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Analytical properties of scattering amplitudes in one-dimensional quantum theory

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Abstract. One-dimensional quantum scattering from a local potential barrier is considered. Analytical properties of the scattering amplitudes have been investigated by means of the integral equations equivalent to the Schrödinger equations. The transition and reflection amplitudes are expressed in terms of two complex functions of the incident energy, which are similar to the Jost function in partial-wave scattering. These functions are entire for finite-range potentials and meromorphic for exponentially decreasing potentials. The analytical properties result from the locality of the potential in the wave equation and represent the effect of causality in the time dependence of the scattering process.

1. Introduction

The problem of the *tunnelling time* has attracted considerable attention for decades [1–4]. It is indeed important to understand the effect of *causality* on particle and wave propagation. The problem is that in the conventional time-independent formalism the causality manifests itself indirectly, i.e. in the analytical properties of the transition amplitudes as functions of (complex) energy. The relations between causality and analyticity were intensively investigated in the 1960s when the concept of the S-matrix dominated in particle physics [5, 6]. At that time, however, the analysis was aimed mainly at three-dimensional scattering processes and for central-symmetric potentials in particular [7, 8]. Partial-wave scattering amplitudes in the complex energy plane were also considered in the theory of multichannel nuclear reactions [9]. The analytical properties of the scattering matrix have also been used in various fields. For example, in the theory of multi-terminal mesoscopic conductance the properties of the multi-probe S-matrix were used [10] to obtain the conductance and to establish the time ordering of the incoming and outgoing lead states. In another work [11], the low-frequency behaviour of dynamic conductance was related to the phase-delay times for the carrier transmission and reflection, which are given by the energy derivatives of the S-matrix elements. The most important feature of the transition amplitudes for various physical processes in the energy representation is their analyticity in the upper half of the complex plane. Sometimes one can find out more about singularities in the lower half-plane, by investigating dynamical equations specific for the physical problem, such as the Schrödinger equation for scattering.

One-dimensional 'scattering', i.e. the potential-barrier problem, is somewhat more complicated than scattering from a force centre, since the system has two channels, corresponding to two waves running in opposite directions to the potential region in the

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final state. Thus instead of one analytical function, the partial-wave scattering amplitude, one deals with two analytical functions, the transmission and reflection amplitudes. (The unitarity condition holds in both cases.) The familiar arguments from scattering theory must be extended properly to the one-dimensional case. The analytical properties of the one-dimensional S-matrix were discussed, in particular, by Faddeev [12, 13] and Newton [14] in view of the inverse problem. The singularities in the complex energy plane, caused by bound and quasi-bound states, were considered more recently [15–17].

The purpose of the present work is to investigate the location and character of singularities in the scattering amplitudes, owing to the potential shape. The investigation is based upon the Schrödinger equation with a local potential. This enables one to reveal the general features of the amplitudes, depending on the character of the vanishing of the potential outside its domain. The analytical properties are essential for application to a spacetime picture of the barrier transmission.

In section 2, the 2×2 scattering and transition matrices are introduced and related to the resolvent of the Schrödinger operator. Next, in section 3, two complex functions are defined for the potential barrier problem, which are related to elements of the monodromy matrix. Their role is similar to that of the Jost function in S-wave potential scattering. These functions have nice analytical properties, which are proven in section 4 by means of Volterra-type integral equations. It is shown, in particular, that the functions have no singularities in the whole complex energy plane (except for infinity), if the potential has a finite range. Singularities appear if the potential behaves exponentially in the asymptotics, and the slope of the exponent determines the distance to the singularies nearest to the real energy axis. Some examples are given in the appendix.

2. Transition operator and the S-matrix

The evolution operator is given by the Laplace transform of the resolvent of the Hamiltonian $\hat{H}$,

$$\exp(-\mathrm{i}t\hat{H}) = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_\infty} \hat{G}_\varepsilon \mathrm{e}^{-\mathrm{i}\varepsilon t}\,\mathrm{d}\varepsilon \qquad \hat{G}_\varepsilon \equiv (\hat{H}-\varepsilon)^{-1}. \tag{1}$$

Here Γ_∞ is the contour in the complex ε-plane, running from $-\infty$ to $+\infty$ *above* the real axis, where the singularities are situated. In scattering problems, the Hamiltonian is the sum of a potential operator and the kinetic energy, with the eigenvectors describing free particle states,

$$\hat{H} \equiv \hat{H}_0 + \hat{V} \qquad \hat{H}_0|\boldsymbol{k}\rangle = \epsilon(k)|\boldsymbol{k}\rangle. \tag{2}$$

In non-relativistic scattering theory, we shall use the units where $\epsilon(k) = k^2$. The transition operator $\hat{H}_\varepsilon$ is introduced as follows

$$\hat{G}_\varepsilon = \hat{G}^{(0)}_\varepsilon - \hat{G}^{(0)}_\varepsilon \hat{H}_\varepsilon \hat{G}^{(0)}_\varepsilon \qquad \hat{G}^{(0)}_\varepsilon \equiv (\hat{H}_0 - \varepsilon)^{-1}. \tag{3}$$

It can be expressed directly in terms of the resolvent $\hat{G}_\varepsilon$,

$$\hat{H}_\varepsilon = \hat{V} - \hat{V}\hat{G}_\varepsilon\hat{V}. \tag{4}$$

As follows from the time-inversion symmetry (the reciprocity principle),

$$\langle\boldsymbol{k}|\hat{H}_\varepsilon|\boldsymbol{k}_0\rangle = \langle-\boldsymbol{k}_0|\hat{H}_\varepsilon|-\boldsymbol{k}\rangle. \tag{5}$$

It is easy to see, using the standard definition of the scattering operator $\hat{S}$, that its matrix elements are expressed in terms of the transition operator on the energy shell,

$$\begin{aligned}\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}_0\rangle &\equiv \lim_{t\to\infty}\langle \boldsymbol{k}|\exp(\tfrac{1}{2}\mathrm{i}t\hat{H}_0)\exp(-\mathrm{i}t\hat{H})\exp(\tfrac{1}{2}\mathrm{i}t\hat{H}_0)|\boldsymbol{k}_0\rangle \\ &= \delta(\boldsymbol{k}-\boldsymbol{k}_0) - 2\pi\mathrm{i}\delta[\epsilon(k)-\epsilon(k_0)]T_{\nu\nu_0}(\varepsilon). \qquad (6)\end{aligned}$$

Here the scattering amplitude is given by

$$T_{\nu\nu_0}(\varepsilon) \equiv \langle \boldsymbol{k}|\hat{H}_\varepsilon|\boldsymbol{k}_0\rangle \qquad \epsilon(k) = \varepsilon = \epsilon(k_0) \qquad (7)$$

where $\nu \equiv \boldsymbol{k}/k$, and the standard normalization is used: $\langle \boldsymbol{k}|\boldsymbol{k}_0\rangle = \delta(\boldsymbol{k}-\boldsymbol{k}_0)$.

In the one-dimensional case $\boldsymbol{k} = \nu k$, where $\nu = \pm 1$, corresponding to two possible directions of motion for a given energy, and

$$\delta(\boldsymbol{k}-\boldsymbol{k}_0) = v\delta[\epsilon(k)-\epsilon(k_0)]\delta_{\nu\nu_0} \qquad v = \mathrm{d}\epsilon/\mathrm{d}k. \qquad (8)$$

The elements of $\hat{S}$ and $\hat{T}$ (on the energy shell) are given by 2×2 matrices S and T,

$$\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}_0\rangle = v\delta[\epsilon(k)-\epsilon(k_0)]S_{\nu\nu_0} \qquad S \equiv I - \frac{2\pi\mathrm{i}}{v}T. \qquad (9)$$

By definition, if $\hat{S}$ exists, it is a unitary operator. This fact implies a unitarity condition on the scattering amplitude, which reads

$$SS^\dagger = I \qquad \frac{1}{2\pi\mathrm{i}}(T-T^\dagger) = -\frac{1}{v}TT^\dagger. \qquad (10)$$

As we will show, the analytical properties of $T(\varepsilon)$ follow from the locality of the potential, and equation (4).

3. General properties of the transition amplitudes

We consider the Schrödinger equation,

$$\hat{H}\psi = \kappa^2\psi \qquad \hat{H} = -(\mathrm{d}/\mathrm{d}x)^2 + V(x) \qquad (11)$$

where $-\infty < x < \infty$, and the potential is local, i.e. $|V(x)| = o(1/x)$ as $|x| \to \infty$. In the coordinate representation, the resolvent can be expressed in terms of two fundamental solutions of the Schrödinger equation, $y_\pm(x)$, satisfying the proper boundary conditions at $\pm\infty$, respectively,

$$\langle x|\hat{G}_\varepsilon|x_0\rangle = \frac{y_-(x_<)y_+(x_>)}{w(y_-,y_+)} \qquad x_{>/<} = \max/\min(x,x_0) \qquad (12)$$

$$y_\pm(x) \to \mathrm{e}^{\pm\mathrm{i}\kappa x} \qquad \text{as } x\to\pm\infty \qquad (13)$$

$$w(y_-,y_+) \equiv y_-'y_+ - y_-y_+' = \text{constant}.$$

As soon as $\varepsilon \equiv \kappa^2$ is introduced in the Laplace transform (1) for the *upper* half of the complex plane, the solutions $y_\pm$ defined above vanish at $\pm\infty$, respectively. Thus one has the properly defined resolvent for the elliptic operator $\hat{H}$ satisfying the Sommerfeld radiation condition at infinity [18].

For large $|x|$, where the potential vanishes, the asymptotics of the fundamental solutions are given by

$$\begin{aligned} y_-(x) &= a\mathrm{e}^{-\mathrm{i}\kappa x} + b\mathrm{e}^{\mathrm{i}\kappa x} \qquad \text{for } x\to+\infty \qquad (14)\\ y_+(x) &= b'\mathrm{e}^{-\mathrm{i}\kappa x} + c\mathrm{e}^{\mathrm{i}\kappa x} \qquad \text{for } x\to-\infty.\end{aligned}$$

In principle, the solutions are defined by (13) for $\mathrm{Re}\,\kappa > 0$ and $\mathrm{Im}\,\kappa \to +0$, yet the analytical continuation to the whole complex κ-plane is considered in the following. For real potentials

$V(x)$, the complex conjugate functions $\overline{y^{\kappa}_{\pm}(x)}$ are also solutions of the Schrödinger equation, satisfying the boundary conditions conjugate to (13). Calculating the Wronskians (which are independent of x) at $x \to \pm\infty$ for various pairs of the solutions, one gets a number of relations between the complex parameters a, b, b', c:

$$w(y_-, y_+) = -2\mathrm{i}\kappa a = -2\mathrm{i}\kappa c : a = c \tag{15}$$

$$w(y_-, \bar{y}_-) = \text{constant} : |a|^2 - |b|^2 = 1 \tag{16}$$

$$w(y_+, \bar{y}_+) = \text{constant} : |c|^2 - |b'|^2 = 1$$

$$w(y_-, \bar{y}_+) = \text{constant} : b' = -\bar{b}. \tag{17}$$

Expressing $\overline{y_\pm}$ in terms of the fundamental solutions, one has

$$\bar{y}_- = \frac{\bar{b}}{a} y_- + \frac{1}{a} y_+ \qquad \bar{y}_+ = \frac{1}{a} y_- - \frac{b}{a} y_+. \tag{18}$$

The analytical continuation of these solutions to the complex κ plane, by $\overline{y^{\kappa}_{\pm}(x)} \equiv y^{-\bar{\kappa}}_{\pm}(x)$, implies a symmetry of $a(\kappa)$ and $b(\kappa)$ with respect to the imaginary κ-axis,

$$\overline{a(\kappa)} = a(-\bar{\kappa}) \qquad \overline{b(\kappa)} = b(-\bar{\kappa}). \tag{19}$$

Thus, the asymptotics of the solutions depend only on two complex functions $a(\kappa)$ and $b(\kappa)$, satisfying one real condition (16), and subject to the symmetry (19). The transition amplitudes, elements of the S-matrix and T-matrix, and of the monodromy matrix [19], are given in terms of these two functions.

If the potential is displaced, b gets a phase shift,

$$V(x) \to V(x-d) \qquad a \to a \qquad b \to b\mathrm{e}^{-2\mathrm{i}\kappa d}. \tag{20}$$

For symmetric potentials one gets an additional relation,

$$V(x) \equiv V(-x) \qquad y_-(-x) \equiv y_+(x) \colon a = c, b' = b \tag{21}$$

so that b is pure imaginary, in view of (17).

As soon as the resolvent is known from (12), the elements of the transition operator in the momentum representation are obtained immediately, by (4),

$$\langle k|\hat{H}_\varepsilon|k_0\rangle = \tilde{V}(q) - \frac{1}{2\pi}\iint \mathrm{d}x\,\mathrm{d}x_0 \mathrm{e}^{-\mathrm{i}kx+\mathrm{i}k_0x_0} V(x)\langle x|\hat{G}_\varepsilon|x_0\rangle V(x_0) \tag{22}$$

where $q = k - k_0$, and

$$\tilde{V}(q) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} V(x)\mathrm{e}^{-\mathrm{i}qx}\,\mathrm{d}x. \tag{23}$$

The double Fourier transform in (22) is performed by means of the Schrödinger equation, $Vy = y'' + \kappa^2 y$, leading to the following integrals

$$\int_{-\infty}^{x} \mathrm{e}^{-\mathrm{i}k\xi} V(\xi) y_-(\xi)\,\mathrm{d}\xi = (\eta'_- + \mathrm{i}k\eta_-)\mathrm{e}^{-\mathrm{i}kx} + (\kappa^2 - k^2)\int_{-\infty}^{x} \mathrm{e}^{-\mathrm{i}k\xi}\eta_-(\xi)\,\mathrm{d}\xi \tag{24}$$

$$\int_{x}^{\infty} \mathrm{e}^{-\mathrm{i}k\xi} V(\xi) y_+(\xi)\,\mathrm{d}\xi = -(\eta'_+ + ik\eta_+)\mathrm{e}^{-\mathrm{i}kx} + (\kappa^2 - k^2)\int_{x}^{\infty} \mathrm{e}^{-\mathrm{i}k\xi}\eta_+(\xi)\,\mathrm{d}\xi \tag{25}$$

where we have introduced the functions $\eta_\pm(x)$ vanishing at $\pm\infty$,

$$\eta_\pm(x) \equiv y_\pm(x) - \mathrm{e}^{\pm\mathrm{i}\kappa x}. \tag{26}$$

The result is

$$\langle k|\hat{H}_\varepsilon|k_0\rangle = \frac{1}{2\pi \mathrm{i}w}\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-\mathrm{i}qx} V(x)\left[\left(\kappa - \frac{q}{2}\right) y_+(x)\mathrm{e}^{-\mathrm{i}\kappa x} + \left(\kappa + \frac{q}{2}\right) y_-(x)\mathrm{e}^{\mathrm{i}\kappa x}\right]$$
$$-\frac{\kappa^2 - \frac{1}{2}(k^2 + k_0^2)}{2\pi w}\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-\mathrm{i}qx}(\eta_+\eta_-' - \eta_-\eta_+')$$
$$-(\kappa^2 - k^2)(\kappa^2 - k_0^2)\frac{1}{2\pi}\iint \mathrm{d}x\, \mathrm{d}x_0 \mathrm{e}^{-\mathrm{i}kx + \mathrm{i}k_0x_0} g(x, x_0) \quad (27)$$

where $w = -2\mathrm{i}\kappa a$, and

$$g(x, x_0) \equiv \eta_-(x_<)\eta_+(x_>)/w. \quad (28)$$

On the energy shell where $k^2 = \kappa^2 = k_0^2$, the contributions from the integrals vanish in equations (24)–(27), and one has

$$T = \frac{1}{2\pi a}\begin{pmatrix} \alpha & \beta \\ \bar{\beta} & \alpha \end{pmatrix} \qquad S = \frac{1}{a}\begin{pmatrix} 1 & b \\ -\bar{b} & 1 \end{pmatrix} \quad (29)$$

where

$$\alpha \equiv \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-\mathrm{i}\kappa x} V(x) y_+(x) = \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{\mathrm{i}\kappa x} V(x) y_-(x) \quad (30)$$
$$\beta \equiv \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{\mathrm{i}\kappa x} V(x) y_+(x) = \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-\mathrm{i}\kappa x} V(x) y_-(x)$$
$$a \equiv 1 - \frac{\alpha}{2\mathrm{i}\kappa} \qquad b \equiv \frac{\beta}{2\mathrm{i}\kappa}. \quad (31)$$

The functions $\alpha(\kappa)$ and $\beta(\kappa)$ are free of a pole at $\kappa = 0$, and are related by the unitarity condition,

$$\alpha - \bar{\alpha} = \frac{\mathrm{i}}{2\kappa}(\alpha\bar{\alpha} - \beta\bar{\beta}). \quad (32)$$

The transmission and reflection amplitudes are $S_{++} = 1/a$ and $S_{+-} = b/a$, respectively, and $\det S = \bar{a}/a$. (The latter equality supports the analogy of a to the Jost function. If there is no reflection, $b = 0$, then $a = \mathrm{e}^{-\mathrm{i}\delta}$, where $\delta(\kappa)$ is a real phase shift.) Besides, if the potential is even, the matrices S and T are symmetrical.

Note that because of the relations (15)–(17) the monodromy matrix [19] composed of a, b is quasi-unitary,

$$M = \begin{pmatrix} \bar{a} & -\bar{b} \\ -b & a \end{pmatrix} \qquad MEM^\dagger = E \qquad E = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (33)$$

Under a displacement of the potential, equation (20), M is transformed to

$$M \to DMD^\dagger \qquad D = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{e}^{-2\mathrm{i}\kappa d} \end{pmatrix}. \quad (34)$$

If $V(x) = V_1(x - d_1) + V_2(x - d_2)$, $d_2 > d_1$, and the potential domain consists of two intervals separated by a forceless gap, one has the following superposition rule,

$$M = D_1M_1D_1^\dagger D_2M_2D_2^\dagger :$$
$$a = a_1a_2 + b_1\bar{b}_2\mathrm{e}^{2\mathrm{i}\kappa(d_2-d_1)} \qquad b = a_1b_2\mathrm{e}^{-2\mathrm{i}\kappa d_2} + \bar{a}_2b_1\mathrm{e}^{-2\mathrm{i}\kappa d_1} \quad (35)$$

which is a consequence of equations (14) and (20).

4. Integral equations and the analytical properties

4.1. Volterra equation and series solutions

Analytical properties of the transition amplitudes can be derived from the integral equation satisfied by the fundamental solutions $y_\pm(x)$,

$$y_\pm(x) = \mathrm{e}^{\pm \mathrm{i}\kappa x} + \frac{1}{\kappa}\int_{\pm\infty}^{x} \sin\kappa(x-\xi)V(\xi)y_\pm(\xi)\mathrm{d}\xi. \tag{36}$$

These equations are of the Volterra type, so the solution exists and admits an analytical continuation to complex κ for local potentials. In order to separate asymptotic oscillations of the solutions, let us introduce new functions (the integrals are evaluated by equations (24) and (25) for $k = \pm\kappa$),

$$A_-(x) \equiv \int_{-\infty}^{x} \mathrm{e}^{\mathrm{i}\kappa\xi} V(\xi)y_-(\xi)\,\mathrm{d}\xi = (y'_- - \mathrm{i}\kappa y_-)\mathrm{e}^{\mathrm{i}\kappa x} + 2\mathrm{i}\kappa$$

$$B_-(x) \equiv \int_{-\infty}^{x} \mathrm{e}^{-\mathrm{i}\kappa\xi} V(\xi)y_-(\xi)\,\mathrm{d}\xi = (y'_- + \mathrm{i}\kappa y_-)\mathrm{e}^{-\mathrm{i}\kappa x} \tag{37}$$

$$A_+(x) \equiv \int_{x}^{\infty} \mathrm{e}^{-\mathrm{i}\kappa\xi} V(\xi)y_+(\xi)\,\mathrm{d}\xi = -(y'_+ + \mathrm{i}\kappa y_+)\mathrm{e}^{-\mathrm{i}\kappa x} + 2\mathrm{i}\kappa$$

$$B_+(x) \equiv \int_{x}^{\infty} \mathrm{e}^{\mathrm{i}\kappa\xi} V(\xi)y_+(\xi)\,\mathrm{d}\xi = -(y'_+ - \mathrm{i}\kappa y_+)\mathrm{e}^{\mathrm{i}\kappa x}. \tag{38}$$

It is easy to see that

$$\frac{\mathrm{d}y_\pm}{\mathrm{d}x} = \pm\mathrm{i}\kappa\left(1 - \frac{1}{2\mathrm{i}\kappa}A_\pm(x)\right)\mathrm{e}^{\pm\mathrm{i}\kappa x} \mp \frac{1}{2}B_\pm(x)\mathrm{e}^{\mp\mathrm{i}\kappa x}$$

$$y_\pm(x) = \left(1 - \frac{1}{2\mathrm{i}\kappa}A_\pm(x)\right)\mathrm{e}^{\pm\mathrm{i}\kappa x} + \frac{1}{2\mathrm{i}\kappa}B_\pm(x)\mathrm{e}^{\mp\mathrm{i}\kappa x} \tag{39}$$

so A and B have definite limits at $x \to \pm\infty$, cf equations (30),

$$\alpha \equiv A_+(-\infty) = A_-(+\infty) \qquad \beta \equiv B_-(+\infty) = \overline{B_+(-\infty)} \tag{40}$$

$$A_\pm(\pm\infty) = 0 = B_\pm(\pm\infty).$$

The pairs of functions (A, B) satisfy a system of first-order differential equations with zero initial conditions at infinity. Setting the equations into the integral form, one gets from (37), in particular, for A_- and B_-,

$$A_-(x) = \int_{-\infty}^{x} V(\xi)\left(1 - \frac{1}{2\mathrm{i}\kappa}A_-(\xi) + \frac{1}{2\mathrm{i}\kappa}B_-(\xi)\mathrm{e}^{2\mathrm{i}\kappa\xi}\right)\mathrm{d}\xi \tag{41}$$

$$B_-(x) = \int_{-\infty}^{x} V(\xi)\left(\left(1 - \frac{1}{2\mathrm{i}\kappa}A_-(\xi)\right)\mathrm{e}^{-2\mathrm{i}\kappa\xi} + \frac{1}{2\mathrm{i}\kappa}B_-(\xi)\right)\mathrm{d}\xi. \tag{42}$$

This form is especially suitable for the perturbative expansion of α and β, namely,

$$\alpha(\kappa) = \int_{-\infty}^{+\infty} V(\xi)\,\mathrm{d}\xi + \frac{1}{\kappa}\int_{-\infty}^{+\infty}\mathrm{d}\xi_2\int_{-\infty}^{\xi_2}\mathrm{d}\xi_1 V(\xi_2)V(\xi_1)\mathrm{e}^{\mathrm{i}\kappa(\xi_2-\xi_1)}\sin\kappa(\xi_2-\xi_1) + \cdots \tag{43}$$

$$\beta(\kappa) = \int_{-\infty}^{+\infty} V(\xi)\mathrm{e}^{-2\mathrm{i}\kappa\xi}\,\mathrm{d}\xi + \frac{1}{\kappa}\int_{-\infty}^{+\infty}\mathrm{d}\xi_2\int_{-\infty}^{\xi_2}\mathrm{d}\xi_1 V(\xi_2)V(\xi_1)\mathrm{e}^{-\mathrm{i}\kappa(\xi_2+\xi_1)}\sin\kappa(\xi_2-\xi_1) + \cdots. \tag{44}$$

Using these expansions, one gets a sort of Padé approximation for the S-matrix in (29). Note that as $\kappa \to 0$, one has $\alpha - \beta \to 0$ while α and β are regular, so expanding in powers of κ one can get, for short-range potentials, an analogue of the effective-range approximation [8].

4.2. Analytical properties

The perturbative series are also used to prove the analytical properties. First of all, one can extend to equation (36) the standard arguments of scattering theory [8], which are based upon the inequality

$$|\sin\kappa(x-\xi)| \leqslant C\frac{|\kappa x|}{1+|\kappa x|}\mathrm{e}^{|\operatorname{Im}\kappa|(x-\xi)} \tag{45}$$

where $x > \xi$, and C is a constant. Thus one proves that the $y_\pm(\kappa)$ are analytical in the domain in the complex κ-plane where

$$\int_{-\infty}^{x} \exp\left[-\xi(|\operatorname{Im}\kappa| \pm \operatorname{Im}\kappa)\right] V(\xi)\,\mathrm{d}\xi < \infty.$$

In particular, if $V(x) \equiv 0$ for $x < x_-$, for some x_-, there is no irregularity as $x \to -\infty$. Similarly, the limit $x \to +\infty$ is considered. The fundamental solutions are analytical in κ, as soon as these two limits are regular.

One may modify the method instead and apply it directly to the functions we are interested in, given by equations (41) and (42). The substitution

$$A_-(x) = f(x)\mathrm{e}^{\mathrm{i}w(x)} \qquad B_-(x) = g(x)\mathrm{e}^{-\mathrm{i}w(x)} \qquad w(x) \equiv \frac{1}{2\kappa}\int_{-\infty}^{x}\mathrm{d}\xi\, V(\xi) \tag{46}$$

eliminates the diagonal terms from the differential equations, and they are reduced to

$$f' = f_0 + P_+(x)g \qquad f_0 = V(x)\mathrm{e}^{-\mathrm{i}w(x)} \tag{47}$$

$$g' = g_0 + P_-(x)f \qquad g_0 = V(x)\exp[-2\mathrm{i}\kappa x + \mathrm{i}w(x)]. \tag{48}$$

Here

$$P_\pm(x) \equiv \pm\frac{V(x)}{2\mathrm{i}\kappa}\exp\left(\pm 2\mathrm{i}[\kappa x - w(x)]\right) \tag{49}$$

and the initial conditions are $f(-\infty) = 0 = g(-\infty)$. Note that $f(x)$ and $g(x)$ have limits as $x \to \infty$, which are α and β, up to conjugate phase shifts, provided that the potential is integrable, and $w(\infty)$ is finite. The solution to equations (47) and (48) is given by the series

$$f = \sum_{n=1}^{\infty} f_n \qquad f_1(x) = \int_{-\infty}^{x}\mathrm{d}\xi\, f_0(\xi) \qquad f_{n+1}(x) = \int_{-\infty}^{x}\mathrm{d}\xi\, P_+(\xi)g_n(\xi) \tag{50}$$

$$g = \sum_{n=1}^{\infty} g_n \qquad g_1(x) = \int_{-\infty}^{x}\mathrm{d}\xi\, g_0(\xi) \qquad g_{n+1}(x) = \int_{-\infty}^{x}\mathrm{d}\xi\, P_-(\xi)f_n(\xi). \tag{51}$$

Upper bounds for f_n and g_n for positive and integrable potentials can be obtained by iteration. From equations (50) and (51), one gets for even n,

$$f_n(x) = \int_{\Delta_n} P_+(\xi_{n-1})P_-(\xi_{n-2})\cdots P_+(\xi_1)g_0(\xi_0)\prod_{m=0}^{n-1}\mathrm{d}\xi_m$$

$$g_n(x) = \int_{\Delta_n} P_-(\xi_{n-1})P_+(\xi_{n-2})\cdots P_-(\xi_1)f_0(\xi_0)\prod_{m=0}^{n-1}\mathrm{d}\xi_m \tag{52}$$

and for odd n,

$$f_n(x) = \int_{\Delta_n} P_+(\xi_{n-1}) P_-(\xi_{n-2}) \cdots P_-(\xi_1) f_0(\xi_0) \prod_{m=0}^{n-1} \mathrm{d}\xi_m$$

$$g_n(x) = \int_{\Delta_n} P_-(\xi_{n-1}) P_+(\xi_{n-2}) \cdots P_+(\xi_1) g_0(\xi_0) \prod_{m=0}^{n-1} \mathrm{d}\xi_m. \tag{53}$$

The integrations take place in the domain $\Delta_n : -\infty < \xi_0 < \xi_1 < \cdots < \xi_{n-1} < x$. If we assume that $V(x) \geqslant 0$, $\kappa w(x)$ is a real, bounded and non-decreasing function of x. For $\mathrm{Im}\,\kappa > 0$, we shall use the following inequalities,

$$|P_+(\xi_i) P_-(\xi_j)| \leqslant \frac{V(\xi_i)}{|2\kappa|} \frac{V(\xi_j)}{|2\kappa|} \qquad \xi_i > \xi_j$$

$$|P_+(\xi_1) g_0(\xi_0)| \leqslant \frac{V(\xi_1)}{|2\kappa|} |f_0(\xi_0)|$$

$$|f_0(\xi_0)| \leqslant V(\xi_0)$$

$$|P_-(\xi)| \leqslant \frac{V(\xi)}{|2\kappa|} |\mathrm{e}^{-2\mathrm{i}\kappa\xi}| |\mathrm{e}^{2\mathrm{i}w(x)}| \qquad \xi < x. \tag{54}$$

Similarly, for $\mathrm{Im}\,\kappa < 0$,

$$|P_-(\xi_i) P_+(\xi_j)| \leqslant \frac{V(\xi_i)}{|2\kappa|} \frac{V(\xi_j)}{|2\kappa|} \qquad \xi_i > \xi_j$$

$$|P_-(\xi_1) f_0(\xi_0)| \leqslant \frac{V(\xi_1)}{|2\kappa|} |g_0(\xi_0)|$$

$$|g_0(\xi_0)| \leqslant V(\xi_0) |\mathrm{e}^{-2\mathrm{i}\kappa\xi_0}|$$

$$|P_+(\xi)| \leqslant \frac{V(\xi)}{|2\kappa|} |\mathrm{e}^{2\mathrm{i}\kappa\xi}| |\mathrm{e}^{-2\mathrm{i}w(x)}| \qquad \xi < x. \tag{55}$$

Using these inequalities one can show that, in the upper half of the complex κ-plane,

$$|f_n(x)| \leqslant |2\kappa| \frac{|w(x)|^n}{n!}$$

$$|g_n(x) \mathrm{e}^{-2\mathrm{i}w(x)}| \leqslant |2\kappa| \frac{|w(x)|^{n-1}}{(n-1)!} |u_-(x)| \tag{56}$$

while in the lower half of the complex κ-plane,

$$|f_n(x) \mathrm{e}^{2\mathrm{i}w(x)}| \leqslant |2\kappa| \frac{|w(x)|^{n-2}}{(n-2)!} |u_-(x) u_+(x)|$$

$$|g_n(x)| \leqslant |2\kappa| \frac{|w(x)|^{n-1}}{(n-1)!} |u_-(x)| \tag{57}$$

where

$$u_\pm(x) \equiv \frac{1}{2\kappa} \int_{-\infty}^{x} \mathrm{d}\xi\, V(\xi) \exp(\pm 2\mathrm{i}\kappa\xi). \tag{58}$$

It is assumed that the integrals exist for real κ and have definite limits as $x \to \infty$ (the Fourier transform of V).

For positive and integrable potentials, $f(x)$ and $g(x)$, and thus $\alpha(\kappa)$ and $\beta(\kappa)$, are given in terms of infinite series which are absolutely convergent in the domain where the corresponding Fourier transforms of $V(x)$ exist, equation (58). Thus $\alpha(\kappa)$ and $a(\kappa)$ are analytical in the upper half κ-plane. The singularities of $\alpha(\kappa)$ and $\beta(\kappa)$ appear if the integrals in equation (58) diverge as $x \to \infty$, which may be only at some values κ below the real axis, at finite distances from it.

4.3. Finite-range potentials

The functions $\alpha(\kappa)$ and $\beta(\kappa)$ are entire, if $V(x) = 0$ outside an interval (x_-, x_+). The analyticity is an immediate result of equations (56)–(58), since $u_\pm$ are finite for potentials with a finite support.

A more direct proof, as well as additional information on the analytic continuation into the complex κ-plane, can be obtained from explicit expressions for $a(\kappa)$ and $b(\kappa)$. Let us introduce two real (for real κ) solutions of the Schrödinger equation, $z_0(x)$ and $z_1(x)$, specified by the following initial conditions,

$$\begin{aligned} z_0(x_-) &= 1 \qquad z_0'(x_-) = 0 \\ z_1(x_-) &= 0 \qquad z_1'(x_-) = 1. \end{aligned} \tag{59}$$

From the continuity of the wavefunction and of its first derivative at $x = x_\pm$, one gets the following expressions for a and b,

$$\begin{aligned} a &= \frac{\exp(\mathrm{i}\kappa(x_+ - x_-))}{2\mathrm{i}\kappa}[-\zeta_0' + \mathrm{i}\kappa(\zeta_0 + \zeta_1') + \kappa^2\zeta_1] \\ b &= \frac{\exp(\mathrm{i}\kappa(x_+ + x_-))}{2\mathrm{i}\kappa}[\zeta_0' - \mathrm{i}\kappa(\zeta_0 - \zeta_1') + \kappa^2\zeta_1] \end{aligned} \tag{60}$$

where $\zeta_{0,1} \equiv z_{0,1}(x_+)$. As soon as ζ and ζ' are analytical functions of κ^2, by the Poincaré theorem [7], $\alpha(\kappa)$ and $\beta(\kappa)$ are also analytical in the whole complex κ-plane.

For large $|\kappa|$ and smooth $V(x)$, one can use the semiclassical approximation,

$$\begin{aligned} \zeta_0 &= \sqrt{\frac{p_-}{p_+}}\cos\theta \qquad \zeta_0' = -\sqrt{p_-p_+}\sin\theta \\ \zeta_1 &= \frac{1}{\sqrt{p_-p_+}}\sin\theta \qquad \zeta_1' = \sqrt{\frac{p_+}{p_-}}\cos\theta \end{aligned} \tag{61}$$

where

$$\theta(\kappa) \equiv \int_{x_-}^{x_+} \sqrt{\kappa^2 - V(x)}\,\mathrm{d}x \qquad p_\pm \equiv \sqrt{\kappa^2 - V(x_\pm)}. \tag{62}$$

In this approximation one gets

$$\begin{aligned} a &= \frac{\exp(\mathrm{i}\kappa(x_+ - x_-))}{2\mathrm{i}\kappa\sqrt{p_-p_+}}[(\kappa^2 + p_-p_+)\sin\theta + \mathrm{i}\kappa(p_- + p_+)\cos\theta] \\ b &= \frac{\exp(\mathrm{i}\kappa(x_+ + x_-))}{2\mathrm{i}\kappa\sqrt{p_-p_+}}[(\kappa^2 - p_-p_+)\sin\theta - \mathrm{i}\kappa(p_- - p_+)\cos\theta]. \end{aligned} \tag{63}$$

Note that this result is exact for the square-well barrier, equation (68), and analytical continuation to the complex plane is possible. Asymptotical locations of zeros of a in the complex κ-plane are given by the equation

$$\exp[-2\mathrm{i}\theta(\kappa)] = \frac{(\kappa - p_-)(\kappa - p_+)}{(\kappa + p_-)(\kappa + p_+)}. \tag{64}$$

Evidently, there are no zeros in the upper half-plane for $V(x) \geqslant 0$.

4.4. Exponentially decreasing potentials

If $V(x) \propto \exp(\mp 2s_\pm x)$ as $x \to \pm\infty$ ($s_\pm > 0$ are constant); $\alpha(\kappa)$ and $\beta(\kappa)$ are no longer entire functions. The singularities appear when $V(x)$ is not small enough to suppress

$\exp(\pm 2\mathrm{i}\kappa x)$, so the integral in equation (58) diverges at $\pm\infty$. The singularities nearest to the real axis appear at $\mathrm{Im}\,\kappa = -s_\pm$ for f and $\alpha(\kappa)$, and at $\mathrm{Im}\,\kappa = \pm s_\pm$ for g and $\beta(\kappa)$.

Explicit expressions for $a(\kappa)$ and $b(\kappa)$, revealing their singularities, can be obtained, assuming that

$$\begin{aligned} V(x) &= v_-^2 \exp(2s_-(x - x_-)) \qquad x < x_- \\ V(x) &= v_+^2 \exp(-2s_+(x - x_+)) \qquad x > x_+ \end{aligned} \tag{65}$$

where $v_\pm$ are constants. The solution to the Schrödinger equation for $x_- < x < x_+$ is still a linear combination of z_0 and z_1, specified by (59), while for $x < x_-$ and $x > x_+$ it is given by linear combinations of the appropriate Bessel functions. Using the matching conditions for the wavefunction at $x_\pm$, one gets

$$\begin{aligned} a = -&\frac{\exp(\mathrm{i}\kappa(x_+ - x_-))}{2\mathrm{i}\kappa}\Gamma(1+\nu_+)\Gamma(1+\nu_-)(\sigma_+/2)^{-\nu_+}(\sigma_-/2)^{-\nu_-}[\zeta_0' J_{\nu_+}(\sigma_+)J_{\nu_-}(\sigma_-) \\ &+\mathrm{i}v_+\zeta_0 J'_{\nu_+}(\sigma_+)J_{\nu_-}(\sigma_-) + \mathrm{i}v_-\zeta_1' J_{\nu_+}(\sigma_+)J'_{\nu_-}(\sigma_-) \\ &-v_+v_-\zeta_1 J'_{\nu_+}(\sigma_+)J'_{\nu_-}(\sigma_-)] \\ b = &\frac{\exp(\mathrm{i}\kappa(x_+ + x_-))}{2\mathrm{i}\kappa}\Gamma(1+\nu_+)\Gamma(1-\nu_-)(\sigma_+/2)^{-\nu_+}(\sigma_-/2)^{\nu_-}[\zeta_0' J_{\nu_+}(\sigma_+)J_{-\nu_-}(\sigma_-) \\ &+\mathrm{i}v_+\zeta_0 J'_{\nu_+}(\sigma_+)J_{-\nu_-}(\sigma_-) + \mathrm{i}v_-\zeta_1' J_{\nu_+}(\sigma_+)J'_{-\nu_-}(\sigma_-) \\ &-v_+v_-\zeta_1 J'_{\nu_+}(\sigma_+)J'_{-\nu_-}(\sigma_-)] \end{aligned} \tag{66}$$

where $\nu_\pm = -\mathrm{i}\kappa/s_\pm$ and $\sigma_\pm = \mathrm{i}v_\pm/s_\pm$. The singularities are the poles of the Γ functions, as soon as $(\sigma/2)^{-\nu}J_\nu(\sigma)$ is known [20] to be an entire function in both σ and ν, while ζ and ζ' are analytical functions of κ^2, by the Poincaré theorem. Thus, both $a(\kappa)$ and $b(\kappa)$ have infinite series of equidistant poles on the imaginary axis: at $\kappa = -\mathrm{i}ns_\pm$ for $a(\kappa)$ (the poles are double if $s_- = s_+$), and at $\kappa = \mp\mathrm{i}ns_\pm$ for $b(\kappa)$ (where n is any positive integer).

The minimal distance of the singularities from the real κ-axis, which was derived from the integral equations, is non-zero for every potential with an asymptotic exponential decline. The results of equation (66) are less general. If the assumption of equation (65) is relaxed, the poles can move off the imaginary axis, as one can see in equation (72) below.

4.5. Singularities of the S-matrix

The singularities of the T- and S-matrices are of physical importance, when the time-dependent process is considered. They are given by zeros of $a(\kappa)$ as well as by the poles of $b(\kappa)$, which do not coincide with those of $a(\kappa)$.

As was proven in section 4.2, for positive and integrable potentials, $a(\kappa)$ is analytical in the upper half κ-plane, which is a result of causality; $\beta(\kappa)$, and thus $b(\kappa)$, may have singularities at finite distances above and below the real κ-axis.

The pattern of singularities of $a(\kappa)$ and $b(\kappa)$ in the complex κ-plane is determined by the asymptotic decline of the potential. For potentials having an asymptotic decline faster than exponential (e.g. finite-range potentials, and the Gaussian barrier), no singularities appear for finite κ. For potentials with exponential asymptotics, the distance from the real κ-axis to the nearest singularities is determined by the slope of the potential at $\pm\infty$.

It is important that $a(\kappa)$ has no zeros in the upper half-plane. As soon as the function is analytical, the number of its zeros is given by the integral

$$N = \frac{1}{2\pi\mathrm{i}}\oint_C \frac{\mathrm{d}a}{a} \tag{67}$$

where the contour C encloses the upper half of the complex plane. For positive and integrable potentials $\alpha(\kappa)$ is limited in the upper half-plane, so $a(\kappa) \to 1$ as $\kappa \to \infty$, and the integral is zero.

The location of zeros of $a(\kappa)$ in the lower half of the complex κ-plane depends on the specific barrier considered. For finite-range potentials the asymptotic distribution of zeros is given by equation (64). Other examples are considered in the appendix.

5. Conclusion

We have considered the one-dimensional problem, assuming that the potential is non-negative everywhere. The barrier transmission and reflection amplitudes are described in terms of two analytical functions $\alpha(\kappa)$ and $\beta(\kappa)$, equations (29)–(31). Both the functions are entire if the potential vanishes outside a finite interval on the x-axis. For potentials decreasing exponentially, singularities appear at finite distances to the real axis, corresponding to the decrease rates at $\pm\infty$. For $\alpha(\kappa)$, all the singularities are in the lower half-plane, while for $\beta(\kappa)$, the front slope controls the singularities in the upper half-plane, and the back slope controls those in the lower half. Poles of the S-matrix are given by zeros of $a(\kappa) \equiv 1 - \alpha/2\mathrm{i}\kappa$. It is proven that for any non-negative potential they are all in the lower half-plane.

The causality in the transmission and reflection processes manifests itself in the analytical properties of the transition amplitudes. These properties have been employed for the spacetime description of the tunnelling through a potential barrier in the Wigner phase-space representation [21].

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Appendix. Examples

A number of examples may be found in standard textbooks, e.g. [22].

(i) *Square barrier*: $V(x) = V_0$ for $|x| < x_0$, $V(x) = 0$ for $|x| > x_0$.

$$a(\kappa) = \frac{1}{4\kappa p}[(\kappa+p)^2\exp(2\mathrm{i}(\kappa-p)x_0) - (\kappa-p)^2\exp(2\mathrm{i}(\kappa+p)x_0)]$$

$$\beta = V_0\frac{\sin 2x_0 p}{p} \tag{68}$$

where $p = \sqrt{\kappa^2 - V_0}$. One can see that these functions depend, actually, on p^2, so there is no cut in the κ-plane. Zeros of a are given by (complex) solutions of the equation

$$\exp(-4\mathrm{i}px_0) = \left(\frac{\kappa-p}{\kappa+p}\right)^2. \tag{69}$$

This equation has no roots for $\mathrm{Im}\,\kappa > 0$. If V_0 is small enough, there are two roots on the imaginary κ-axis. Other roots appear in pairs, and their asymptotical position is given by

$$\mathrm{Re}\,p = \pm\frac{\pi}{2x_0}n \qquad \mathrm{Im}\,p = -\frac{1}{x_0}\log\frac{2\mathrm{Re}\,p}{V_0} \tag{70}$$

where $n \gg 1$ is an integer.

(ii) *Exponential barrier*: $V(x) = V_0 \exp(-|x/x_0|)$,

$$a = -\frac{[\Gamma(1+\nu)]^2}{x_0\kappa}\left(\frac{z}{2\mathrm{i}}\right)^{1-4\nu} J'_\nu(z)J_\nu(z)$$
$$b = \frac{2\pi\sqrt{V_0}}{\sinh 2\pi\kappa}[J'_\nu(z)J_{-\nu}(z) + J_\nu(z)J'_{-\nu}(z)] \tag{71}$$

where $J_\nu(z)$ is the Bessel function, $\nu = -2\mathrm{i}\kappa$, and $z = 2\mathrm{i}x_0\sqrt{V_0}$.

(iii) *The Pöschl–Teller barrier:* $V(x) = V_0/\cosh^2(x/x_0)$.

$$a = \mathrm{i}\frac{\Gamma^2(1-\mathrm{i}\kappa x_0)}{\kappa x_0\Gamma(\frac{1}{2}+\mathrm{i}\sigma-\mathrm{i}\kappa x_0)\Gamma(\frac{1}{2}-\mathrm{i}\sigma-\mathrm{i}\kappa x_0)} \qquad b = -\mathrm{i}\frac{\cosh\pi\sigma}{\sinh\pi\kappa x_0} \tag{72}$$

where $\sigma = \sqrt{V_0x_0^2 - \frac{1}{4}}$. The function $a(\kappa)$ has zeros at $\kappa x_0 = -\mathrm{i}(n+\frac{1}{2}) \pm \sigma$, and (double) poles at $\kappa x_0 = -\mathrm{i}(n+1)$, while β has (simple) poles at $\kappa x_0 = \pm \mathrm{i}n$, $n = 1, 2, \ldots$. (Note that σ is imaginary for $2x_0 < V_0^{-1/2}$.)

(iv) *Narrow barrier*: $V(x) = v_0\delta(x)$. This is the limit one gets as $V_0 \to \infty$, $x_0 \to 0$, $2x_0V_0 = v_0$, from the three preceding cases. Now both the entire functions are just constant,

$$\alpha = \beta = v_0 \tag{73}$$

and $a(\kappa)$ has one zero at $\kappa = -\mathrm{i}v_0/2$.

(v) *A double barrier*: $V(x) = V_1(x-d_1) + V_2(x-d_2)$. The case of two non-overlapping barriers is described by equation (35); α and β remain entire functions. As is well known, new zeros may appear in $a(\kappa)$ close to the real axis, corresponding to metastable states of the particle trapped between the barriers. A special case is that of a symmetrical double barrier, where $a_1 = a_2 \equiv \cosh\rho\,\mathrm{e}^{-\mathrm{i}\delta}$ and $b_1 = -\bar{b}_2 \equiv \sinh\rho\,\mathrm{e}^{\mathrm{i}\gamma}$. Now

$$a = \cosh^2\rho\,\mathrm{e}^{-2\mathrm{i}\delta} + \sinh^2\rho\,\mathrm{e}^{2\mathrm{i}\kappa d}$$
$$b = \mathrm{i}\sinh 2\rho\cos(\kappa d + \delta + \gamma) \tag{74}$$

where d is the distance between the barrier centres. It is easy to see that the reflection may vanish at certain resonance values of the energy, independently of the reflection from a single barrier.

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