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On the quantum mechanical scattering from a potential step

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Abstract

The problem of finding the exact spacetime particle's propagator in the presence of a potential step (interface between different materials) is revisited. In contrast to the conventional Feynman path-integral approach, integration over all energy values of the particle's spectral density matrix (discontinuity of the energy-dependent Green's function across the real energy axis) is suggested for obtaining the exact spacetime propagator. The energy-dependent Green's functions are found in the framework of the multiple scattering theory (MST). The problem of finding the step-localized energy-dependent potentials responsible for the particle's reflection from and transmission through a potential step, which are needed for MST application, is solved. The obtained exact result for the particle's propagator is expressed in terms of integrals of elementary functions and has a significantly simpler form than that reported earlier. The obtained expressions allow easy evaluation of all limiting cases, including the case of the infinitely large potential step, as well as simple numerical visualization. The square of the absolute value of the propagator, which represents the relative transition probability density between two spacetime points, is plotted and discussed in detail for the cases of particle reflection and transmission.

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(Some figures in this article are in colour only in the electronic version)

One of the key differences between the classical and quantum mechanics is that there always exists a nonzero probability of reflection of a quantum particle at a potential landscape inhomogeneity at any value of the particle's total energy as well as a probability of the particle's penetration into a classically forbidden region of energy. These effects stem from the wave properties of a particle which reveal themselves when the de Broglie wavelength is large compared to the range of the potential energy inhomogeneity and are not surprising from the conventional wave theory point of view. From the particle propagation point of view, the partial reflection from and transmission through a potential inhomogeneity may be explained by the quantum mechanical rules of computing the probabilities of different events. These

rules represent the quantum mechanical generalization of the Huygens–Fresnel principle and were introduced by Feynman as the path-integral formalism [1].

It states that a wavefunction of a single particle moving in a perturbing potential $V(\mathbf{r}, t)$ may be presented as

$$\Psi(\mathbf{r}, t) = \int \mathrm{d}\mathbf{r}' K(\mathbf{r}, t; \mathbf{r}', t_0)\Psi(\mathbf{r}', t_0). \tag{1}$$

Equation (1) shows (in accordance with the Huygens–Fresnel principle) that the wavefunction $\Psi(\mathbf{r}, t)$ at the spacetime point $(\mathbf{r}, t)$ is the sum of contributions of all points of space where the wavefunction $\Psi(\mathbf{r}', t_0)$ at $t = t_0$ is nonzero. The propagator $K(\mathbf{r}, t; \mathbf{r}', t_0)$ is the probability amplitude for the particle's transition from the initial spacetime point $(\mathbf{r}', t_0)$ to the final point $(\mathbf{r}, t)$ by means of all possible paths. It provides the information for the full particle's dynamics and resolves the corresponding time-dependent Schrödinger equation.

Thus, the problem is to find the propagator $K(\mathbf{r}, t; \mathbf{r}', t_0)$ for the given potential $V(\mathbf{r}, t)$. In some cases, for example, when the potential is quadratic in the space variable, the kernel $K(\mathbf{r}, t; \mathbf{r}', t_0)$ may be calculated exactly. In the case when the potential changes smoothly enough, the quasi-classical approximation can be employed. The list of exact solutions for the propagator $K(\mathbf{r}, t; \mathbf{r}', t_0)$ is, however, very short.

The time-independent one-dimensional step potential

$$V(x) = U\theta(x), \tag{2}$$

where $\theta(x)$ is the Heaviside step function, does not fall into any of the above-mentioned categories. On the other hand, this rather academic one-dimensional problem of quantum mechanical scattering of a particle from a potential step has acquired reality and important practical implementation in the newly emerged field of nanoscience and nanotechnology. Such potential approximates, e.g. the potential step at the perfect interfaces of layered nanostructures made of alternating magnetic and nonmagnetic layers, have been attracting a good deal of interest especially since the discovery of the giant magnetoresistance (GMR) [2] and tunneling magnetoresistance (TMR) [3, 4] effects. These effects, which stem, particularly, from the quantum mechanical scattering from a potential well and transmission through a potential barrier, have led to very important commercial applications. Thus, understanding of the particle (electron) full spacetime dynamics in the presence of the step-type potential (2) becomes important not only from the scientific point of view.

The problem of finding even one-dimensional spacetime propagator $K(x, t; x', t_0)$ in the presence of the potential (2) has turned out rather difficult to solve in contrast to the textbook problem of solution to the corresponding time-independent Schrödinger equation. The former has been resolved in [5] by the path decomposition expansion method (see also the recent paper [6]). The exact formula for this propagator is very complicated, expressed in terms of integrals of special functions and is not easily tractable. More simple is the case with the δ-function barrier potential

$$V(x) = a\delta(x), \tag{3}$$

for which the propagator was found in [7]. However, even in this case the propagator is not expressible in terms of elementary functions.

In this paper we suggest a rather simple and more physically appealing method of computing the propagator for potentials (2) and (3). The idea is to first find the energy-dependent Green's function and then to obtain the spacetime propagator by integrating the discontinuity of this Green's function across the real energy axis (the spectral density matrix) over all possible particle energies. In contrast to the path-integral formalism, where the time slicing of each spacetime particle's trajectory leads to the functional integration over

all possible trajectories, the suggested approach may be viewed as the energy-sliced one. The problem will be considered in the three-dimensional case but with the step potential (2) changing in one direction, which may model the potential profile in the layered nanostructures with perfect interfaces. In this case, finding the energy-dependent Green's function reduces to the one-dimensional energy- and $\mathbf{k}_\parallel$-resolved problem ($\mathbf{k}_\parallel$ is the parallel-to-interface component of the particle wave vector $\mathbf{k}$). We will show that the reflection from and transmission through the potential step (2) can be calculated in the framework of the multiple scattering theory (MST) with the energy- and $\mathbf{k}_\parallel$-dependent δ-function potentials localized at the interface. The obtained δ-like potentials describing the quantum scattering from a potential step provide a clear picture of the particle's scattering taking place at the interface located at $x = 0$, and make it convenient to calculate the energy-dependent Green's function and the spacetime propagator especially when scattering from more than one interface which needs to be accounted for and other sources of scattering mix the particle's states with different $\mathbf{k}_\parallel$ (i.e. when $\mathbf{k}_\parallel$ is no longer conserved). Such a situation is typical for real multilayers with disordered interfaces [8–10] and for the Casimir effect [11]. The exact spacetime propagator obtained in this paper for a particle in the presence of the step potential (2) is expressed in a substantially more simple form (of the integrals of elementary functions) compared to those in the cited papers and allows for its relatively simple analysis and numerical modeling. Particularly, an analytical solution for the infinitely high step ($U \to \infty$) is obtained. The corresponding transition probabilities between two spacetime points for various regions divided by the interface at $x = 0$ are pictured by numerical calculations and discussed in detail.

The time-dependent retarded propagator $K(t; t') = \theta(t - t') \exp\left[-\frac{\mathrm{i}}{\hbar} H(t - t')\right]$ will be calculated with use of the following definition:

$$K(t; t') = \theta(t - t') \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E(t-t')} [G(E + \mathrm{i}\varepsilon) - G(E - \mathrm{i}\varepsilon)] \, \mathrm{d}E, \qquad \varepsilon \to +0, \tag{4}$$

where

$$G(E) = \frac{1}{E - H} \tag{5}$$

is the resolvent operator, E stands for the energy and H is the Hamiltonian of the system under consideration. Correspondingly, $G(E \pm \mathrm{i}\varepsilon) = G^{\pm}(E)$ defines the retarded (G^+) or the advanced (G^-) Green's function. The E-resolving Fourier transformation (4) is useful for the calculation of the propagator $K(t; t')$ when the Green's functions $G^{\pm}(E)$ may be found for each value of E, i.e. when the considered processes are energy-conserved as is the case considered in this paper.

We are generally looking for the spacetime propagator $K(\mathbf{r}, t; \mathbf{r}', 0) = \langle \mathbf{r} | K(t; 0) | \mathbf{r}' \rangle$ defining the probability amplitude for a particle transition from the initial point $(\mathbf{r}', 0)$ to the final destination $(\mathbf{r}, t)$ in the presence of the step potential (2). As a model of the three-dimensional system with the potential (2), we will consider two semi-infinite layers of different homogeneous materials divided by an interface located at the $x = 0$ plane with the potential energy $V(x) = 0$ for $x < 0$ and $V(x) = U > 0$ for $x > 0$. For such a geometry, it is convenient to present the r-representation of the resolvent operator $G_0(\mathbf{r}, \mathbf{r}'; E) = \langle \mathbf{r} | \frac{1}{E - H_0} | \mathbf{r}' \rangle$ corresponding to the free particle described by the Hamiltonian $H_0 = -\frac{\hbar^2}{2m} \nabla^2$ and the Green's function with the Hamiltonian H, $G(\mathbf{r}, \mathbf{r}'; E) = \langle \mathbf{r} | \frac{1}{E - H} | \mathbf{r}' \rangle$, as follows:

$$\begin{aligned} G_0(\mathbf{r}, \mathbf{r}'; E) &= \frac{1}{A} \sum_{\mathbf{k}_\parallel} \mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel (\rho - \rho')} G_0(x, x'; E; \mathbf{k}_\parallel), \\ G(\mathbf{r}, \mathbf{r}'; E) &= \frac{1}{A} \sum_{\mathbf{k}_\parallel \mathbf{k}'_\parallel} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel \rho - \mathbf{k}'_\parallel \rho')} G(x, x'; E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel), \end{aligned} \tag{6}$$

where $\rho = (y, z)$ is a two-dimensional parallel-to-interface vector and A is the area of the interface. The Green's function given by the second line of (6) accounts for the possible nonconserving of $\mathbf{k}_\parallel$ in the case of an imperfect interface. Thus, the problem is reduced to finding the one-dimensional Green's function dependent on the angle of the particle motion relative to the interface defined by vectors $\mathbf{k}_\parallel$ and $\mathbf{k}'_\parallel$. The one-dimensional retarded Green's function $G_0(x, x'; E; \mathbf{k}_\parallel)$ corresponding to the free particle is (see e.g. [12])

$$\begin{aligned} G^+_{0>}(x, x'; E; \mathbf{k}_\parallel) &= \frac{1}{\mathrm{i}\hbar v^\perp_>(E, \mathbf{k}_\parallel)} \exp\left[\mathrm{i}k^\perp_>(E, \mathbf{k}_\parallel)|x - x'|\right], \qquad x > 0, \quad x' > 0 \\ G^+_{0<}(x, x'; E; \mathbf{k}_\parallel) &= \frac{1}{\mathrm{i}\hbar v^\perp_<(E, \mathbf{k}_\parallel)} \exp\left[\mathrm{i}k^\perp_<(E, \mathbf{k}_\parallel)|x - x'|\right], \qquad x < 0, \quad x' < 0, \end{aligned} \tag{7}$$

where according to (2), perpendicular to the interface velocity and wave vector are

$$\begin{aligned} &v^\perp_{>(<)}(E, \mathbf{k}_\parallel) = \hbar k^\perp_{>(<)}(E, \mathbf{k}_\parallel)/m, \\ &k^\perp_>(E, \mathbf{k}_\parallel) = \sqrt{\frac{2m}{\hbar^2}(E - U) - \mathbf{k}^2_\parallel}, k^\perp_<(E, \mathbf{k}_\parallel) = \sqrt{\frac{2m}{\hbar^2}E - \mathbf{k}^2_\parallel}. \end{aligned} \tag{8}$$

When $U = 0$, the Green's functions (7) are defined in the entire domain of x, x' with $k^\perp(E, \mathbf{k}_\parallel) = k^\perp_>(E, \mathbf{k}_\parallel) = k^\perp_<(E, \mathbf{k}_\parallel)$.

To compare the results with the known one-dimensional ones and to make the presentation of suggested approach more clear, we will first consider a strictly one-dimensional problem with the potential (2) which can then be easily generalized to the introduced model three-dimensional system by accounting for different possible $\mathbf{k}_\parallel$ as it follows from (6)–(8). Thus, we will first calculate $K(x, t; x', 0) = \langle x|K(t; 0)|x'\rangle$ which is determined by the Green's function $G(x,x'; E) = \langle x|\frac{1}{E-H}|x'\rangle$ according to (4) and (5). The 'free' Green's function $G^+_0(x,x'; E) = \langle x|\frac{1}{E-H_0}|x'\rangle$ with $H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is then given by equations (7) and (8) with $\mathbf{k}_\parallel = 0$.

If the Hamiltonian can be presented as $H = H_0 + H_i$, where

$$H_i(x) = H_i\delta(x) \tag{9}$$

describes the localized (at the interface point $x = 0$) perturbation of the 'free' motion given by H_0, it is convenient to expand the Green's function $G(x, x'; E)$ in the MST perturbation series

$$G(x, x'; E) = [\theta(x)\theta(x') + \theta(-x)\theta(-x')]G_0(x, x'; E) + G_0(x, 0; E)T(E)G_0(0, x'; E), \tag{10}$$

where we have taken into consideration that the first 'free' motion term is absent when x and x' are defined at different sides of $x = 0$ (i.e. the first term is not zero for the reflection process but vanishes for the transmission process). Here, the scattering (from the interface) t-matrix is defined as

$$T(E) = H_i + H_iG_0(0, 0; E)H_i + \cdots, \tag{11}$$

where H_i in (9) and the interface Green's function $G_0(0, 0; E)$ (7) can be defined differently for reflection and transmission processes (see below).

Note that the scattering from the interface is an energy (E)-conserved process, and in the E-resolved multiple-scattering processes, given by expansion (11), H_i may depend on E (i.e. $H_i = H_i(E)$). Thus, we envision that the quantum mechanical reflection from and transmission through a perfect potential step (2) may be described by the E-dependent δ-function potential, i.e. for each E

$$H_{i>(<)}(x, E) = H_{i>(<)}(E)\delta(x), \qquad H_{i><}(x, E) = H_{i><}(E)\delta(x), \tag{12}$$

where $H_{i>(<)}(E)$ is the reflection potential amplitude, index $>$ or $<$ indicates its possible dependence on the side of the particle's incidence with respect to the interface: right ($>$) or left ($<$), and $H_{i><}(E)$ is the transmission potential amplitude. Thus, the problem is to find $H_{i>(<)}(E)$ and $H_{i><}(E)$ corresponding to the quantum mechanical reflection from and transmission through the potential step (2).

The perturbation series (11) in the case of potential (12) is easily exactly summed up yielding

$$T_{>(<)}(E) = \frac{H_{i>(<)}(E)}{1 - G_{0>(<)}(E)H_{i>(<)}(E)}, \qquad T_{><}(E) = \frac{H_{i><}(E)}{1 - G_{0><}(E)H_{i><}(E)}, \tag{13}$$

where the retarded Green's functions at the interface for considered reflection and transmission processes are defined as

$$\begin{aligned} &G^{+}_{0>(<)}(E) = G^{+}_{0>(<)}(0,0;E) = 1/\mathrm{i}\hbar v^{\perp}_{>(<)}(E) \\ &G^{+}_{0><}(0,0;E) = G^{+}_{0><}(E) = \left[G^{+}_{0>}(E)G^{+}_{0<}(E)\right]^{1/2} = 1/\mathrm{i}\hbar\sqrt{v^{\perp}_{>}(E)v^{\perp}_{<}(E)} \end{aligned} \tag{14}$$

in accordance with (7) and $v^{\perp}_{>(<)}(E)$ is defined by (8) with $\mathbf{k}_{\parallel} = 0$.

Let us define the energy-dependent amplitude of the potential (12) responsible for the quantum mechanical reflection from, $H_{i>(<)}(E)$, and transmission through, $H_{i><}(E)$, the potential step (2) as follows:

$$\begin{aligned} H_{i>}(E) &= \frac{\mathrm{i}\hbar}{2}\left[v^{\perp}_{>}(E) - v^{\perp}_{<}(E)\right], \\ H_{i<}(E) &= \frac{\mathrm{i}\hbar}{2}\left[v^{\perp}_{<}(E) - v^{\perp}_{>}(E)\right], \\ H_{i><}(E) &= \frac{2\mathrm{i}\hbar v^{\perp}_{>}(E)v^{\perp}_{<}(E)}{\left[\sqrt{v^{\perp}_{>}(E)} + \sqrt{v^{\perp}_{<}(E)}\right]^2}, \end{aligned} \tag{15}$$

where $H_{i>(<)}(E)$ corresponds to the particle incoming to the interface from the right (left). This potential is a Hermitian one in the sense that it does not lead to any dissipation: the Schrödinger equation with the potential defined by (12), (15) is invariant under the transformation $t \to -t$ $\left(v^{\perp}_{>(<)} \to -v^{\perp}_{>(<)}\right), i \to -i$ and, therefore, describes a reversible process.

From (14) and (15) we have for the reflection $T^{+}_{>(<)}(E)$ and transmission $T^{+}_{><}(E)$ the t-matrix (13) corresponding to the retarded Green's function

$$T^{+}_{>(<)}(E) = \mathrm{i}\hbar v^{\perp}_{>(<)}r_{>(<)}, \qquad T^{+}_{><}(E) = \mathrm{i}\hbar\sqrt{v^{\perp}_{>}v^{\perp}_{<}}t, \tag{16}$$

where $r_{>(<)}(E)$ and $t(E)$ are the standard reflection to the right (left) of the interface and transmission amplitudes

$$\begin{aligned} r_{>}(E) &= \frac{k^{\perp}_{>} - k^{\perp}_{<}}{k^{\perp}_{>} + k^{\perp}_{<}}, \qquad r_{<}(E) = \frac{k^{\perp}_{<} - k^{\perp}_{>}}{k^{\perp}_{>} + k^{\perp}_{<}}, \\ t(E) &= \frac{2\sqrt{k^{\perp}_{>}k^{\perp}_{<}}}{k^{\perp}_{>} + k^{\perp}_{<}}, \end{aligned} \tag{17}$$

and the argument E is omitted in $v^{\perp}_{>(<)}$, $k^{\perp}_{>(<)}$ for brevity. Substituting (7) and (16) into (10), we obtain the Green's function in the presence of the step potential (2) as follows:

$$
\begin{aligned}
G^{+}(x,x';E) &= \frac{1}{\mathrm{i}\hbar v_{<}^{\perp}}[\mathrm{e}^{\mathrm{i}k_{<}^{\perp}|x-x'|} + r_{<}\,\mathrm{e}^{-\mathrm{i}k_{<}^{\perp}(x+x')}], \qquad x<0, \quad x'<0\\
G^{+}(x,x';E) &= \frac{1}{\mathrm{i}\hbar v_{>}^{\perp}}[\mathrm{e}^{\mathrm{i}k_{>}^{\perp}|x-x'|} + r_{>}\,\mathrm{e}^{\mathrm{i}k_{>}^{\perp}(x+x')}], \qquad x>0, \quad x'>0,\\
G^{+}(x,x';E) &= \frac{1}{\mathrm{i}\hbar\sqrt{v_{>}^{\perp}v_{<}^{\perp}}}\,\mathrm{e}^{-\mathrm{i}k_{<}^{\perp}x}\,t\,\mathrm{e}^{\mathrm{i}k_{>}^{\perp}x'}, \qquad x<0, \quad x'>0,\\
G^{+}(x,x';E) &= \frac{1}{\mathrm{i}\hbar\sqrt{v_{>}^{\perp}v_{<}^{\perp}}}\,\mathrm{e}^{\mathrm{i}k_{>}^{\perp}x}\,t\,\mathrm{e}^{-\mathrm{i}k_{<}^{\perp}x'}, \qquad x>0, \quad x'<0.
\end{aligned}
\tag{18}
$$

The result (18) was obtained in [8, 9] by the conventional matching procedure. When $k_{>}^{\perp} = k_{<}^{\perp} = k^{\perp}$ and, therefore, $r_{>(<)} = 0$, $t(E) = 1$, equations (18) reduce to the 'free' propagator.

It is rather interesting that the quantum mechanical reflection from and transmission through the potential step (2) may be described by the scattering potentials, given by (12) and (15), which are localized at the interface. The obtained potentials also provide a clear physical picture of the particle reflection and transmission as a multiple scattering by these potentials as well as a useful and simple mathematical tool for the calculation of the particle propagator in the framework of the perturbation expansion (11), especially when several (generally disordered) interfaces should be taken into consideration (see [10]).

To obtain the propagator $K(x,t;x',0)$, we also need the advanced Green's function, which is connected to the retarded one by the following relation (see e.g. [12]):

$$
G^{-}(x,x';E) = [G^{+}(x',x;E)]^{*}. \tag{19}
$$

Noting that the Green's functions (18) are symmetric with regard to permutation $x \leftrightarrows x'$, we take that the retarded and advanced Green's functions are related as

$$
G^{-}(x,x';E) = [G^{+}(x,x';E)]^{*}. \tag{20}
$$

In equation (4) the energy integration includes the states with $E < 0$ which, however, should not contribute to the propagator because these states are forbidden at the selected origin of energy $E = 0$ (see (2) and (8), where $U \geqslant 0$). One can check, with the help of (17), (18) and (20), that this is actually the case, because for such states both $k_{>}^{\perp}(v_{>}^{\perp})$ and $k_{<}^{\perp}(v_{<}^{\perp})$ are imaginary and both terms in (4) cancel each other at $E < 0$. Thus, the integration in (4) may be performed in the energy range $[0, +\infty]$. To secure the convergence of the integral over E in (4), it is useful to switch to the imaginary time $t \to -\mathrm{i}t$ and then switch back to the real time in the result.

Integration of the Green's function (7) (with $\mathbf{k}_{\parallel} = 0$ for the considered one-dimensional case) over E according to (4) with account for (20) yields the following known result for the 'free' propagator, i.e. the propagator corresponding to the incoming particles from the left and right (see [13]):

$$
\begin{aligned}
K_0(x,t;x',0) &= \theta(t)\left(\frac{m}{2\pi\mathrm{i}\hbar t}\right)^{1/2}\exp\left[\frac{\mathrm{i}m(x-x')^2}{2\hbar t}\right], \qquad x<0, \qquad x'<0\\
K_0(x,t;x',0) &= \theta(t)\left(\frac{m}{2\pi\mathrm{i}\hbar t}\right)^{1/2}\exp\left[\frac{\mathrm{i}m(x-x')^2}{2\hbar t}\right]\exp\left(-\frac{\mathrm{i}}{h}Ut\right), \qquad x>0, \quad x'>0.
\end{aligned}
\tag{21}
$$

Contribution of reflection from the step potential to this propagator $\Delta_r K(x,t;x',0)$ can be found in the same way using the second right-hand-side terms of equation (18) first two lines. The result of integration over E is for $x<0, x'<0$

$$\Delta_r K(x,t;x',0) = \theta(t)\left(\frac{m}{2}\right)^{1/2}\frac{1}{\pi\hbar}\frac{1}{U} \times\left\{\int_0^\infty \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\times\cos\left[\frac{\sqrt{2mE}(x+x')}{\hbar}\right]\left(2\sqrt{E}-\frac{U}{\sqrt{E}}\right)\mathrm{d}E -2\int_U^\infty \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\times\cos\left[\frac{\sqrt{2mE}(x+x')}{\hbar}\right]\sqrt{E-U}\,\mathrm{d}E -2\int_0^U \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\sin\left[\frac{\sqrt{2mE}(x+x')}{\hbar}\right]\sqrt{U-E}\,\mathrm{d}E\right\}, \quad x<0, \quad x'<0. \tag{22}$$

For $x>0, x'>0$, the result reads

$$\Delta_r K(x,t;x',0) = \theta(t)\left(\frac{m}{2}\right)^{1/2}\frac{1}{\pi\hbar}\frac{1}{U} \times\left\{2\int_0^U \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\exp\left[-\frac{\sqrt{2m(U-E)}(x+x')}{\hbar}\right]\sqrt{E}\,\mathrm{d}E+\int_U^\infty \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\cos \times\left[\frac{\sqrt{2m(E-U)}(x+x')}{\hbar}\right]\left(2\sqrt{E}-\sqrt{E-U}-\frac{E}{\sqrt{E-U}}\right)\mathrm{d}E\right\}. \tag{23}$$

The propagator $K_t(x,t;x',0)$ corresponding to the transition through the interface with a potential step (2) is calculated in a similar manner using (4) and the third and fourth lines of (18). The result is

$$K_t(x,t;x',0) = \theta(t)\frac{(2m)^{1/2}}{\pi\hbar}\frac{1}{U} \times\left\{\int_0^U \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\exp\left[-\frac{\sqrt{2m(U-E)}x'}{\hbar}\right] \times\left[\cos\left(\frac{\sqrt{2mE}x}{\hbar}\right)\sqrt{E}-\sin\left(\frac{\sqrt{2mE}x}{\hbar}\right)\sqrt{U-E}\right]\mathrm{d}E +\int_U^\infty \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\cos\left[\frac{\sqrt{2m}}{\hbar}(\sqrt{E}x-\sqrt{E-U}x')\right](\sqrt{E}-\sqrt{E-U})\,\mathrm{d}E\right\}, \quad x<0, \quad x'>0. \tag{24}$$

For $x>0, x'<0$, the space variables x, x' in (24) should be interchanged ($x \rightleftarrows x'$).

Prior to numerical evaluation of the integrals in (22), (23) and (24), it is instructive to check these results in some limiting cases. First of all, it can be verified that $\Delta_r K(x,t;x',0)=0$ and $K_t(x,t;x',0)=K_0(x,t;x',0)$ when $U=0$. However, it is interesting to note that there is no expansion in small U: the coefficients of expansion of (22), (23) and (24) become divergent in the second order in U, but at $U=0$ all terms of expansion containing U vanish.

In the opposite limiting case $U\to\infty$ (this case is conveniently checked by taking the substitution $t\to -\mathrm{i}t$), $K_t^\infty(x,t;x',0)=0$, $K^\infty(x,t;x',0)=K_0^\infty(x,t;x',0)+\Delta_r^\infty K(x,t;x',0)=0$ at $x>0, x'>0$ and

$$K^\infty(x,t;x',0) = K_0(x,t;x',0)+\Delta_r^\infty K(x,t;x',0) = \theta(t)\left(\frac{m}{2\pi\mathrm{i}\hbar t}\right)^{1/2}\left\{\exp\left[\frac{\mathrm{i}m(x-x')^2}{2\hbar t}\right]-\exp\left[\frac{\mathrm{i}m(x+x')^2}{2\hbar t}\right]\right\}, \quad x<0, \quad x'<0. \tag{25}$$

It is seen that propagator (25) vanishes either at $x = 0$ or at $x' = 0$. This is because the incoming wave is cancelled by the reflecting wave when their phase difference is equal to π and this happens at $|x - x'| = x + x'$, i.e. at the interface. Thus, the incoming particle cannot reach the interface with $U = \infty$. It is also interesting to consider how the probability amplitude (25) vanishes when a particle approaches the interface starting from some point (x'). The dependence of (25) on x at $x \to 0$ is linear ($\sim x$). Thus, the derivative of propagator (25) on x is not continuous at the interface (although the propagator itself is continuous). This fact is natural when the potential leap (2) at the interface is infinite. It is worth noting that in this case one cannot use the standard matching procedure for finding the Green's (wave)functions (18). In this case the reflection and transmission potentials (12), (15) allow for finding these Green's functions in the framework of MST as it has been demonstrated above.

For consistency reason, it is also needed to obtain the propagator along the interface $K(0, t; 0, 0)$, i.e. $K(x, t; x', 0)$ at $x = x' = 0$. From equations (21)–(24), we have the known result for the partial propagator

$$K(0, t; 0, 0) = \theta(t) \left(\frac{m\hbar}{2\pi}\right)^{1/2} \frac{1}{(it)^{3/2}} \frac{1}{U} (1 - \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} Ut}), \tag{26}$$

which is the important ingredient of the path decomposition expansion method [5, 6]. This result demonstrates the continuity of the propagator at $x = 0$.

It is important that the propagator given by (21)–(24) is expressed in terms of the integrals (some of which can be calculated analytically) of elementary functions. This allows a relatively simple visualization of the results using numerical calculations. We calculate and plot the square of the absolute value of the propagator, $|K(x, t; x', 0)|^2$, which defines the relative probability density of finding the particle at the (x, t) spacetime point if it starts at (x', t') point. On the other hand, $|K(x, t; x', 0)|^2 \, \mathrm{d}x$ may be interpreted as the density of particles at the point $(x.t)$ emitted by the source at x' and at $t = 0$.

In figure 1, we present as a reference the well-known result for $|K_0(x, t; x', 0)|^2$, i.e. for the 'free' particle (see e.g. [1]). For this case the relative probability density to find the particle at the point (x, t) is space-homogeneous and decreases with time as $1/t$. Figure 2 presents $|K(x, t; x', 0)|^2$ for a potential step height $U = 1$ eV and $x < 0$, $x' < 0$, i.e. for the case when the electronic waves incoming to and reflected from the potential step (interface) at $x = 0$ interfere in the left semispace. One can see that the relative probability density changes radically compared to the free motion case. As a result of the interference of the incident and reflected waves, this quantity remains substantial only in a specific time interval depending on the initial point x' and the destination point x. The closer either x or x' is to the potential step ($x = 0$) the shorter time is needed for the constructive interference to occur to form the peak of $|K(x, t; x', 0)|^2$. The amplitude of $|K(x, t; x', 0)|^2$ peak increases toward the potential step at $x = 0$ where the conditions for interference of the incoming wave with $|x - x'|$ spatial dependence and the reflected one with $x + x'$ spatial argument are most favorable. The relative probability density of the particle transmission from the left semispace to the right one for the same values of x' and U as those used for plotting figure 2 is shown in figure 3. Similarly to the case of reflection, a substantial transmission through the potential step takes place in the time interval where the probability to reach the interface is large while, as expected, this period of time which is related to the time 'needed to reach' the potential step is similar to that in the case of reflection. At the same time, the amplitude of the peak of $|K_t(x, t; x', 0)|^2$ corresponds to the amplitude of $|K(x, t; x', 0)|^2$ at the interface (cf figure 2). The homogeneity of $|K_t(x, t; x', 0)|^2$ at $x > 0$ can be explained by the dispersion of the wave packet formed at the left semispace due to the interference of the incoming and reflected waves.

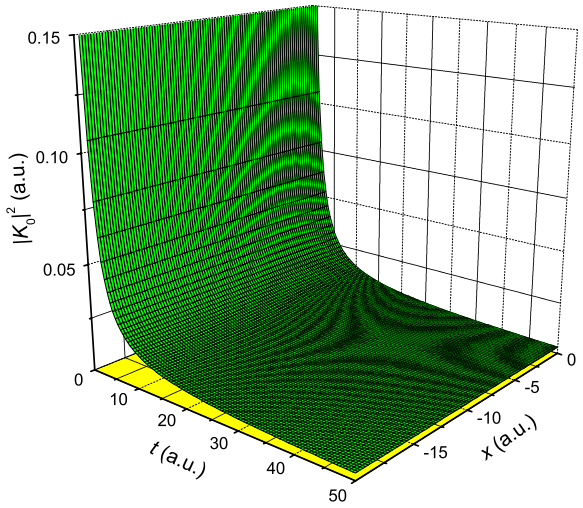

Figure 1. The square of the absolute value of the 'free' particle propagator plotted as a function of time and position in the one-dimensional case.

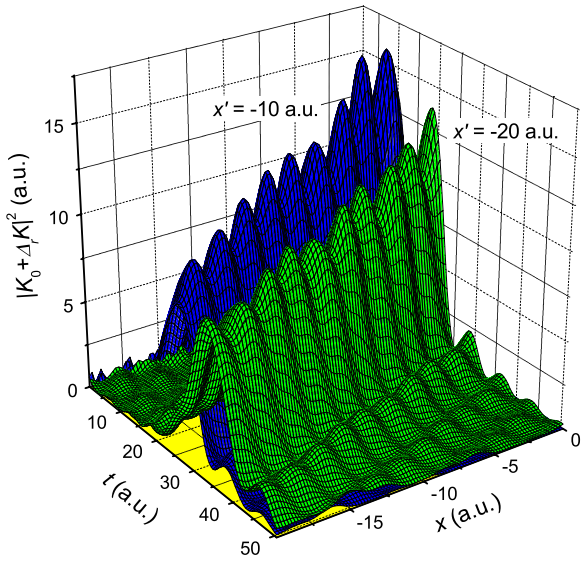

Figure 2. Relative one-dimensional probability density for the particle reflection at the potential step $U = 1$ eV plotted as a function of time and coordinate of the particle destination point for two different starting positions x'.

Now we will generalize consideration to the model three-dimensional system described above and for which the propagator $K(\mathbf{r}, t; \mathbf{r}', 0) = \langle \mathbf{r}|K(t; 0)|\mathbf{r}'\rangle$ can be obtained with the use of equations (4)–(8). In this case the localized (at the interface plane $x = 0$) perturbation of the 'free' motion, given by $H_0 = -\frac{\hbar^2}{2m}\Delta$ can depend on the two-dimensional vector parallel to the interface, $\rho = (y, z)$,

$$H_i(x, \rho) = H_i(\rho)\delta(x) \tag{27}$$

(compare with (9)) and MST perturbation series defined by (10) and (11) should be generalized as

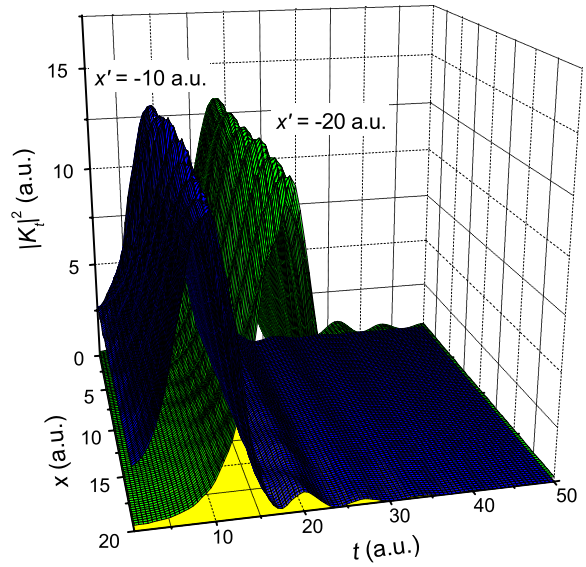

Figure 3. Relative one-dimensional probability density for the particle transmission through the potential step $U = 1$ eV plotted as a function of time and coordinate of the particle destination point for two different starting positions x'.

$$
\begin{aligned}
G(x, x'; E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel) &= [\theta(x)\theta(x') + \theta(-x)\theta(-x')]G_0(x, x'; E; \mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel} \\
&\quad + G_0(x, 0; E; \mathbf{k}_\parallel)T(E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel)G_0(0, x'; E; \mathbf{k}'_\parallel), \\
T(E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel) &= H_{i\mathbf{k}_\parallel \mathbf{k}'_\parallel} + \sum_{\mathbf{k}_{1\parallel}} H_{i\mathbf{k}_\parallel \mathbf{k}_{1\parallel}} G_0(0, 0; E; \mathbf{k}_{1\parallel}) H_{i\mathbf{k}_{1\parallel} \mathbf{k}'_\parallel} + \cdots,
\end{aligned}
\tag{28}
$$

where $H_{i\mathbf{k}_\parallel \mathbf{k}'_\parallel} = < \mathbf{k}_\parallel | H_i(\rho) | \mathbf{k}'_\parallel > = \frac{1}{A} \int \mathrm{d}\rho \exp[-\mathrm{i}(\mathbf{k}_\parallel - \mathbf{k}'_\parallel)\rho] H_i(\rho)$ is the matrix element of $H_i(\rho)$ in the $\mathbf{k}_\parallel$-representation (here E-dependence of H_i is omitted for brevity). The ρ-dependence of the interface potential can be caused by the imperfections located at the interface plane $x = 0$. If the interaction Hamiltonian does not depend on $\rho[H_i(\rho) = H_i(E)]$, then$H_{i\mathbf{k}_\parallel \mathbf{k}'_\parallel} = H_i(E)\delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel}$ and $T(E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel) = T(E; \mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel}$, i.e. the series (28) describes specular $\mathbf{k}_\parallel$-conserved and $\mathbf{k}_\parallel$-resolved multiple scatterings from a perfect interface (the scattering at the interface does not mix different $\mathbf{k}_\parallel$), and the scattering amplitude H_i in (27) may be different for different $\mathbf{k}_\parallel$. In this case, the quantum mechanical reflection from and transmission through a perfect potential step (2) may be described by the E- and $\mathbf{k}_\parallel$-dependent δ-function potential, i.e. for each E and $\mathbf{k}_\parallel$ we have, instead of (12),

$$
\begin{aligned}
H_{i>(<)}(x, E, \mathbf{k}_\parallel) &= H_{i>(<)}(E, \mathbf{k}_\parallel)\delta(x), \\
H_{i><}(x, E, \mathbf{k}_\parallel) &= H_{i><}(E, \mathbf{k}_\parallel)\delta(x),
\end{aligned}
\tag{29}
$$

where $H_{i>(<)}(E, \mathbf{k}_\parallel)$ and $H_{i><}(E, \mathbf{k}_\parallel)$ are defined by (15) with $v^{\perp}_{>(<)}(E; \mathbf{k}_\parallel)$ (8). The perturbation series (28) in the case of energy- and $\mathbf{k}_\parallel$-conserving potential (29) is exactly summed up yielding

$$
\begin{aligned}
&T_{>(<)}(E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel) = T_{>(<)}(E; \mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel}, \qquad T_{><}(E; \mathbf{k}_\parallel, \mathbf{k}'_\parallel) = T_{><}(E; \mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel} \\
&T_{>(<)}(E; \mathbf{k}_\parallel) = \frac{H_{i>(<)}(E, \mathbf{k}_\parallel)}{1 - G_{0>(<)}(E; \mathbf{k}_\parallel)H_{i>(<)}(E, \mathbf{k}_\parallel)}, \\
&T_{><}(E; \mathbf{k}_\parallel) = \frac{H_{i><}(E, \mathbf{k}_\parallel)}{1 - G_{0><}(E; \mathbf{k}_\parallel)H_{i><}(E, \mathbf{k}_\parallel)},
\end{aligned}
\tag{30}
$$

where the retarded Green's functions at the interface for considered reflection and transmission processes are defined by equation (14), and where all quantities now depend on $\mathbf{k}_\parallel$.

Thus, for a perfect $\mathbf{k}_\parallel$-conserving interface plane $x = 0$, the Green's function (28) is diagonal in $\mathbf{k}_\parallel$-representation, and all left- and right-hand sides of formulas from (15) to (20) acquire $\mathbf{k}_\parallel$-dependence (as in equations (28)–(30)) via $\mathbf{k}_\parallel$-dependence of $v^\perp_{>(<)}\left(k^\perp_{>(<)}\right)$ (8). Now, to obtain the propagator $K(\mathbf{r}, t; \mathbf{r}', 0)$, an additional integration over $\mathbf{k}_\parallel$ should be performed in accordance with (6). As a result, we have the three-dimensional expressions for $K_0(\mathbf{r}, t; \mathbf{r}', 0)$, $\Delta_r K(\mathbf{r}, t; \mathbf{r}', 0)$, $K_t(\mathbf{r}, t; \mathbf{r}', 0)$ and $K(\rho, t; \rho', 0)$ given by equations (21)–(25), and (26), accordingly, multiplied by the factor $(m/2\pi \mathrm{i}\hbar t)\exp[\mathrm{i}m(\rho - \rho')^2/2\hbar t]$.

It is easy to verify that the reflection and transmission (generally $\mathbf{k}_\parallel$-dependent) amplitudes (17) can be expressed as follows:

$$\begin{aligned} r_{>(<)}(E; \mathbf{k}_\parallel) &= \left[G^+_{0>(<)}(E; \mathbf{k}_\parallel)\right]^{-1} G^+(E; \mathbf{k}_\parallel) - 1, \\ t(E, \mathbf{k}_\parallel) &= \left[G^+_{0><}(E; \mathbf{k}_\parallel)\right]^{-1} G^+(E; \mathbf{k}_\parallel), \end{aligned} \tag{31}$$

where $G^+(E; \mathbf{k}_\parallel) = G^+(0, 0; E; \mathbf{k}_\parallel)$ is the Green's function (18) defined at the interface $x = 0$ as

$$G^+(E; \mathbf{k}_\parallel) = G^+_{0>(<)}(E; \mathbf{k}_\parallel) + G^+_{0>(<)}(E; \mathbf{k}_\parallel) T^+_{>(<)}(E; \mathbf{k}_\parallel) G^+_{0>(<)}(E; \mathbf{k}_\parallel) \tag{32}$$

for the reflection process or

$$G^+(E; \mathbf{k}_\parallel) = G^+_{0><}(E; \mathbf{k}_\parallel) T^+_{><}(E; \mathbf{k}_\parallel) G^+_{0><}(E; \mathbf{k}_\parallel) \tag{33}$$

for the transmission process. Making use of (14), (16) and (17), we have from (32) and (33) the same result, as expected,

$$G^+(E; \mathbf{k}_\parallel) = \frac{2}{\mathrm{i}\hbar\left(v^\perp_> + v^\perp_<\right)}. \tag{34}$$

Advantage of equations (31) relating the reflection and transmission amplitudes to the complete Green's function at the interface reveals itself when it is necessary to consider scattering from more than one (disordered) interface. In this case these formulas are easily generalized to the $\mathbf{k}_\parallel$-nonconserving situation and the complete Green's function may be calculated from the MST perturbation expansion (28) (see [9, 10]).

In summary, a relatively simple form of solution, compared to that given by the path-integral approach, to the problem of finding the exact spacetime propagator for a particle moving in the presence of a potential step (interface) is found and visualized by numerical calculation. The suggested approach is based on the MST for the energy-dependent Green's function, the discontinuity of which across the real energy axis (spectral density matrix) is integrated over the entire energy range to yield the spacetime propagator. The MST effectively works with the obtained reflection from and transmission through a potential step interface (step)-localized scattering potentials, which allow treating these processes as the particle multiple scatterings at a potential step. It seems that this approach solves the considered problem more easily and effectively (than those known to us) and provides more insight into the physics of particle quantum mechanical scattering at a potential step. In the same way, the solution to the case with potential (3) [7] may be easily obtained. By switching to the imaginary time, the obtained results would describe the corresponding diffusion processes or the density matrix for the particles at a given temperature. The presented results are also expected to be useful in the studies of various effects in magnetic multilayers for spintronics applications.

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