Wave functions and characteristic times for transmission and reflection

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Abstract.
We present a renewed wave-packet analysis based on the following ideas: if a quantum one-particle scattering process and the corresponding state are described by an indivisible wave packet to move as a whole at all stages of scattering, then they are elementary; otherwise, they are combined; each combined process consists from several alternative elementary ones to proceed simultaneously; the corresponding (normed) state can be uniquely presented as the sum of elementary ones whose (constant) norms give unit, in sum; Born’s formula intended for calculating the expectation values of physical observables, as well as the standard timing procedure are valid only for elementary states and processes; only an elementary time-dependent state can be considered as the quantum counterpart to some classical one-particle trajectory. By our approach, tunneling a non-relativistic particle through a static one-dimensional potential barrier is a combined process consisting from two elementary ones, transmission and reflection. In the standard setting of the problem, we find an unique pair of solutions to the Schrödinger equation, which describe separately transmission and reflection. On this basis we introduce (exact and asymptotic) characteristic times for transmission and reflection.

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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 timing the motion of the center of "mass" (CM) of the corresponding wave packet to describe the process, does not provide a clear prescription both to interpret the scattering of finite in \( x \) space wave packets and to introduce characteristic times for a tunneling particle. The latter is known as the tunneling time problem (TTP) which has been of great interest for the last decades.

As is known (see [7]), the main difficulties to arise in interpreting the wave-packet’s tunneling are connected to the fact that there is no causal link between the transmitted (or reflected) and incident wave packets. One of the visual consequences of this is that the average particle’s kinetic energy for the transmitted, reflected and incident wave packets is different. For example, in the case of an opaque rectangular barrier, the velocity of the CM of the transmitted wave packet is larger than that of the incident one. It is evident that this fact needs a proper physical explanation. As was pointed out in [7], 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.

One has to point also to the well-known Hartman effect [3] related to the acceleration of the CM of the transmitted wave packet, to superluminal velocities (see also [8]). In many respects, the present interpretation of this property of wave packets is still controversial.

Note, in the case of wide (strictly speaking, infinite) in \( x \) space wave packets the average kinetic energy of particles, before and after the interaction, is the same. However, it is evident that a causal link between the transmitted and incident wave packets does not appear in this limiting case. Perhaps, this fact is a basic reason by which many physicists appraise the phase times introduced in the SWPA as ill-defined. At least, a 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 to deal with the CM of a wave packet, in the same or different setting the tunneling problem, a variety of alternative approaches (see reviews [1, 9, 10, 11, 12, 13] and references therein) to introduce various characteristic times for a tunneling particle have also been developed. Among the alternative concepts, of interest are that of the dwell time [14, 15, 16, 17], that of the Larmor time [18, 19, 20, 21, 22] to give the way of measuring the dwell time, and the concept of the time of arrival which is based on introducing either a suitable time operator (see, for example, [23, 24, 25, 26, 27]) or the positive operator valued measure (see review [12]). Besides, of importance are the studies of the temporal aspects of tunneling on the basis of the Feynman, Bohmian
and Wigner approaches to deal with the random trajectories of particles (see, for example, \cite{28, 29, 30, 31, 32} and references therein). One should also mention the papers \cite{33, 34, 35} where the TTP is studied beyond the framework of the standard setting the scattering problem.

We have to stress however that in the standard setting, when the initial wave packet may include a zero-momentum component, none of the alternative approaches have led to commonly accepted characteristic times (see \cite{1, 9, 10, 11, 12, 13}). The recent papers \cite{36, 37}, which present new versions of the dwell time (see \cite{36}) and complex tunneling times (see \cite{37}), evidence too that up to now there are no preferable time concepts for a tunneling particle.

There is an opinion that the TTP, in the standard setting of the one-dimensional scattering problem, is ill-defined, since it does not include the measurement process. We think that such an opinion is very questionable. Of course, in some cases the measurement process can essentially modify the original scattering one, and hence the study of its possible influence on the temporal aspects of this scattering process can be very useful (see, for instance, \cite{38} and the review \cite{12} where this question is deeply analyzed). At the same time, to state that any measurement-independent setting of the TTP is ill-defined is unacceptable, in principle. Otherwise, all Hamiltonians to describe a measurement-independent scattering processes (including the motion of a free particle, and the tunneling process) would be considered as ones having no physical sense. We have to stress that any quantum scattering process, like classical one, proceeds, irrespective of our assistance, in some space-time framework. So that quantum theory should give a clear and unambiguous prescription to define both the spatial and temporal limits of this process.

The main question of the TTP, which implies an unique answer, is that of the (average) time spent by a quantum particle inside a finite barrier region. There is a particular case when answering this question is trivial. We have in mind tunneling a particle through the $\delta$-potential barrier. Indeed, one can \textit{a priori} say that this characteristic time should be equal to zero for this potential. For the probability to find a particle in its barrier region is equal to zero.

Note, the TTP is very often (see, for example, \cite{39}) treated as the problem of introducing characteristic times for a \textit{wave packet} passing through a quantum-mechanical barrier. As is seen, from the very outset, this formulation implies timing a lengthy object whose spatial size is comparable with (or even much more than) the width of the potential barrier. Such a vision of the TTP is of wide spreading. Therefore it is no mere chance that a nonzero phase transmission time obtained in the SWPA for the $\delta$-potential is viewed by many physicists as a fully expected result, which allegedly says about the non-locality of a quantum scattering process. However, this result, being derived in the SWPA on the basis of timing the motion of the CM of a wave packet, is \textit{a priori} inconsistent: any selected point of a wave packet should cross instantaneously the point-like support of the $\delta$-potential.

As regards the non-locality of tunneling, the example of the $\delta$-potential shows
explicitly that the time spent by a quantum particle in the barrier region provides insufficient information about a quantum one-particle scattering process. It is useful also to define the time interval when the probability to find a particle crossing through the barrier region is sufficiently large. The necessity in the additional time scale is associated eventually with the fact that the time of arrival of a particle at some point can be predicted, in quantum theory, with the error amounting to the half-width of the corresponding wave packet. It is this characteristic time that must be derived, for a particle, with taking into account of the wave-packet’s width. This time, which can be treated as the time of the interaction of a quantum ensemble of particles with the barrier, is always greater than the time spent in the barrier region by each particle of this ensemble. It is this quantity that must be nonzero for the $\delta$-potential.

So, due to the uncertainty in finding the position of a tunneling particle, the (average) time spent by the particle in the barrier region is insufficient to give a full information about its interaction with the barrier. However, there is once more peculiarity of a quantum description of the one-dimensional scattering of a particle, which drastically complicates solving the TTP. Indeed, in classical theory, in timing a scattering particle for a given initial condition, we deal with the only trajectory of a particle, that corresponds either transmission or reflection. However, in quantum description we deal with a wave function to include information about both the alternative possibilities. Therefore every physicist setting to the TTP has firstly to resolve the dilemma, whether he has to introduce individual (transmission and reflection) times or whether he must solve the TTP with no distinguishing between transmission and reflection.

One should recognize that at present this question is still open. Most of the time concepts, such as the time of arrival as well as the dwell, Larmor and phase tunneling times suggest introducing individual characteristic times for transmission and reflection. As is pointed out by Nussenzveig (see [13]), “...[if some characteristic time] does not distinguish between reflected and transmitted particles, [this is] usually taken as a defect ...”. At the same time, Nussenzveig himself believes (ibid) that ”...[a joint description of the whole ensemble of tunneling particles] is actually a virtue, since transmission and reflection are inextricably intertwined; ...only the characteristic times averaged over transmitted and reflected particles have a physical sense”.

An intrigue is that there are forcible arguments in both the cases. On the one hand, quantum mechanics, as it stands, indeed provides no prescription to separate to-be-transmitted and to-be-reflected particles at the early stages of scattering. Thus, having no information about the behaviour of both the kinds of particles in the barrier region, it is impossible to find the average time spent, in this region, by particles of each kind. A knowledge about their behavior after the scattering event is insufficient for this purpose.

On the other hand, the final state of a tunneling particle evidences that tunneling consists in fact from two alternative processes - transmission and reflection. Born’s formula underlying the statistical interpretation of quantum mechanics fails in this case:
the average values of the particle’s position and momentum calculated over the whole ensemble of particles, cannot be interpreted as the expectation values of these quantities. We consider that this fact is a poor background for introducing characteristic times averaged over transmitted and reflected particles.

In fact, the above controversy says that usual quantum mechanics does not provide both a joint and separate description of transmitted and reflected particles. It enables one to study in detail the temporal behavior of wave packets to describe the tunneling process. However, it gives no basis to extract from these detailed data the expectation values of the particle’s position and momentum, as well as to introduce its characteristic times. Its basic tools - Born’s formula for calculating the expectation values, and the standard timing procedure - proved to be usefulness in studying a tunneling particle.

The main idea of this paper is that in order to learn to calculate expectation values of physical observables for a tunneling particle (and solve the TTP, on this basis) one needs to correct our understanding of the nature of a quantum one-particle scattering state and the correspondence principle. Now it is generally accepted that any quantum time-dependent one-particle state can be considered, in principle, as the quantum counterpart to some classical one-particle trajectory. However, generally speaking, this is not the case.

In this approach, all quantum one-particle scattering processes described by the Schrödinger equation are divided into two classes - combined and elementary. If the wave packet to describe a quantum one-particle scattering process represents at some time a disconnected object (or, in other words, when the set of spatial points, where the probability to find a particle is nonzero, is disconnected), then we deal with a combined process. Otherwise, the process is elementary. Only in the last case, Born’s formula and the standard timing procedure are applicable. By our approach, only an elementary time-dependent one-particle scattering state can be considered as the quantum counterpart to some classical one-particle trajectory. As regards a combined time-dependent state, it can be associated with several one-particle trajectories.

On the basis of this idea we develop a renewed wave-packet analysis in which we treat the one-particle one-dimensional scattering of a particle on a static potential barrier as a combined process consisting from two alternative ones, transmission and reflection. We hope that this approach will be useful for a deeper understanding of the nature of quantum one-particle scattering processes and, in particular, the tunneling effect.

The paper is organized as follows. In Section 2 we pose a complete one-dimensional scattering problem for a particle. Shortcomings of the SWPA are analyzed in Section 3. In Section 4 we present a renewed wave-packet analysis in which transmission and reflection are treated separately. In Section 5 we define the average (exact and asymptotic) transmission and reflection times and consider the cases of rectangular barriers and δ-potentials. In the last section some aspects of our approach are discussed in detail.
2. Setting the problem for a completed scattering

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 \( \Psi_{left}^{(0)}(x) \) 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

\[
\langle \Psi_{left}^{(0)} | \hat{x} | \Psi_{left}^{(0)} \rangle = 0, \quad \langle \Psi_{left}^{(0)} | \hat{p} | \Psi_{left}^{(0)} \rangle = \hbar k_0 > 0, \quad \langle \Psi_{left}^{(0)} | \hat{x}^2 | \Psi_{left}^{(0)} \rangle = l_0^2,
\]

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.

Since we study a complete scattering, an important restriction should be imposed on the rate of spreading the incident wave packet. Namely, we will suppose that the average velocity \( \hbar k_0 / m \) is large enough, so that the parts of the incident wave packet lying behind its CM, within the wave-packet’s half-width, move toward the barrier together with the CM; \( m \) is the particle’s mass.

As is known, the formal solution to the temporal one-dimensional Schrödinger equation (OSE) of the problem can be written as \( e^{-iHt/\hbar} \Psi_{in}(x) \). In order to solve explicitly this equation we will use here the variant (see [40]) of the well-known transfer matrix method [41] that allows one to calculate the tunneling parameters, as well as to connect the amplitudes of outgoing and corresponding incoming waves, for any system of potential barriers.

Let \( E \) be the energy of a particle. Then for the wave function \( \Psi_{full} \) to describe its stationary state in the out-of-barrier regions we have

\[
\Psi_{full}(x; k) = A_{in}(k)e^{ikx} + B_{out}(k)e^{-ikx}
\]

for \( x \leq a \), and

\[
\Psi_{full}(x; k) = A_{out}(k)e^{ikx} + B_{in}(k)e^{-ikx},
\]

for \( x > b \); here \( k = \sqrt{2mE/\hbar} \); \( A_{in}(k) \) should be found from the initial condition; \( B_{in}(k) = 0 \). The coefficients entering this solution are connected by the transfer matrix \( Y \):

\[
\begin{pmatrix} A_{in} \\ B_{out} \end{pmatrix} = Y \begin{pmatrix} A_{out} \\ B_{in} \end{pmatrix}; \quad Y = \begin{pmatrix} q & p \\ p^* & q^* \end{pmatrix};
\]

that can be expressed (see [40]) in terms of the real tunneling parameters \( T, J \) and \( F \):

\[
q = \frac{1}{\sqrt{T(k)}} \exp \left[ i(kd - J(k)) \right]; \quad p = \sqrt{\frac{R(k)}{T(k)}} \exp \left[ i \left( \frac{\pi}{2} + F(k) - ks \right) \right];
\]

\( T(k) \) (the real transmission coefficient) and \( J(k) \) (phase) are even and odd functions, respectively; \( F(-k) = \pi - F(k) \); \( R(k) = 1 - T(k) \); \( s = a + b \). One can easily show that for a particle impinging the barrier from the left

\[
B_{out}/A_{in} \equiv b_{out} = p^*/q, \quad A_{out}/A_{in} \equiv a_{out} = 1/q.
\]
We will suppose that the tunneling parameters have already been calculated (in the case of many-barrier structures, for this purpose one can use the recurrence relations obtained in [40] 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 [42]. Thus, definitions of characteristic times in this approach can be done in terms of the in and out asymptotes of the tunneling problem.

Note, 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. But 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 asymptote \( \Psi_{\text{in}}(x, t) \) and out asymptote \( \Psi_{\text{out}}(x, t) \) can be written, for the problem at hand, as follows

\[
\Psi_{\text{in}}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_{\text{in}}(k, t) e^{ikx} dk, \quad f_{\text{in}}(k, t) = A_{\text{in}}(k) \exp[-iE(k)t/\hbar]; \quad (6)
\]

\[
\Psi_{\text{out}}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f_{\text{out}}(k, t) e^{ikx} dk, \quad f_{\text{out}}(k, t) = f_{\text{tr}}(k, t) + f_{\text{ref}}(k, t); \quad (7)
\]

\[
f_{\text{tr}}(k, t) = \sqrt{T(k)} A_{\text{in}}(k) \exp[i(J(k) - kd - E(k)t/\hbar)]; \quad (8)
\]

\[
f_{\text{ref}}(k, t) = \sqrt{R(k)} A_{\text{in}}(-k) \exp[-i(J(k) - F(k) - \pi/2 + 2ka + E(k)t/\hbar)] \quad (9)
\]

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

For a completed scattering we have

\[
\Psi_{\text{full}}(x, t) \approx \Psi_{\text{in}}(x, t) \quad \text{when} \quad t = 0; \quad \Psi_{\text{full}}(x, t) = \Psi_{\text{out}}(x, t) \quad \text{when} \quad t \to \infty.
\]

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

For the average particle’s position, well before the scattering event, we have

\[
< \hat{x} >_{\text{in}} = \frac{\hbar k_{0}}{m} t \quad (10)
\]

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

\[
< \hat{Q} >_{\text{in}} = \frac{< f_{\text{in}} | \hat{Q} | f_{\text{in}} >}{< f_{\text{in}} | f_{\text{in}} >};
\]

similar notations are used below for the transmitted and reflected wave packets). The averaging separately over the transmitted and reflected wave packets yields

\[
< \hat{x} >_{\text{out}}^{\text{tr}} = \frac{\hbar}{m} < k >_{\text{out}}^{\text{tr}} - < J'(k) >_{\text{out}}^{\text{tr}} + d; \quad (11)
\]

\[
< \hat{x} >_{\text{out}}^{\text{ref}} = \frac{\hbar}{m} < k >_{\text{out}}^{\text{ref}} + < J'(k) - F'(k) >_{\text{out}}^{\text{ref}} + 2a \quad (12)
\]

(hereinafter the prime denotes the derivative with respect to \( k \)). Exps. (10) — (12) yield the basis for defining the asymptotic tunneling times in the SWPA.
3. Timing the particle’s motion in the framework of the standard wave-packet analysis

For the following it is convenient to derive again the SWPA’s tunneling times. Their derivation is known to be based on the standard in quantum mechanics timing procedure which is dictated by the correspondence principle. Namely, 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 value of the position of a particle (or, what is equivalent, from studying the temporal behavior of the CM of a wave packet to describe its state). Besides, quantum theory implies calculating the error of the timing, which should be based on the analysis of the temporal dependence of the mean-square deviation for the position operator.

The standard timing procedure is evident to imply that the average value of the particle’s position has its primary physical sense (as the most probable position of a particle) at all stages of its motion. For instance, for a free particle whose state is described by a Gaussian-like wave packet, this requirement is fulfilled and, as a consequence, no problem arises in timing its motion. However, an essentially different situation arises in the case of a tunneling particle. Now, following the CM of a wave packet to describe the whole ensemble of tunneling particles becomes meaningless at some stages of scattering. In particular, after the scattering event, when we deal with two scattered (transmitted and reflected) wave packets, the averaging over the whole ensemble of particles has no physical sense. By this reason the above timing procedure cannot be applied in this case.

Of course, at late times one can attempt to define individual average positions of transmitted and reflected particles. However, in timing, this implies a separate description of both the subensembles at the first stage of scattering, what is widely accepted to be impossible in conventional quantum mechanics. As a result, it is not clear how to apply the above timing procedure both to the whole ensemble and to its parts, transmitted and reflected particles. This question remains open in the SWPA. In this section, following this approach, we will simply take the incident wave packet as the counterpart to the transmitted (reflected) one at the initial stage of scattering.

So, let \(Z_1\) be the spatial 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 the 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

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

(13)

Then, considering (10) and (11), one can write the ”transmission time” \(\Delta t_{tr}\) \((\Delta t_{tr} = \)
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\[ \Delta t_{tr} = \frac{m}{\hbar} \left[ \frac{< J' >_{out}}{< k >_{out}^c} + \frac{L_1}{k_0} + a \left( \frac{1}{< k >_{out}^c} - \frac{1}{k_0} \right) \right]. \]  

(14)

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

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

(15)

From equations (10), (12) and (15) it follows that the "reflection time" \( \Delta t_{ref} (\Delta t_{ref} = t'_2 - t'_1) \) can be written as

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

(16)

Note, the average 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, when

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

we have

\[ < k >_{tr} = k_0 + \frac{< T' >_{in}}{4l_0^2 < T >_{in}}; \]

\[ < -k >_{ref} = k_0 + \frac{< R' >_{in}}{4l_0^2 < R >_{in}}. \]  

(17)

(18)

Let

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

then relations (17) and (18) can be written in the form (note that \( R' = -T' \))

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

(19)

As is seen, quantities (14) and (16) cannot serve as characteristic times for a particle. Due to the last terms in these expressions the above times depend 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, when the difference \( < k >_{tr}^c - k_0 \) is sufficiently large. The numerical modeling of tunneling shows in this case a premature appearance of the CM of the transmitted packet behind the barrier, what just points to the lack of a causal link between the transmitted and incident wave packets (see [11, 12, 13]).

As was shown in [11, 12], 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 (14) and (16) tend to zero when \( l_0 \to \infty \), with the ratio \( l_0/a \) being fixed, can be proved with help of Exps. (17) and (18) (note that the limit \( l_0 \to \infty \) with a fixed value of \( a \) is...
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unacceptable in this analysis, because it contradicts the initial condition $a \gg l_0$ for a completed scattering).

However, one has to stress that in the limit $l_0 \to \infty$ the incident and transmitted (reflected) wave packets are causally disconnected, as in the general case. As before, the former cannot be considered as the counterpart to the transmitted (or reflected) wave packet at the initial stage of scattering. The inconsistency of introducing the phase times in the SWPA is seen explicitly in the particular case of the $\delta$-potential. As is known, the phase transmission time is nonzero in this case. This result is usually treated as the evidence of a non-local character of tunneling a particle. However, one has to bear in mind the fact that in the SWPA this nonzero time describes the motion of the wave-packet’s CM. Thus, this result is clearly erroneous, since any point of a moving wave packet should cross instantly the spatial region of a zero width.

At the same time we have to stress that, although Exps. (14) and (16) cannot be applied to a particle, they notwithstanding correctly describe the relative motion of the transmitted (or reflected) and incident wave packets. Thus, the main problem is that quantum mechanics, as it stands, does not provide a clear prescription to interpret properly the behaviour of these packets as applied to a particle. To clarify this question is the main goal of our study.

4. A renewed wave-packet analysis

4.1. Tunneling a quantum particle as a combined process consisting from two alternative elementary ones, transmission and reflection

4.1.1. Born’s formula underlying the statistical interpretation of a wave function and the problem of defining the expectation values of physical observables for a tunneling particle. As is seen from the previous section, modeling the tunneling process in terms of wave packets meets a paradoxical situation. On the one hand, since this process is one-particle, the corresponding time-dependent state of a quantum particle is supposed to be the quantum analogue of a classical one-particle trajectory. On the other hand, the average values of the particle’s position and momentum calculated for this one-particle state, by Born’s formula, cannot be interpreted as the expectation values of these quantities.

However, as is well-known, this formula is an integral part of Born’s statistical interpretation of a wave function. Therefore the above controversy means that the wave function to describe the one-particle tunneling process cannot be associated with the motion of a single quantum particle. This is seen also from the fact that at late times this function represents the superposition of the transmitted and reflected wave packets. The naive statistical interpretation of this wave function (as that to describe the motion of a single particle), which ignores the above controversy, leads to the non-local pseudo-effect: transmitted and reflected particles of the ensemble are inextricably intertwined even after the scattering event. Of course, the above fact that Born’s formula is not
applicable to this case says that this "non-locality" as well as the above interpretation of wave function have no physical sense.

The above situation is similar to that to arise in the well-known two-slits experiment where the beam of mutually non-interacting, identically prepared particles diffracts on an opaque screen with two slits. As is known, a wave packet to describe this (one-particle) process passes, like usual waves, through both the slits. As in the above case, the naive statistical interpretation of this wave function (as that to describe the stochastic motion of a single particle) "permits" the particle to pass simultaneously through both the slits; for both the events are inextricably intertwined in this interpretation. That is, again we arrive at the pseudo-effect of non-locality.

4.1.2. Elementary and combined one-particle scattering states and processes. So, scattering a wave packet on the potential barrier as well as its scattering on the slits in an opaque screen, each cannot be associated unambiguously with the motion of a single quantum particle. This is true also for any one-particle quantum scattering process which involves either several sinks or several sources of particles, or several possible channels of motion. In all non-relativistic scattering processes, a quantum particle is evident to be an indivisible object. And, though we can say nothing, before measuring, about the position of the particle, we can say a priori that this object can be emitted only by one source of particles, can move only along one scattering channel and can be absorbed only by one sink of particles. This property should be considered as a distinctive of the motion of a single quantum particle. It is evident that the behaviour of wave packets in the case of the tunneling process and above diffraction on slits does not guarantee the fulfillment of this property.

By our approach, all quantum one-particle scattering processes and the corresponding time-dependent states fall into two classes - elementary and combined. Namely, if the above property is fulfilled, we deal with elementary ones. Otherwise, a quantum one-particle scattering process and the corresponding state are combined. Unlike an elementary process, a combined one implies several alternative scattering channels for a particle. The motion of a particle along each channel should be described by the corresponding wave function to obey the Schrödinger equation and the corresponding boundary conditions to distinguish this channel from others. The wave function to describe a combined process is the sum of those to describe all elementary ones involved in the former.

Note, since all elementary processes involved in the same combined one are mutually exclusive, a particle can take part only in one of them. This means that the whole quantum ensemble of particles involved in the combined scattering process can be uniquely decomposed into the subensembles of particles taking part only in one of the elementary processes: the sum of norms of wave functions to describe the elementary processes is equal to unit. The number of particles in each subensemble is evident to be constant in time.

We have to stress that only elementary one-particle states can be viewed as the
quantum analogue of classical ones. To calculate the expectation values of the position
and momentum of a particle is meaningful only for elementary processes. In this case
one can calculate the trajectory of the wave-packet’s CM. It can be used then for timing
a quantum particle. As regards a combined process, making use of Born’s formula has
no physical sense in this case. Such a process can be associated with several CM’s
trajectories, rather than with one. The number of these trajectories is equal to that of
elementary processes involved in the combined one.

So, by our approach tunneling a non-relativistic quantum particle through an one-
dimensional static potential barrier is a combined process consisting from two alternative
elementary ones, transmission and reflection. Our next step is to find two solutions
to the Schrödinger equations to describe separately transmission and reflection. The
wave function for transmission will be named further as the transmission wave function
(TWF), and that for reflection will be named as the reflection wave function (RWF).

The main thing which should be taken into account in finding these solutions is that
the RWF should describe only reflected particles, and the TWF does only transmitted
particles. In both the cases, stationary solutions should contain one incoming and one
outgoing wave. In this paper we show that such solutions do exist.

4.2. 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 4.1 their sum represents the wave function to describe, in the problem
at hand, the combined 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 $t$,

$$
\Psi_{full}(x, t) = \Psi_{tr}(x, t) + \Psi_{ref}(x, t) \tag{20}
$$

where $\Psi_{full}(x, t)$ is the full wave function to describe all particles (see section 4.1). In the
limit $t \to \infty$

$$
\Psi_{tr}(x, t) = \Psi_{out}^{tr}(x, t); \quad \Psi_{ref}(x, t) = \Psi_{out}^{ref}(x, t) \tag{21}
$$

where $\Psi_{out}^{tr}(x, t)$ and $\Psi_{out}^{ref}(x, t)$ are the transmitted and reflected wave packets whose
Fourier-transforms presented in (8) and (9).

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 $\Psi_{ref}(x; k)$ and $\Psi_{tr}(x; k)$ for the
spatial region $x \leq a$. In this region let

$$
\Psi_{ref}(x; k) = A_{in} \left( A_{in}^{ref} e^{ikx} + B_{out}^{ref} e^{-ikx} \right) \tag{22}
$$

$$
\Psi_{tr}(x; k) = A_{in} \left( A_{in}^{tr} e^{ikx} + B_{out}^{tr} e^{-ikx} \right) \tag{23}
$$

where $A_{in}^{tr} + A_{in}^{ref} = 1$, $B_{out}^{tr} + B_{out}^{ref} = p^*/q$. 

In its turn, for $\Psi_{tr}$ in the form $x$ it, we have to study both the solutions in the region $\text{ref}$.

As a result, we obtain for $\Psi_{tr}$

$$|A_{in}^{\text{ref}}|^2 - |B_{out}^{\text{ref}}|^2 = 0. \quad (24)$$

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

$$|A_{in}^{tr}|^2 - |B_{out}^{tr}|^2 = \frac{\hbar k}{m} T(k) \quad (25)$$

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

Taking into account that $\Psi_{tr} = \Psi_{full} - \Psi_{ref}$ let us now exclude $\Psi_{tr}$ from Eq. (25).

As a result, we obtain for $\Psi_{ref}$ the equation

$$\text{Re} \left( A_{in}^{\text{ref}} - B_{out}^{\text{ref}} b_{out}^* \right) = 0. \quad (26)$$

Eq. (26) guarantees the coincidence of the probability flux for $\Psi_{full}(x)$ and $\Psi_{tr}(x)$.

From condition (21) for $\Psi_{ref}(x; k)$ it follows that $B_{out}^{\text{ref}}(k) = b_{out}(k) \equiv p^*/q$ (see (5)).

Then Eq. (26) yields that $\text{Re}(A_{in}^{\text{ref}}) = R$, and Eq. (24) leads to $|A_{in}^{\text{ref}}|^2 = |B_{out}^{\text{ref}}|^2 = |p^*/q|^2 = R$. Thus, $A_{in}^{\text{ref}} = \sqrt{R}(\sqrt{R} \pm i\sqrt{T}) \equiv \sqrt{R}\exp(i\lambda)$; $\lambda = \pm \arctan(\sqrt{T}/R)$.

As is seen, the superposition of the incoming waves to describe transmission and reflection for a given $E$ yields the incoming wave of unite amplitude, which describes the whole ensemble of incident particles. In this case, not only $A_{in}^{tr} + A_{in}^{\text{ref}} = 1$, but also $|A_{in}^{tr}|^2 + |A_{in}^{\text{ref}}|^2 = 1!$

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

$$\Psi_{ref}(x; k) = -2\sqrt{R}A_{in} \sin \left( k(x - a) + \frac{1}{2} \left( \lambda - J + F - \frac{\pi}{2} \right) \right) e^{i\phi(+)} \quad (27)$$

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 reflection. To select it, we have to study both the solutions in the region $x \geq b$ where they can be written in the form

$$\Psi_{ref}(x; k) = A_{in} \left( A_{out}^{\text{ref}} e^{ikx} + B_{in}^{\text{ref}} e^{-ikx} \right); \quad (28)$$

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

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

$$\Psi_{ref}(x; k) = \mp 2\sqrt{R}A_{in} \sin \left[ k(x - b) + \frac{1}{2} \left( J + F + \frac{\pi}{2} - \lambda \right) \right] e^{i\phi(+)}. \quad (29)$$
For the following it is convenient to go over to the variable $x'$: $x = x_{mid} + x'$, where \( x_{mid} = (a + b)/2 \). Then, for $x' \leq -d/2$, we have

\[
\Psi_{ref}(x') = -2\sqrt{RA_m}\sin\left[\frac{1}{2}(kd + \lambda - \frac{\pi}{2}) + \frac{F}{2} + kx'\right]e^{i\phi},
\]

for $x' \geq d/2$ —

\[
\Psi_{ref}(x') = \pm 2\sqrt{RA_m}\sin\left[\frac{1}{2}(kd + \lambda - \frac{\pi}{2}) - \frac{F}{2} - kx'\right]e^{i\phi}.
\]

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

\[
\Psi_{ref}(x_0) = -2\sqrt{RA_m}\sin\left[\frac{1}{2}(kd + \lambda - \frac{\pi}{2} + F) + kx_0\right]e^{i\phi} \quad (30)
\]

\[
\Psi_{ref}(-x_0) = \pm 2\sqrt{RA_m}\sin\left[\frac{1}{2}(kd + \lambda - \frac{\pi}{2} + F) + kx_0 - F\right]e^{i\phi} \quad (31)
\]

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. (30) and (31), one of the above two stationary solutions $\Psi_{ref}(x'; k)$ is odd in the out-of-barrier region, but another function is even. Namely, when $F = 0$ the upper sign in (31) 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 $\Psi_{ref}(x'; k)$.

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 $\Psi_{ref}(x'; k)$ 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 time-dependent wave function formed only from the odd (or even) stationary solutions $\Psi_{ref}(x'; k)$, should be equal to zero at the barrier’s midpoint. This means that particles impinging a symmetric barrier from the left 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 $\Psi_{ref}(x'; k)$. In this case the corresponding probability density is everywhere continuous, including the point $x' = 0$, and the probability flux is everywhere equal to zero.

As regards the searched-for TWF, $\Psi_{tr}(x; k)$, it can be found now from the expression $\Psi_{tr}(x; k) = \Psi_{full}(x; k) - \Psi_{ref}(x; k)$. 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 $x = x_{mid}$, though the first derivative of $\Psi_{tr}(x; k)$ on $x$ 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. (30) and (31), for asymmetric potential barriers, both the solutions $\Psi_{ref}(x'; k)$ 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,
Wave functions and characteristic times for transmission and reflection

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 time-dependent 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 the wave functions \( \Psi_{\text{full}} \), \( \Psi_{\text{tr}} \) and \( \Psi_{\text{ref}} \) in the case of symmetric barriers, we have considered the case of the rectangular barrier of height \( V_0 \). In this case, the stationary-state wave function \( \Psi_{\text{ref}}(x;k) \), for \( a \leq x \leq x_{\text{mid}} \), reads as

\[
\Psi_{\text{ref}} = 2\sqrt{RA_m}e^{i\phi(\pm)}\left[ \cos(ka + \phi(-)) \sinh(kd/2) - \frac{\kappa}{\kappa} \sin(ka + \phi(-)) \cosh(kd/2) \right] \sinh\left(\kappa(x - x_{\text{mid}})\right)
\]

where \( \kappa = \sqrt{2m(V_0 - E)/ \hbar} \) (\( E < V_0 \)); and

\[
\Psi_{\text{ref}} = -2\sqrt{RA_m}e^{i\phi(\pm)}\left[ \cos(ka + \phi(-)) \sin(kd/2) + \frac{\kappa}{\kappa} \sin(ka + \phi(-)) \cos(kd/2) \right] \sin(\kappa(x - x_{\text{mid}}))
\]

where \( \kappa = \sqrt{2m(E - V_0)/ \hbar} \) (\( E \geq V_0 \)). In both cases \( \Psi_{\text{ref}}(x;k) \equiv 0 \) for \( x \geq x_{\text{mid}} \).

We have calculated the spatial dependence of the probability densities \( |\Psi_{\text{full}}(x,t)|^2 \) (dashed line), \( |\Psi_{\text{tr}}(x,t)|^2 \) (open circles) and \( |\Psi_{\text{ref}}(x,t)|^2 \) (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 \( \Psi_{\text{full}}(x,0) \) represents the Gaussian wave packet with \( l_0 = 7.5nm \); the average kinetic energy is equal to 0.25eV, 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 \( \Psi_{\text{full}} \) (remind that the latter, unlike the former, cannot be unambiguously interpreted as the expectation value of the particle’s position). 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 \( < T >_{\text{in}} \approx 0.149 \). For the well \( < T >_{\text{in}} \approx 0.863 \).

We have to stress once more that, by our approach, the initial state of a tunneling particle can be presented as the superposition of those for transmission and reflection: \( \Psi_{\text{full}}(x,0) = \Psi_{\text{tr}}(x,0) + \Psi_{\text{ref}}(x,0) \). One might say that it is meaningless to define the
initial state of transmitted particles, since it is impossible to predict the future of a
starting particle. However, the destination of quantum theory is to predict the behavior
of the quantum ensembles of identically prepared particles, rather than that of one
particle. Main thing is that $\Psi_{tr}(x,0)$ is the only initial wave packet, for the given
potential $V(x)$, which evolves isometrically (causally) into the transmitted one, and
$\Psi_{ref}(x,0)$ is the only one which evolves isometrically into the reflected wave packet. A
more detailed discussion of some aspects of the separation of transmission and reflection
is given in the last section of the paper.

5. Exact and asymptotic tunneling times for transmission and reflection

5.1. Exact tunneling times

So, we have found two causally evolving wave packets to describe the subensembles
of transmitted and reflected particles at all stages of tunneling. 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 the wave packets to describe separately reflection and
transmission, at all stages of its motion.

Let $t_1^{tr}$ and $t_2^{tr}$ be such moments of time that

$$\frac{<\Psi_{tr}(x,t_1^{tr})|\hat{x}|\Psi_{tr}(x,t_1^{tr})>}{<\Psi_{tr}(x,t_1^{tr})|\Psi_{tr}(x,t_1^{tr})>} = a - L_1; \quad (34)$$

$$\frac{<\Psi_{tr}(x,t_2^{tr})|\hat{x}|\Psi_{tr}(x,t_2^{tr})>}{<\Psi_{tr}(x,t_2^{tr})|\Psi_{tr}(x,t_2^{tr})>} = b + L_2, \quad (35)$$

where $\Psi_{tr}(x,t)$ describes transmission. Then, one can define the transmission time
$\Delta t_{tr}(L_1,L_2)$ as the difference $t_2^{tr}(L_2) - t_1^{tr}(L_1)$ where $t_1^{tr}(L_1)$ is the smallest root of Eq. (34), and $t_2^{tr}(L_2)$ is the largest root of Eq. (35).

Similarly, for reflection, let $t$ be such that

$$\frac{<\Psi_{ref}(x,t)|\hat{x}|\Psi_{ref}(x,t)>}{<\Psi_{ref}(x,t)|\Psi_{ref}(x,t)>} = a - L_1, \quad (36)$$

then the reflection time $\Delta t_{ref}(L_1)$ can be defined as $\Delta t_{ref}(L_1) = t_2^{ref} - t_1^{ref}$ where $t_1^{ref}$ is the smallest root, and $t_2^{ref}$ is the largest root of Eq. (36) (of course, if they exist, for
the wave-packet’s CM may do not enter the barrier region).

It is important to emphasize that, due to conserving the norms of $\Psi_{tr}(x,t)$ and
$\Psi_{ref}(x,t)$ both the characteristic times are non-negative for any distances $L_1$ and $L_2.$
Both the definitions are valid 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. Both the characteristic times show, in fact, the time spent by the
corresponding CM in the barrier region. Of course, one has to bear in mind that in the
case of reflection the CM of the wave packet may turn back without entering the barrier
region: in this case $\Delta t_{ref}(0) = 0$. Of course, if $L_1$ is larger than the wave-packet’s width,
$\Delta t_{ref}(L_1) \neq 0.$
5.2. 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 \( \Delta t_{ref}(L_1) \) in more explicit form. Indeed, in this case, instead of the exact subensemble’s wave functions, we can use the corresponding in asymptotes derived in \( k \)-representation. Indeed, now the “full” in asymptote, like the corresponding out asymptote, represents the sum of two wave packets:

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

(37)

\[
\alpha = 1 \text{ if } \Lambda \geq 0; \text{ otherwise } \alpha = -1. 
\]

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

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

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 \( <k>_{tr}^{in} \) and \( <k>_{ref}^{in} \)) is equal to that for large times:

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

Besides, at early times

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

(39)

(40)

As it follows from Exps. (39) and (40), 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:

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

(41)

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. Of great importance here is that \( x_{start}^{tr} \) and \( x_{start}^{ref} \) are the initial values of \( <\hat{x}>_{in}^{tr} \) and \( <\hat{x}>_{in}^{ref} \), respectively, which have the status of expectation values of the particle’s position. They behave causally in time. As regards the average starting point for the whole ensemble of particles, its coordinate is the initial value of \( <\hat{x}>_{in} \) which behaves non-causally; for this quantity is not an expectation value of the particle’s position (see also the last section of this paper). By this reason the (asymptotic) phase times obtained in the SWPA should be considered as ill-defined quantities, for any wave packets.
Let us take into account Expns. (40) and (11) 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 \( t_{tr1} \) and \( t_{tr2} \), which correspond to the extreme points \( Z_1 \) and \( Z_2 \), respectively, read now as

\[
\langle \hat{x} \rangle_{in} (t_{tr1}) = a - L_1; \quad \langle \hat{x} \rangle_{out} (t_{tr2}) = b + L_2.
\]

Considering (39) and (11), we obtain from here that now the transmission time is

\[
\tau_{tr}(L_1, L_2) \equiv t_{tr2} - t_{tr1} = \frac{m}{\hbar} \left( < J' >_{out}^{tr} - < J' >_{in}^{tr} + L_1 + L_2 \right). \tag{42}
\]

Similarly, for the reflection time \( \tau_{ref}(L_1) \) (\( \tau_{ref} = t_{ref2} - t_{ref1} \)), we have

\[
\langle \hat{x} \rangle_{in}^{ref} (t_{ref1}) = a - L_1; \quad \langle \hat{x} \rangle_{out}^{ref} (t_{ref2}) = a - L_1.
\]

Considering (40) and (12), one can easily show that

\[
\tau_{ref}(L_1) \equiv t_{ref2} - t_{ref1} = \frac{m}{\hbar} \left( < J' - F' >_{out}^{ref} - < J' >_{in}^{ref} + 2L_1 \right). \tag{43}
\]

The inputs \( \tau_{as}^{tr}(\tau_{as}^{tr} = \tau_{tr}(0, 0)) \) and \( \tau_{as}^{ref}(\tau_{as}^{ref} = \tau_{ref}(0, 0)) \) will be named below as the asymptotic transmission and reflection times for the barrier region, respectively:

\[
\tau_{as}^{tr} = \frac{m}{\hbar} \left( < J' >_{out}^{tr} - < J' >_{in}^{tr} \right), \tag{44}
\]

\[
\tau_{as}^{ref} = \frac{m}{\hbar} \left( < J' - F' >_{out}^{ref} - < J' >_{in}^{ref} \right). \tag{45}
\]

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

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

\[
d_{eff}^tr = < J' >_{out}^{tr} - < J' >_{in}^{tr}, \quad d_{eff}^ref = < J' - F' >_{out}^{ref} - < J' >_{in}^{ref}, \tag{46}
\]

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

5.3. 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 expectation value, \( x_{start}(k) \), of the 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 momentum \( \hbar k_0 \) 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 [10, 13]), one can show that, for the below-barrier case \((E \leq V_0)\),

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

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

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

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

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

where \( \kappa = \sqrt{2m(V-E)/\hbar^2}; \beta = 1 \) 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 \( d_{\text{eff}} \to d \) and \( x_{\text{start}}(k) \to 0 \), in the limit \( k \to \infty \).

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. Note, for wells, the values of \( d_{\text{eff}} \) and, as a consequence, the corresponding asymptotic 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 \( d_{\text{eff}} \approx d \). 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 \cdot \frac{k^2 - \beta \kappa_0^2 \sin^2(\kappa d/2)}{4k^2 \kappa^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^2 + \kappa_0^4 \sin^2(\kappa d)}
\]

for \( E \geq V_0 \).

It is important that for the \( \delta \)-potential, \( V(x) = W \delta(x - a) \), we have \( d_{\text{eff}} \equiv 0 \). That is, like the dwell and Larmor times, \( x_{\text{start}}^* = 0 \) in this case. Thus, though the ensemble of identically prepared particles spends nonzero time to pass through this potential, each quantum particle of the ensemble spends no time in its barrier region. While the quantum ensemble of particles interacts with the \( \delta \)-potential, there is a nonzero probability to find a particle near this barrier.

Note, unlike the first derivative of \( \Psi_{\text{full}}(x, t) \) with respect to \( x \), that of \( \Psi_{\text{tr}}(x, t) \) has equal values in the limits \( x \to a \pm 0 \). The average force calculated for a particle in the state \( \Psi_{\text{tr}}(x, t) \) is zero, for this potential. That is, \( \Psi_{\text{tr}}(x, t) \) describes that part
of the incident wave packet, which does not experience the action of the $\delta$-potential. Transmitting particles start, on the average, from the point $x_{\text{start}}(k)$,

$$x_{\text{start}}(k) = -\frac{2m\hbar^2 W}{\hbar^2 k^2 + m^2 W^2};$$

and moves then freely.

6. Discussion and conclusions

The problem of introducing characteristic times for a tunneling particle as that of calculating the expectation values of its position and momentum

The main idea underlying this paper is that tunneling a particle through an one-dimensional static potential barrier is a combined stochastic process consisting from two alternative elementary ones - transmission and reflection. We showed that the wave function to describe the tunneling process can be uniquely decomposed into two solutions of the Schrödinger equation for the given potential, which describe separately transmission and reflection. We found both the solutions in the case of symmetric potential barriers and introduced, according to the standard timing procedure, the average (exact and asymptotic) transmission and reflection times.

By our approach, in the most cases, quantum one-particle scattering processes are just combined. Each of them represents a complex stochastic process consisting from several alternative elementary ones. The decomposition of a combined process into elementary ones can be performed uniquely. Accordingly, the wave function to describe the combined process can be uniquely presented as a sum of those to describe all the elementary ones.

The main peculiarity of combined states is that the averaging over such states of the particle’s position and momentum, with help of Born’s formula intended for calculating the expectation values of physical observables, does not give in reality expectation values of these quantities. Both the average values behave non-causally in time. Strictly speaking, in the case of combined states, the particle’s position and momentum (though their operators are Hermitian) lost their primary status of physical observables! As a result, timing a particle in such states is meaningless too. Only for elementary quantum processes and states Born’s formula and the timing procedure are valid. In other words, only for elementary states the particle’s position and momentum (and other physical quantities with linear Hermitian operators) have their primary status of observables, and, as consequence, there is no problem to time the motion of a particle being in such states.

About some aspects of a superposition of the probability fields As is shown, the peculiarity of the wave functions for transmission and reflection is that each of them contains only one incident and only one scattered wave packets. At the same time it is evident that if a particle was prepared in the combined state $\Psi_{tr}(x, 0)$, then this packet would be divided by the barrier into two parts. Of course, in the case considered the
initial combined state of a particle is $\Psi_{\text{full}}(x, 0)$ but not $\Psi_{\text{tr}}(x, 0)$. Nevertheless, we have to clear up the principal difference taking place between a wave function to describe a combined process and those to describe elementary ones involved in the former.

Let, for the given potential, in addition to the problem at hand where the amplitudes of incoming and outgoing waves are, respectively,

$$a_{\text{in}} = 1, \quad b_{\text{out}} = \frac{p}{q}, \quad a_{\text{out}} = \frac{1}{q}, \quad b_{\text{in}} = 0,$$

we have two auxiliary scattering problems with amplitudes

$$a_{\text{ref}}^{\text{in}} = \frac{|p|^2}{|q|^2}, \quad b_{\text{out}}^{\text{ref}} = \frac{p}{q}, \quad a_{\text{out}}^{\text{ref}} = 0, \quad b_{\text{in}}^{\text{ref}} = \frac{p}{|q|^2},$$

and

$$a_{\text{tr}}^{\text{in}} = \frac{1}{|q|^2}, \quad b_{\text{out}}^{\text{tr}} = 0, \quad a_{\text{out}}^{\text{tr}} = \frac{1}{q}, \quad b_{\text{in}}^{\text{tr}} = -\frac{p}{|q|^2},$$

(the transfer matrix $T$ is evident to be the same for all three problems).

Note that in the first auxiliary problem the only outgoing wave coincides with the reflected wave arising in (47). And, in the second one, the only outgoing wave coincides with the transmitted wave in (47). It is evident that the sum of these two functions results just in that to describe the state of a particle in the original tunneling problem.

As is seen, the main peculiarity of the superposition of these two probability fields is that due to interference their incoming waves in the region $x > b$ fully annihilate each other (note that in the corresponding reverse motion they are outgoing waves). The corresponding flux of particles is reoriented into the region $x < a$. Thus, the initial probability fields (48) and (49) associated with the transmitted and reflected wave packets are radically modified under the superposition. In this case, the wave packet connected causally to the transmitted (reflected) one is just $\Psi_{\text{tr}}(x, t)$ ($\Psi_{\text{ref}}(x, t)$).

Thus, we see that the sum of wave functions (48) and (49) can be presented as that of the stationary-states RWF and TWF. As a result of reorienting 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 $|a_{\text{in}}^{\text{ref}}|^2 = R^2$ (see (48)) to $|a_{\text{in}}^{\text{ref}}|^2 + |b_{\text{in}}^{\text{ref}}|^2 = R^2 + TR = R$ (in the RWF). In the case of transmission, the corresponding quantity increases from the initial value $|a_{\text{in}}^{\text{tr}}|^2 = T^2$ (see (49)) to $|a_{\text{in}}^{\text{tr}}|^2 + |b_{\text{in}}^{\text{tr}}|^2 = T^2 + TR = T$ (in the TWF).

As is seen, in contrast to probability fields (48) and (49), $\Psi_{\text{tr}}(x, t)$ and $\Psi_{\text{ref}}(x, t)$ should be considered as an inseparable pair: they cannot evolve separately. Of course, in this case one would doubt the reality of these fields. Indeed, they cannot be observed separately. And, besides, being involved in the combined state, they cannot be directly observed, at early stages of scattering, because of interference. However, for any combined process, namely the interference between wave fields to describe elementary sub-processes provides all needed information to justify their existence.

Indeed, let $|\Psi_{\text{full}}(x, t)|^2$ be the result of measuring $|\Psi_{\text{full}}(x, t)|^2$. Then, using the distributions $|\Psi_{\text{tr}}(x, t)|^2$ and $|\Psi_{\text{ref}}(x, t)|^2$ calculated beforehand, we can extract, from
the experiment data, the difference $|\Psi^{exp}_{full}(x, t)|^2 - |\Psi_{tr}(x, t)|^2 - |\Psi_{ref}(x, t)|^2$ to describe interference between the wave fields $\Psi_{tr}(x, t)$ and $\Psi_{ref}(x, t)$. By our approach, it must have two important properties: 1) the integral of this difference over the region $(-\infty, \infty)$ must be zero; 2) this difference must be nonzero only for the first stages of scattering, and only for $x \leq x_{mid}$. The first property means that the whole ensemble of particles, in this scattering problem, can be indeed divided into two subensembles described by the distributions $|\Psi_{tr}(x, t)|^2$ and $|\Psi_{ref}(x, t)|^2$. The second property means that one of them is indeed connected causally to the transmitted wave packet, and another evolves causally into the reflected one. This means, in turn, that the above decomposition is unique.

Note, this property is inherent only to combined processes. The elementary states $\Psi_{tr}(x, t)$ and $\Psi_{ref}(x, t)$, themselves represent decompositions into the orthogonal stationary states. However, the latter cannot be treated as elementary states. For the interference between them does not have the above two properties. They cannot be separated, in principle.

So, the wave functions $\Psi_{tr}(x, t)$ and $\Psi_{ref}(x, t)$ describe two real processes to proceed simultaneously. Taking into account the fact that a wave function describes the beam (or, ensemble) of identically prepared particles, rather than a single quantum particle, one can interpret the found decomposition of $\Psi_{full}(x, t)$ as follows. Namely, $\Psi_{tr}(x, t)$ describes that part of the beam of mutually non-interacted particles prepared in the state $\Psi_{full}(x, 0)$, which is transmitted through the barrier. Similarly, $\Psi_{ref}(x, t)$ does the reflected part of this beam.

At early times these parts of the beam move in the same spatial region. At this stage of scattering, the study of the motion of both parts is reduced to the analysis of the interference between them. At all stages they evolve irrespective of each other, not "seeing" their own counterparts; just $\Psi_{tr}(x, t)$ ($\Psi_{ref}(x, t)$) is causally connected to the transmitted (reflected) wave packet considered separately, but not $\Psi_{full}(x, t)$. As well as in the superposition of free moving wave packets they do not destroy each other (after their meeting in some spatial region they move unaltered), in the superposition of the modified wave fields $\Psi_{tr}(x, t)$ and $\Psi_{ref}(x, t)$ they do not influence each other, too.

It is not surprising that particles of both parts start, on the average, from the spatial points to differ from the average starting point calculated for the whole beam of particles. Firstly, $\langle \hat{x} \rangle_{in} \neq \langle T \rangle < \hat{x} >_{in}^{tr} + < R > < \hat{x} >_{in}^{ref}$ due to interference; here $\langle T \rangle$ and $\langle R \rangle$ are the norms of $\Psi_{tr}(x, t)$ and $\Psi_{tr}(x, t)$, respectively. And, what is more important, among these three average quantities, only $\langle \hat{x} \rangle_{in}^{tr}$ and $\langle \hat{x} \rangle_{in}^{ref}$ have the physical meaning of the expectation values of the particle’s position. The behaviour of $\langle \hat{x} \rangle_{in}$, being averaged over two alternative processes, is not causal. It cannot be interpreted as the expectation value of the particle’s position.

The main point of our research is that any combined state represents a superposition of elementary states which are distinguishable. As a consequence, by our approach, the experimental study of the probability density for a particle taking part in a combined process means, in fact, the observation of the interference between the elementary states
involved in the combined process. However, maxima and minima of the interference pattern behave non-causally. Or, more correctly, only when we know all information about each elementary state, which just behaves causally, we can unambiguously interpret the behaviour of the interference pattern.

All this takes place, in particular, in the case of tunneling. By this approach, the non-causal behaviour of a tunneling wave packet (which have been pointed out by [7]) is explained by the fact that tunneling is a combined process. An exhaustive explanation of this quantum effect can be achieved only in the framework of a separate description of transmission and reflection. For only these processes are elementary, and, as a consequence, namely they (and the corresponding probability densities) behave causally.

About the perspective of studying the temporal and other aspects of quantum one-particle scattering processes A simple analysis shows that the definitions of the asymptotic tunneling times given in our approach differ essentially from their analogs known in the literature. At this point we have to note once more that a correct timing of transmitted and reflected particles implies the availability of a complete information about these subensembles of particles at all stages of scattering. Making use, in the alternative approaches, of the incident wave packet as the counterpart to the transmitted (or reflected) wave packet at the first stage of scattering is clearly an inconsistent step. For the former does not connected causally to the transmitted (or reflected) one (see also [4]). Just the wave functions for transmission and reflection found in our approach provides all needed information. Thus, we think that our definitions of tunneling times have a more solid basis.

Of course, a final decision in the long-lived controversy in solving the TTP should be made by a reliable experiment. In this connection, we have to note that the main ideas of such approaches as [20], [38] and others whose formalism involves the peculiarities of the measurement process, may be very useful in the following study of the tunneling and other scattering processes treated as combined ones. Indeed, the fact that our definitions of the tunneling times do not coincide, for example, with those obtained in [20] and [38] does not mean at all that the main ideas underling our and these approaches contradict each other. Rather they are mutually complementary. We think that namely in combination all these ideas will be useful in studying quantum scattering processes.

So, it would be very useful to define the Larmor time and time-of-arrival distribution on the basis of wave functions for transmission and reflection. It is evident that the influence of an external magnetic field (or absorbing potential) on transmitted and reflected particles should be different. Hence, the study of the interference between transmission and reflection, at the first stages of scattering, might permit us to check both our idea of separating these elementary processes and ways [20, 38] of introducing characteristic times, which differ from the standard timing procedure. For the first case, for this purpose, the same magnetic field (or absorbing potential) might be localized in two equivalent spatial regions lying on the same distance from the midpoint of a
symmetric potential barrier. In this case, the symmetry of the original potential remains unaltered, and there is no principal problem to find the wave functions for transmission and reflection.

As regards further development of our approach, it can be applied, in principle, to any potential localized in the finite spatial region. In one dimension, it is applicable to the potential steps and asymmetric potential barriers. No principal difficulties should arise also in separating transmission and reflection in the case of quasi-one-dimensional structures, when the potential energy of a particle depends only on one coordinate. As regards the scattering problem with two slits in the opaque screen, it seems to involve four elementary processes, transmission and reflection for the first and second slits. Besides, scattering a particle on a point-like obstacle, with a spherically symmetrical potential, seems to involve two alternative elementary processes. In this case there is a plain to separate both the processes. This plain must be parallel to the vectors $\vec{r}_0$ and $[\vec{r}_0 \times \vec{p}_0]$ and pass through the obstacle; here $\vec{r}_0$ and $\vec{p}_0$ are the average position and momentum of a particle calculated for its initial combined state.

Of course, in the general case the problem of decomposing some combined process into alternative elementary ones may be technically complicated. This task should be considered, in every case, separately.

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Figure captions

\Figure{\label{fig1}}The $x$-dependence of $|\Psi_{\text{full}}(x,t)|^2$ (dashed line) which represents the Gaussian wave packet with $l_0=7.5 \text{ nm}$ and the average kinetic particle’s energy $0.25 \text{ eV}$, as well as $|\Psi_{\text{tr}}(x,t)|^2$ (open circles) and $|\Psi_{\text{ref}}(x,t)|^2$ (solid line) for the rectangular barrier ($V_0=0.3 \text{ eV}$, $a=500 \text{ nm}$, $b=505 \text{ nm}$); $t=0$.}

\Figure{\label{fig2}}The same as in \ref{fig1}, but $t=0.4 \text{ ps}$.}

\Figure{\label{fig3}}The same as in \ref{fig1}, but $t=0.42 \text{ ps}$.}

\Figure{\label{fig4}}The $x$-dependence of $|\Psi_{\text{full}}(x,t)|^2$ (dashed line) which represents the Gaussian wave packet with $l_0=7.5 \text{ nm}$ and the average kinetic particle’s energy $0.25 \text{ eV}$, as well as $|\Psi_{\text{tr}}(x,t)|^2$ (open circles) and $|\Psi_{\text{ref}}(x,t)|^2$ (solid line) for the rectangular well ($V_0=-0.3 \text{ eV}$, $a=500 \text{ nm}$, $b=505 \text{ nm}$); $t=0$.}

\Figure{\label{fig5}}The same as in \ref{fig4}, but $t=0.4 \text{ ps}$.}

\Figure{\label{fig6}}The same as in \ref{fig4}, but $t=0.43 \text{ ps}$.}

\Figure{\label{fig7}}The same functions for the barrier region; parameters are the same as for \ref{fig2}.}

\Figure{\label{fig8}}The same functions for the barrier region; parameters are the same as for \ref{fig5}.}
