Wave functions and tunneling times for one-dimensional transmission and reflection.

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Abstract

It is shown that in the case of the one-particle one-dimensional scattering problem for a given time-independent potential, for each state of the whole quantum ensemble of identically prepared particles, there is an unique pair of (subensemble’s) solutions to the Schrödinger equation, which, as we postulate, describe separately transmission and reflection: in the case of nonstationary states, for any instant of time, these functions are orthogonal and their sum describes the state of all particles; evolving with constant norms, one of them approaches at late times the transmitted wave packet and another approaches the reflected packet. Both for transmission and reflection, 1) well before and after the scattering event, the average kinetic energy of particles is the same, 2) the average starting point differs, in the general case, from that for all particles. It is shown that for reflection, in the case of symmetric potential barriers, the domain of the motion of particles is bounded by the midpoint of the barrier region. We define (exact and asymptotic) transmission and reflection times and show that the basic results of our formalism can be, in principle, checked experimentally.

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1 Introduction

For a long time tunneling a particle through an one-dimensional time-independent 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) [1, 2, 3, 4, 5] (see also [6]), in which the study of the temporal aspects of tunneling is reduced to following the centers of "mass" (CMs) of wave packets, does not provide a clear prescription both how to interpret properly the scattering of finite in $x$ space wave packets and how to introduce characteristic times for a tunneling particle. All these questions constitute the main content of the so-called tunneling time problem (TTP) which have been of great interest for the last decades.

As is known, the main peculiarity of the tunneling of finite wave packets is that the average particle’s kinetic energy for the transmitted, reflected and incident wave packets is different. For example, in the case of tunneling through an opaque rectangular barrier, the average velocity of the transmitted particle is larger than that of the incident particle. It is evident that this fact needs a proper explanation. As was pointed out in [7, 8], it would be strange to interpret the above property of wave packets as the evidence of accelerating a particle (in the asymptotic regions) by the static potential barrier. Besides, in this case there is no causal link between the transmitted and incident wave packets (see [7, 8]).

As regards wide (strictly speaking, infinite) in $x$ space wave packets, the average kinetic energy of particles, before and after the interaction, is the same. But now the uncertainty in defining the CM’s position and, consequently, corresponding asymptotic times is very large. As a result, the most of physicists considers the characteristic times introduced in the SWPA as quantities having no physical sense. The review [1] devoted to the TTP seems to be the last one in which the SWPA is considered in a positive context.

Apart from the SWPA, in the same or different setting the tunneling problem, a variety of alternative approaches (see reviews [1, 8, 9, 10, 11, 12] and references therein) to advance different characteristic times for a tunneling particle have also been developed. Among the alternative conceptions, of interest are that of the dwell time [13, 14, 15, 16], that of the Larmor time [17, 18, 19, 20, 21] to give the way of measuring the dwell time, and the conception of the time of arrival which is based on introducing either a suitable time operator (see, for example, [22, 23, 24, 25, 26]) or the positive operator valued measure [11]. Besides, of interest are attempts to study the temporal aspects of tunneling in the frame of the Feynman, Bohmian and Wigner approaches to deal with the random trajectories of particles (see, for example, [27, 28, 29, 30, 31] and references therein). One should also mention the papers [32, 33, 34] where the TTP is studied in the framework of a nonstandard setting the scattering problem. But again, for a particle whose initial state is described by a Gaussian-like wave packet, none of the alternative approaches have not yet led to commonly accepted characteristic times (see the reviews [1, 8, 9, 10, 11, 12]).

Note, unlike the SWPA, in all these approaches theoretical efforts have been aimed
at elaborating some rule of timing the motion of a quantum particle. As was said in [11], "... up to now the interest of theoreticians [to the TTP] has been motivated ... by a fundamental lacuna of quantum theory, namely the absence of a clear prescription to incorporate time observables into its formalism". However, in our opinion, there is no necessity in such a prescription: time in quantum mechanics has the status of a parameter, and, hence, there is no room here for time observables (or, time operators). And, what is more important, the rule of timing the particle's motion have already been available in quantum theory, and this rule is dictated by the correspondence principle.

By the analogue with classical mechanics where timing the particle's motion is reduced to the analysis of the function $x(t)$ ($x$ is the particle's position, $t$ is time), in quantum mechanics characteristic times for a particle should be derived from studying the temporal dependence of the expectation (average) value of the position operator for a particle in a given state (or, what is equivalent, from studying the temporal behavior of the CM of the corresponding wave packet). Besides, from the analysis of the temporal dependence of the mean-square deviation for this operator (or, from the analysis of the temporal behavior of the corresponding leading and trailing edges of the wave packet) one can take into account uncertainty in the particle's position, and thereby evaluate the error of the above timing.

However, one has to bear in mind the following. The above timing procedure suggests that the average value of the position operator has its primary physical sense, as the most probable position of a particle, at all stages of its motion. For a free particle whose state is described by a Gaussian-like wave packet, this requirement is fulfilled and, thus, no problem arises in timing its motion. An essentially different situation takes place in the case of a tunneling particle. Now, following the CM of the wave packet to describe the state of the whole ensemble of particles becomes meaningless at some stages of scattering. In particular, after the scattering event, when we deal, in fact, with two scattered (transmitted and reflected) wave packets, the averaging over the whole ensemble of particles has no physical sense. Of course, in this case there is a possibility to define the individual average positions of transmitted and reflected particles. However, in timing, such averaging suggests the separate description of both the subensembles at early times, what is widely accepted to be impossible in quantum mechanics. As was pointed out in [12], "... transmission and reflection are inextricably intertwined".

So, quantum theory provides the needed rule of timing the motion of a particle, but it conflicts with the existing viewpoint that transmission and reflection are allegedly inseparable (namely this obstacle have remained to overcome in the SWPA). However, in our opinion, there is no basis for such a viewpoint. For none of the principles of quantum mechanics forbids such a separation. In reality, the main problem is that quantum theory, as it stands, does not provide the way of separating transmission and reflection. In our opinion, just the absence of the corresponding mathematical formalism is a fundamental lacuna in quantum theory.

In this paper, in the framework of the conventional quantum mechanics, we show
that, at least in one dimension, transmission and reflection can be described separately. It is surprising that such a description needs no innovation. As it has turned out, the separation of transmission and reflection is provided by the intrinsic property of the Schrödinger equation, which have been overlooked before. Namely, we show that in the standard setting the one-dimensional scattering problem for a given potential the Schrödinger equation possesses, in addition to the solution to describe the state of the whole ensemble of particle, an unique pair of other solutions which, as we postulate, describe separately transmission and reflection. The basis for such a postulate is that, for any instant of time, the subensemble’s nonstationary-state wave functions are mutually orthogonal and their sum describes the state of the whole ensemble of particles; one of them causally evolves into the transmitted wave packet, and another approaches at late times the reflected one. The main peculiarity of stationary-state wave functions for transmission and reflection is that, for a given energy of particle, there is a point in the barrier region where these everywhere continuous functions have discontinuous first spatial derivatives. Nevertheless, this point is not a sink or source of particles for each subensemble. So that the norms of the corresponding wave packets are constant in time.

Note, at present there is a paradoxical situation. Although the tunneling phenomenon have been known for a long time, the properties of tunneling proper have remained, in fact, unstudied. The point is that the "full" wave function to describe the state of a particle in the one-dimensional scattering problem relates to all particles of the quantum ensemble, rather than to transmitted particles only. In this connection, we hope that the formalism presented here will be useful for a deeper understanding of the tunneling process and, in particular, Hartman effect [3] widely discussed in the literature (see, for example, [35]).

The paper is organized as follows. In Section 2 we pose a complete one-dimensional scattering problem for a particle, and display explicitly shortcomings to arise in the SWPA in solving the TTP. In Section 3 we present a renewed wave-packet analysis in which transmission and reflection are treated separately. In Section 4 we define the average (exact and asymptotic) transmission and reflection times and consider, in details, the cases of rectangular barriers and δ-potentials.

2 Setting the problem for a completed scattering

2.1 Backgrounds

Let us consider a particle tunneling 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 $\Psi_{in(0)}(x)$. The function is proposed to belong to the set $S_\infty$ consisting from infinitely differentiable functions vanishing exponentially in the limit $|x| \to \infty$. The Fourier-transform of such functions are known to belong to the set $S_\infty$ as well. In this case the position and momentum
operators both are well-defined. Without loss of generality we will suppose that
\[ <\Psi^{(0)}_{left}|\hat{x}\Psi^{(0)}_{left}> = 0, \quad <\Psi^{(0)}_{left}|\hat{p}\Psi^{(0)}_{left}> = \hbar k_0 > 0, \quad <\Psi^{(0)}_{left}|\hat{x}^2\Psi^{(0)}_{left}> = l_0^2, \]
here \( l_0 \) is the wave-packet’s half-width at \( t = 0 \) (\( l_0 << a \)); \( \hat{x} \) and \( \hat{p} \) are the operators of the particle’s position and momentum, respectively.

An important restriction should be imposed also on the rate of spreading the incident wave packet. Namely, we will suppose that the average velocity \( \bar{\hbar k_0}/m \) is large enough, so that in the incident wave packet its parts lying behind the CM within the wave-packet’s half-width move toward the barrier.

As is known, the formal solution to the temporal one-dimensional Schrödinger equation (OSE) of the problem can be written as \( e^{-i\hat{H}t/\hbar}\Psi_{in}(x) \). To solve explicitly this equation, we will use here the variant (see [36]) of the well-known transfer matrix method [37] that allows one to calculate the tunneling parameters, as well as to connect the amplitudes of the outgoing and corresponding incoming waves, for any system of potential barriers. The state of a particle with the wave-number \( k \) can be written in the form
\[
\Psi_{full}(x; k) = A_{in}(k)e^{ikx} + B_{out}(k)e^{-ikx},
\]
for \( x \leq a \), and
\[
\Psi_{full}(x; k) = A_{out}(k)e^{ikx} + B_{in}(k)e^{-ikx},
\]
for \( x > b \), where \( A_{in}(k) \) should be found from the initial condition; \( B_{in}(k) = 0 \). The coefficients entering this solution are connected by the transfer matrix \( Y \):
\[
\begin{pmatrix} A_{in} \\ B_{out} \end{pmatrix} = Y \begin{pmatrix} A_{out} \\ B_{in} \end{pmatrix}; \quad Y = \begin{pmatrix} q & p \\ p^* & q^* \end{pmatrix};
\]
which can be expressed in terms of the real tunneling parameters \( T, J \) and \( F \),
\[
q = \frac{1}{\sqrt{T(k)}} \exp [i(kd - J(k))]; \quad p = \sqrt{\frac{R(k)}{T(k)}} \exp \left[ i \left( \frac{\pi}{2} + F(k) - ks \right) \right];
\]
\( T(k) \) (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 the tunneling parameters have already been known explicitly. To find them, one can use the recurrence relations obtained in [36] just for these real parameters.
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 the corresponding in or out asymptote [38]. Thus, definitions of characteristic times in this approach can be done in terms of the in and out asymptotes of the tunneling problem.

Note that in asymptote in the one-dimensional scattering problem represents an one-packet object to converge, well before the scattering event, with the incident wave packet, while out asymptote represents the superposition of two non-overlapped wave packets to converge, at $t \to \infty$, with the transmitted and reflected ones. It is easy to show that in the problem at hand in asymptote, $\Psi_{in}(x, t)$, and out asymptote, $\Psi_{out}(x, t)$, can be written as follows

$$\Psi_{in}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_{in}(k, t)e^{ikx}dk, \quad f_{in}(k, t) = A_{in}(k) \exp[-iE(k)t/\hbar];$$  \hspace{1cm} (5)$$

$$\Psi_{out}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} [f_{tr}(k, t) + f_{ref}(k, t)] e^{ikx}dk, \quad f_{out}(k, t) = f_{out}^{tr}(k, t) + f_{out}^{ref}(k, t);$$ \hspace{1cm} (6)$$

$$f_{out}^{tr}(k, t) = \sqrt{T(k)}A_{in}(k) \exp[i(J(k) - k\beta - E(k)t/\hbar)];$$ \hspace{1cm} (7)$$

$$f_{out}^{ref}(k, t) = \sqrt{R(k)}A_{in}(-k) \exp[-i(J(k) - F(k) - \pi/2 + 2ka + E(k)t/\hbar)] \quad (8)$$

where $E(k) = \hbar^2 k^2/2m$.

For a completed scattering we have

$$\Psi_{full}(x, t) \approx \Psi_{in}(x, t) \quad \text{when} \quad t = 0,$$

$$\Psi_{full}(x, t) = \Psi_{out}(x, t) \quad \text{when} \quad t \to \infty.$$

It is obvious that the larger is the distance $a$, the more correct is the approximation for $\Psi_{full}(x, t)$ at $t = 0$.

For particles starting (on the average) from the origin, we have

$$<\hat{x}>_{in} = \frac{\hbar k_0}{m} t$$ \hspace{1cm} (9)$$

(hereinafter, for any Hermitian operator $\hat{Q}$)

$$<\hat{Q}>_{in} = \frac{<f_{in}|\hat{Q}|f_{in}>}{<f_{in}|f_{in}>};$$
similar notations are used below for the transmitted and reflected wave packets). The averaging separately over the transmitted and reflected wave packets yields

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

(10)

\[ \langle \hat{x} \rangle_{\text{ref}}^{\text{out}} = \frac{\hbar t}{m} < k >_{\text{ref}}^{\text{out}} + \langle J'(k) - F'(k) >_{\text{ref}}^{\text{out}} + 2a \]  

(11)

(hereinafter the prime denotes the derivative with respect to \( k \)). Exps. (9) — (11) yield the basis for defining the asymptotic tunneling times in the SWPA.

2.2 Problems of the standard wave-packet analysis

To display explicitly some shortcomings of the SWPA, let us derive again the SWPA’s tunneling times. 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 [4], 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

\[ \langle \hat{x} \rangle_{\text{in}}^{\text{tr}} (t_1) = a - L_1; \quad \langle \hat{x} \rangle_{\text{tr}}^{\text{out}} (t_2) = b + L_2. \]  

(12)

Then, considering (9) and (10), one can write the ”transmission time” \( \Delta t_{\text{tr}} \) \((\Delta t_{\text{tr}} = t_2 - t_1)\) for the given interval in the form

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

(13)

Similarly, for the reflected packet, let \( t_1' \) and \( t_2' \) be such instants of time that

\[ \langle \hat{x} \rangle_{\text{in}}^{\text{ref}} (t_1') = \langle \hat{x} \rangle_{\text{ref}}^{\text{out}} (t_2') = a - L_1. \]  

(14)

From equations (9), (11) and (14) it follows that the ”reflection time” \( \Delta t_{\text{ref}} \) \((\Delta t_{\text{ref}} = t_2' - t_1')\) can be written as

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

(15)
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 is described by the Gaussian wave packet, we have

$$A_{in}(k) = A \exp(-l_0^2(k - k_0)^2), \quad A = \left(\frac{l_0^2}{\pi}\right)^{1/4}.$$ 

On can show that in this case

$$< k >_{tr} = k_0 + \frac{< T >_{in}}{4l_0^2 < T >_{in}}; \quad \quad (16)$$

$$< -k >_{ref} = k_0 + \frac{< R >_{in}}{4l_0^2 < R >_{in}}. \quad \quad (17)$$

Let

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

then relations (16) and (17) can be written in the form

$$< T >_{in} < (\Delta k)_{tr} = - < R >_{in} < (\Delta k)_{ref} = \frac{< T >_{in}}{4l_0^2}. \quad \quad (18)$$

Note that $R' = -T'$.  

As is seen, quantities (13) and (15) 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 \cite{1, 4, 5, 15} shows in this case a premature appearance of the CM of the transmitted packet behind the barrier, what points to the lack of a causal link between the transmitted and incident wave packets (see \cite{8}).

As was shown in \cite{1, 4}, this effect disappears in the limiting case $l_0 \to \infty$. For example, in the case of Gaussian wave packets the fact that the last terms in (13) and (15) tend to zero when $l_0 \to \infty$, with the ratio $l_0/a$ being fixed, can be proved with help of Exps. (16) and (17) (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, at first glance, in the limit $l_0 \to \infty$ the SWPA seems to provide correct characteristic times for a particle. However, as will be seen from our formalism, even in this case, the above times are poorly defined. The point is that the above definitions of tunneling times for transmission and reflection are based on the implicit assumption that particles of both the subensembles start, on the average, from the origin as those of a whole quantum ensemble. As will be seen from the following, this is not the case.
Note, the fact that Exps. (13) and (15) 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 principal shortcoming of the above approach is that it is meaningless to compare the motion of the transmitted (or reflected) wave packet with that of the incident one since they are related to different ensembles of particles and, as a consequence, there is no causal relationship between them. The right procedure of a separate timing of transmitted particles suggests the availability of such initial wave packet to evolve causally into the transmitted one.

3 Separate description of transmission and reflection in the one-dimensional scattering problem

For a long time the processes of transmission and reflection in a quantum scattering have been accepted to be inseparable, in principle. However, in this paper we show that, at least in the one-dimensional case, there are sound reasons to consider these processes separately.

3.1 Wave function of a tunneling particle as a sum of wave functions to describe separately transmission and reflection

According to quantum scattering theory, in one dimension, stationary-state wave functions for a particle impinging the barrier from the left (or from the right) possess one incoming and two outgoing waves. That is, in this case we deal, in fact, with one-source two-sinks scattering problems.

Let for the problem at hand the amplitude of incoming wave, \( a_{in} \), be equal to unit, then the amplitudes of all four waves read as

\[
a_{in} = 1, \quad b_{out} = \frac{p^*}{q}, \quad a_{out} = \frac{1}{q}, \quad b_{in} = 0
\]  

(note, \( B_{out} = b_{out}A_{in} \), \( A_{out} = a_{out}A_{in} \), \( B_{in} = b_{in}A_{in} \)). Let us also consider two auxiliary (two-sources one-sink) scattering tasks in which the amplitudes of incoming and outgoing waves are

\[
a_{in}^{ref} = \frac{|p|^2}{|q|^2}, \quad b_{out}^{ref} = \frac{p^*}{q}, \quad a_{out}^{ref} = 0, \quad b_{in}^{ref} = \frac{p^*}{|q|^2};
\]  

and

\[
a_{in}^{tr} = \frac{1}{|q|^2}, \quad b_{out}^{tr} = 0, \quad a_{out}^{tr} = \frac{1}{q}, \quad b_{in}^{tr} = -\frac{p^*}{|q|^2}
\]
(the transfer matrix (3) is common for all three tasks).

Note that in the first auxiliary task the only outgoing wave coincides with the reflected wave arising in the problem at hand (see (19)). And, in the second task, the only outgoing wave coincides with the transmitted wave in (19). It is evident that the sum of these two functions results just in that to describe the state of a particle in the initial tunneling problem.

As is seen, the main peculiarity of the superposition of these two states is that due to interference the incoming waves, in the region $x > b$, disappear entirely (note that in the corresponding reverse motion they are outgoing waves). Figuratively speaking, interference reorients these waves into the region $x < a$. That is, in this superposition the probability fields of both sinks are radically reconstructed due to interference. Namely, they transform into fields with one outgoing and one incoming waves.

Hereinafter, the wave function in which an incoming wave is associated with the reflected wave of solution (19) will be referred to as the reflection wave function (RWF). Similarly, the wave function in which an incoming wave is related to the transmitted wave of (19) will be referred to as the transmission wave function (TWF). We postulate that, in the considered scattering problem, namely the nonstationary-state TWF and RWF describe, respectively, the transmission and reflection processes. As will be shown below, both the functions evolve in time with constant norms; at late times the TWF (RWF) coincides with the transmitted (reflected) wave packet.

Thus, we see that the sum of wave functions (20) and (21) can be presented as that of the stationary-state RWF and TWF. Under the reconstruction of the probability fields, the squared amplitude of the incoming wave (in the region $x < a$) associated with reflection increases due to interference from the initial value $|a_{in}^{ref}|^2 (= R^2)$ (see (20)) to $|a_{in}^{ref}|^2 + |b_{in}^{ref}|^2 (= R^2 + TR = R)$ (in the RWF). In the case of transmission the corresponding quantity increases from the initial value $|a_{in}^{tr}|^2 (= T^2)$ (see (21)) to $|a_{in}^{tr}|^2 + |b_{in}^{tr}|^2 (= T^2 + TR = T)$ (in the TWF).

Of course, the above postulate suggests the availability of a proper pair of solutions to the Schrödinger equation. The main thing which should be taken into account in finding these solutions is that the RWF describes the states of reflected particles only, and the TWF relates only to transmitted particles. As was said above, in both the cases, stationary solutions should contain one incoming and one outgoing wave. In this paper we show that such solutions do exist.

### 3.2 Wave functions for one-dimensional transmission and reflection

So, let $\Psi_{tr}$ and $\Psi_{ref}$ be the searched-for TWF and RWF, respectively. In line with subsection 3.1, their sum represents the wave function to describe, in the problem at hand, the state of the whole ensemble of particles. Hence, from the mathematical point of view our task now is to find such solutions $\Psi_{tr}$ and $\Psi_{ref}$ to the Schrödinger equation that
for any $t$,

$$\Psi_{\text{full}}(x, t) = \Psi_{\text{tr}}(x, t) + \Psi_{\text{ref}}(x, t)$$

(22)

where $\Psi_{\text{full}}(x, t)$ is the full wave function to describe all particles (see section 2). In the limit $t \to \infty$

$$\Psi_{\text{tr}}(x, t) = \Psi_{\text{tr}}^{\text{out}}(x, t); \quad \Psi_{\text{ref}}(x, t) = \Psi_{\text{ref}}^{\text{out}}(x, t)$$

(23)

where $\Psi_{\text{tr}}^{\text{out}}(x, t)$ and $\Psi_{\text{ref}}^{\text{out}}(x, t)$ are the transmitted and reflected wave packets whose Fourier-transforms presented in (7) and (8).

As is known, searching for the wave functions in the case of the time-independent potential $V(x)$ is reduced to the solution of the corresponding stationary Schrödinger equation. For a given $k$, let us find firstly the functions $\Psi_{\text{ref}}(x; k)$ and $\Psi_{\text{tr}}(x; k)$ for the spatial region $x \leq a$. In this region let

$$\Psi_{\text{ref}}(x; k) = A_{\text{in}}(k) \left( A_{\text{in}}^{\text{ref}}(k) e^{ikx} + B_{\text{out}}^{\text{ref}}(k) e^{-ikx} \right)$$

(24)

$$\Psi_{\text{tr}}(x; k) = A_{\text{in}}(k) \left( A_{\text{in}}^{\text{tr}}(k) e^{ikx} + B_{\text{out}}^{\text{tr}}(k) e^{-ikx} \right)$$

(25)

where $A_{\text{in}}^{\text{tr}} + A_{\text{in}}^{\text{ref}} = 1$, $B_{\text{out}}^{\text{tr}} + B_{\text{out}}^{\text{ref}} = b_{\text{out}}$.

Since the RWF describes the state of reflected particles only, the probability flux for $\Psi_{\text{ref}}(x; k)$ should be equal to zero, i.e.,

$$|A_{\text{in}}^{\text{ref}}|^2 - |B_{\text{out}}^{\text{ref}}|^2 = 0.$$  

(26)

In its turn, for $\Psi_{\text{tr}}(x; k)$ we have

$$|A_{\text{in}}^{\text{tr}}|^2 - |B_{\text{out}}^{\text{tr}}|^2 = \frac{\hbar k}{m} T(k)$$

(27)

(the probability flux for the full wave function $\Psi_{\text{full}}(x; k)$ and for $\Psi_{\text{tr}}(x; k)$ should be the same).

Taking into account that $\Psi_{\text{tr}} = \Psi_{\text{full}} - \Psi_{\text{ref}}$ let us now exclude $\Psi_{\text{tr}}$ from Eq. (27). As a result, we obtain for $\Psi_{\text{ref}}$ the equation

$$\text{Re} \left( A_{\text{in}}^{\text{ref}} a_{\text{in}}^* - B_{\text{out}}^{\text{ref}} b_{\text{out}}^* \right) = 0.$$  

(28)

The physical meaning of Eq. (28) is that the function $\Psi_{\text{ref}}(x)$, with zero probability flux, is such that the sum of the stationary-state RWF and any other stationary-state wave function with a nonzero probability flux does not change the value of the latter.
From condition (23) for $\Psi_{ref}(x; k)$ it follows that $B_{out}^{ref}(k) = b_{out}(k) \equiv p^*/q$ (see (19)). Then Eq. (28) yields $Re(A_{in}^{ref}) = R$, and Eq. (26) leads to $|A_{in}^{ref}|^2 = |B_{out}^{ref}|^2 = |p^*/q|^2 = R$. Thus, $A_{in}^{ref} = \sqrt{R}(\sqrt{R} \pm i\sqrt{T}) \equiv \sqrt{R} \exp(i\lambda)$; $\lambda = \pm \arctan(\sqrt{T}/R)$.

So, there are two solutions to satisfy the above requirements for $\Psi_{ref}(x; k)$, in the region $x \leq a$. Considering Exps. (4) for the elements $q$ and $p$, we have

$$\Psi_{ref}(x; k) = -2\sqrt{R}A_{in} \sin \left( k(x - a) + \frac{1}{2} \left( \lambda - J + F - \frac{\pi}{2} \right) \right) e^{i\phi(+)}$$

(29)

where

$$\phi(\pm) = \frac{1}{2} \left[ \lambda \pm \left( J - F - \frac{\pi}{2} + 2ka \right) \right].$$

Now we have to show that only one of these solutions describes the state of the subensemble of reflected particles. To select it, we have to study both the solutions in the region $x \geq b$ where they can be written in the form

$$\Psi_{ref}(x; k) = A_{in}(k) \left( A_{out}^{ref}(k) e^{ikx} + B_{in}^{ref}(k) e^{-ikx} \right)$$

(30)

where

$$A_{out}^{ref} = \sqrt{R} e^{i\phi(+)}; \quad B_{in}^{ref} = \sqrt{R} e^{i\phi(-)}; \quad G = q e^{-i\phi(-)} - p^* e^{i\phi(-)}.$$

Considering Exps. (4) as well as the equality $\exp(i\lambda) = \sqrt{R} \pm i\sqrt{T}$, one can show that

$$G = \mp i \exp \left[ i \left( kb - \frac{1}{2} \left( J + F + \frac{\pi}{2} - \lambda \right) \right) \right];$$

here the signs ($\mp$) correspond to those in the expression for $\lambda$. Then, for $x \geq b$, we have

$$\Psi_{ref}(x; k) = \pm 2\sqrt{R}A_{in} \sin \left[ k(x - b) + \frac{1}{2} \left( J + F + \frac{\pi}{2} - \lambda \right) \right] e^{i\phi(+)}.$$  

(31)

For the following it is convenient to go over to the variable $x'$: $x = x_{mid} + x'$ where $x_{mid} = (a + b)/2$. Then we have, for $x' \leq -d/2$,

$$\Psi_{ref}(x'; k) = -2\sqrt{R}A_{in} \sin \left[ \frac{1}{2} (kd + \lambda - J - F) + \frac{F}{2} + kx' \right] e^{i\phi(+)};$$

for $x' \geq d/2$ —

$$\Psi_{ref}(x'; k) = \pm 2\sqrt{R}A_{in} \sin \left[ \frac{1}{2} (kd + \lambda - J - F) - \frac{F}{2} - kx' \right] e^{i\phi(+)}.$$  

From these expressions it follows that for any point $x' = x_0$ ($x_0 \leq -d/2$) we have

$$\Psi_{ref}(x_0) = -2\sqrt{R}A_{in} \sin \left[ \frac{1}{2} (kd + \lambda - J - F) + kx_0 \right] e^{i\phi(+)}$$

(32)
\[
\Psi_{\text{ref}}(-x_0) = \pm 2\sqrt{RA}\sin \left[ \frac{1}{2}(kd + \lambda - J - \frac{\pi}{2} + F) + kx_0 - F \right] e^{i\phi(+)}.
\] (33)

Let us consider the case of symmetric potential barriers: \(V(x') = V(-x')\). For such barriers the phase \(F\) is equal to either 0 or \(\pi\). Then, as is seen from Exps. (32) and (33), one of the above two stationary solutions \(\Psi_{\text{ref}}(x'; k)\) is odd in the out-of-barrier region, but another function is even. Namely, when \(F = 0\) the upper sign in (33) corresponds to the odd function, the lower gives the even solution. On the contrary, when \(F = \pi\) the second root \(\lambda\) leads to the odd function \(\Psi_{\text{ref}}(x'; k)\).

It is evident that in the case of symmetric barriers both the functions keep their “out-of-barrier” symmetry in the barrier region as well. Thus, the odd solution \(\Psi_{\text{ref}}(x'; k)\) is equal to zero at the point \(x' = 0\). Of importance is the fact that this property takes place for all values of \(k\). In this case the probability flux, for any nonstationary-state wave function formed only from the odd (or even) stationary solutions \(\Psi_{\text{ref}}(x'; k)\), should be equal to zero at the barrier’s midpoint. This means that for particles impinging a symmetric barrier from the left they are reflected by the barrier without penetration into the region \(x' \geq 0\). In its turn, this means that the searched-for stationary-state RWF should be zero in the region \(x' \geq 0\), but in the region \(x' \leq 0\) it must be equal to the odd function \(\Psi_{\text{ref}}(x'; k)\). In this case the corresponding probability density is everywhere continuous, including the point \(x' = 0\), and the probability flux is everywhere equal to zero.

Of importance is the fact that the above property of reflection admits, in principle, experimental checking. Indeed, since reflected particles does not penetrate into the region \(x \geq x_{\text{mid}}\) of the symmetric barrier, the switching on an infinitesimal magnetic field in this region must not influence the spin of these particles. For checking this property, one can use the experimental scheme presented in [19].

As regards the searched-for TWF, \(\Psi_{\text{tr}}(x; k)\), it can be found now from the expression \(\Psi_{\text{tr}}(x; k) = \Psi_{\text{full}}(x; k) - \Psi_{\text{ref}}(x; k)\). This function is everywhere continuous, and the corresponding probability flux is everywhere constant (we have to stress once more that this quantity has no discontinuity at the point \(x = x_{\text{mid}}\), though the first derivative of \(\Psi_{\text{tr}}(x; k)\) is discontinuous at this point). Thus, as in the case of the RWF, wave packets formed from the stationary-state TWF should evolve in time with a constant norm.

As is seen from Exps. (32) and (33), for asymmetric potential barriers, both the solutions \(\Psi_{\text{ref}}(x'; k)\) are neither even nor odd functions. Nevertheless, it is evident that for any given value of \(k\) one of these solutions has opposite signs at the barrier’s boundaries. This means that, for any \(k\), there is at least one point in the barrier region, at which this function is equal to zero. However, unlike the case of symmetric barriers, the location of such a point depends on \(k\). Therefore the behavior of the nonstationary-state RWF in the barrier region is more complicated for asymmetric barriers. Now the most right turning point for reflected particles lies, as in the case of symmetric barriers, in the barrier region, but this point does not coincide in the general case with the midpoint of this region.
To illustrate the temporal behavior of all the three wave functions, i.e., $\Psi_{full}$, $\Psi_{tr}$ and $\Psi_{ref}$, we have considered the case of rectangular barriers. In this case, the stationary-state wave function $\Psi_{ref}(x; k)$, for $a \leq x \leq x_{mid}$, reads as

$$
\Psi_{ref} = 2\sqrt{RA} e^{i\phi(+)} [\cos(ka + \phi(-)) \sinh(\kappa d/2) \\
- \frac{k}{\kappa} \sin(ka + \phi(-)) \cosh(\kappa d/2)] \sinh(\kappa(x - x_{mid}))
$$

(34)

where $\kappa = \sqrt{2m(v_0 - E)/\hbar}$ (the below-barrier case); and

$$
\Psi_{ref} = -2\sqrt{RA} e^{i\phi(+)} [\cos(ka + \phi(-)) \sin(\kappa d/2) \\
+ \frac{k}{\kappa} \sin(ka + \phi(-)) \cos(\kappa d/2)] \sin(\kappa(x - x_{mid}))
$$

(35)

where $\kappa = \sqrt{2m(E - v_0)/\hbar}$ (the above-barrier case). In both cases $\Psi_{ref}(x; k) \equiv 0$ for $x \geq x_{mid}$.

We have calculated the spatial dependence of the probability densities $|\Psi_{full}(x, t)|^2$ (dashed line), $|\Psi_{tr}(x, t)|^2$ (open circles) and $|\Psi_{ref}(x, t)|^2$ (solid line) for the rectangular barrier ($V_0 = 0.3eV$, $a = 500nm$, $b = 505nm$) and well ($V_0 = -0.3eV$, $a = 500nm$, $b = 505nm$). Figures 1 ($t = 0$), 2 ($t = 0.4ps$) and 3 ($t = 0.42ps$) display results for the barrier, and figures 4 ($t = 0$), 5 ($t = 0.4ps$) and 6 ($t = 0.43ps$) display results for the well. In both the cases, the function $\Psi_{full}(x, 0)$ represents the Gaussian wave packet with $l_0 = 7.5nm$; the average kinetic energy is equal to 0.25$eV$, both for the barrier and well. Besides, in both cases, the particle’s mass is 0.067$m_e$ where $m_e$ is the mass of an electron.

As is seen from figures 1 and 4, the average starting points for the RWF and TWF differ from that for $\Psi_{full}$. The main peculiarity of the transmitting wave packet is that it is slightly compressed in the region of the barrier, and stretched in the region of the well. Figure 7 shows that, at the stage of the scattering event ($t = 0.4ps$; see also figure 2), the probability to find a transmitting particle in the barrier region is larger than in the neighborhood of the barrier. This means that in the momentum space this packet becomes wider when the ensemble of particles enters the barrier region. For the well (see figure 8) there is an opposite tendency. Note that for the barrier $< T >_{in} \approx 0.149$. For the well $< T >_{in} \approx 0.863$.

3.3 Connection of the wave functions for reflection and transmission with the eigenvectors of the scattering matrix

Of importance is the fact that there are other two settings of the tunneling problem for the given potential $V(x)$ when the subensemble’s states described by the RWF and TWF
arise explicitly. Indeed, let us find such solutions to the Schrödinger equation, for a given potential $V(x)$, for which

$$\begin{pmatrix} a_{out} \\ b_{out} \end{pmatrix} = S \begin{pmatrix} a_{in} \\ b_{in} \end{pmatrix}$$

where $S$ is a constant. This means that the amplitudes of incoming waves should obey the characteristic equation

$$S \begin{pmatrix} a_{in} \\ b_{in} \end{pmatrix} = S \begin{pmatrix} a_{in} \\ b_{in} \end{pmatrix} = \begin{pmatrix} q^{-1} & -p/q \\ p^*/q & q^{-1} \end{pmatrix}$$

where $S$ is the scattering matrix.

It is easy to show that the solutions of this equation can be written in the form

$$S = \frac{1 + i\mu|p|}{q}; \quad \begin{pmatrix} a_{in} \\ b_{in} \end{pmatrix} = c(\mu) \begin{pmatrix} i\mu p/|p| \\ 1 \end{pmatrix}$$

where $\mu = \pm 1$; $c(\mu)$ and $c(-\mu)$ are arbitrary constants.

Now let us find such values of $c(\mu)$ and $c(-\mu)$ at which $b_{out} = p^*/q$. It easy to show that all four amplitudes read, in this case, as

$$a_{in} = \frac{i\mu|p|}{1 + i\mu|p|} \equiv \sqrt{T}(\sqrt{R} + i\mu\sqrt{T}); \quad b_{out} = \frac{p^*}{q};$$

$$a_{out} = \frac{i\mu|p|}{q} = \frac{i\mu|p|}{p} \cdot \frac{p^*}{q}; \quad b_{in} = \frac{p^*}{1 + i\mu|p|} = \frac{p^*}{i\mu|p|} \sqrt{T}(\sqrt{R} + i\mu\sqrt{T}).$$

One of two solutions with these amplitudes is evident to coincide, for $x < a$, with the RWF found in subsection 3.2. This means that in the case of symmetric potential barriers this function, like the RWF, is equal to zero at the midpoint of the barrier region, for any value of $k$. In this two-sources scattering problem, both the incident wave packets does not cross the above point. In fact, we deal here with the ideal bilateral reflection of particles from the midpoint of the barrier region, which is described by the sum of two the RWFs.

In a similar way, for the same eigenvalue of the scattering matrix, one can find such values of $c(\mu)$ and $c(-\mu)$ at which $a_{out} = 1/q$:

$$a_{in} = \frac{1}{1 + i\mu|p|} \equiv \sqrt{T}(\sqrt{T} - i\mu\sqrt{R}); \quad b_{out} = -\frac{i\mu|p|}{p} \cdot \frac{1}{q};$$

$$a_{out} = \frac{1}{q}; \quad b_{in} = -\frac{i\mu|p|}{p} \cdot \frac{1}{1 + i\mu|p|} \equiv -\frac{i\mu|p|}{p} \cdot \sqrt{T}(\sqrt{T} - i\mu\sqrt{R}).$$
As is seen, the stationary-state TWF appears explicitly in the solution with amplitudes (39). In the case of symmetric potential barriers this solution is evident to represent a sum of two continuous wave functions whose probability fluxes are continuous too. For one of them the amplitudes of incoming and outgoing waves are, respectively, \( a_{\text{in}} (= \sqrt{T(\sqrt{T} - i\mu\sqrt{R})}) \) and \( a_{\text{out}} (= 1/q) \). For another function these amplitudes are, respectively, \( b_{\text{in}} (= -(i\mu|p|/p) \cdot \sqrt{T(\sqrt{T} - i\mu\sqrt{R})}) \) and \( b_{\text{out}} (= -(i\mu|p|/p) \cdot (1/q)) \). The first (second) function is just the TWF to describe the ideal transmission of particles impinging the barrier from the left (right). The corresponding nonstationary-state wave functions are evident to evolve in time with a constant norm.

So, each of the above ”two-sources” wave functions generated by eigenvectors of the scattering matrix represent a sum of two causally evolved ”one-source” wave functions. One of them describes the state of a particle impinging the barrier from the left. Another function relates to particles moving to the right of the barrier. In the case of (38) both the one-source wave packets are ideally reflected by the barrier. And, in the case of (39) both one-source wave packets are ideally transmitted by it. These two auxiliary tunneling problems give us the basis to verify the formalism presented in this paper.

Note also that the stationary-state RWF and TWF, for the problem at hand, should correspond to the same value of \( \mu \), i.e., to the same eigenvalue of the scattering matrix. As regards another eigenvalue, in the case of reflection it generates the even function which does not fit as a RWF (see subsection 3.2). That is, only one of the eigenvalues of the scattering matrix is associated with the RWF and TWF of the scattering problem considered.

4 Exact and asymptotic tunneling times for transmission and reflection

4.1 Exact tunneling times

So, we have found two causally evolved wave packets to describe the subensembles of transmitted and reflected particles in the considered tunneling problem, at all stages of the scattering process. As is shown, the motion of these packets can be, in principle, observed experimentally. It is evident that the given formalism may serve as the basis to solve the tunneling time problem, since now one can follow the CMs of wave packets, which describe separately reflection and transmission, at all instants of time.

Let \( t_{1r}^r \) and \( t_{2r}^r \) be such instants of time that

\[
\frac{\langle \Psi_{tr}(x,t_{1r}^r)|\hat{x}|\Psi_{tr}(x,t_{1r}^r) \rangle}{\langle \Psi_{tr}(x,t_{2r}^r)|\hat{x}|\Psi_{tr}(x,t_{2r}^r) \rangle} = a - L_1; \quad (40)
\]

\[
\frac{\langle \Psi_{tr}(x,t_{1r}^r)|\hat{x}|\Psi_{tr}(x,t_{1r}^r) \rangle}{\langle \Psi_{tr}(x,t_{2r}^r)|\hat{x}|\Psi_{tr}(x,t_{2r}^r) \rangle} = b + L_2, \quad (41)
\]
where $\Psi_{tr}(x, t)$ is the subensemble’s wave function found above for transmission. Then, one can define the transmission time $\Delta t_{tr}(L_1, L_2)$ as the difference $t_{tr}^2(L_2) - t_{tr}^1(L_1)$ where $t_{tr}^1(L_1)$ is the smallest root of Eq. (40), and $t_{tr}^2(L_2)$ is the largest root of Eq. (41).

Similarly, for reflection, let $t_{ref}^1(L_1)$ and $t_{ref}^2(L_2)$ be such instants of time $t$ that

$$
\langle \Psi_{ref}(x, t) | \hat{x} | \Psi_{ref}(x, t) \rangle = a - L_1,
$$

(42)

Then the reflection time $\Delta t_{ref}(L_1)$ can be defined as $\Delta t_{ref}(L_1) = t_{ref}^2 - t_{ref}^1$ where $t_{ref}^1(L_1)$ is the smallest root, and $t_{ref}^2(L_2)$ is the largest root of Eq. (42) (of course, if they exist).

It is important to emphasize that, due to conserving the number of particles in both the subensembles, both these quantities are non-negative for any distances $L_1$ and $L_2$. Both the definitions are valid, in particular, when $L_1 = 0$ and $L_2 = 0$. In this case the quantities $\Delta t_{tr}(0, 0)$ and $\Delta t_{ref}(0)$ yield, respectively, exact transmission and reflection times for the barrier region. Of course, one has to take into account that in the case of reflection the CM of the wave packet may turn back without entering the barrier region.

### 4.2 Asymptotic tunneling times

It is evident that in the general case the above average quantities can be calculated only numerically. At the same time, for sufficiently large values of $L_1$ and $L_2$, one can obtain the tunneling times $\Delta t_{tr}(L_1, L_2)$ and $\Delta t_{tr}(L_1, L_2)$ in more explicit form. Indeed, in this case, instead of the exact subensemble’s wave functions, we can use the corresponding asymptotes derived in $k$-representation. Indeed, now the ”full” in asymptote, like the corresponding out asymptote, represents the sum of two wave packets:

$$
f_{in}(k, t) = f_{in}^{tr}(k, t) + f_{in}^{ref}(k, t); \quad f_{in}^{tr}(k, t) = \sqrt{T(k)}A_{in}(k) \exp[i(\Lambda(k) - \alpha \frac{\pi}{2} - E(k)t/\hbar)];
$$

(43)

$$
f_{in}^{ref}(k, t) = \sqrt{R(k)}A_{in}(k) \exp[i(\Lambda(k) - E(k)t/\hbar)];
$$

(44)

$\alpha = 1$ if $\Lambda \geq 0;$ otherwise $\alpha = -1$. Here the function $\Lambda(k)$ coincides, for a given $k$, with one of the functions, $\lambda(k)$ or $-\lambda(k)$, for which $\Psi_{ref}(x; k)$ is an odd function (see above). One can easily show that for both the roots

$$
|\Lambda'(k)| = \frac{|T'|}{\sqrt{2RT}}.
$$

A simple analysis in the $k$-representation shows that well before the scattering event the average kinetic energy of particles in both subensembles (with the average wave numbers $< k >_{in}^{tr}$ and $< k >_{in}^{ref}$) is equal to that for large times:

$$
< k >_{out}^{tr} = < k >_{in}^{tr}, \quad < k >_{out}^{ref} = - < k >_{in}^{ref}.
$$

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Besides, at early times

\[
< \hat{x} >_{in}^{tr} = \frac{\hbar t}{m} < k >_{in}^{tr} - < \Lambda'(k) >_{in}^{tr}; \quad (45)
\]

\[
< \hat{x} >_{in}^{ref} = \frac{\hbar t}{m} < k >_{in}^{ref} - < \Lambda'(k) >_{in}^{ref}. \quad (46)
\]

As it follows from Exps. (45) and (46), the average starting points \( x_{start}^{tr} \) and \( x_{start}^{ref} \), for the subensembles of transmitted and reflected particles, respectively, differ from that for all particles:

\[
x_{start}^{tr} = - < \Lambda'(k) >_{in}^{tr}, \quad x_{start}^{ref} = - < \Lambda'(k) >_{in}^{ref}. \quad (47)
\]

The implicit assumption made in the SWPA that incident, as well as transmitted and reflected particles start, on the average, from the same point does not agree with this result. By our approach, this is the main reason why the asymptotic transmission and reflection times obtained in the SWPA should be considered as ill-defined quantities, for any wave packets.

Let us take into account Exps. (45), (46) and again analyze the motion of a particle in the above spatial interval covering the barrier region. In particular, let us calculate the transmission time, \( \tau_{tr} \), spent (on the average) by a particle in the interval \([Z_1, Z_2]\). It is evident that the above equations for the arrival times \( t_{1tr}^{tr} \) and \( t_{2tr}^{tr} \), which correspond the extreme points \( Z_1 \) and \( Z_2 \), respectively, read now as

\[
< \hat{x} >_{in}^{tr} (t_{1tr}^{tr}) = a - L_1; \quad < \hat{x} >_{out}^{tr} (t_{2tr}^{tr}) = b + L_2.
\]

Considering (45) and (10), we obtain from here that now the transmission time is

\[
\tau_{tr}(L_1, L_2) \equiv t_{2tr}^{tr} - t_{1tr}^{tr} = \frac{m\hbar}{k} < k >_{in}^{tr} \left( < J' >_{out}^{tr} - < \Lambda' >_{in}^{tr} + L_1 + L_2 \right). \quad (48)
\]

Similarly, for the reflection time, \( \tau_{ref}(L_1) \) \( (\tau_{ref} = t_{2ref}^{ref} - t_{1ref}^{ref}) \), we have

\[
< \hat{x} >_{in}^{ref} (t_{1ref}^{ref}) = a - L_1; \quad < \hat{x} >_{out}^{ref} (t_{2ref}^{ref}) = a - L_1.
\]

Considering (46) and (11), one can easily show that

\[
\tau_{ref}(L_1) \equiv t_{2ref}^{ref} - t_{1ref}^{ref} = \frac{m\hbar}{k} < k >_{in}^{ref} \left( < J' - F' >_{out}^{ref} - < \Lambda' >_{in}^{ref} + 2L_1 \right). \quad (49)
\]

The inputs \( \tau_{tr}^{as} (\tau_{tr}^{as} = \tau_{tr}(0, 0)) \) and \( \tau_{ref}^{as} (\tau_{ref}^{as} = \tau_{ref}(0, 0)) \) will be named below as the asymptotic transmission and reflection times for the barrier region, respectively.
\[ \tau_{as}^{tr} = \frac{m}{\hbar} \left( < J' >_{out}^{tr} - < \Lambda' >_{in}^{tr} \right), \tag{50} \]

\[ \tau_{as}^{ref} = \frac{m}{\hbar} \left( < J' >_{out}^{ref} - < \Lambda' >_{in}^{ref} \right) \tag{51} \]

Here the word "asymptotic" points to the fact that these quantities were obtained with making use of the in and out asymptotes for the subensembles investigated. Unlike the exact tunneling times the asymptotic times may be negative by value.

The corresponding lengths \(d_{eff}^{tr}\) and \(d_{eff}^{ref}\),

\[ d_{eff}^{tr} = < J' >_{out}^{tr} - < \Lambda' >_{in}^{tr}, \quad d_{eff}^{ref} = < J' >_{out}^{ref} - < \Lambda' >_{in}^{ref} \tag{52} \]

can be treated as the effective widths of the barrier for transmission and reflection, respectively.

### 4.3 Average starting points and asymptotic tunneling times for rectangular potential barriers and \(\delta\)-potentials

Let us consider the case of a rectangular barrier (or well) of height \(V_0\) and obtain explicit expressions for \(d_{eff}(k)\) (now, both for transmission and reflection, \(d_{eff}(k) = J'(k) - \Lambda'(k)\) since \(F'(k) \equiv 0\)) which can be treated as the effective width of the barrier for a particle with a given \(k\). Besides, we will obtain the corresponding expressions for the coordinate, \(x_{start}(k)\), of the average starting point for this particle: \(x_{start}(k) = -\Lambda'(k)\). It is evident that in terms of \(d_{eff}\) the above asymptotic times for a particle with the well-defined average momentum \(k_0\) read as

\[ \tau_{as}^{tr} = \tau_{as}^{ref} = \frac{md_{eff}(k_0)}{\hbar k_0}. \]

Using the expressions for the real tunneling parameters \(J\) and \(T\) (see [36, 39]), one can show that, for the below-barrier case \((E \leq V_0)\),

\[ d_{eff}(k) = \frac{4}{\kappa} \left[ k^2 + \kappa_0^2 \sinh^2(\kappa d/2) \right] \left[ \kappa_0^2 \sinh(\kappa d) - k^2 \kappa d \right] \]

\[ x_{start}(k) = -\kappa_0^2 (\kappa^2 - k^2) \sinh(\kappa d) + k^2 \kappa d \cosh(\kappa d) \]

where \(\kappa = \sqrt{2m(V_0 - E)}/\hbar^2\); for the above-barrier case \((E \geq V_0)\) —

\[ d_{eff}(k) = \frac{4}{\kappa} \left[ k^2 - \beta \kappa_0^2 \sin^2(\kappa d/2) \right] \left[ k^2 \kappa d - \beta \kappa_0^2 \sin(\kappa d) \right] \]

\[ x_{start}(k) = \kappa_0^2 (\kappa^2 - k^2) \sinh(\kappa d) - k^2 \kappa d \cosh(\kappa d) \]
\[ x_{\text{start}}(k) = -2\beta \frac{\kappa_0^2}{\kappa} \cdot \left( \frac{\kappa^2 + k^2}{4k^2 + \kappa_0^4 \sin^2(\kappa d)} \right) \]

where \( \kappa = \sqrt{2m(E - V_0)/\hbar^2}; \beta = 1 \) if \( V_0 > 0 \), otherwise, \( \beta = -1 \). In both the cases \( \kappa_0 = \sqrt{2m|V_0|/\hbar^2} \).

It is important to stress that, in the limit \( k \to \infty \), \( d_{\text{eff}} \to d \) and \( x_{\text{start}}(k) \to 0 \). This property guarantees that for infinitely narrow in \( x \)-space wave packets the average starting points for both subensembles will coincide with that for all particles. It is important also that for wells the values of \( d_{\text{eff}} \) and, as a consequence, the corresponding tunneling times are negative, in the limit \( k \to 0 \), when \( \sin(\kappa_0 d) < 0 \).

Note that for sufficiently narrow barriers and wells, namely when \( \kappa d \ll 1 \), we have \( d_{\text{eff}} \approx d \). That is, particles tunnel, on the average, classically through such barriers. For the starting point we have

\[ x_{\text{start}}(k) \approx -\frac{\kappa_0^2}{2k^2} d, \quad x_{\text{start}}(k) \approx -\beta \frac{\kappa_0^2}{2k^2} d \]

for \( E \leq V_0 \) and \( E \geq V_0 \), respectively.

For wide barriers and wells, when \( \kappa d \gg 1 \), we have \( d_{\text{eff}} \approx 2/\kappa \) and \( x_{\text{start}}(k) \approx 0 \), for \( E \leq V_0 \); and

\[ d_{\text{eff}} \approx 4k^2 d \cdot \frac{k^2 - \beta \kappa_0^2 \sin^2(\kappa d/2)}{4k^2 + \kappa_0^4 \sin^2(\kappa d)} \quad x_{\text{start}}(k) \approx \frac{2\beta \kappa_0^2 k^2 d \cos(\kappa d)}{4k^2 + \kappa_0^4 \sin^2(\kappa d)}, \]

for \( E \geq V_0 \).

It is interesting to note that for the \( \delta \)-potential \( V(x) = W \delta(x - a) \) \( d_{\text{eff}} \equiv 0 \). This means that, contrary to the phase tunneling time, the tunneling times defined here equal to zero for this potential. As regards the starting point \( x_{\text{start}}(k) \) in the case of the \( \delta \)-potential, we have

\[ x_{\text{start}}(k) = -\frac{2m \hbar^2 W}{\hbar^2 k^2 + m^2 W^2}. \]

Thus, we see that, for example, in the case of \( \delta \)-wells \( (W < 0) \) particles in each subensemble start, on the average, with an advance in comparison with those of the whole quantum ensemble.

\section{Conclusion}

A separate description of transmission and reflection is commonly accepted to contradict the principles of quantum mechanics. However, in this paper we argue that this is not the case, at least in the one-dimensional one-particle scattering problem. We show that the
wave function to describe, in this problem, the state of the whole ensemble of identically prepared particles can be uniquely presented as the sum of two functions (named here as the TWF and RWF) to obey the Schrödinger equation. In the case of nonstationary case, these functions are mutually orthogonal. At late times the TWF coincides with the transmitted wave packet, and the RWF approaches the reflected one. We postulate that namely the TWF and RWF are the wave functions to describe, respectively, transmission and reflection in the considered scattering process.

There is also a widely accepted viewpoint (see, for example, page 106 in [40] and page 17 in [41]) that all solutions to the stationary one-dimensional Schrödinger equation, for a finite potential, must be everywhere continuous together with their spatial derivatives; otherwise, the points where this requirement is violated contain allegedly sinks or sources of particles. However, in this paper we show that the above requirement for ”physical” solutions to the Schrödinger equation is, in reality, excessive. The main peculiarity of the presented stationary-state wave functions for transmission and reflection is that there is a point in the barrier region where these everywhere continuous functions have discontinuous first spatial derivatives (in the case of symmetric potential barriers this takes place at the midpoint of the barriers). Nevertheless, for each subensemble, this point contains neither sink nor source of particles: both for transmission and reflection, the probability current density for each stationary-state wave function is constant on the spatial axis, and the norm of wave packets formed from these functions is constant in time.

We show that, in the case of a symmetric potential barrier, reflected particles impinging the barrier from the left do not penetrate into the spatial domain lying to the right of the midpoint of the barrier region. This means, in particular, that the switching on an infinitesimal magnetic field in this domain must not influence the spin of these particles.

Besides, for the given potential we formulate two scattering problem in which the RWF and TWF arise separately and, as a consequence, there is another possibility to check experimentally our approach. In both the scattering problems the amplitudes of incoming waves form the eigenvectors of the scattering matrix for the given potential.

On the basis of the above formalism we define average (exact and asymptotic) transmission and reflection times. The exact tunneling times are always non-negative. In the case of rectangular barriers and $\delta$-potentials, for both the subensembles, we derive explicit expressions for the asymptotic tunneling times and for the average starting points. These times differ essentially from those arising in the SWPA.

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Figure captions

Fig. 1 The $x$-dependence of $|\Psi_{full}(x,t)|^2$ (dashed line) which represents the Gaussian wave packet with $l_0 \approx 7.5nm$ and the average kinetic particle’s energy $0.25eV$, as well as $|\Psi_{tr}(x,t)|^2$ (open circles) and $|\Psi_{ref}(x,t)|^2$ (solid line) for the rectangular barrier ($V_0 = 0.3eV$, $a = 500nm$, $b = 505nm$); $t = 0$.

Fig. 2 The same as in Fig. 1, but $t = 0.4ps$.

Fig. 3 The same as in Fig. 1, but $t = 0.42ps$.

Fig. 4 The $x$-dependence of $|\Psi_{full}(x,t)|^2$ (dashed line) which represents the Gaussian wave packet with $l_0 = 7.5nm$ and the average kinetic particle’s energy $0.25eV$, as well as $|\Psi_{tr}(x,t)|^2$ (open circles) and $|\Psi_{ref}(x,t)|^2$ (solid line) for the rectangular well ($V_0 = -0.3eV$, $a = 500nm$, $b = 505nm$); $t = 0$.

Fig. 5 The same as in Fig. 4, but $t = 0.4ps$.

Fig. 6 The same as in Fig. 4, but $t = 0.43ps$.

Fig. 7 The same functions for the barrier region; parameters are the same as for Fig. 2.

Fig. 8 The same functions for the barrier region; parameters are the same as for Fig. 5.
