Asymptotes and characteristic times for transmission and reflection.

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A complete one-dimensional scattering of a spinless particle on a time-independent potential barrier is considered. To describe separately transmitted and reflected particles in the corresponding subsets of identical experiments, we introduce the notions of scattering channels for transmission and reflection. We find for both channels the (unitary) scattering matrices and reconstruct, by known out asymptotes (i.e., by the transmitted and reflected wave packets), the corresponding in asymptotes. Unlike the out asymptotes for transmission and reflection, their in asymptotes represent nonorthogonal functions. As is shown, the position distributions of to-be-transmitted and to-be-reflected particles, except their average positions, are unpredictable. At the same time, the momentum distributions of these particles are physically meaningful and can be observed to the full. We show that both the subensembles of particles must start (on the average) from the same spatial point, and the momentum distributions of to-be-scattered and scattered particles must be the same for each scattering channel. Taking into account these properties, we define the (individual) delay times for transmission and reflection for wave packets of an arbitrary width. Besides, to estimate the duration of the scattering event, we derive the expression for a (total) scattering time.

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INTRODUCTION

For a long time tunneling a spinless particle through a one-dimensional static potential barrier was considered in quantum mechanics as a representative of well-understood phenomena. However, now it has been realized that this is not the case. The inherent to quantum theory standard wave-packet analysis (SWPA) (see, for example, [1–3]) does not provide a clear prescription both how to interpret properly the temporal behavior of finite in $x$ space wave packets and how to introduce characteristic times for a tunneling particle.

As is known, the main peculiarity of the tunneling of finite wave packets is that the average particle’s momentum for the transmitted, reflected and incident wave packets are different. It is evident that this fact needs in a proper explanation. As was pointed out in [4], it would be strange to interpret the above property of wave packets as the evidence of accelerating a particle (in the asymptotic regions) by a static potential barrier. Besides, in this case there is no causal link between the transmitted and incident wave packets (see [4]), and the tunneling times introduced in the SWPA are ill-defined [1,4].

Perhaps, no problems in this approach arise only for wide (strictly speaking, infinite) in $x$ space wave packets, when the average kinetic energy of particles, before and after the interaction, is the same. In this case the asymptotic phase times [1–3,6] are formally well-defined.

Apart from the SWPA, the variety of alternative approaches to solving the tunneling time problem (TTP) have also been developed (see, for example, [1–20] and references therein). However again, a clear agreement between these approaches and the SWPA have been achieved only for wide wave packets. In the general case all the attempts have not yet led to commonly accepted quantities which would describe a tunneling particle in the standard setting the tunneling problem [1,4,5]. As regards the interpretation of the above peculiarity of the tunneling of finite wave packets, as we are aware this question was of no interest in these approaches.

However, we think the question of timing a tunneling particle cannot be solved without of a proper understanding of the behavior of tunneling wave packets. In this paper we develop the approach, in which both the questions are closely connected. Its basis is the formalism of a separate description of transmitted and reflected particles at the stage preceding the scattering event. We show that such a description is needed and quite admissible in quantum theory.

The necessity in the separate description follows from the fact that when $t \to \infty$ the transmitted and reflected wave packets are localized, in the case of a completed scattering, in the disjoint spatial regions. By the ensemble (statistical) interpretation of quantum mechanics, this means that the whole (infinite) set of identical experiments on tunneling, in which scattered particles are detected far from the barrier, is divided into two separate parts. One of them includes experiments in which a particle is transmitted through the barrier: we will say that it moves in this case along the transmission channel. In another part, a particle is reflected by the barrier: similarly, we will say that it moves in such experiments along the reflection channel.

In each experiment a particle is evident to pass all the distance between the particle’s source and detector. So that at the initial stage of scattering we deal in fact with the subensembles of to-be-transmitted (STP) and to-be-reflected (SRP) particles. Of course, the formalism of quantum mechanics, as it stands, does not suggest a separate description of the STP and SRP. The states of these particles cannot be described in terms of orthogonal wave functions. However, it is evident that just the STP and SRP should be causally connected with the subensembles of transmitted and reflected particles, respectively. Thus, to clear up the above acceleration of finite wave packets, one needs to study the dynamics of these subensembles both after and before the scattering event.

As will be shown in this paper, the principles of quantum mechanics admit a separate description of the STP and SRP. One can uniquely introduce the non-orthogonal in asymptotes for transmission and reflection. Being "unphysical" from the viewpoint of the conventional quantum description, they in reality possess some properties typical for "physical" (orthogonal) quantum states. In particular, the number of particles in each subensemble should be conserved. The momentum distributions of to-be-transmitted and to-be- reflected particles are physically meaningful and should be experimentally observed. In particular, the energy distribution of particles in the asymptotic regions, to the left and to the right of the barrier, should be the same for each scattering channel. At the same time, due to the statistical dependency of these subensembles, their position distributions cannot be, in full, reproducible in experiment. Only the average positions of to-be-transmitted and to-be-reflected particles can be uniquely determined and verified experimentally.

Taking into account the properties of the in asymptotes for transmission and reflection, we offer our interpretation to the behavior of finite wave packets in tunneling and define delay times for transmission and reflection. Besides, apart from the separate description of transmitted and reflected particles, we introduce a total scattering time to estimate the duration of the scattering event.

The paper is organized as follows. In Section I we find total in and out asymptotes for a tunneling particle, and display explicitly shortcomings to arise in the SWPA in solving the TTP. In Section II we introduce the notion of in asymptotes for transmission and reflection and define the corresponding (individual) delay times which can be verified experimentally. The (total) scattering time to describe the duration of the scattering event, as well as its start and finish instants of time are derived in Section III. In addition, we find here the restrictions on the wave-packet’s parameters which must be fulfilled for a completed scattering. The expressions for the asym-
totic expectation values of the position and wave-number operators as well as for their mean-square deviations are presented in Appendix.

1. SETTING THE PROBLEM FOR A COMPLETED SCATTERING

A. Backgrounds

Let us consider a particle that tunnels through the time-independent potential barrier \( V(x) \) confined to the finite spatial interval \([a, b]\) \((a > 0)\); \(d = b - a\) is the barrier width. Let its in state, \(\Psi_{in}(x)\), at \(t = 0\) be the normalized function \(\Psi_{lef}^{(0)}(x)\) when it moves from the left, or \(\Psi_{right}^{(0)}(x)\), otherwise. Both functions belong to the set \(S_\infty\) to consist from infinitely differentiable functions vanishing exponentially in the limit \(|x| \to \infty\). The Fourier-transforms of such functions are known to belong to the set \(S_\infty\), too. In this case the position and momentum operators both are well-defined. Without loss of generality we will suppose that

\[
< \Psi_{lef}^{(0)} | \hat{x} | \Psi_{lef}^{(0)} > = 0, \quad < \Psi_{lef}^{(0)} | \hat{p} | \Psi_{lef}^{(0)} > = \hbar k_0 > 0,
\]

\[
< \Psi_{lef}^{(0)} \hat{x}^2 \Psi_{lef}^{(0)} > = l_0^2, \quad \Psi_{right}^{(0)}(x) \equiv \Psi_{lef}^{(0)}(x_r - x)
\]

(that is, the function \(\Psi_{right}^{(0)}(x)\) is centered at the point \(x = x_r\); here \(l_0\) is the wave-packet’s half-width at \(t = 0\) \((l_0 < a)\); \(l_0 < x_r - b\); \(\hat{x}\) and \(\hat{p}\) are the operators of the particle’s position and momentum, respectively.

Besides, let \(\hat{H}\) be the Hamiltonian, \(\hat{H} = \hat{H}_0 + V(x)\) where \(\hat{H}_0\) describes a free particle. Let also \(\hat{H}_0^{ref}\) be the Hamiltonian to describe the ideal reflection of a free particle off the potential wall located at the middle point of the interval \([a, b]\), i.e., at \(x_{midp} = (a + b)/2\).

An important restriction should be imposed on the rate of spreading the incident wave packet. We must be sure that at early times the quantum ensemble of particles moves, as a whole, toward the barrier. In particular, at the initial stage of scattering, the probability to find a particle at the initial point should diminish in time. This does not at all mean that the incident wave packet must not contain waves with \(p \leq 0\) \((p \geq 0)\), if the initial state of a particle is described by the function \(\Psi_{lef}^{(0)}(\Psi_{right}^{(0)})\). This condition is fulfilled when the back front of the incident wave-packet, which is away from the center of mass (CM) of the wave packet at the distance equal to the wave-packet’s half-width, moves toward the barrier. Such a behavior takes place only if the packet’s spreading is ineffective enough (see condition (3.6) in Section III).

B. Stationary states

As is known, the formal solution to the temporal one-dimensional Schrödinger equation (OSE) of the problem at hand can be written as \(e^{-i\hat{H}t/\hbar}\Psi_{in}(x)\). To solve explicitly this equation, we will use here the transfer matrix method (TMM) [24] that allows one to calculate the tunneling parameters for any system of potential barriers. The state of a particle with the wave-number \(k\) can be written in the form

\[
\Psi_{lef} = \left[ A^{(+)}_{in}(k) \exp(ikx) + A^{(-)}_{out}(k) \exp(-ikx) \right] \times \exp[-iE(k)t/\hbar],
\]

for \(x < a\); and for \(x > b\) we have

\[
\Psi_{right} = \left[ A^{(+)}_{out}(k) \exp(ikx) + A^{(-)}_{in}(k) \exp(-ikx) \right] \times \exp[-iE(k)t/\hbar].
\]

Here \(E(k) = \hbar^2 k^2/2m\). The coefficients entering this solution are connected by the transfer matrix \(Y\) (see [24]):

\[
\begin{pmatrix}
A^{(+)}_{in} \\
A^{(-)}_{out}
\end{pmatrix} = Y \begin{pmatrix}
A^{(+)}_{out} \\
A^{(-)}_{in}
\end{pmatrix}; \quad Y = \begin{pmatrix}
q & p & q^* & p^* \\
p & q & p^* & q^*
\end{pmatrix};
\]

where

\[
q = \frac{1}{\sqrt{T(k)}} \exp[-i(J(k) - kd)];
\]

\[
p = \frac{\sqrt{R(k)}}{T(k)} \exp[i(\frac{\pi}{2} + F(k) - ks)];
\]

\(T(k)\) (the real transmission coefficient) and \(J(k)\) (phase) are even and odd functions of \(k\), respectively: \(F(-k) = \pi - F(k)\); \(R(k) = 1 - T(k)\); \(s = a + b\). Note that the functions \(T(k)\), \(J(k)\) and \(F(k)\) contain all needed information about the influence of the potential barrier on a particle. We will suppose that these functions have already been known explicitly. To find them, one can use the recurrence relations obtained in [24].

The amplitudes of the outgoing and corresponding incoming waves are connected by the scattering matrix \(S\):

\[
A_{out} = SA_{in}; \quad S = \begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix};
\]

\[
A_{in} = \begin{pmatrix}
A^{(+)}_{in} \\
A^{(-)}_{in}
\end{pmatrix}; \quad A_{out} = \begin{pmatrix}
A^{(+)}_{out} \\
A^{(-)}_{out}
\end{pmatrix};
\]

here

\[
S_{11} = S_{22} = q^{-1} = \sqrt{T(k)} \exp[i(J - kd)],
\]

\[
S_{12} = -\frac{p}{q} = \sqrt{R(k)} \exp[i(J + F - \frac{\pi}{2} - 2kb)]
\]

\[
S_{21} = \frac{p^*}{q} = \sqrt{R(k)} \exp[i(J - F - \frac{\pi}{2} + 2ka)].
\]
Note that the scattering matrix can be uniquely presented as the sum of two non-unitary matrices to describe separately transmission and reflection,

\[ S = \Pi_{tr} + \Pi_{ref} \]  

(1.6)

where

\[ \Pi_{tr} = S_{tr}P_{tr}, \quad \Pi_{ref} = S_{ref}P_{ref}; \]

\[ S_{tr} = \Delta_{tr}S_{tr}^{(0)}, \quad S_{ref} = \Delta_{ref}S_{ref}^{(0)} \]  

(1.7)

(\( S_{tr} \) and \( S_{ref} \) are unitary matrices);

\[ P_{tr} = I\sqrt{T}; \quad P_{ref} = I\sqrt{R}; \]  

(1.8)

\[ S_{tr}^{(0)} = I; \quad S_{ref}^{(0)} = \left( \begin{array}{cc} 0 & -e^{-iks} \\ -e^{iks} & 0 \end{array} \right) ; \]  

(1.9)

\[ \Delta_{tr} = I \exp[i(J - kd)]; \]

\[ \Delta_{ref} = \left( \begin{array}{cc} e^{iF} & 0 \\ 0 & e^{-iF} \end{array} \right) \exp[i(J + \pi/2 - kd)]; \]  

(1.10)

where \( I \) is the unit matrix; \( S_{tr}^{(0)} \) and \( S_{ref}^{(0)} \) are the scattering matrix to correspond the Hamiltonians \( \hat{H}_0 \) and \( \hat{H}_0^{ref} \), respectively.

### C. Total in and out asymptotes

As is known, solving the TTP is reduced in the SWPA to timing a particle beyond the scattering region where the exact solution of the OSE approaches to the corresponding in or out asymptote [21]. Thus, definitions of characteristic times for a tunneling particle can be obtained in terms of the in and out asymptotes of the tunneling problem. To find them, we have to go over to the temporal scattering problem and consider two independent cases,

\[ A_{in} = \left( \begin{array}{c} A_{m}^{(+)}(k) \\ 0 \end{array} \right), \quad A_{in} = \left( \begin{array}{c} 0 \\ A_{m}^{(-)}(k) \end{array} \right), \]  

(1.11)

when the incident particle moves toward the barrier from the left (the left-side case) or from the right (the right-side case), respectively.

Note that in both the cases the in asymptotes represent one-packet objects to converge, at \( t \to -\infty \), with the corresponding incident packets, while the out asymptotes represent a superposition of two non-overlapped wave packets to converge, at \( t \to \infty \), with the superposition of the transmitted and reflected ones. It is easy to show that in the first case the in and out asymptotes, in \( k \) space, can be written for both scattering channels as follows

\[ f_{in}(k, t) = A_{in}^{(+)}(k) \exp[-iE(k)t/\hbar]; \]  

(1.12)

\[ f_{out}(k, t) = f_{out}^{tr}(k, t) + f_{out}^{ref}(k, t) \]  

(1.13)

where

\[ f_{out}^{tr}(k, t) = \sqrt{T(k)}A_{in}^{(+)}(k) \exp[i(J(k) - kd - E(k)t/\hbar)]; \]  

(1.14)

\[ f_{out}^{ref}(k, t) = \sqrt{R(k)}A_{in}^{(-)}(k) \exp[-i(J(k) - F(k) - \pi/2 - 2ka + E(k)t/\hbar)]. \]  

(1.15)

For particles starting, on the average, at the origin (the left-side case), we have (see Appendix)

\[ < \dot{x} >_{in} = \frac{\hbar k_0}{m} \]  

(1.16)

The averaging separately over the transmitted and reflected wave packets yields

\[ < \dot{x} >_{out}^{tr} = \frac{\hbar t}{m} < k >_{out}^{tr} - < J'(k) >_{out}^{tr} + d; \]  

(1.17)

\[ < \dot{x} >_{out}^{ref} = \frac{\hbar t}{m} < k >_{out}^{ref} + < J'(k) >_{out}^{ref} + 2a \]  

(1.18)

(hereinafter the prime denotes the derivative with respect to \( k \)).

Similarly, for the right-side case, we have

\[ f_{in}(k, t) = A_{in}^{(-)}(k) \exp[-iE(k)t/\hbar]; \]  

(1.19)

\[ f_{out}^{tr}(k, t) = \sqrt{T(k)}A_{in}^{(-)}(k) \exp[-i(J(k) - kd + E(k)t/\hbar)]; \]  

(1.20)

\[ f_{out}^{ref}(k, t) = \sqrt{R(k)}A_{in}^{(-)}(k) \exp[i(J(k) + F(k) - \pi/2 - 2kb - E(k)t/\hbar)]. \]  

(1.21)

Hence

\[ < \dot{x} >_{in} = x_r - \frac{\hbar k_0}{m} \]  

(1.22)

\[ < \dot{x} >_{out}^{tr} = x_r + \frac{\hbar t}{m} < k >_{out}^{tr} + < J'(k) >_{out}^{tr} - d; \]  

(1.23)

\[ < \dot{x} >_{out}^{ref} = -x_r + \frac{\hbar t}{m} < k >_{out}^{ref} - < J'(k) + F'(k) >_{out}^{ref} + 2b. \]  

(1.24)
D. Paradoxes of the standard wave-packet analysis

To display explicitly the basic shortcoming of the SWPA, let us derive again the SWPA’s tunneling times. For this purpose it is sufficient to consider the left-side case.

Let \( Z_1 \) be a point to lie at some distance \( L_1 \) (\( L_1 \gg l_0 \) and \( a - L_1 \gg l_0 \)) from the left boundary of the barrier, and \( Z_2 \) be a point to lie at some distance \( L_2 \) (\( L_2 \gg l_0 \)) from its right boundary. Following [2], let us define the difference between the times of arrival of the CMs of the incident and transmitted packets at the points \( Z_1 \) and \( Z_2 \), respectively (this time will be called below as the "transmission time"). Analogously, let the "reflection time" be the difference between the times of arrival of the CMs of the incident and reflected packets at the same point \( Z_1 \).

Thus, let \( t_1 \) and \( t_2 \) be such instants of time that

\[
< \hat{x} >_{\text{in}}(t_1) = a - L_1; \quad < \hat{x} >_{\text{out}}(t_2) = b + L_2. \tag{1.25}
\]

Then, considering (1.16) and (1.17), one can write the "transmission time" \( \Delta t_{tr} \) (\( \Delta t_{tr} = t_2 - t_1 \)) for the given interval in the form

\[
\Delta t_{tr} = \frac{m}{\hbar} \left[ \frac{< J' >_{\text{out}}^{tr} + L_2}{< k >_{\text{out}}^{tr}} + \frac{L_1}{k_0} \right. \\
+ a \left( \frac{1}{< k >_{\text{out}}^{tr}} - \frac{1}{k_0} \right) \right]. \tag{1.26}
\]

Similarly, for the reflected packet, let \( t'_1 \) and \( t'_2 \) be such instants of time that

\[
< \hat{x} >_{\text{in}}(t'_1) = < \hat{x} >_{\text{out}}^{ref}(t'_2) = a - L_1. \tag{1.27}
\]

From equations (1.16), (1.18) and (1.27) it follows that the "reflection time" \( \Delta t_{ref} \) (\( \Delta t_{ref} = t'_2 - t'_1 \)) can be written as

\[
\Delta t_{ref} = \frac{m}{\hbar} \left[ \frac{< J' >_{\text{out}}^{ref} - L_1}{< k >_{\text{out}}^{ref}} + \frac{L_1}{k_0} \right. \\
+ a \left( \frac{1}{< k >_{\text{out}}^{ref}} - \frac{1}{k_0} \right) \right]. \tag{1.28}
\]

Note that the expectation values of \( k \) for all three wave packets coincide only in the limit \( l_0 \to \infty \) (i.e., for particles with a well-defined momentum). In the general case these quantities are distinguished. For example, for a particle whose initial state, in the left-side case (1.11), is described by the Gaussian wave packet (GWP),

\[
A_{\text{in}}^{(+)}(k) = \frac{l_0}{\sqrt{\pi}} \exp(-l_0^2(k - k_0)^2),
\]

we have

\[
< k >_{tr} = k_0 + \frac{< T' >_{\text{in}}}{4l_0^2} < R >_{\text{in}}. \tag{1.29}
\]

Let

\[
< k >_{tr} = k_0 + (< \Delta k >_{tr}), \quad < k >_{ref} = k_0 + (< \Delta k >_{ref}),
\]

then relations (1.29) and (1.30) can be written in the form

\[
\bar{T} \cdot (< \Delta k >_{tr}) = -\bar{R} \cdot (< \Delta k >_{ref}) = \frac{< T' >_{\text{in}}}{4l_0^2}. \tag{1.31}
\]

Note that \( R' = -R \).

As we can see, in the general case each characteristic time (1.26) and (1.28) cannot serve as characteristic times for a particle. Due to the last terms in these expressions the above times depend essentially on the initial distance between the wave packet and barrier, with \( L_1 \) being fixed. These terms are dominant for the sufficiently large distance \( a \). Moreover, one of them must be negative. For example, for the transmitted wave packet it takes place in the case of the under-barrier tunneling through an opaque rectangular barrier. The numerical modelling of tunneling [1-3,15] shows in this case a premature appearance of the CM of the transmitted packet behind the barrier, which points to the lack of a causal link between the transmitted and incident wave packets (see [4]).

As was shown in [1,2], this effect disappears in the limiting case \( l_0 \to \infty \). In the case of Gaussian wave packets, the fact that the last terms in (1.26) and (1.28) tend to zero when \( l_0 \to \infty \), with the ratio \( l_0/a \) being fixed, can be proved with help of Exps. (1.29) and (1.30) (note that the limit \( l_0 \to \infty \) with a fixed value of \( a \) is unacceptable in this analysis, because it contradicts the initial condition \( a \gg l_0 \) for a completed scattering). Thus, in the limit \( l_0 \to \infty \) the SWPA formally provides characteristic times for a particle.

Note, the fact that Exps. (1.29) and (1.30) cannot be applied to particles does not at all mean that they are erroneous. These expressions correctly describe the relative motion of the transmitted (or reflected) and incident wave packets. The main problem is to understand what particle’s dynamics underlies such a behavior of wave packets.

II. FORMALISM OF SEPARATE DESCRIPTION OF TRANSMITTED AND REFLECTED PARTICLES

A. In and out asymptotes for transmission and reflection

We think that the principle mistake made in the SWPA in deriving the individual tunneling times is that the incident wave packet cannot be used as a counterpart neither to the transmitted nor to reflected wave packet,
when they are treated separately. This step is physically meaningless because the incident packet describes the whole quantum ensemble of particles (or, the whole set of the corresponding identical experiments), while the transmitted packet, for example, represents only its part. The former can be used as a reference only for the transmitted and reflected packets taken jointly. As regards the separate description of transmitted particles, for example, it makes sense to compare their motion only with that of to-be-transmitted particles mentioned in Introduction. This means that in order to develop a separate description of both scattering channels, one needs to find the in and out asymptotes for transmission and reflection, if they exist.

Let us show that decomposition (1.6) permits us to find uniquely such asymptotes. Indeed, let

\[ A_{\text{out}}^{\text{tr}} = \text{P}_{\text{tr}} A_{\text{in}}; \quad A_{\text{out}}^{\text{ref}} = \text{P}_{\text{ref}} A_{\text{in}}. \]

Considering (1.7) we can rewrite these relations as follows,

\[ A_{\text{out}}^{\text{tr}} = \text{S}_{\text{tr}} A_{\text{in}}^{\text{tr}}; \quad A_{\text{out}}^{\text{ref}} = \text{S}_{\text{ref}} A_{\text{in}}^{\text{ref}}, \tag{2.1} \]

where

\[ A_{\text{in}}^{\text{tr}} = \text{P}_{\text{tr}} A_{\text{in}}; \quad A_{\text{in}}^{\text{ref}} = \text{P}_{\text{ref}} A_{\text{in}}. \tag{2.2} \]

The pairs \((A_{\text{in}}^{\text{tr}}, A_{\text{out}}^{\text{tr}})\) and \((A_{\text{in}}^{\text{ref}}, A_{\text{out}}^{\text{ref}})\) related by the unitary matrices \(S_{\text{tr}}\) and \(S_{\text{ref}}\), respectively, will be treated further as the amplitudes of incoming and outgoing waves to describe transmission and reflection. Since the amplitudes of outgoing waves are known, relations (2.1) can be used for reconstructing those of incoming waves,

\[ A_{\text{in}}^{\text{tr}} = S_{\text{tr}}^{-1} A_{\text{out}}^{\text{tr}}; \quad A_{\text{in}}^{\text{ref}} = S_{\text{ref}}^{-1} A_{\text{out}}^{\text{ref}}. \]

Then it is easy to show that in the left-side case the searched-for in asymptotes can be written, in \(k\) space, as follows

\[ f_{\text{in}}^{\text{tr}}(k, t) = \sqrt{T(k)} A_{\text{in}}^{(+)}(k) \exp[-iE(k)t/\hbar]; \tag{2.3} \]

\[ f_{\text{in}}^{\text{ref}}(k, t) = \sqrt{R(k)} A_{\text{in}}^{(-)}(k) \exp[-iE(k)t/\hbar]; \tag{2.4} \]

Thus, for the left-side case (see (1.11),

\[ < \hat{x} >^{\text{tr}}_{\text{in}} = \frac{\hbar t}{m} < k >^{\text{tr}}_{\text{in}}; \tag{2.5} \]

\[ < \hat{x} >^{\text{ref}}_{\text{in}} = \frac{\hbar t}{m} < k >^{\text{ref}}_{\text{in}}; \tag{2.6} \]

Similarly, for the right-side case, we have

\[ f_{\text{in}}^{\text{tr}}(k, t) = \sqrt{T(k)} A_{\text{in}}^{(+)}(-k) \exp[-iE(k)t/\hbar]; \tag{2.7} \]

\[ f_{\text{in}}^{\text{ref}}(k, t) = \sqrt{R(k)} A_{\text{in}}^{(-)}(-k) \exp[-iE(k)t/\hbar]. \tag{2.8} \]

As a consequence,

\[ < \hat{x} >^{\text{tr}}_{\text{in}} = \frac{\hbar t}{m} < k >^{\text{tr}}_{\text{in}}; \tag{2.9} \]

\[ < \hat{x} >^{\text{ref}}_{\text{in}} = \frac{\hbar t}{m} < k >^{\text{ref}}_{\text{in}}. \tag{2.10} \]

Note that the separate treating of the out asymptotes for transmission and reflection have been of usual practice. They are the transmitted and reflected wave packets that coincide, in the limit \(t \to \infty\), with these asymptotes. For these orthogonal states which describe mutually exclusive events, the probabilities \(T\) and \(R\) satisfy relation (A10): \(T + R = 1\). Besides, according to (A13),

\[ < k^n >_{\text{out}} = \bar{T} < k^n >_{\text{tr}} + \bar{R} < (k^n)^{\text{ref}} >_{\text{out}}. \]

It is important to emphasize that similar probabilistic rules take place also for \(f_{\text{in}}^{\text{tr}}(k, t)\) and \(f_{\text{in}}^{\text{ref}}(k, t)\) to evolve along the in asymptotes for transmission and reflection, respectively:

\[ < f_{\text{in}}^{\text{tr}} | f_{\text{in}}^{\text{tr}} > = < f_{\text{in}}^{\text{tr}} | f_{\text{in}}^{\text{ref}} > + < f_{\text{in}}^{\text{ref}} | f_{\text{in}}^{\text{ref}} >, \tag{2.11} \]

\[ < k^n >_{\text{in}} = \bar{T} < k^n >_{\text{in}} + \bar{R} < k^n >_{\text{in}}^{\text{ref}}, \tag{2.12} \]

\[ < \hat{x} >_{\text{in}} = \bar{T} < \hat{x} >_{\text{in}} + \bar{R} < \hat{x} >_{\text{in}}^{\text{ref}}. \tag{2.13} \]

However, because of the nonorthogonality of \(f_{\text{in}}^{\text{tr}}\) and \(f_{\text{in}}^{\text{ref}}\), there are no similar probabilistic rules for higher moments of the operator \(\hat{x}\).

For each scattering channel we have

\[ < f_{\text{in}}^{\text{tr}} | f_{\text{in}}^{\text{tr}} > = < f_{\text{in}}^{\text{tr}} | f_{\text{in}}^{\text{ref}} > = \bar{T}; \tag{2.14} \]

and

\[ < f_{\text{in}}^{\text{ref}} | f_{\text{in}}^{\text{ref}} > = < f_{\text{in}}^{\text{ref}} | f_{\text{in}}^{\text{ref}} > = \bar{R}; \tag{2.15} \]

that is, the number of particles in each subensemble is the same before and after the scattering event. Besides,

\[ < \hat{k} >_{\text{in}}^{\text{tr}} = < \hat{k} >_{\text{out}}^{\text{tr}} \tag{2.16} \]

and

\[ < \hat{k} >_{\text{in}}^{\text{ref}} = - < \hat{k} >_{\text{out}}^{\text{ref}}; \tag{2.17} \]

which point to the conservation of the average momentum of transmitted and reflected particles in the asymptotic spatial regions.
B. Ideal and nonideal passage of particles in the scattering channels

So, in the tunneling problem considered as a two-channel scattering, the transmission and reflection channels (or, what is equivalent, two subsets of identical experiments, each includes only transmitted or reflected particles) are described by Exp. (2.11) - (2.17). A simple analysis shows that it is convenient to distinguish a nonideal and ideal passage of particles along the scattering channels. The ideal passage in the transmission channel is characterized by the Hamiltonian \( H_0 \) and by the unit scattering matrix \( S^{(0)}_t \) describing a free particle. By the ideal reflection is meant the reflection of a free particle off the absolutely opaque potential wall located at the point \( x_{midp} \), which is described by the Hamiltonian \( \tilde{H}^{ref}_0 \) and scattering matrix \( S^{(0)}_r \) (see (1.9)).

In the general case, the scattering channels are always nonideal. A nonideal passage of a particle along transmission and reflection channels is described by the unitary matrices \( S_t \) and \( S_r \), respectively. As is seen from (1.7) and (1.10), in this case a particle stay longer in the scattering region than in the case of ideal scattering. In the subset of experiments where particles are transmitted, the influence of the potential barrier on a particle is equivalent, in the asymptotic regions, to that of a reflectionless potential. In another subset its effect is similar to that of some potential structure with the above opaque potential. In another subset its effect is similar to that of a reflectionless potential, and to the one-channel scattering processes: the transmission and reflection channels is described by the unitary matrix \( \pi \). This implies that only the first moment of all the moments of the position operator for the STP and SRP, excepting the first moment, cannot be obtained in quantum mechanics. For example, the properties of transmitted and reflected particles at early times cannot be obtained in quantum mechanics. This implies that only the first moment of the position operator may be used in defining individual characteristic times for transmission and reflection.

C. Delay times for transmitted and reflected particles

Because of the influence of the potential barrier a transmitted or reflected particle is delayed (on the average), in the scattering region, relatively to a particle moving freely in the scattering channel with the same in asymptote. For an observer investigating only transmitted or reflected particles, it is important to estimate the corresponding time and spatial delays. In particular, by the sign of the time delay one can ascertain whether the potential barrier investigated is repulsive or attractive with respect to the given subensemble of particles.

At the beginning let us define the delay times for transmission and reflection for the left-side case. As it follows from expressions (1.17) and (2.5), the transmitted and corresponding free particles arrive (on the average) at the same point \( Z_T \) (see ID), at the instants \( t^{tr} \) and \( t^{free} \), respectively, such that

\[
< \hat{x} >^{tr}_{in} (t^{tr}) = < \hat{x} >^{free}_{out} (t^{tr}) = b + L_T. \tag{2.18}
\]

Then for transmitted particles the delay time \( \tau^{tr}_{del} \) can be defined as

\[
\tau^{tr}_{del} = \frac{m}{\hbar} \langle < J' >^{tr} - d \rangle \tag{2.19}
\]

(since the average values of the tunneling parameters over the in and out states are the same for both scattering channels, hereinafter we will substitute \(< \ldots >^{tr,ref} \) for \(< \ldots >^{tr,ref} \).

Similarly, from expressions (1.18) and (2.6) it follows that the reflected and corresponding ideally reflected particles arrive (on the average) at the same point \( Z_T \) at the instants \( t^{ref} \) and \( t^{free} \), respectively, such that

\[
< \hat{x} >^{ref}_{in} (t^{ref}) = < \hat{x} >^{free}_{out} (t^{ref}) = a - L_1. \tag{2.20}
\]

As a result, the delay time, \( \tau^{(-)}_{del} \), for reflection can be written in the form

\[
\tau^{(-)}_{del} = \frac{m}{\hbar} \langle < J' - F' >^{ref} - d \rangle. \tag{2.21}
\]

Analogously, for the right-side case the delay time for reflection is given by

\[
\tau^{(+)\ref}_{del} = \frac{m}{\hbar} \langle < J' + F' >^{ref} - d \rangle \tag{2.22}
\]

It is obvious that the transmission delay times for the left- and right-side cases should be always equal. However, the equality \( \tau^{(-)}_{del} = \tau^{(+)}_{del} \) takes place only for symmetrical potential barriers for which \( F'(k) \equiv 0 \).

Note that the expressions \( < J' >^{tr} - d \) and \( < J' - F' >^{ref} - d \) (or \( < J' + F' >^{ref} - d \)) can be treated as the spatial delays for the subensembles of transmitted and reflected particles, respectively.
D. About the verification of the individual properties of to-be-transmitted and to-be-reflected particles.

So, quantum theory quite admits a separate description of transmitted and reflected particles at the stage preceding the scattering event. As was shown, there can be uniquely determined, by known out asymptotes, in asymptotes to describe individually to-be-transmitted and to-be-reflected particles. The peculiarity of such description is that these partial wave functions, being non-orthogonal, provide only such physical characteristics as the momentum distributions, the average positions and the delay times for to-be-transmitted and to-be-reflected particles. Contrary to wave functions to describe the whole quantum ensembles of free particles, the position distributions calculated over its to-be-transmitted and to-be-reflected parts have, by our formalism, no physical sense. These distributions should not be reproducible (except the average positions), in the repeated series of identical experiments.

Of course, a problem is that the dealing with the subensembles of to-be-transmitted and to-be-reflected particles have not been inherent in quantum mechanics. In particular, one may doubt in that the particle subensembles described by non-orthogonal wave functions can be, in principle, distinguishable. Besides, by the above formalism the reverse motion of the transmitted wave packet should describe only particles which must pass through the barrier. However, this property seems to contradict the rigorous results of one-dimensional quantum theory. As is known, in the general case only a part of incident particles may pass through the barrier. Another part should be reflected by it. So that there is the necessity to remove all these doubts and to show that the above formalism is indeed in agreement with the principles of quantum theory and can be experimentally verified.

We will proceed from the natural assumption that in each single experiment with a tunneling particle the latter interacts twice with an experimental device: this takes place at the initial instant of time when the particle is emitted in a given state by an appropriate source, and at the final instant when it is absorbed by the detector to measure the particle’s final state. Note that to emit a free particle in the given state means, in fact, to emit a particle with random (unpredictable) values of the particle’s momentum and position to belong the given distributions. To be sure that a particle is indeed emitted in the given state, in each single experiment an experimenter should obtain (in the same or in the different series of identical experiments with the particle) the values of the particle’s momentum and position not only for the final but also for the initial instant of time. Due to time reversal, both the instants of time should be equivalent in the sense that in the case of the reverse motion the experimental data for the initial and final states should switch their roles. Thus, from the above it follows that the division of experimental data for scattered particles, in the corresponding infinite set of identical experiments, should lead automatically to that of data for to-be-scattered particles, thereby providing the momentum and position distributions for to-be-transmitted and to-be-reflected particles. So that, the subensembles of to-be-transmitted and to-be-reflected are quite distinguishable.

To end this question, we have once more to pay reader’s attention on the status of the partial momentum and position distributions. The former is reproducible, that is, one can carry out the several series of identical experiments, and the momentum distributions for transmission and reflection should be the same for these series. A cardinally different situation should take place for their position distributions. They are not reproducible, excepting the average positions of to-be-transmitted and to-be-reflected particles. The position distributions for transmission and reflection obtained in two different series of identical experiments may be different. For the given instant of time, only the average positions of to-be-scattered particles for each channel should be reproduced in this case.

Our next aim is to illustrate the difference between the cases when the same wave packet, in one case, describes the whole ensemble of particles, and in another case it does only a part. For this purpose it is interesting to analyze the reverse motion of the transmitted and reflected wave packets. Namely, let us consider three closely connected solutions with the following in and out asymptotes:

1) the reverse motion of the transmitted wave packet -
\[ f^{(1)}_{in}(k,t) = [f^{(1)}_{out}(-k,t)]^*, \quad f^{(1)}_{out}(k,t) = [g_1(-k,t)]^* \]
where
\[ g_1(k,t) = \left[ T(k)A^{(+)in}_{in}(k) - \sqrt{R(k)}T(k)A^{(+)in}_{in}(-k) \right.\]
\[ \times \exp[-i(\frac{\pi}{2} + F(-k) + ks)] \exp(-iE(k)t/\hbar); \quad (2.23) \]

2) the reverse motion of the reflected wave packet -
\[ f^{(2)}_{in}(k,t) = [f^{(2)}_{out}(-k,t)]^*, \quad f^{(2)}_{out}(k,t) = [g_2(-k,t)]^* \]
where
\[ g_2(k,t) = \left[ R(k)A^{(+)in}_{in}(k) + \sqrt{R(k)}T(k)A^{(+)in}_{in}(-k) \right.\]
\[ \times \exp[-i(\frac{\pi}{2} + F(-k) + ks)] \exp(-iE(k)t/\hbar); \quad (2.24) \]

3) the combined reverse motion -
\[ f^{(3)}_{in}(k,t) = f^{(1)}_{in}(k,t) + f^{(2)}_{in}(k,t), \quad f^{(3)}_{out}(k,t) = [f_{in}(-k,t)]^* \quad (2.25) \]

(it is evident that the last asymptotes describe the motion that is reverse with respect to the left-side case (see (1.11)).
As is seen from (2.23) and (2.24), the second terms in the right (and left) and then reflected by (transmitted through) data to describe particles impinging on the barrier from the right (left) case the function of the scattering event. Before this instant the state of a particle evolves in the vicinity of the total in asymptote. One can say that in order to define the function of the total in asymptote. That is, the set of the experimentally obtained solutions to (3.1) - (3.2) can be written in the form (see expressions (A19) and (A20).

Each of equations (3.1) - (3.3) have two roots. A simple analysis shows that in the case of (3.1) one has to take the smallest root. But in the case of (3.2) and (3.3) only the biggest root has a physical sense. So, the searched-for solutions to (3.1) - (3.2) can be written in the form

\[ t_{\text{start}} = \frac{m}{\hbar} \cdot \frac{a k_0 - \sqrt{l_{\text{tr}}^2 k_0^2 + (a^2 - l_{\text{tr}}^2) < (\delta k)^2 >_{\text{tr}}}}{k_{\text{tr}} - < (\delta k)^2 >_{\text{in}}} \]

(3.4)

(remind that \( a \gg l_0 \)); for \( n = 1, 2 \)

\[ t_{\text{end}}^{(n)} = \frac{m}{\hbar} \left( \frac{b_n k_n - \chi_n}{k_n^2 - \delta k_n^2} \right) \sqrt{\sigma_n k_n^2 + \chi_n^2 - 2k_n b_n \chi_n + (b_n^2 - \sigma_n) \delta k_n^2} ; \]

\[ k_{1,2} = < k >_{(\text{tr,ref})}, \quad \delta k_{1,2} = \sqrt{< (\delta k)^2 >_{(\text{tr,ref})}} \]

(see also expressions (A19) and (A25) for transmission, and (A20) and (A26) for reflection).

The maximal time, \( t_{\text{end}}^{(1)} \) or \( t_{\text{end}}^{(2)} \), we take as the end time, \( t_{\text{end}} \), of scattering. Then the total scattering time, \( t_{\text{scatt}} \), can be defined as the difference \( t_{\text{end}} - t_{\text{start}} \).

A simple analysis shows that this quantity is strictly positive when the inequalities

\[ k_0 > \sqrt{< (\delta k)^2 >_{\text{in}}}, \quad (3.6) \]

and

\[ k_n > \delta k_n ; \quad n = 1, 2 \]

(3.7)

are fulfilled. They should be considered as the conditions of a completed scattering. In this case, with the sufficient accuracy, one can say that all incident particles start at \( t = 0 \) toward the barrier, and the transmitted and reflected packets occupy, in the limit \( t \to \infty \), disjoint spatial regions. For a completed scattering the hierarchy \( t_{\text{end}} > t_{\text{start}} > 0 \) is obvious to be true. The second inequality is satisfied due to (3.6). The first one is valid, since the quantum ensemble of particles cannot leave the barrier region before entering it: the number of particles in the whole quantum ensemble is constant. In this case it is important to note that, in the limit \( k_{\text{tr}}^2 \to < (\delta k)^2 >_{\text{in}} \),...
\[ t_{\text{start}} = \frac{m(a^2 - l_0^2)}{2\hbar k_0 a} \approx \frac{ma}{2\hbar k_0}. \]

That is, expression (3.4) has no singularity in this limit.

One can easily show that there is an optimal value of \( l_0 \) at which \( \tau_{\text{scatt}} \) is minimal: in the limit \( l_0 \to \infty \), the scattering time grows together with \( l_0 \), but at small values of this parameter this time is large because of the fast spreading of the wave packet. If requirements (3.7) are violated, the transmitted and reflected packets must be overlapped at \( t \to \infty \) due to their spreading. As a result, the scattering event becomes incomplete.

In the limit \( l_0 \to \infty \), i.e., for narrow (in \( k \)-space) wave packets, expressions (3.4) - (3.5) are essentially simplified. In this case \( k_2 = k_1 = k_0 \) and terms with \( <(\delta k)^2> \), \( <(\delta k)(\delta J')> \) and \( <(\delta k)(\delta F')> \) may be neglected. Taking into account only the dominant terms in (3.4) - (3.5), we obtain

\[ t_{\text{start}} = \frac{m}{\hbar k_0}(a - l_0); \]

\[ t_1 - t_{\text{start}} = \frac{m}{\hbar k_0} l_{\text{scat}}^{(1)}, \quad t_2 - t_{\text{start}} = \frac{m}{\hbar k_0} l_{\text{scat}}^{(2)} \quad (3.8) \]

where

\[ l_{\text{scat}}^{(1)} = l_0 + <J'>_{\text{tr}} + \sqrt{\sigma_1} \quad (3.9) \]

\[ l_{\text{scat}}^{(2)} = l_0 + <J' - F'>_{\text{ref}} + \sqrt{\sigma_2}. \quad (3.10) \]

The maximum of these differences should be taken as the total scattering time \( \tau_{\text{scatt}} \) and the corresponding quantity, \( l_{\text{scat}}^{(1)} \) or \( l_{\text{scat}}^{(2)} \), may be treated, in this particular case, as the scattering length. Note, for the right-side case the sign of \( F'(k) \), in the expressions for scattering time and length, is opposite. For symmetric potential barriers this derivative is equal to zero for all \( k \).

**CONCLUSION**

One of the main aims of this paper was to argue that in the case of a one-dimensional completed scattering the conventional quantum theory quite admits a separate description of transmitted and reflected particles at the stage preceding the scattering event. We introduced the notion of the transmission and reflection channels and showed that for each channel one can define an unique (unitary) scattering matrix. By the known out asymptotes describing separately transmitted and reflected particles, these matrices enable one to reconstruct uniquely in asymptotes to describe separately to-be-transmitted and to-be-reflected particles. As was shown, the momentum distribution and the number of particles calculated over the in and out asymptotes, for each channel, should be the same. Besides, in both scattering channels particles were shown to start, on the average, from the same point. As regards the second and higher moments of the position operator, they cannot be determined separately for these two subensembles of particles.

On this basis we proposed characteristic times to describe tunneling a spinless particle through a time-independent potential barrier. We introduced the individual delay times for transmission and reflection. Besides, to estimate the duration of the scattering event, we derived the expression for the (total) scattering time. All three tunneling times can be applied for wave packets of an arbitrary width. They were obtained in terms of the mean values of the particle’s momentum and phase times calculated over the incident, transmitted or reflected wave packets. In addition, we found the conditions to be satisfied for a completed scattering.

**APPENDIX: EXPECTATION VALUES OF OPERATORS OVER IN AND OUT-STATES**

Let us consider the left-side case (see Exp. (1.11) and calculate all needed moments of the position and momentum operators over the incident, transmitted and reflected wave packets. In the limit \( t \to -\infty \) we have to deal with the incident one to move along in asymptote (1.12). In the limit \( t \to \infty \) we have to consider transmitted and reflected packets to correspond to separate out asymptotes (1.14) and (1.15) (separate in asymptotes (2.3) and (2.4) can be treated by the same manner). Let us write down these wave functions in the form

\[ \Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} df(k, t)e^{ikx}, \quad (A1) \]

\[ f(k, t) = M(k)\exp(i\xi(k, t)) \]

(remind that \( f(k, t) \in S_{\text{scat}} \)): \( M(k) \) and \( \xi(k, t) \) are the real functions. In particular, for the incident packet (1.12) we have

\[ M_{\text{in}}(k) = |A^{(+)}_{\text{in}}(k)|; \quad \xi_{\text{in}}(k, t) = -\frac{\hbar k^2t}{2m}. \quad (A2) \]

For the transmitted (1.14) and reflected (1.15) packets,

\[ M_{\text{tr}}(k) = \sqrt{T(k)}M_{\text{in}}(k); \]

\[ \xi^{tr}_{\text{in}}(k, t) = \xi_{\text{in}}(k, t) + J(k) - kd; \quad (A3) \]

\[ M_{\text{ref}}(k) = \sqrt{R(k)}M_{\text{in}}(k); \]

\[ \xi^{ref}_{\text{in}}(-k) = \xi_{\text{in}}(k, t) + 2ka + J(k) - F(k) - \frac{\pi}{2}. \quad (A4) \]

Fourier transformation (A1)-(A4) enables one to determine the time dependence of the expectation value \( <\hat{Q}> \) for any Hermitian operator \( \hat{Q} \), at the stages preceding and following the scattering event.
\[ <\hat{Q}> = \frac{<\Psi|\hat{Q}|\Psi>}{<\Psi|\Psi>}, \quad (A5) \]

where \(\Psi\) is one of the above wave functions (for a subensemble of particles this value acquires the status of a conditional probability).

Note that for the incident and reflected packets the integrals in (A5) should be calculated, strictly speaking, over the interval \((-\infty, a]\). For the transmitted packet, one needs to integrate over the interval \([b, \infty)\). Expressions (A1)-(A4) for these packets are valid only for the corresponding spatial region and corresponding stage of scattering. However, taking into account that the body of each packet is located, in the limit \(t \to \infty\) or \(t \to -\infty\), in its “own” spatial region, we may extend the integration in (A5) onto the whole \(OX\)-axis. Due to this step the description of these packets becomes very simple. As regards a mistake introduced in the formalism, one can expect that it is sufficiently small; in any case, the farther is the packet from the barrier at the initial time, the smaller is this mistake. It vanishes in the limits \(t \to \mp \infty\) when the particle’s state moves along the in and out asymptotes. Thus, the \(k\)-representation provides a suitable basis for the calculation of desired characteristics of all three packets.

1. **Normalization**

So, within the above accuracy, the norms of these functions are constant beyond the scattering region,
\[ <\Psi(x, t)|\Psi(x, t)> = \int_{-\infty}^{\infty} dk M^2(k). \quad (A6) \]

Then for each packet we have the following norms. Since \(\Psi_{r(0)}^{(0)}\) is normalized function, we have
\[ <\Psi_{r(0)}|\Psi_{r(0)}> = \int_{-\infty}^{\infty} dk M^2_{in}(k) = 1. \quad (A7) \]

For the transmitted packet,
\[ <f_{out}^t|f_{out}^t> = \int_{-\infty}^{\infty} dk |M_{out}^t(k)|^2 \]
\[ = \int_{-\infty}^{\infty} dk T(k) M_{in}^2(k) \equiv <T(k)>_{in} \equiv \hat{T}. \quad (A8) \]

For the reflected packet,
\[ <f_{out}^{ref}|f_{out}^{ref}> = \int_{-\infty}^{\infty} dk |M_{out}^{ref}(k)|^2 \]
\[ = \int_{-\infty}^{\infty} dk R(k) M_{in}^2(-k). \]

Having made an obvious change of variables, we obtain
\[ <f_{out}^{ref}|f_{out}^{ref}> = <R(k)>_{in} \equiv \hat{R}. \quad (A9) \]

From (A7) - (A9) it follows that
\[ \hat{T} + \hat{R} = 1. \quad (A10) \]

2. **The expectation values of the operators \(\hat{k}^n\) (\(n\) is the positive number)**

Since in the \(k\)-representation \(\hat{k}\) is a multiplication operator, for any number \(n\) we have
\[ <\Psi|\hat{k}^n|\Psi> = \int_{-\infty}^{\infty} dk M^2(k) k^n. \quad (A11) \]

Now we can treat separate packets. From (A11) and (A3) it follows that
\[ <f_{out}^t|f_{out}^t> = <f_{in}|T(k)k^n|f_{in}>. \]

In a similar way we find also that
\[ <f_{out}^{ref}|f_{out}^{ref}> = (-1)^n <f_{in}|R(k)k^n|f_{in}> \]
and, hence,
\[ <T(k)k^n>_{in} = \hat{T} <k^n>_{tr}, \]
\[ <R(k)k^n>_{in} = (-1)^n \hat{R} <k^n>^{ref}. \quad (A12) \]

As a consequence, the next relationship is obvious to be valid
\[ <k^n>_{in} = \hat{T} <k^n>_{out} + \hat{R} <(-k)^n>_{out}. \quad (A13) \]

3. **The expectation values of the operator \(\hat{x}\)**

We begin again with expressions to be common for all three packets. Since \(\hat{x} = i \frac{\partial}{\partial k}\) we have
\[ <\Psi|\hat{x}|\Psi> = i \int_{-\infty}^{\infty} dk f^*(k, t) \frac{\partial f(k, t)}{\partial k} = \]
\[ = i \int_{-\infty}^{\infty} dk M(k) \frac{dM(k)}{dk} - \int_{-\infty}^{\infty} dk M^2(k) \frac{\partial \xi(k, t)}{\partial k}. \quad (A14) \]

Since the first term here is equal to
\[ \frac{i}{2} M^2(k)|^{\infty}_{-\infty} = 0, \]
we have
\[ <\Psi|\hat{x}|\Psi> = - \int_{-\infty}^{\infty} dk M^2(k) \frac{\partial \xi(k, t)}{\partial k} \]
\[ \equiv <f|\frac{\partial \xi(k, t)}{\partial k}|f> \quad (A15) \]

For the incident and transmitted packets, taking into account expressions (A2) and (A3) for \(\xi(k, t)\), we obtain
\[ <\hat{x}>_{in} = \frac{\hbar}{m} k_0, \quad (A16) \]
\[ <\hat{x}>_{out} = \frac{\hbar}{m} <k>_{out} - <J'(k)>_{out} + d. \quad (A17) \]
Since the functions $J'(k)$ and $F'(k)$ are even, from (A4) it follows that

$$<\hat{x}>_{out}^{ref} = 2a + J'(k) - F'(k) >_{out}^{ref} - \frac{\hbar t}{m} < k >_{out}^{ref}.$$  

(A18)

Let, at the instant $t$, $L_{tr}$ be the distance between the CM of the transmitted packet and the nearest boundary of the barrier, i.e., $L_{tr} = <\hat{x}>_{tr} - b$. Similarly, let $L_{ref}$ be the distance between the CM and the corresponding barrier’s boundary for the reflected packet at the same instant: $L_{ref} = a - <\hat{x}>_{ref}$. From (A17) and (A18) it follows that

$$L_{tr}(t) = \frac{\hbar t}{m} < k >_{tr} - b_1,$$

(A19)

$$L_{ref}(t) = \frac{\hbar t}{m} < - k >_{ref} - b_2$$

(A20)

where $\bar{b}_1 = < J'(k) >_{out}^{tr} + a$, $\bar{b}_2 = < J'(k) >_{out}^{ref} >_{out}^{ref} + a$.

4. The mean-square deviations in $x$-space

Let us derive firstly the expression for all packets. We have

$$<\Psi|\hat{x}^2|\Psi> = -\int_{-\infty}^{\infty} dk f^*(k,t) \frac{\partial^2 f(k,t)}{\partial k^2}. $$

Since

$$\frac{\partial^2 f(k,t)}{\partial k^2} = [M'' - M(\xi')^2 + i(2M'\xi' + M'') ] e^{i\xi}, $$

we have

$$<\Psi|\hat{x}^2|\Psi> = \int_{-\infty}^{\infty} dk M[M(\xi')^2 - M'']$$

$$- i \int_{-\infty}^{\infty} dk [(M')^2 + M^2 \xi''].$$

(A21)

One can easily show that the last integral in (A21) is equal to zero. Therefore

$$<\Psi|\hat{x}^2|\Psi> = \int_{-\infty}^{\infty} dk M^2(k)[\xi'(k,t)]^2$$

$$+ \int_{-\infty}^{\infty} dk [M'(k)]^2.$$  

(A22)

Let, for any operator $\hat{Q}$, $< (\delta \hat{Q})^2 >$ be the mean-square deviation: $\delta \hat{Q} = \hat{Q} - < \hat{Q} >$. For the operator $\hat{x}$ we have

$$< (\delta \hat{x})^2 > = < (\ln' M)^2 > + < (\delta \xi')^2 >.$$  

(A23)

Now we are ready to find these quantities for each packet. Using (A23) and expressions (A2)-(A4), one can show that for incident packet

$$< (\delta \hat{x})^2 >_{in} = (ln' A)^2 >_{in} + \frac{\hbar^2 t^2}{m^2} < (\delta k)^2 >_{in}$$

(A24)

(here the first term is equal to $l^2_0$, in accordance with the initial condition); for the transmitted packet

$$< (\delta \hat{x})^2 >_{out}^{tr} = \sigma_1 - 2\frac{\hbar t}{m} \chi_1 + \frac{\hbar^2 t^2}{m^2} < (\delta k)^2 >_{out}^{tr},$$

(A25)

for the reflected packet

$$< (\delta \hat{x})^2 >_{out}^{ref} = \sigma_2 - \frac{\hbar t}{m} \chi_2 + \frac{\hbar^2 t^2}{m^2} < (\delta k)^2 >_{out}^{ref};$$

(A26)

where

$$\sigma_1 = (ln' M_{out}^{tr})^2 >_{out}^{tr} + < (\delta J')^2 >_{out}^{tr};$$

$$\sigma_2 = (ln' M_{out}^{ref})^2 >_{out}^{ref} + < (\delta J' - \delta F')^2 >_{out}^{ref};$$

$$\chi_1 = < (\delta J')(\delta k) >_{out}^{tr}, \chi_2 = - < (\delta J' - \delta F')(\delta k) >_{out}^{ref}.$$
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