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SCATTERING OF A QUANTUM PARTICLE ON THE POTENTIAL STEP: CHARACTERISTIC TIMES FOR THE TRANSMISSION AND REFLECTION

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We present a new model of scattering a quantum particle on the potential step, which reconstructs the prehistory of the subensembles of transmitted and reflected particles by their final states. Unlike the conventional one this model predicts the existence of a transitional spatial region behind the potential step where the probability to find reflected particles is nonzero and the average velocity of transmitted particles monotonously varies between asymptotic values. For both subprocesses we define the dwell and asymptotic group times.

Keywords: *potential step, dwell time, group velocity*

1 Introduction

As far as we know, to date there are at least two approaches [1, 2] in the tunneling time literature (TTL) that deal directly with the temporal aspects of scattering a non-relativistic quantum particle by the potential step (see also the recent paper [3] where the approach [2] is generalized onto relativistic particles). Both approaches are treated in the TTL as realistic ones since they define the transmission and reflection times with making use of clock models which imply a direct measurement of these scattering times.

Our purpose is to show that these models violate the causality principle and their results can hardly be called realistic. We begin with the most striking result whose essence is the following (see [2]). When the particle's energy is less by an infinitesimal magnitude than the height of the potential step (situated for example at the point $x = a$) the average time of staying a particle in the spatial region $x > a$ located behind the step diverges; that is, in this case the particle takes (on average) an infinite time to bounce back into the region $(-\infty, a]$. However, when its energy is higher by an infinitesimal magnitude than the step height, the particle bounces off the step instantaneously.

Davies emphasizes the paradoxicality of this result. But he believes that it creates no interpretational problems since this discontinuity occurs just at that point on the energy scale where the clock model [2] is unreliable because of its limited resolution.

But such an explanation is not convincing since the reflection time defined in this model exhibits strange physical properties not only at this point. This occurs at all energies exceeding the step height: according to this model, the reflection time is nonzero when the particle's energy is less than the step height; whilst otherwise it equals strictly to zero. That is, this model says, in fact, that the probability to find reflected particles in the spatial region behind the step is nonzero when this region is classically forbidden, but zero when this region is classically accessible.

Note that this consequence of [2] is in a full agreement with the conventional quantum-mechanical model (CQM) of scattering a particle on the potential step. Under this model, when the particle energy is less by an infinitesimal magnitude than the step height, the probability to find reflected particles, at a finite distance behind the step, is nonzero. However, if its energy exceeds the step height by an infinitesimal magnitude, then this probability equals strictly to zero everywhere in this region (where only the transmitted wave exists).

That is, according to the CQM, in the first case, reflected particles are able to penetrate (due to their wave properties) into the classically forbidden spatial region. While in the second case (when this region becomes classically accessible, and the difference in energy, in the comparison with the first case, is infinitesimal) they cannot. Such energy dependence of the probability density, in the CQM, is evident to contradict the very spirit of quantum mechanics. So that the strange behavior of the reflection time in the clock model [2], based fully on the CQM, is a consequence of the latter.

Another argument against the CQM is that it, in principle, does not allow one to introduce the transmission and reflection times in accordance with the causality principle. To show this, let us analyze in detail the presented in [2] idea of introducing the transmission time: "To achieve this, the particle is coupled (weakly) to a quantum clock. The coupling is chosen to be non-zero only when the particle's position lies within a given spatial interval... Initially the clock pointer is set to zero. After a long time,

when the particle has traversed the spatial region of interest with high probability, the position of the clock pointer is measured. The change in position yields the expectation value for the time of flight of the particle between the two fixed points."

Note that this clock model has been designed for timekeeping a *scattering* particle, but its key features have been illustrated in [2] by the example of a *free* particle. That is, per se, the dynamics of free and scattering particles are treated in [2] as qualitatively identical. But this is not; this model, being true in the case of a free particle, violates the causality principle in the case of a particle scattering by the potential step or rectangular barrier.

To see the principal difference between the timekeeping of the quantum dynamics of free and scattering particles, one has to take into account the following two points. First, the mentioned coupling between a quantum clock and a particle in the stationary state is realized in [2] as a coupling between the clock and the phase of the wave function that describes the particle's state. Second, when "the spatial region of interest" is empty the incident wave, that traverses it, never splits into parts. Whilst, when this region contains the potential step or rectangular barrier, the incident wave splits here into two waves – transmitted and reflected.

The latter means that at the initial stage of scattering the clock pointer is coupled in this model to the phase of the *incident* wave (that describes the whole ensemble of particles, without distinguishing its to-be-transmitted and to-be-reflected parts), while at the final stage it is coupled to the phase of the *transmitted* wave (that describes only the transmitted part of the incident ensemble). That is, in this model, the procedure of setting to zero of the clock pointer is based, in fact, on the implicit assumption that the average departure times of the whole ensemble of particles and its to-be-transmitted part (causally connected to the transmitted subensemble), coincide with each other. But this is not (see [4]). So that the clock model [2] violates the causality principle. To correctly perform this procedure for clocks used for measuring the transmission (reflection) time, one needs first to restore the whole prehistory of the subensemble of transmitted (reflected) particles by the transmitted (reflected) wave.

One more crucial point, that should be taken into account in studying the temporal aspects of both subprocesses, is that the transmission and reflection times, even being properly defined, cannot be *directly* measured because of interference between these subprocesses. Neither the measurement of these characteristic times nor the unambiguous interpretation of measurement data can be properly realized without a quantum-mechanical model of

the scattering process, that would able to 'see' the dynamics of each subprocess at all stages of scattering. In particular, the key point of all such measurements – zero setting of the clock pointer – cannot be correctly performed if the dynamics of each subprocess at the initial stage of scattering is unknown.

In the papers [5–8] we suggest, by the example of scattering a particle by symmetric potential barriers, the technique of restoring the individual prehistory of the subensembles of transmitted and reflected particles by their final states. The main idea of this approach is to present the total wave function that describes this process as a superposition of two "subprocess wave functions" (SWFs) that describe the dynamics of each subprocess at all stages of scattering. According to this approach, any characteristic time and expectation value of any one-particle physical observable can be calculated *only* for subprocesses.

This idea contradicts the conventional practice of a quantum-mechanical description of scattering a particle by 1D potential barriers. And its proponents claim that any decomposition into SWFs of the total wave function – the solution of the scattering problem, continuous everywhere together with its first spatial derivative – is inadmissible. Only this wave function they say should be used for calculating any physical quantities; no part of the total wave function can be used for that.

However, as was shown above, characteristic times for the potential step cannot be correctly calculated on the basis of the total wave function. Moreover, even the transmission and reflection coefficients cannot be calculated on its basis: the incident wave that is used for this purpose is just a part of the total wave function. Besides, for the final stage of a time-dependent scattering, it is clearly pointless to calculate the expectation values of the particle's position and momentum on the basis of the total wave function, because it represents at this stage the superposition of the transmitted and reflected wave packets occupying macroscopically distinct spatial regions.

So that the validity of this practice is an illusion, in fact, and the idea to apply the decomposition technique [5] to the potential step is quite motivated.

2 Backgrounds

We begin with the CQM. Let a particle with a given momentum $\hbar k$ impinges from the left on the potential step of height V_0, situated at the point $x = a$ ($a > 0$). The total wave function $\Psi_{tot}(x, k)$ to describe this scattering process when $E > V_0$, where $E = \hbar^2 k^2/2m$, is

$$\Psi_{tot}(x,k) = \begin{cases} e^{ikx} + B e^{-ikx} & x < a, \\ A e^{i\kappa x} & x > a, \end{cases} \tag{1}$$

$$A = \frac{2k}{k+\kappa}e^{i(k-\kappa)a}, \quad B = \frac{k-\kappa}{k+\kappa}e^{2ika}; \quad (2)$$

$$\kappa = k\sqrt{1 - \beta(\kappa_0/k)^2}, \ \kappa_0 = \sqrt{2m|V_0|}/\hbar, \ \beta = sgn(V_0);$$

the corresponding transmission and reflection coefficients are

$$T = \frac{4k\kappa}{(k+\kappa)^2}, \quad R = \left(\frac{k-\kappa}{k+\kappa}\right)^2.$$

The wave function $\Psi_{tot}(x,t)$ to describe a time-dependent scattering process is

$$\Psi_{tot}(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathcal{A}(k)\Psi_{tot}(x,k)e^{-iE(k)t/\hbar}dk; \quad (3)$$

$\mathcal{A}(k)$ is the Gaussian function

$$\mathcal{A}(k) = (2l_0^2/\pi)^{1/4}\exp[-l_0^2(k-k_0)^2]$$

for example. In this setting of the problem, at the initial time $t = 0$

$$\bar{x}_{tot}(0) = 0, \quad \bar{p}_{tot}(0) = \hbar\bar{k}, \quad \overline{x^2}_{tot}(0) = l_0^2 \quad (4)$$

hereinafter, for the average value of any physical observable F and localized state Ψ_B^A we will use two equivalent notations:

$$\bar{F}_B^A(t) \equiv <F>_B^A(t) = \frac{<\Psi_B^A|\hat{F}|\Psi_B^A>}{<\Psi_B^A|\Psi_B^A>},$$

if $\bar{F}_B^A(t)$ is constant its argument will be omitted. We assume that the parameters l_0 and $\bar{k}$ obey the conditions that are necessary for a one-dimensional *completed* scattering (OCS): the rate of scattering the transmitted and reflected wave packets exceeds the rate of widening each packet, so that the transmitted and reflected wave packets non-overlap each other at the final stage of scattering, i.e., when $t \to \infty$. We also assume that the origin of coordinates, which is the starting point of the "center of mass" (CM) $\bar{x}_{tot}(t)$ of the wave packet $\Psi_{tot}(x,t)$, lies far enough from the potential step: $a \gg l_0$.

At the initial stage of the OCS, i.e., long before the scattering event,

$$\Psi_{tot}(x,t) \simeq \Psi_{inc}(x,t) =$$
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathcal{A}(k)\ e^{i[kx-iE(k)t/\hbar]}dk. \quad (5)$$

At the final stage of the OCS, i.e., long after the scattering event,

$$\Psi_{tot}(x,t) = \Psi_{tr}(x,t) + \Psi_{ref}(x,t); \quad (6)$$

$$\Psi_{tr}(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathcal{A}(k)A(k)\ e^{i[\kappa x - E(k)t/\hbar]}dk,$$

$$\Psi_{ref}(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathcal{A}(k)B(k)\ e^{-i[kx+E(k)t/\hbar]}dk.$$

Our next step is to present the scattering process described by $\Psi_{tot}(x,t)$ as a complex process consisting of two alternative subprocesses, transmission and reflection, described at all stages of scattering by the SWFs $\psi_{tr}(x,t)$ and $\psi_{ref}(x,t)$, respectively.

3 The total wave function as a superposition of two SWFs

3.1 Physical requirements imposed on the SWFs

According to [5], the uniqueness of partitioning this time-dependent scattering process into subprocesses, for any function $\mathcal{A}(k)$, is provided by the uniqueness of presenting the total stationary state $\Psi_{tot}(x,k)$ in the form of a superposition of the SWFs $\psi_{tr}(x,k)$ and $\psi_{ref}(x,k)$. The latter, in its turn, is provided by physically motivated requirements imposed on the SWFs.

The first requirement follows from the fact that at the final stage of scattering the total wave function $\Psi_{tot}(x,t)$ represents the superposition of two nonoverlapping wave packets, transmitted and reflected (see (6)). Thus, to provide the fulfilment of this property for any function $\mathcal{A}(k)$, the stationary SWFs must be such that, for any values of x and k,

(a) $\psi_{tr}(x,k) + \psi_{ref}(x,k) = \Psi_{tot}(x,k)$.

In this case, the time-dependent SWFs

$$\psi_{tr,ref} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathcal{A}(k)\psi_{tr,ref}(x,k)e^{-iE(k)t/\hbar}dk \quad (7)$$

are evident to obey the equality

$$\Psi_{tot}(x,t) = \psi_{tr}(x,t) + \psi_{ref}(x,t). \quad (8)$$

Next requirement is dictated by the very nature of the SWFs:

(b) each SWF must have only one incoming wave and only one outgoing wave; the outgoing wave of $\psi_{tr}(x,k)$ is $Ae^{i\kappa x}$ and that of $\psi_{ref}(x,k)$ is Be^{-ikx} (see (1)).

As is known, for $E > V_0$ there is no solution to the stationary Schrödinger equation, which would be everywhere continuous together with its first spatial derivative and simultaneously possess one incoming wave and one outgoing wave. Thus, we must so weaken the continuity conditions of the SWFs that they would ensure, on the one hand, the existence of a nontrivial resolution of the decomposition problem and, on the other hand, a causal relationship between the incoming and outgoing waves in each SWF.

Namely, we believe that an incoming wave and outgoing wave of each stationary SWF represent two different solutions to the Schrödinger equation (for the same potential step), that are joined together at some spatial point $x_c(k)$ according to the following requirement:

(c) at the point $x_c(k)$ where the incoming and outgoing waves of each stationary SWF are joined to each other, the SWF must be continuous together with the corresponding probability current density.

According to the (b) and (c) requirements, the SWF $\psi_{ref}(x,k)$ must be zero in the region $x > x_c(k)$ because its incoming and outgoing waves move to the left of the point $x_c(k)$. Thus, $\psi_{ref}(x,k)$ is a currentless wave function and the point $x_c(k)$, that plays in this model the role of an extreme right turning point for reflected particles, is evident to coincide with some zero of this function. The right zero obeys the following requirement:

(d) for any given value of k the point $x_c(k)$ must coincide with such a zero of the currentless wave function $\psi_{ref}(x,k)$, at which the absolute value of $dx_c(k)/dk$ is less than at other zeros of this function.

The crucial difference between the k dependence of the sought-for zero and others is most noticeable in the limiting cases $k \to \kappa_0 + 0$ when $V_0 > 0$, and $k \to 0$ when $V_0 < 0$. As will be seen from the following, for the step potential the point $x_c(k)$ always lies behind the step, i.e., in the region $x > a$. Thus, according to our approach, the interval $[a, x_c(k)]$ is accessible for reflected particles; hereinafter, it will be referred to as 'the transitional region'. Note that, according to the CQM, reflected particles can enter the region $x > a$ only when $V_0 > 0$ and $E < V_0$ (see Introduction and Section 4.3).

Our next step is to realize the above program of decomposing the total wave function into SWFs.

3.2 Wave functions for transmission and reflection

Note that, due to the (b) and (c) requirements, the search of the SWFs $\psi_{tr}(x,k)$ and $\psi_{ref}(x,k)$ reduces in fact to finding the amplitudes of their incoming waves as well as to finding the position of the point x_c. In this case the (a), (b) and (c) requirements uniquely determine these amplitudes. Indeed, according to the (b) and (c) requirements, both SWFs in the region $x < a$ can be written in the form

$$\psi_{tr}(x,k) = A_{tr}e^{ikx}, \qquad (9)$$
$$\psi_{ref}(x,k) = A_{ref}e^{ikx} + Be^{-ikx};$$

and in the region $x > x_c(k)$ they are

$$\psi_{tr}(x,k) = Ae^{i\kappa x}, \qquad \psi_{ref}(x,k) = 0. \qquad (10)$$

As the probability current densities of the incoming and outgoing waves of each SWF are equal,

$$|A_{tr}|^2 = \frac{\kappa}{k}|A|^2 = T, \qquad |A_{ref}|^2 = |B|^2 = R. \qquad (11)$$

Thus, the complex amplitudes A_{tr} and A_{ref} can be written in the form $A_{tr} = \sqrt{T}e^{i\mu}$ and $A_{ref} = \sqrt{R}e^{i\nu}$, where μ and ν are unknown phases. Since $A_{tr} + A_{ref} = 1$, what follows from the (a) requirement, these phases obey the equation $\sqrt{T}e^{i\mu} + \sqrt{R}e^{i\nu} = 1$. Solving this equation for any given value of k, we obtain two pairs of roots:

$$\mu_1 = \lambda - \frac{\pi}{2}, \quad \nu_1 = \lambda; \quad \mu_2 = -\lambda + \frac{\pi}{2}, \quad \nu_2 = -\lambda;$$
$$\lambda = \arctan\sqrt{T/R} = 2\arctan\sqrt{(\kappa/k)^\beta}. \qquad (12)$$

However, only the pair of amplitudes

$$A_{ref} = \sqrt{R}\exp(i\beta\lambda), \qquad (13)$$
$$A_{tr} = \sqrt{T}\exp\left[i\beta\left(\lambda - \frac{\pi}{2}\right)\right].$$

gives $\psi_{ref}(x,k)$ whose zero in the region $x > a$, nearest to the step, obeys the (d) requirement and hence can serve as the extreme right turning point x_c. For $x < a$ this function is determined by the expression (see also (9))

$$\psi_{ref}(x,k) = \sqrt{R}e^{i(ka+\beta\lambda/2)}$$
$$\times \left[e^{i[k(x-a)+\beta\lambda/2]} + \beta e^{-i[k(x-a)+\beta\lambda/2]}\right]. \qquad (14)$$

In the transitional region $[a, x_c(k)]$ it can be written in the form

$$\psi_{ref} = C\sin\left[\kappa(x - x_c)\right], \quad x_c = a + \frac{1}{\kappa}\arctan\sqrt{\frac{\kappa}{k}}; \quad (15)$$
$$C = -2i^{\frac{\beta-1}{2}}\sqrt{\frac{k}{\kappa}}R\,\exp\left[i\left(ka + \beta\frac{\lambda}{2}\right)\right].$$

Note that in the limiting cases we have

- $V_0 > 0$ and $k \to \kappa_0 + 0$ ($\kappa \to 0$): $(x_c - a) \to (\kappa\kappa_0)^{-1/2}$ and $\kappa(x_c - a) \to 0$;

- $V_0 < 0$ and $k \to 0$: $(x_c - a) \to \pi/(2\kappa_0)$ and $\kappa(x_c - a) \to \pi/2$;

- $k \to \infty$: $(x_c - a) \to +0$ and $\kappa(x_c - a) \to \pi/4$ for both signs of V_0.

As is seen, when $V_0 > 0$ the length $x_c - a$ tends to infinity as $\kappa^{-1/2}$ in the limit $\kappa \to 0$. Note that $\kappa(x_c - a) \to 0$ in this case! For all other zeros, the corresponding lengths increase in this limit as κ^{-1}.

Thus, according to our model, the probability to find reflected particles to the right of the step is nonzero for both signs of V_0. And this takes place in the transitional region $[a, x_c(k)]$. The CQM does not imply the existence of such a region. This model says that for $V_0 > 0$ the penetration depth of reflected particles is infinite for $E \to V_0 - 0$ but zero for $E \to V_0 + 0$ (see [2]). As it will be shown below, in our model this quantity is infinite in both these limits (see Exps. (17) and (21)).

Note also that for the alternative pair of roots in (12) the corresponding function $\psi_{ref}^{alt}(x,k)$ is nonzero at the point x_c; but its first spatial derivative is zero here. For both signs of V_0, there is no zero of $\psi_{ref}^{alt}(x,k)$ which would lie between the step $x = a$ and zero $x_c(k)$ of the function $\psi_{ref}(x,k)$.

4 Characteristic times for transmission and reflection

Since the dynamics of both subprocesses is now known in all spatial regions, we can proceed to studying their temporal aspects. Our aim is to define for each subprocess the dwell and asymptotic group times. The former will be defined on the basis of the flow velocity concept for the stationary scattering problem. The latter will be defined on the basis of the group velocity concept for narrow in k space wave packets (the value of l_0 is assumed to be large enough).

4.1 Dwell times for transmission and reflection

In the case of transmission the flow velocity $v_{tr-flow}(x,k)$ at any point x is

$$v_{tr-flow}(x,k) = \frac{I_{tr}}{|\psi_{tr}(x,k)|^2}; \qquad (16)$$

$$I_{tr} = I_{tot} = \frac{\hbar k}{m} T(k).$$

In the regions $x \leq a$ and $x \geq x_c$ the flow velocity of transmitted particles coincides with the 'free-particle' velocities $v_k = \hbar k/m$ and $v_\kappa = \hbar\kappa/m$, respectively. In the transitional region $[a, x_c]$ it varies monotonously between these two asymptotic values. When $V_0 > 0$ ($V_0 < 0$), the average velocity of transmitted particles in this region is higher (smaller) than v_κ. Thus, since a particle is free (in the above sense) outside the transitional region, it is sufficient to consider in detail only this region.

The transmission dwell time for this region is defined as

$$\tau_{tr-dwell} = \frac{1}{I_{tr}} \int_a^{x_c} |\psi_{tr}(x,k)|^2 dx.$$

As regards reflected particles, the flow velocity concept is inapplicable for revealing their average velocity in the transitional region because $I_{ref} = 0$. Therefore the reflection dwell time for the transitional region is defined here in line with [9]:

$$\tau_{ref-dwell} = \frac{1}{I_{ref}^{inc}} \int_a^{x_c} |\psi_{ref}(x,k)|^2 dx; \ I_{ref}^{inc} = \frac{\hbar k}{m} R(k).$$

Considering the equality

$$\psi_{tr}(x,k) = \Psi_{tot}(x,k) - \psi_{ref}(x,k)$$

and Exps. (15) for $\psi_{ref}(x,k)$, we obtain dwell times for both subprocesses:

$$\tau_{tr-dwell} = \frac{m}{2\hbar k\kappa^3} \left[(\kappa^2 + k^2) \arctan \sqrt{\frac{\kappa}{k}} - \beta\kappa_0^2 \frac{\sqrt{k\kappa}}{k+\kappa} \right],$$

$$\tau_{ref-dwell} = \frac{2m}{\hbar\kappa^2} \left[\arctan \sqrt{\frac{\kappa}{k}} - \frac{\sqrt{\kappa k}}{k+\kappa} \right].$$

Thus, if $\tau_{free} = (x_c - a)/v_\kappa$ then $\tau_{tr-dwell} - \tau_{free}$ (which will be denoted as $\tau_{tr-dwell-del}$) is the dwell delay time for transmission:

$$\tau_{tr-dwell-del} = \frac{m(\kappa - k)}{2\hbar k\kappa^3} \left[(\kappa - k) \arctan \sqrt{\frac{\kappa}{k}} + \sqrt{k\kappa} \right].$$

This quantity is negative for $V_0 > 0$, but positive for $V_0 < 0$. This agrees with the fact that the flow velocity $v_{tr-flow}(x,k)$ in the transitional region is greater than v_κ, when $V_0 > 0$, but less than v_κ, when $V_0 < 0$.

As regards reflected particles, by analogy with [2] we introduce for them the effective penetration depth. Assuming that reflected particles move in the region $x > a$ with the velocity v_k and $\tau_{ref-dwell} = 2l_{depth}/v_k$, we obtain

$$l_{depth} = \frac{k}{\kappa^2} \left[\arctan \sqrt{\frac{\kappa}{k}} - \frac{\sqrt{\kappa k}}{k+\kappa} \right]. \qquad (17)$$

Thus, the *average* turning point for reflected particles lies always to the left of their *extreme right* turning point: $a + l_{depth}(k) \leq x_c(k)$. For $V_0 > 0$ the penetration depth $l_{depth}(k)$ diverges in the limit $k \to \kappa_0 + 0$ ($\kappa \to 0$) as $\kappa^{-1/2}$. But $l_{depth} = 0$ in the limit $k \to 0$ for $V_0 < 0$. In both cases, $\kappa l_{depth} \to (\pi - 2)/4$ and $\kappa(x_c - a) \to \pi/4$ when $k \to \infty$.

So, for a particle scattering at the potential step the flow velocity concept leads in our approach to nonzero transmission and reflection delay times.

4.2 Group times for transmission and reflection

Our next step is to study the temporal aspects of both subprocesses on the basis of the group velocity concept. More precisely, we intend here to determine asymptotic group times for narrow wave packets peaked at the point $\bar{k}$, where $\bar{k} \neq 0$ when $V_0 < 0$, and $\bar{k} \neq \kappa_0$ when $V_0 > 0$; hereinafter, dealing with such packets, we will omit the top dash in the notation $\bar{k}$.

Before doing so, we want to note that, for studying the time-dependent SWFs (7), it is suitable to rewrite the stationary SWFs $\psi_{tr}(x,k)$ and $\psi_{ref}(x,k)$ in terms of 'usual' solutions of the Schrödinger equation, which are continuous everywhere on the OX axis together with their first spatial derivatives. Indeed, let $\Phi_{ref}(x,k)$ be the wave function determined by Exp. (14) in the region $x < a$ and by Exps. (15)

everywhere in the region $x > a$. Then the SWFs $\psi_{ref}(x,k)$ and $\psi_{tr}(x,k)$ can be written as $\psi_{ref}(x,k) = \Phi_{ref}(x,k)\theta(x_c(k) - x)$ and $\psi_{tr}(x,k) = \Psi_{tot}(x,k) - \Phi_{ref}(x,k)\theta(x_c(k)-x)$, where $\theta(x)$ is the Heaviside step function.

Since we are interested in *asymptotic* scattering times, let us consider the asymptotically large interval $[0, a+L]$ where $L \gg l_0$ and let $\psi_{tr}^{inc}(x,t)$ and $\psi_{ref}^{inc}(x,t)$ be wave packets to describe the transmission and reflection subprocesses at the initial stage of scattering. These are (see (13))

$$\psi_{tr}^{inc} = \frac{-i\beta}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{A}(k)\sqrt{T(k)}\, e^{i[kx+\beta\lambda(k)-E(k)t/\hbar]}dk,$$

$$\psi_{ref}^{inc} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{A}(k)\sqrt{R(k)}\, e^{i[kx+\beta\lambda(k)-E(k)t/\hbar]}dk.$$

These wave packets differ from the incident one $\Psi_{inc}(x,t)$ (5) to describe the whole scattering process. And in the general case the average departure time t_{dep}^{tr} (t_{dep}^{ref}) of transmitted (reflected) particles from the point $x = 0$ does not coincide with the departure time t_{dep}^{tot} of the whole ensemble of particles; in our setting of the problem $t_{dep}^{tot} = 0$ (see (4)). Thus, the procedure of zero setting, for clocks used in [2] for 'measuring' the transmission and reflection times, is justified only in those cases when t_{dep}^{tr} and t_{dep}^{ref} coincide with t_{dep}^{tot}.

As regards the scattered packets $\psi_{tr}^{fin}(x,t)$ and $\psi_{ref}^{fin}(x,t)$, they coincide with the scattered parts of $\Psi_{tot}(x,t)$ (see (6)): $\psi_{tr}^{fin}(x,t) \equiv \Psi_{tr}(x,t)$ and $\psi_{ref}^{fin}(x,t) \equiv \Psi_{ref}(x,t)$. Thus, in our model and in the CQM, the average *time of arrival* t_{arr}^{tr} of transmitted particles at the point $x = a+L$ *is the same*! This is also true for the time of arrival t_{arr}^{ref} of reflected particles at the point $x = 0$.

Note, the definition of the transmitted wave packet $\psi_{tr}^{fin}(x,t)$ is valid at those points x that lie far enough from the turning points $x_c(k)$ of all waves that constitute this packet. At the first blush, this requirement cannot be fulfilled in the general case because $x_c(k) \to \infty$ in the limits $k \to 0$ ($V_0 < 0$) and $k \to \kappa_0 + 0$ ($V_0 > 0$). However this is not the case, because $T(k)x_c(k) \to 0$ in both these limits. The effective length $< x_c >_{tr} -a$ of the transitional region is finite for any transmitted wave packet with the weighted function $\mathcal{A}(k)$ exponentially decreasing in the limit $|k| \to \infty$. That is, in the general case $\psi_{tr}^{fin}(x,t)$ is defined for such x that $< x_c >_{tr} +l_0 \ll x$.

As in the model of symmetric potential barriers (see [5–7]), calculations carried out for the potential step show that the norms $\mathcal{T}$ and $\mathcal{R}$ of $\psi_{tr}(x,t)$ and $\psi_{ref}(x,t)$, respectively, take the same constant values at the initial and final stages of scattering:

$$< \psi_{tr}^{inc}|\psi_{tr}^{inc} >= \int_{-\infty}^{\infty} |\mathcal{A}(k)|^2 T(k)dk \equiv \mathcal{T}_{as},$$

$$< \psi_{ref}^{inc}|\psi_{ref}^{inc} >= \int_{-\infty}^{\infty} |\mathcal{A}(k)|^2 R(k)dk \equiv \mathcal{R}_{as}.$$

Moreover, $\mathcal{T}_{as} + \mathcal{R}_{as} = 1$. This means that the transmission and reflection subprocesses behave as *alternative* ones not only at the final stage of scattering (when the scattered wave packets do not overlap each other) but also at the initial stage (when the incident wave packets $\psi_{tr}^{inc}(x,t)$ and $\psi_{ref}^{inc}(x,t)$ interfere with each other). We have to stress that this is true for wave packets of any width.

However, $\mathcal{T} + \mathcal{R} \neq 1$ at the very stage of scattering, and there are two reasons why the transmission and reflection subprocesses cannot be considered now as alternative.

One of them has been discussed in [5–7] by the example of symmetric potential barriers, where it leads to the nonconservation of the norm $\mathcal{T}$. Its essence is that the (a)–(d) requirements ensure the balance of the input $(I_{tr}(x,k)|_{x=x_c-0})$ and output $(I_{tr}(x,k)|_{x=x_c+0})$ probability flow densities only in the stationary case, i.e., only for every single wave $\psi_{tr}(x,k)$ in the wave packet $\psi_{tr}(x,t)$. However, for the packet itself, the interaction between its main 'harmonic' $\psi_{tr}(x,\bar{k})$ and 'subharmonics' $\psi_{tr}(x,k)$ leads to the imbalance between the time-dependent input and output flow densities at the point x_c: $d\mathcal{T}/dt = I_{tr}(x,t)|_{x=x_c+0} - I_{tr}(x,t)|_{x=x_c-0} \neq 0$.

This effect influences the velocity of the CM of the wave packet $\psi_{tr}(x,t)$. In the case of a narrow packet $\psi_{tr}(x,t)$ peaked at the point k, this influence is maximal when the leading or trailing front of the packet crosses the point $x_c(k)$, i.e., when the role of its subharmonics is essential. Specifically, when the leading front crosses this point, it serves, depending on the parameters V_0 and k, as a source (or sink) of particles. This leads to acceleration (or deceleration) of the CM of the wave packet $\psi_{tr}(x,t)$. When the trailing front crosses this point, it serves conversely as a sink (or source), leading again to the acceleration (or deceleration) of the CM. Thus, this acceleration (or deceleration) effect, that has no relation to the average velocity of to-be-transmitted *particles*, is accumulated in the course of the OCS. At the same time the total change of the 'number of particles' involved in the transmission subprocess is strictly zero.

Other reason of violating the equality $\mathcal{T} + \mathcal{R} = 1$ is associated with the fact that, unlike symmetric barriers when the function $x_c(k)$ is constant on the k scale, for the step potential the function $x_c(k)$ is not constant. Now, for the wave packet $\psi_{ref}(x,t)$ with the small width Δk ($\Delta k \sim l_0^{-1}$) we have

$$I_{ref}(x,t)|_{x=x_c(k)-0} \sim \frac{dx_c(k)}{dk}\, \Delta k \neq 0,$$

while $I_{ref}(x,t)|_{x=x_c(k)+0} = 0$. Due to imbalance between these flows the norm $\mathcal{R}$ now varies at the very

stage of scattering (for symmetric barriers $\mathcal{R}$ is strictly constant (see [5])).

It is evident that, in addition to $\mathcal{R}$, the second effect influences also the norm $\mathcal{T}$. And, unlike the first effect, its influence on this norm is maximal when the CM of the packet $\psi_{tr}(x,t)$ crosses the point $<x_c>_{tr}$. Of course, the smaller is Δk, the smaller is its influence.

Let further $l_0 \gg |x'_c(k)/x_c(k)|$ and $x_c(k) - a \ll l_0 \ll a + L - x_c(k)$; here the prime denotes the derivative with respect to k. For such narrow packets the second effect is negligible and $<x_c>_{tr} \approx <x_c>_{ref} \approx x_c(k)$.

In this case the CM's dynamics for both subprocesses is described, at the initial and final stages of scattering, by the expressions

$$<x>_{tot}^{inc} = \frac{\hbar k}{m}t, \quad <x>_{tr}^{inc} = <x>_{ref}^{inc} = \frac{\hbar k}{m}t - \beta \lambda',$$

$$<x>_{tr}^{fin} = \frac{\hbar \kappa}{m}t + a\left(1 - \frac{\kappa}{k}\right), \quad <x>_{ref}^{fin} = -\frac{\hbar k}{m}t + 2a.$$

As it follows from them, the CMs of the narrow wave packets $\psi_{tr}(x,t)$ and $\psi_{ref}(x,t)$ start from the same point

$$<x>_{tr}^{inc}(0) = <x>_{ref}^{inc}(0) = x_{start} = -\beta \lambda',$$

which differs from the initial position of the CM of the total wave packet: $<x>_{tot}^{inc}(0) = \bar{x}_{tot}(0) = 0$ (see (4)). As a result, the departure times t_{dep}^{tr}, t_{dep}^{ref} and t_{dep}^{tot} of the CMs of the wave packets $\psi_{tr}(x,t)$, $\psi_{ref}(x,t)$ and $\Psi_{tot}(x,t)$, respectively, are determined by the expressions

$$t_{dep}^{tr} = t_{dep}^{ref} = t_{dep} = \beta\frac{\lambda'(k)}{v_k} = \frac{m(k-\kappa)}{\hbar(k\kappa)^{3/2}}, \tag{18}$$

while $t_{dep}^{tot} = 0$. As regards the arrival times t_{arr}^{tr} and t_{arr}^{ref}, they are

$$t_{arr}^{ref} = \frac{2a}{v_k}, \quad t_{arr}^{tr} = \frac{a}{v_k} + \frac{L}{v_\kappa}. \tag{19}$$

Thus, the group transmission and reflection times for the interval $[0, a+L]$ are, respectively, $\Delta t_{tr} = t_{arr}^{tr} - t_{dep}$ and $\Delta t_{ref} = t_{arr}^{ref} - t_{dep}$. Considering Eqs. (18) and (19), we obtain for them

$$\Delta t_{tr} = \frac{a}{v_k} + \frac{L}{v_\kappa} - \beta\frac{\lambda'}{v_k}, \quad \Delta t_{ref} = \frac{2a}{v_k} - \beta\frac{\lambda'}{v_k}.$$

Excluding expressions related to the 'free' regions $[0, a]$ and $[x_c(k), a+L]$, we obtain the *asymptotic* (extrapolated) group times $\tau_{tr-group}$ and $\tau_{ref-group}$ for transmission and reflection, respectively:

$$\tau_{tr-gr} = (x_c - a)/v_\kappa - t_{dep} = \tau_{free} - t_{dep},$$

$$\tau_{ref-gr} = -t_{dep}.$$

However, according to the clock model [2], these characteristic times should be defined as follows: $\tau_{tr-gr}^{Dav} = \tau_{free}$ and $\tau_{ref-gr}^{Dav} = 0$. That is, the 'zero

setting' procedure in this model is based in fact on the implicit assumption that the departure times of the CMs of the transmitted and reflected packets coincide with that of the total wave packet, and hence $t_{dep} = 0$. This means that the delay times for both subprocesses are zero in this model. In particular, in line with [2], reflected particles with $E > V_0$ bounce off the step instantaneously. This takes place even in the limit $E \to V_0 + 0$ for $V_0 > 0$.

In our approach the group delay time for the CM of the reflected wave packet is nonzero in the general case. This delay is fully determined by the group reflection time: $\tau_{tr-gr-del} = \tau_{tr-gr} = -t_{dep}$. For the transmitted CM the delay time is $\tau_{tr-gr-del} = \tau_{tr-gr} - t_{free} = -t_{dep}$. So that, in the last analysis, for the potential step we obtain

$$\tau_{tr-gr-del} = \tau_{ref-gr-del} = -t_{dep} = \frac{m(\kappa - k)}{\hbar(k\kappa)^{3/2}}. \tag{20}$$

For $V_0 > 0$ both group delay times are negative; for $V_0 < 0$ they are positive.

4.3 Scattering times for the total reflection

Let us now consider the case when $V_0 > 0$ and $E < V_0$, i.e., when transmission is absent: $T(k) \equiv 0$ in the region $(0, \kappa_0]$. Now, in Exps. (1)

$$A = \frac{2k}{k+i\kappa}e^{(\kappa+ik)a}, \quad B = \frac{k-i\kappa}{k+i\kappa}e^{2ika},$$

where $\kappa = \sqrt{\kappa_0^2 - k^2}$. For this one-channel scattering the SWF ψ_{ref} transforms into the total wave function Ψ_{tot}, and $\psi_{tr} \equiv 0$. Thus, $\psi_{ref}(x,k) = e^{ikx} + Be^{-ikx}$ for $x < a$, and $\psi_{ref}(x,k) = Ae^{-\kappa x}$ for $x > a$.

Calculations yield that now

$$\tau_{ref-dwell} = \frac{\int_a^\infty |\psi_{ref}(x,k)|^2 dx}{I_{ref}^{inc}}$$

$$= \frac{2mk}{\hbar\kappa\kappa_0^2} = \frac{2l_{depth}}{v_k}, \quad l_{depth} = \frac{k^2}{\kappa\kappa_0^2}. \tag{21}$$

As regards the group reflection time, since now $\lambda \equiv 0$ we have $t_{dep}(k) \equiv 0$ and $\tau_{ref-group} = 2m/\hbar k\kappa = 2/\kappa v_k$ as in the clock model [2].

On the basis of this expression Davies defines the length scale $d = 1/\kappa$ and treats it as "the expectation value for the penetration depth of the particle into the potential step" [2]. But our analysis shows that this interpretation is unjustified.

5 On the average penetration depth of reflected particles into the potential step

By our approach, only the parameter l_{depth} defined on the basis of the reflection *dwell* time can play the role of the average penetration depth of reflected particles into the potential step. Both quantities behave equally only in the limit $k \to \kappa_0 - 0$, when they tend to ∞.

While, everywhere in the region $k > \kappa_0$ as well as in the long-wave region $k \to 0$ their properties differ cardinally.

When $k > \kappa_0$ the probability to find reflected particles behind the step is nonzero in our model; this takes place in the transitional region $[a, x_c(k)]$. But in the model [2], based on the CQM, this probability is strictly zero in the region $x > a$, including the limiting case $k \to \kappa_0 + 0$. That is, within the CQM (which does not imply the existence of any transitional region in this scattering problem), the "penetration depth" $d(k)$ has an infinite discontinuity at the point $k = \kappa_0$ when $V_0 > 0$. This means that the probability to find a to-be-reflected particle in the region $x > a$ (at some finite distance from the point $x = a$) changes abruptly when the particle energy is shifted by an infinitesimal magnitude from $E = V_0 - 0$ to $E = V_0 + 0$. Such an abrupt change of the quantum probability contradicts the very spirit of quantum mechanics. In our model, the penetration depth $l_{depth}(k)$ diverges in both one-side limits, $k \to \kappa_0 - 0$ and $k \to \kappa_0 + 0$.

Not less strange behavior of $d(k)$ takes place when $k \to 0$. In this case $d \to 1/\kappa_0$. As is obvious, this contradicts the fact that the probability to find a reflected particle in the region $x > a$ is strictly zero in this limit! Unlike the 'group' penetration depth d, the 'dwell' penetration depth l_{depth} tends to zero in this case.

6   Conclusion

Scattering a quantum particle on the potential step consists of two subprocesses when $E > V_0$. In this case, neither characteristic time nor expectation value of a physical observable can be calculated within the framework of the CQM, because this model does not 'see' the dynamics of each subprocess at all stages of scattering. It allows neither direct nor indirect measurement of these quantities. The former is impossible because of interference between the subprocesses. The latter is impossible since this implies the knowledge of the time evolution of each subprocess at all stages of scattering.

In this paper we present an alternative model of this process, that uniquely reconstructs the prehistory of the transmitted and reflected subensembles of particles by their final states. Unlike the CQM this model predicts the existence of a transitional region

behind the potential step, where the probability to find reflected particles is nonzero. This region starts at the point $x = a$ where the potential step is situated and ends at the point x_c that serves as an extreme turning point for reflected particles. The average velocity of transmitted particles in this region monotonously changes between the asymptotic values v_k and v_κ.

We define scattering times for each subprocess – the dwell time (in the time-independent case) and asymptotic group time (for narrow wave packets). Among these two concepts only the former allows one to reveal the average times of staying the subensembles of transmitted and reflected particles in the transitional region.

As it turns out, in the time-dependent case the transmission and reflection subprocesses are not strictly alternative at the very stage of scattering – the rule $\mathcal{T} + \mathcal{R} = 1$ is violated at this stage. More precisely, this takes place when the leading and trailing fronts of the narrow wave packet $\psi_{tr}(x, t)$ cross the point x_c, i.e., when the role of its 'subharmonics' $(k \neq \bar{k})$ is essential. In these two cases the velocity of the wave-packet's CM depends not only on the average velocity of particles, but also on the character of changing the norm $\mathcal{T}$.

Thus, on the one hand, the presented decomposition technique confirms once more the well-known truth – at the micro-level, quantum probability is irreducible to classical one; the "either-or" rule $\mathcal{T} + \mathcal{R} = 1$, that must be fulfilled for alternative subprocesses from the viewpoint of classical probability theory, does not hold at the very stage of scattering a quantum particle on the potential step. On the other hand, it shows that, at the asymptotically large distances from the step, the properties of quantum probability in this scattering problem are compatible with those of classical one. That is, our quantum-mechanical model respects the correspondence principle.

The following pressing task is to elaborate the Larmor-clock procedure for the potential step, which could serve as a basis for the indirect measurement of the dwell times of both subprocesses.

Acknowledgement

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РАССЕЯНИЕ КВАНТОВОЙ ЧАСТИЦЫ НА ПОТЕНЦИАЛЬНОЙ СТУПЕНЬКЕ: ХАРАКТЕРИСТИЧЕСКИЕ ВРЕМЕНА ДЛЯ ПРОХОЖДЕНИЯ И ОТРАЖЕНИЯ

Представлена новая модель рассеяния квантовой частицы на потенциальной ступеньке, которая восстанавливает предысторию прошедших и отраженных частиц по их конечным состояниям. В отличие от общепринятой модели данная модель предсказывает существование переходной пространственной области позади потенциальной ступеньки, где вероятность найти отражающиеся частицы не равна нулю, а средняя скорость проходящих частиц монотонно изменяется между асимптотическими значениями. Для обоих подпроцессов определены время пребывания и асимптотическое групповое время рассеяния.

Ключевые слова: *потенциальная ступенька, время пребывания, групповая скорость.*

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