm{e}^{-ilx} & \text{for} \quad x \le a \\ \mathrm{e}^{-irx} + \varrho_q^-\,\mathrm{e}^{irx} & \text{for} \quad x \ge b\ . \end{cases}$$

The factors are chosen such that $j = const.$ implies $|\tau_q^\pm|^2 + |\varrho_q^\pm|^2 = 1$. We obtain the following expression for the transfer matrix $M_q(a,\, b)$:

$$\begin{pmatrix} \sqrt{\frac{r}{l}}\ \mathrm{Re}\,\dfrac{\mathrm{e}^{i(la-rb)} + \varrho_q^+\,\mathrm{e}^{-i(la+rb)}}{\tau_q^+} & \dfrac{1}{\sqrt{lr}}\ \mathrm{Im}\,\dfrac{\mathrm{e}^{i(la-rb)} + \varrho_q^+\,\mathrm{e}^{-i(la+rb)}}{\tau_q^+} \\ -\sqrt{lr}\ \mathrm{Im}\,\dfrac{\mathrm{e}^{i(la-rb)} - \varrho_q^+\,\mathrm{e}^{-i(la+rb)}}{\tau_q^+} & \sqrt{\frac{l}{r}}\ \mathrm{Re}\,\dfrac{\mathrm{e}^{i(la-rb)} - \varrho_q^+\,\mathrm{e}^{-i(la+rb)}}{\tau_q^+} \end{pmatrix}.$$

The relations $\tau_q^- = \tau_q^+ \neq 0$ and $\varrho_q^- = -\,\varrho_q^{+*}\,\dfrac{\tau_q^+}{\tau_q^{+*}}$ are proved as in Section 3, and Lemma 2 for $V_z(x) = V(x-z)$ generalizes to

$$\tau_{q,z}^\pm = \mathrm{e}^{i(l-r)z}\,\tau_q^\pm \qquad \varrho_{q,z}^+ = \mathrm{e}^{i2lz}\,\varrho_q^+ \qquad \varrho_{q,z}^- = \mathrm{e}^{-i2rz}\,\varrho_q^- \ .$$

The simplest and most important example is the potential step with $V(x) = v_l$ for $x < 0$ and $V(x) = v_r$ for $x > 0$. We have $a = b = 0$ and $M_q(0,0) = 1$, thus (analogous to (9))

$$\frac{1+\varrho_q^+}{\tau_q^+} = \sqrt{\frac{l}{r}} \qquad \frac{1-\varrho_q^+}{\tau_q^+} = \sqrt{\frac{r}{l}}\,, \qquad \text{thus}$$

$$\tau_q^\pm = \frac{2\sqrt{lr}}{l+r} \qquad \varrho_q^+ = \frac{l-r}{l+r} = -\,\varrho_q^- \ .$$

The formulas for multiple reflections remain the same:

Theorem 5
Consider $-\infty < a \le b \le c \le d < \infty$ *and* $v_l,\, v_m,\, v_r \in \mathbb{R}$. *The potential* V *shall be locally integrable and satisfy* $V(x) = v_l$ *for* $x < a$, $V(x) = v_m$ *for* $b < x < c$ *and* $V(x) = v_r$ *for* $x > d$. *Define potentials* $V_{1,2}$ *by* $V_1(x) = V(x)$ *for* $x < c$, $V_1(x) = v_m$ *for* $x > b$ *and* $V_2(x) = V(x)$ *for* $x > b$, $V_2(x) = v_m$ *for* $x < c$. *Then for* $q > 0$ *with* $q^2 > v_l,\, v_m,\, v_r$, *the generalized scattering amplitudes for* $p^2 + V$ *are obtained from those of* $p^2 + V_1$ *and* $p^2 + V_2$ *according to*

$$\tau_q^+ = \frac{\tau_{q,1}^+\,\tau_{q,2}^+}{1-\varrho_{q,1}^-\,\varrho_{q,2}^+} \qquad \varrho_q^+ = \varrho_{q,1}^+ + \frac{\varrho_{q,2}^+\,\tau_{q,1}^+\,\tau_{q,1}^-}{1-\varrho_{q,1}^-\,\varrho_{q,2}^+} \ . \tag{19}$$

The proof is the same as for Theorem 3: We have $\psi^+(x) = \psi_1^+(x) + \xi\,\psi_1^-(x)$ for $x \le c$, thus $\varrho^+ = \varrho_1^+ + \xi\sqrt{\frac{m}{l}}\,\tau_1^-$. On the other hand, we have $\psi^+(x) = \eta\,\psi_2^+(x)$ for $x \ge b$, thus $\tau^+ = \eta\sqrt{\frac{m}{l}}\,\tau_2^+$. The condition

$$\Big(\sqrt{\frac{m}{l}}\,\tau_1^+ + \xi\,\varrho_1^-\Big)\begin{pmatrix}1\\ im\end{pmatrix}\mathrm{e}^{imc} + \xi\begin{pmatrix}1\\ -im\end{pmatrix}\mathrm{e}^{-imc}$$
$$= \eta\begin{pmatrix}1\\ im\end{pmatrix}\mathrm{e}^{imc} + \eta\,\varrho_2^+\begin{pmatrix}1\\ -im\end{pmatrix}\mathrm{e}^{-imc}$$

yields a system of linear equations for ξ and η with the solution

$$\eta = \frac{\sqrt{\frac{l}{m}}\,\tau_1^+}{1-\varrho_1^-\,\varrho_2^+} \qquad \xi = \frac{\sqrt{\frac{l}{m}}\,\tau_1^+\,\varrho_2^+}{1-\varrho_1^-\,\varrho_2^+}\ ,$$

and the desired formulas for τ^+ and ϱ^+ are obtained. ∎

Theorem 5 is applied to deduce the scattering amplitudes for the square-well potential from those of step potentials: We have

$$V(x) = \begin{cases} v\,, & |x| < b\\ 0\,, & |x| > b\end{cases} \qquad V_1(x) = \begin{cases} 0\,, & x < -b\\ v\,, & x > -b\end{cases} \qquad V_2(x) = \begin{cases} v\,, & x < b\\ 0\,, & x > b\end{cases},$$

and for $q > 0$ with $q^2 > v$, the scattering amplitudes for the step potentials are

$$\tau^{\pm}_{q,1} = \mathrm{e}^{i(r-q)b}\,\frac{2\sqrt{qr}}{q+r} \qquad \varrho^{+}_{q,1} = \mathrm{e}^{-i2qb}\,\frac{q-r}{q+r} \qquad \varrho^{-}_{q,1} = \mathrm{e}^{i2rb}\,\frac{r-q}{q+r}$$

$$\tau^{\pm}_{q,2} = \mathrm{e}^{i(r-q)b}\,\frac{2\sqrt{qr}}{q+r} \qquad \varrho^{+}_{q,2} = \mathrm{e}^{i2rb}\,\frac{r-q}{q+r} \qquad \varrho^{-}_{q,2} = \mathrm{e}^{-i2qb}\,\frac{q-r}{q+r}$$

with $r = \sqrt{q^2 - v}$. Now (19) yields

$$\tau^{+}_{q} = \frac{\Big(\mathrm{e}^{i(r-q)b}\,\dfrac{2\sqrt{qr}}{q+r}\Big)^2}{1 - \Big(\mathrm{e}^{i2rb}\,\dfrac{r-q}{q+r}\Big)^2} = \frac{4qr\,\mathrm{e}^{-i2qb}}{(q+r)^2\,\mathrm{e}^{-i2rb} - (r-q)^2\,\mathrm{e}^{i2rb}} \tag{20}$$

$$\varrho^{+}_{q} = \frac{\mathrm{e}^{-i2qb}\,\dfrac{q-r}{q+r} + \mathrm{e}^{i2(r-q)b}\,\dfrac{r-q}{q+r}}{1 - \Big(\mathrm{e}^{i2rb}\,\dfrac{r-q}{q+r}\Big)^2} = \frac{(q^2-r^2)\,(\mathrm{e}^{-i2rb} - \mathrm{e}^{i2rb})\,\mathrm{e}^{-i2qb}}{(q+r)^2\,\mathrm{e}^{-i2rb} - (r-q)^2\,\mathrm{e}^{i2rb}} \tag{21}$$

and thus we arrive at the formulas (10). (We have used (13) for ϱ^{+}_{q}.) The scattering amplitudes for a square-well potential are given in terms of multiple reflections at step potentials. (I am not sure if (20) and (21) are known, but textbooks mention multiple reflections in the context of resonance scattering for the square-well potential [9, p. 80]. For a discussion of the time evolution in the resonant case, see [21, p. 86].)

7 The Dirac Operator

Now we consider the Dirac equation for a relativistic electron with mass $m > 0$. The velocity of light shall be $c = 1$. We have the Hilbert space $\mathcal{H} = L^2(\mathbb{R},\,\mathbb{C}^2)$ and two self-adjoint matrices $\alpha,\,\beta \in \mathbb{C}^{2\times 2}$ with $\alpha^2 = \beta^2 = 1$, $\alpha\beta + \beta\alpha = 0$. The free Dirac equation is $i\,\dot{\psi} = H_0\,\psi$ with $H_0 = \alpha p + \beta m = -i\alpha\frac{d}{dx} + \beta m$. The matrix $\alpha p + \beta m$ has the eigenvalues $\pm E$ with $E = +\sqrt{p^2+m^2}$. The corresponding eigenvectors are $w_{p,\pm E} \in \mathbb{C}^2$ with the normalization $w^{+}_{p,\pm E}\,w_{p,\pm E} = E/m$, where the spinor conjugation is given by $\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}^{+} = (w_1^*,\,w_2^*)$. The subspaces $\mathcal{H}_\pm$ of positive/negative energy have the continuum basis $w_{p,\pm E}\,\mathrm{e}^{ipx}$, $p \in \mathbb{R}$. For

$$\widehat{\psi}(p) = b(p)\,\sqrt{\frac{m}{E}}\,w_{p,+E} + c(p)\,\sqrt{\frac{m}{E}}\,w_{p,-E}\ ,$$

the Foldy-Wouthuysen representation of ψ is given by $\widehat{\psi}_{FW}(p) = \begin{pmatrix} b(p) \\ c(p) \end{pmatrix}$. It is the Fourier transform of $\psi_{FW}(\widetilde{x})$, which defines the Newton-Wigner position operator $\widetilde{x}$. In preparing the ground for quantum field theory, one may write

$$\psi(x,\,t) = \frac{1}{\sqrt{2\pi}}\int dp\, b(p)\,\sqrt{\frac{m}{E}}\,w_{p,+E}\,\mathrm{e}^{-iEt+ipx} + c(p)\,\sqrt{\frac{m}{E}}\,w_{p,-E}\,\mathrm{e}^{+iEt+ipx}$$

$$= \frac{1}{\sqrt{2\pi}} \int dp\, b(p) \sqrt{\frac{m}{E}}\, u_p\, \mathrm{e}^{-iEt + ipx} + d^*(p) \sqrt{\frac{m}{E}}\, v_p\, \mathrm{e}^{+iEt - ipx}$$

with $u_p = w_{p,+E}$, $v_p = w_{-p,-E}$ and $d^*(p) = c(-p)$. If $c(p)$ measures the presence of an electron with energy $-E$ and momentum $+p$, then $d^*(p)$ measures the absence of a positron with energy $+E$ and momentum $+p$. Thus the negative energies are removed from the theory by introducing antiparticles. In our one-particle approach, we shall restrict our attention to the scattering of positive energy states.

We are interested in the scattering theory for $H = H_0 + V$, where the potential matrix $V(x) \in \mathbb{C}^{2\times 2}$ is self-adjoint, locally integrable and satisfies some short-range condition. Here we shall assume that $V(x)$ vanishes for $x < a$ and $x > b$. The scattering operator S commutes with H_0 and leaves $\mathcal{H}_\pm$ invariant. With $S_\pm = S|_{\mathcal{H}_\pm}$ we have $H_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$ and $S = \begin{pmatrix} S_+ & 0 \\ 0 & S_- \end{pmatrix}$ in the Foldy-Wouthuysen representation.

The stationary scattering theory for positive energy states can be formulated similar to that of the Schrödinger operator: We have $S_+\, b(p) = \tau_p\, b(p) + \varrho_{-p}\, b(-p)$, and the amplitudes τ_p and ϱ_p are obtained from the asymptotics of continuum eigenfunctions of H as follows: For $q > 0$, $\psi_{\pm q}(x)$ satisfy $-i\alpha\, \psi' + \beta m\, \psi + V(x)\, \psi = +\sqrt{q^2 + m^2}\, \psi$ with the asymptotics

$$\psi_{+q}(x) = \begin{cases} u_{+q}\, \mathrm{e}^{iqx} + \varrho_{+q}\, u_{-q}\, \mathrm{e}^{-iqx} & \text{for} \quad x \le a \\ \tau_{+q}\, u_{+q}\, \mathrm{e}^{iqx} & \text{for} \quad x \ge b \end{cases}$$

$$\psi_{-q}(x) = \begin{cases} \tau_{-q}\, u_{-q}\, \mathrm{e}^{-iqx} & \text{for} \quad x \le a \\ u_{-q}\, \mathrm{e}^{-iqx} + \varrho_{-q}\, u_{+q}\, \mathrm{e}^{iqx} & \text{for} \quad x \ge b\ . \end{cases}$$

We deal exclusively with positive energy states, and $\pm q$ denotes the sign of the momentum. We write $\psi_{\pm q}$ instead of $\psi_q^\pm$ to avoid confusion with the spinor conjugation. Existence and uniqueness can be shown in the same way as for the Schrödinger operator, by employing the current density $j = \psi^+ \alpha\, \psi$. The phase of $\varrho_{\pm q}$ depends on the choice of $u_{\pm q}$ and we assume $u_{-q} = \beta\, u_{+q}$ to fix it. For $\alpha = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ we have $u_p = \begin{pmatrix} \cosh \varphi/2 \\ i\, \sinh \varphi/2 \end{pmatrix}$ with $p = m \sinh \varphi$. Observe that for $q > 0$, u_{+q} and u_{-q} are linearly independent (but not orthogonal).

The formulas for multiple reflections are the same as for $H_0 = p^2$ (Theorem 3):

Theorem 6

Consider $-\infty < a \le b \le c \le d < \infty$ and symmetric potential matrices V_1, $V_2 \in L^1$ with $\operatorname{supp} V_1 \subset [a,\, b]$ and $\operatorname{supp} V_2 \subset [c,\, d]$, and define $V = V_1 + V_2$. Then for $q > 0$ the scattering amplitudes for $\alpha p + \beta m + V$ are obtained from those of $\alpha p + \beta m + V_1$ and $\alpha p + \beta m + V_2$ according to

$$\tau_{+q} = \frac{\tau_{+q,1}\, \tau_{+q,2}}{1 - \varrho_{-q,1}\, \varrho_{+q,2}} \qquad \varrho_{+q} = \varrho_{+q,1} + \frac{\varrho_{+q,2}\, \tau_{+q,1}\, \tau_{-q,1}}{1 - \varrho_{-q,1}\, \varrho_{+q,2}}\ . \tag{22}$$

This can be generalized as in Theorem 5. The proof is the same as for Theorem 3, where equation (16) is replaced by

$$(\tau_{+q,1} + \xi\,\varrho_{-q,1})\,u_{+q}\,\mathrm{e}^{+iqc} + \xi\,u_{-q}\,\mathrm{e}^{-iqc} \;=\; \eta\,u_{+q}\,\mathrm{e}^{+iqc} + \eta\,\varrho_{+q,2}\,u_{-q}\,\mathrm{e}^{-iqc}\;.$$

The high-energy asymptotics for well-behaved scalar potentials V are given by [12]

$$\tau_{\pm q} \;=\; \mathrm{e}^{-i\int_{-\infty}^{\infty}dx\,V(x)} + \mathcal{O}(1/q^2) \qquad \varrho_{\pm q} \;=\; \mathcal{O}(1/q^2)\;, \tag{23}$$

which implies $\tau_q^+ \;=\; \tau_{q,1}^+\,\tau_{q,2}^+ + \mathcal{O}(1/q^4)$, cf. the remarks on equation (14).

The Transfer Matrix

To complete the discussion of one-dimensional Dirac scattering, we shall consider the transfer matrix approach and relations between the amplitudes for $+q$ and $-q$. From now on we assume $\alpha = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The potential matrix can be written as $V \;=\; \widetilde{V} - \alpha\,A$, where $\widetilde{V} \in \mathbb{R}^{2\times 2}$ is symmetric and $A \in \mathbb{R}$. In [22, p. 108], Thaller gives a physical interpretation for different forms of V in three dimensions. $A(x)$ corresponds to a magnetic vector potential, which can be removed by a gauge transformation in one dimension: If $A(x) = \lambda'(x)$, thus $V = \widetilde{V} - \alpha\,\lambda'$, then $H_0 + V = \mathrm{e}^{i\lambda}(H_0 + \widetilde{V})\mathrm{e}^{-i\lambda}$ and we obtain (cf. [11, p. 47] and the proof of [10, Lemma 4.18]):

$$\tau_{\pm q} \;=\; \mathrm{e}^{\pm i\int_{-\infty}^{\infty}ds\,A(s)}\,\widetilde{\tau}_{\pm q} \qquad \varrho_{\pm q} \;=\; \widetilde{\varrho}_{\pm q}\;.$$

If $\int_{-\infty}^{\infty}ds\,A(s) \;=\; 0$, then A has no effect on the scattering operator, and if $\int_{-\infty}^{\infty}ds\,A(s) \;\neq\; 2k\pi$, then we have $\tau_{-q} \neq \tau_{+q}$ (since $\widetilde{\tau}_{-q} = \widetilde{\tau}_{+q}$, see below). Thus we shall assume that $A = 0$ in the following discussion of the transfer matrix. Then the equation

$$-i\alpha\,\psi' + \beta m\,\psi + V(x)\,\psi \;=\; E\,\psi\,, \quad E \;=\; +\sqrt{q^2+m^2}\,, \quad V \in \mathbb{R}^{2\times 2}$$

is real and thus the transfer matrix is real, too. It is defined by its property $\psi(x) \;=\; M_q(x,\,y)\,\psi(y)$ for solutions ψ of the Dirac equation and satisfies

$$\frac{d}{dx}\,M_q(x,\,y) \;=\; F(x)\,M_q(x,\,y) \quad \text{with} \quad F(x) \;=\; i\alpha\,(E - \beta m - V(x))\;.$$

$A = 0$ implies $\operatorname{tr} F(x) = 0$, thus

$$\det M_q(x,\,y) \;=\; \mathrm{e}^{\int_y^x ds\,\operatorname{tr}F(s)}\,\det M_q(y,\,y) \;=\; 1\;.$$

We have $u_q = \begin{pmatrix} \cosh\varphi/2 \\ i\,\sinh\varphi/2 \end{pmatrix}$ for $q = m\sinh\varphi$, and the scattering amplitudes are determined from

$$u_{+q}\,\frac{1}{\tau_{+q}}\,\mathrm{e}^{iq(a-b)} + u_{-q}\,\frac{\varrho_{+q}}{\tau_{+q}}\,\mathrm{e}^{-iq(a+b)} \;=\; M_q(a,\,b)\,u_{+q}\;. \tag{24}$$

Since $M_q(a,\,b)$ is real for $A = 0$, we can employ the same idea as for the Schrödinger operator to find the following representation for $M_q(a,\,b)$, which is similar to (8):

$$\begin{pmatrix} \mathrm{Re}\,\dfrac{\mathrm{e}^{iq(a-b)} + \varrho_q^+\,\mathrm{e}^{-iq(a+b)}}{\tau_q^+} & \dfrac{1}{Q}\,\mathrm{Im}\,\dfrac{\mathrm{e}^{iq(a-b)} + \varrho_q^+\,\mathrm{e}^{-iq(a+b)}}{\tau_q^+} \\ -Q\,\mathrm{Im}\,\dfrac{\mathrm{e}^{iq(a-b)} - \varrho_q^+\,\mathrm{e}^{-iq(a+b)}}{\tau_q^+} & \mathrm{Re}\,\dfrac{\mathrm{e}^{iq(a-b)} - \varrho_q^+\,\mathrm{e}^{-iq(a+b)}}{\tau_q^+} \end{pmatrix} . \tag{25}$$

with $Q = \tanh\varphi/2 = \dfrac{q}{E+m}$. The scattering amplitudes can be computed from $M_q(a,\,b)$ as in (9). We obtain the same relations as (1) for the Schrödinger equation

$$|\tau_{\pm q}|^2 + |\varrho_{\pm q}|^2 = 1 \qquad \tau_{-q} \,=\, \tau_{+q} \,\neq\, 0 \qquad \varrho_{-q} \,=\, -\,\varrho_{+q}^*\,\frac{\tau_{+q}}{\tau_{+q}^*}\,.$$

If $V(-x) = V(x)$ and $\beta\,V(x) = V(x)\,\beta$, then we have $\psi_{-q}(x) = \beta\,\psi_{+q}(-x)$, thus $\tau_{-q} = \tau_{+q}$ and $\varrho_{-q} = \varrho_{+q}$. If $V(-x) = V(x)$ (and $a = -b$), but $\beta\,V(x) \neq V(x)\,\beta$, then we may have $\varrho_{-q} \neq \varrho_{+q}$: In the example of $V(x) = \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix}$ for $|x| < b$ we find that $M = M_q(-b,\,b)$ satisfies $M_{11} \neq M_{22}$. Thus (25) implies that ϱ_{+q}/τ_{+q} is not imaginary, and thus $\varrho_{-q} \neq \varrho_{+q}$.

The Square-Well Potential

Let us consider the example of the square potential well/barrier: $V(x) = v$ for $|x| < b$. It may be treated in the same way as in Section 6, but we shall use the transfer matrix directly. For $E = \sqrt{q^2+m^2} > m + v$ we set $r = \sqrt{(E-v)^2 - m^2} = \sqrt{q^2 - 2Ev + v^2}$ and obtain the transfer matrix

$$M_q(-b,\,b) \;=\; \begin{pmatrix} \cos 2rb & -\,\dfrac{E-v+m}{r}\,\sin 2rb \\ \dfrac{E-v-m}{r}\,\sin 2rb & \cos 2rb \end{pmatrix} .$$

(24) or (25) yields the scattering amplitudes

$$\tau_{\pm q} \;=\; \frac{rq\,\mathrm{e}^{-i2qb}}{rq\,\cos 2rb \,-\, i\,(q^2 - vE)\,\sin 2rb} \qquad \varrho_{\pm q} \;=\; \frac{-imv\sin 2rb\,\mathrm{e}^{-i2qb}}{rq\,\cos 2rb \,-\, i\,(q^2 - vE)\,\sin 2rb}\,. \tag{26}$$

The probabilities for transmission and reflection are given by

$$|\tau_{\pm q}|^2 \;=\; \frac{r^2q^2}{r^2q^2 \,+\, m^2v^2\,\sin^2 2rb} \qquad |\varrho_{\pm q}|^2 \;=\; \frac{m^2v^2\,\sin^2 2rb}{r^2q^2 \,+\, m^2v^2\,\sin^2 2rb}\,.$$

If we reintroduce the velocity of light as a parameter c in the Dirac equation, we obtain $-ic\alpha\,\psi' + \beta mc^2\,\psi + V(x)\,\psi = \sqrt{q^2c^2 + m^2c^4}\,\psi$. Thus we have to replace m by mc and v by v/c in (26). It is well known that S_+ approaches the scattering operator for the Schrödinger equation ($H_0 = \frac{1}{2m}\,p^2$) in the nonrelativistic limit $c \to \infty$ [22, p. 312]. We have $\lim\limits_{c\to\infty} r = \sqrt{q^2 - 2mv} =: R$ and

$$\tau_{\pm q} \to \frac{Rq\,\mathrm{e}^{-i2qb}}{Rq\,\cos 2Rb\,-\,i\,(q^2 - mv)\,\sin 2Rb} \qquad \varrho_{\pm q} \to \frac{-imv\sin 2Rb\,\mathrm{e}^{-i2qb}}{Rq\,\cos 2Rb\,-\,i\,(q^2 - mv)\,\sin 2Rb}\,.$$

For $m = 1/2$ these are the amplitudes obtained for $H_0 = p^2$ in (10). Remember that the phase of $\varrho_{\pm q}$ was fixed by the condition $u_{-q} = \beta\,u_{+q}$.

Finally we consider the high-energy limit $q \to \infty$ of (26) (with $c = 1$). From $r = \sqrt{q^2 - 2v\sqrt{q^2+m^2} + v^2} = q - v + \mathcal{O}(1/q^2)$ and $\dfrac{q^2 - v\sqrt{q^2+m^2}}{qr} = 1 + \mathcal{O}(1/q^4)$ we obtain

$$\tau_{\pm q} \;=\; \mathrm{e}^{i2b(r\,-\,q)} + \mathcal{O}(1/q^4) \;=\; \mathrm{e}^{-i2bv} + \mathcal{O}(1/q^2) \qquad \varrho_{\pm q} \;=\; \mathcal{O}(1/q^2)$$

in accordance with (23).

8 Electromagnetic Waves

Let us return to our original motivation, the scattering of light. Maxwell's equations read

$$\begin{aligned} \operatorname{rot}\mathbf{E} &= -\dot{\mathbf{B}} & \qquad \operatorname{rot}\mathbf{H} &= \dot{\mathbf{D}} \\ \operatorname{div}\mathbf{B} &= 0 & \qquad \operatorname{div}\mathbf{D} &= 0 \\ \mathbf{D} &= \varepsilon(\mathbf{x})\,\mathbf{E} & \qquad \mathbf{B} &= \mu(\mathbf{x})\,\mathbf{H}\,, \end{aligned}$$

where we assume that our medium is an isotropic insulator and we neglect the dependence of ε and μ on the frequency. We further assume that we have a stratified medium, where ε and μ depend only on x, and consider a linearly polarized wave traveling in the x-direction:

$$\mathbf{E}(x,\,y,\,z,\,t) \;=\; \begin{pmatrix} 0 \\ 0 \\ E(x,\,t) \end{pmatrix} \qquad \mathbf{H}(x,\,y,\,z,\,t) \;=\; \begin{pmatrix} 0 \\ H(x,\,t) \\ 0 \end{pmatrix}\,.$$

Then Maxwell's equations reduce to

$$E' \;=\; \mu(x)\,\dot{H} \qquad H' \;=\; \varepsilon(x)\,\dot{E}\,,$$

where E, H, $\dot{E}$, $\dot{H}$ shall be absolutely continuous w.r.t. x. If we assume that in addition $\mu(x) = \mu_0 = const.$, then E' is absolutely continuous, too, and we have

$$E'' \;=\; \mu_0\,\varepsilon(x)\,\ddot{E} \;=\; \frac{1}{c(x)^2}\,\ddot{E}$$

with the velocity of light $c(x) = 1/\sqrt{\mu_0\,\varepsilon(x)}$. If $c(x)$ approaches $c_0 = 1/\sqrt{\mu_0\,\varepsilon_0}$ sufficiently fast for $x \to \pm\infty$, a scattering theory makes sense (cf. [19, p. 197]). A free plane wave is of the form

$$E(x,\,t) \,=\, \mathrm{Re}\,\mathrm{e}^{-i\omega t} F(x) \,=\, \mathrm{Re}\,\mathrm{e}^{-i\omega t\,+\,ikx} G$$

with $\omega = c_0\,|k|$ and $F(x)$, $G \in \mathbb{C}$. The stationary scattering solutions satisfy

$$F'' \,=\, -\mu_0\,\varepsilon(x)\,c_0^2\,k^2\,F \,=\, -n(x)^2\,k^2\,F \tag{27}$$

with the index of refraction $n(x) = c_0/c(x) = \sqrt{\varepsilon(x)/\varepsilon_0}$. For fixed k, this corresponds to the Schrödinger equation $-F'' + V(x)\,F = k^2\,F$ with a potential $V(x) = k^2\,(1 - n(x)^2)$. If $-\infty < a \leq b < \infty$ and $n(x) = 1$ for $x < a$ and $x > b$, then we have solutions $F_k^{\pm}$ of (27) with

$$F_k^+(x) \,=\, \begin{cases} \mathrm{e}^{ikx} + \varrho_k^+\,\mathrm{e}^{-ikx} & \text{for} \quad x \leq a \\ \tau_k^+\,\mathrm{e}^{ikx} & \text{for} \quad x \geq b \end{cases}$$

and analogously for $F_k^-(x)$.

To describe a parallel sheet of glass, take $a = -b$ and $n(x) = 1$ for $|x| > b$ and $n(x) = n$ for $|x| < b$ with a fixed $n > 1$. This corresponds to the square-well potential with $V(x) = v = k^2\,(1 - n^2)$ for $|x| < b$. From the formulas (10) we obtain with $r = kn$

$$\tau_k^+ \,=\, \frac{2n\,\mathrm{e}^{-i2kb}}{2n\,\cos 2knb \,-\, i\,(n^2+1)\,\sin 2knb} \qquad \varrho_k^+ \,=\, \frac{i(n^2-1)\,\sin 2knb\,\mathrm{e}^{-i2kb}}{2n\,\cos 2knb \,-\, i\,(n^2+1)\,\sin 2rb}\,, \tag{28}$$

and the probabilities for transmission and reflection are given by

$$|\tau_k^+|^2 \,=\, \frac{4n^2}{4n^2 \,+\, (n^2-1)^2\,\sin^2 2knb} \qquad\qquad |\varrho_k^+|^2 \,=\, \frac{(n^2-1)^2\,\sin^2 2knb}{4n^2 \,+\, (n^2-1)^2\,\sin^2 2knb}\,.$$

One observes the characteristic dependence on the thickness $2b$, which accounts for the colors of, e.g., a film of oil floating on the surface of water.

The formulas for multiple reflections are the same as for the Schrödinger- and Dirac equation. The electromagnetic case was already treated in [1].

Theorem 7

Consider $-\infty < a \leq b \leq c \leq d < \infty$ and indices of refraction $n_{1,2}(x)$ with $0 < \alpha \leq n_i(x) \leq \beta < \infty$ and $n_1(x) = 1$ for $x \notin [a,\,b]$, $n_2(x) = 1$ for $x \notin [c,\,d]$. Define $n(x) = n_1(x)$ for $x < c$ and $n(x) = n_2(x)$ for $x > b$. Then for $k > 0$, the scattering amplitudes are related by

$$\tau_k^+ = \frac{\tau_{k,1}^+\,\tau_{k,2}^+}{1 \,-\, \varrho_{k,1}^-\,\varrho_{k,2}^+} \qquad \varrho_k^+ = \varrho_{k,1}^+ \,+\, \frac{\varrho_{k,2}^+\,\tau_{k,1}^+\,\tau_{k,1}^-}{1 \,-\, \varrho_{k,1}^-\,\varrho_{k,2}^+}\,. \tag{29}$$

This theorem remains true, if $n(x)$ takes different constant values for $x < a$, $b < x < c$ and $x > d$. Thus we can obtain the amplitudes (28) for the sheet of glass from those for a halfspace of glass. (We have obtained the amplitudes for a square-well potential in terms of those of step potentials in (20)). We have

$$\tau_{k,1}^{\pm} = \tau_{k,2}^{\pm} = \mathrm{e}^{i(n-1)kb}\,\frac{2\sqrt{n}}{n+1} \qquad \varrho_{k,1}^{-} = \varrho_{k,2}^{+} = \mathrm{e}^{i2knb}\,\frac{n-1}{n+1}\ ,$$

$$\begin{aligned} \tau_k^{+} &= \frac{\Big(\mathrm{e}^{i(n-1)kb}\,\frac{2\sqrt{n}}{n+1}\Big)^2}{1 - \Big(\mathrm{e}^{i2knb}\,\frac{n-1}{n+1}\Big)^2} \\ &= \Big(\mathrm{e}^{i(n-1)kb}\,\frac{2\sqrt{n}}{n+1}\Big)\sum_{j=0}^{\infty}\Big(\mathrm{e}^{i2knb}\,\frac{n-1}{n+1}\Big)^{2j}\Big(\mathrm{e}^{i(n-1)kb}\,\frac{2\sqrt{n}}{n+1}\Big)\ , \end{aligned}$$

and analogously for ϱ_k^{+}. The factors can be interpreted as follows: $\frac{n-1}{n+1}$ describes the reflection from the front or back surface of the glass, and e^{i2knb} accounts for the motion through the glass, cf. the remark after Lemma 2. Thus we arrive at Feynman's formulation in terms of probability amplitudes [8].

References

[1] T. Aktosun, A Factorization of the S-Matrix for the Schrödinger Equation and for the Wave Equation in One Dimension, J. Math. Phys. **33**, 3865–3869 (1992).

[2] T. Aktosun, M. Klaus and C. van der Mee, Factorization of Scattering Matrices due to Partitioning of Potentials in One-Dimensional Schrödinger-Type Equations, J. Math. Phys. **37**, 5897–5915 (1996).

[3] S. Albeverio et al., *Solvable Models in Quantum Mechanics*, Springer, New York 1988.

[4] M. Sassoli de Bianchi and M. Di Ventura, On the Number of States Bound by One-Dimensional Finite Periodic Potentials, J. Math. Phys. **36**, 1753–1764 (1995).

[5] M. Sassoli de Bianchi and M. Di Ventura, Differential Equations and Factorization Property for the One-Dimensional Schrödinger Equation with Position-Dependent Mass, Europ. J. Phys. **16**, 260–265 (1995).

[6] M. Sassoli de Bianchi, Comment on "Factorization of Scattering Matrices due to Partitioning of Potentials in One-Dimensional Schrödinger-Type Equations", J. Math. Phys. **38**, 4882–4883 (1997).

[7] P. Exner and M. Tater, Evanescent Modes in a Multiple Scattering Factorization, preprint (1997), to appear in Czech. J. Phys..

[8] R. P. Feynman, *QED — The Strange Theory of Light and Matter*, Princeton University Press 1988.

[9] S. Gasiorowicz, *Quantum Physics*, Wiley, New York

[10] W. Jung, Der geometrische Ansatz zur inversen Streutheorie bei der Dirac-Gleichung, Diploma thesis, RWTH Aachen (1996).

[11] W. Jung, Geometrical Approach to Inverse Scattering for the Dirac Equation, J. Math. Phys. **38**, 39–48 (1997).

[12] W. Jung, The High-Energy Asymptotics of One-Dimensional Quantum Scattering, preprint in preparation (2002).

[13] T. M. Kalotas and A. R. Lee, A New Approach to One-Dimensional Scattering, Am. J. Phys. **59**, 48–52 (1991).

[14] V. Kostrykin and R. Schrader, Scattering Theory Approach to Random Schrödinger Operators in One Dimension, preprint (1997).

[15] E. Kujawski, Additivity of Phase Shifts for Scattering in One Dimension, Am. J. Phys. **39**, 1248–1254 (1971).

[16] I. R. Lapidus, Resonance Scattering from a Double δ-Function Potential, Am. J. Phys. **50**, 663–664 (1982).

[17] D. B. Pearson, *Quantum Scattering and Spectral Theory*, Techniques of Physics **9**, Academic Press, London 1988.

[18] M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic Press, San Diego 1975.

[19] M. Reed and B. Simon, *Methods of Modern Mathematical Physics III: Scattering Theory*, Academic Press, New York 1979.

[20] M. G. Rozman, P. Reineker and R. Thever, One-Dimensional Scattering: Recurrence Relations and Differential Equations for Transmission and Reflection Amplitudes, Phys. Rev. A **49**, 3310–3321 (1994).

[21] F. Schwabl, *Quantenmechanik*, Springer, Berlin Heidelberg 1993.

[22] B. Thaller, *The Dirac Equation*, Springer, Berlin Heidelberg 1992.

[23] K. Vacek, A. Okiji and H. Kasai, Multichannel Ballistic Magnetotransport Through Quantum Wires with Double Circular Bends, Phys. Rev. B **47**, 3695–3705 (1993).