Quantum traversal time

Antônio B. Nassar
Department of Physics, University of California, Los Angeles, California 90024
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The time spent by a quantum particle in a scattering event or a tunneling process (the traversal time) through a rectangular barrier is calculated from the viewpoint of the stochastic formulation of quantum mechanics. Comparison with previous results is also provided.

I. INTRODUCTION

The question of the duration of a quantum-mechanical scattering event and a tunneling process of a particle through a potential barrier has been of considerable interest and debate in the literature.[1-41] Of particular importance in chemical and nuclear physics is the relationship between properties of the collision partners and the collisional time delay: experimental advances in nuclear physics[42] have allowed direct measurement of proton-nuclei time delays, providing useful data for testing various models of nuclear scattering. The interest in the traversal time for tunneling in solid-state physics arises in connection with the field emission of an electron out of a metal surface into the vacuum or into a semiconductor.[17] The ability of the image charge to spread out and respond to the departing electron depends on the duration of the tunneling process.

Calculation of the traversal time by a variety of approaches has led to disparate answers. We allude now to different earlier methods as some examples of the state of the art. As shown by Eisenbud,[40] Bohm,[39] and Wigner,[38] one can calculate the time delay of a scattering event from the energy derivative of the phase shift, which the scattered wave exhibits relative to the incident wave. This (so-called) stationary-phase method has been generalized to a considerable extent by many subsequent authors,[4,8,22-24,30,34,35] for multichannel scattering processes (including inelastic mechanisms[22,26]). (A comprehensive review of time-delay theories can be found in Ref. 12.) It has also been proposed[18] that the time-delay theory is valid for any scattering event irrespective of whether the underlying dynamics is classical or quantum mechanical,[11] thus providing a method for defining a universal phase-shift-like functional that is a characteristic of both quantum and classical systems. This was stressed by the fact that one can derive a classical analogue to the quantum-mechanical Levinson theorem.[16,18] Despite fundamental conceptual dissimilarities to the latter works, our approach exhibits a natural reciprocity between the classical and quantum definitions of the traversal time. In fact, by simply letting $\hbar \rightarrow 0$, in Eq. (29) below, we may recover classical results from quantum ones. In the discussion of Sec. III, we draw some comparisons between our traversal time and the time delay of the stationary-phase method.

Another approach given by Smith,[36] and advanced by others,[24,27,30,33] determines the average dwell time of a particle within the interaction region from a kinetic point of view: the ratio of the number of particles in the barrier to the incident flux determines such a time. Smith has shown that the kinetic definition and the one given by the generalization of the stationary-phase method are essentially identical: the average time delay associated with scattering out of the incident channel or initial state is found from the diagonal elements of a collision operator. This formalism has been greatly advanced by several authors.[8,12,13,15,16,20,21,23] Recently, Osborn and coworkers have carried out formal studies of the relationship between the collisional time delay and system densities of states in N-body scattering. (In particular, see Ref. 10 and references cited therein for a comprehensive analysis of this subject.)

In another approach, Stevens[7] has analyzed the propagation of electromagnetic waves in dispersive and attenuating media (as developed by Brillouin and Sommerfeld) and applied it to the tunneling problem by following the time evolution of a pulselike wave train. A different approach has been given subsequently by Pollak and Miller,[5] who have shown that the collision time may be interpreted as the time average of a flux-flux correlation function. This interpretation leads to a complex traversal time, whose real part is identical to the usual definition as provided by Smith.[36] The imaginary part is identical, in the semiclassical limit, to the imaginary time associated to tunneling. This is also related to what Stevens[7] has suggested to be the signal velocity of the wave packet. For a rectangular barrier, the traversal time inferred from this analysis is linearly proportional to the barrier width.

Baz'[32] and Rybachenko[31] have proposed the use of the Larmor precession as a clock to measure the time taken by a particle to traverse a barrier, wherein an applied magnetic field is confined. By comparing the spin orientation of the transmitted particles with the incident-beam orientation, Rybachenko finds that for an opaque rectangular barrier the traversal time is independent on the barrier width. However, Büttiker[6] has demonstrated that had Rybachenko considered that the polarization of the transmitted and reflected particles also acquired a component parallel to the magnetic field, the traversal time would turn out to be linearly dependent on the barrier width. In yet another recent approach given by Sokoloviski and Baskin,[1] the traversal time is obtained as a matrix element of some classical functional in the Feynman path-integral technique. In general, their main expressions are complex, which led them to claim that the quantum traversal time is not an observable in the usual sense.

In this work, the problem of the traversal time for a scattering event and a tunneling process through a potential barrier is approached from a new perspective: via a stochastic formulation of quantum mechanics.[43–46] We attempt to show here that the concept of quantum traversal time can be developed within a framework that does not depart radically from a classical physical picture. We feel that the method set forth here is an attempt to make the physical picture of the problem more transparent. The formulation of the problem and the calculation of the traversal time is carried out in Sec. II. A comparative discussion of our results with those of previous works is provided in Sec. III.

II. FORMULATION

Within the framework of the stochastic formulation of quantum mechanics, we assume that the quantum particle is subject to an external and a stochastic force, this last being generated by quantum fluctuations resulting from the action of a stochastic invariant thermostat.[43–46] So, the particle's forward (backward) drift velocity $v_+ (v_-)$ can be written as the sum (difference) of a current velocity v and a stochastic velocity u,

$$v_{\pm} = D_{\pm} x(t) = v \pm u \ . \tag{1}$$

$D_{\pm}(\ ) \equiv [\partial(\ )/\partial t] + v_{\pm}[\partial(\ )/\partial x] \pm (\hbar/2m)[\partial^2(\ )/\partial x^2]$ defines the substantial derivatives of the stochastic motion in the forward and backward directions.[43,46] The dynamics of the process $x(t)$ is equivalent to the pair of hydrodynamical equations

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}(vu) - \frac{\hbar}{2m}\frac{\partial^2 v}{\partial x^2} \tag{2}$$

and

$$\frac{\partial v}{\partial t} = -\frac{1}{m}\frac{\partial V}{\partial x} - v\frac{\partial v}{\partial x} + u\frac{\partial u}{\partial x} + \frac{\hbar}{2m}\frac{\partial^2 u}{\partial x^2} \ , \tag{3}$$

such that for each quantum state with the wave function

$$\Psi(x,t) = [\rho(x,t)]^{1/2}\exp[iS(x,t)] \ , \tag{4}$$

we associate

$$v = (\hbar/m)(\partial S/\partial x) \tag{5}$$

and

$$u = (\hbar/2m)(\partial \ln\rho/\partial x) \ , \tag{6}$$

which establish the equivalence with the Schrödinger equation.

Consider now a steady flux of particles with energy E scattered by a static potential well of depth $-V_0$ ($V_0 > 0$) for $0 \le x \le L$ and 0 elsewhere. The wave function describing the particles incident from the left ($x < 0$) is given by $\Psi_L(x,t) = (e^{ikx} + Ae^{-ikx})\exp(-iEt/\hbar)$. The transmitted wave function ($x > L$) is $\Psi_R(x,t) = Be^{ikx}\exp(-iEt/\hbar)$. Here we denote $k^2 \equiv 2mE/\hbar^2$.

In the interaction region, one needs the total density ρ and phase S to obtain the dynamics of the process (1): the stationary solution to the set of equations [(2) and (3)] can be found by first expressing the wave function as

$$\Psi(x,t) = [\rho(x)]^{1/2}\exp\{i[S(x) - (Et/\hbar)]\} \ . \tag{7}$$

Then, by using (5), (6), and (7) (and since v and u are gradient functions), we can readily simplify (2) and (3):

$$2\phi'(x)S'(x) + S''(x)\phi(x) = 0 \ , \tag{8}$$

$$\phi''(x) + q^2\phi(x) = [S'(x)]^2\phi(x) \ , \tag{9}$$

where $\rho(x) \equiv \phi^2(x)$ and $q^2 \equiv 2m(E+V_0)/\hbar^2$.

Integration of (8) implies that

$$S'(x) = C_1/\rho(x) \ , \tag{10}$$

which inserted into (9) gives

$$\phi''(x) + q^2\phi(x) = C_1^2/\phi^3(x) \ . \tag{11}$$

Integration of (11) yields

$$\{[\rho'(x)]^2/4\rho(x)\} + q^2\rho(x) + [C_1^2/\rho(x)] = C_2 \ , \tag{12a}$$

which upon a second integration reduces to[47]

$$\rho(x) = (1/2q^2)\{[C_2^2 - 4q^2C_1^2]^{1/2}\cos 2q(x - x_0) + C_2\} \ . \tag{12b}$$

By matching the boundary conditions, we obtain, at $x = 0$,

$$1 + A = \phi(0)\exp[iS(0)] \ , \tag{13}$$

$$ik(1 - A) = [\phi'(0) + iS'(0)\phi(0)]\exp[iS(0)] \ , \tag{14}$$

and at $x = L$,

$$\phi(L)\exp[iS(L)] = B\exp(ikL) \ , \tag{15}$$

$$[\phi'(L) + iS'(L)\phi(L)]\exp[iS(L)] = ikB\exp(ikL) \ . \tag{16}$$

Eliminating A between (13) and (14), the real and imaginary parts of the resulting expression are

$$2k\sin[S(0)] = \phi'(0) \ , \tag{17}$$

$$2k\cos[S(0)] = \phi(0)[k + S'(0)] \ . \tag{18}$$

Eliminating B between (15) and (16) and collecting the real and imaginary parts of the resulting expression, one has

$$\phi'(L) = 0 \ , \tag{19}$$

$$S'(L) = k \ . \tag{20}$$

The constants of integration C_1, C_2, and x_0 can determined as follows. Substitution of (12b) into (19) implies that

$$x_0 = L \ . \tag{21}$$

Combination of (10) with (20) gives

$$\rho(L) = C_1/k \ . \tag{22}$$

By inserting (22) into (12a), and with the help of (19), we find that

$$C_2 = kC_1[1+(q/k)^2] \ . \tag{23}$$

By substituting (23) into (12b), we are left with

$$\rho(x) = (C_1/k)\{1-[1-(q/k)^2]\cos^2 q(x-L)\}/(q/k)^2 \ . \tag{24}$$

Squaring and adding (17) and (18), we obtain

$$4k^2 = [\phi'(0)]^2 + \phi^2(0)[k+S'(0)]^2 \ , \tag{25}$$

which combined with (10), (12a), and (23) yields

$$[3+(q/k)^2]C_1 = k\{4-\rho(0)[1-(q/k)^2]\} \ . \tag{26}$$

Now, (23) and (26) determine C_1,

$$(C_1/k) = 4(q/k)^2/\{[1+(q/k)^2]^2 - [1-(q/k)^2]^2\cos^2 qL\} \ , \tag{27a}$$

which is the transmission coefficient [see (15) and (22)]

$$T = |B|^2 = (C_1/k) \ . \tag{27b}$$

In turn, from (1), (5), (6), (10), (12b), and (27) we obtain

$$v_\pm(x) = (\hbar/m)(\{2k(q/k)^2 \pm q[1-(q/k)^2]\sin 2q(x-L)\}/\{[1+(q/k)^2]-[1-(q/k)^2]\cos 2q(x-L)\}) \ . \tag{28}$$

Next, we define for the *stationary regime* the quantum scattering traversal time by conceptually keeping reciprocity with the classical physical picture, namely,

$$\tau_s \equiv \int_0^L dx/\sqrt{(2/m)K} = \int_0^L dx/[(v_+^2+v_-^2)/2]^{1/2} \ . \tag{29}$$

The key point here is that both the forward and backward velocities of the particle contribute equally to the traversal kinetic motion: the kinetic energy $K=(m/2)[(v_+^2+v_-^2)/2]=(m/2)(v^2+u^2)$. Thus, with the help of Eq. (28), we have

$$\tau_s = \left[\frac{mk}{2\hbar q^2}\right]\int_0^L dx \frac{(r^2+1)+(r^2-1)\cos 2q(x-L)}{(1+\{(r^2-1)[\sin 2q(x-L)]/2r\}^2)^{1/2}} \ , \tag{30a}$$

where $r \equiv (q/k) = \sqrt{(E+V_0)/E}$.

When the integral (30a) is carried out, we find that[48]

$$\tau_s = (m/2\hbar q^2)(F[\alpha;\beta] + \ln|\{|r^2-1|[\sin(2qL)]/2r\} + \{1+[(r^2-1)(\sin 2qL)/2r]^2\}^{1/2}|) \ , \tag{30b}$$

where $F[\alpha;\beta]$ is the elliptic integral of first kind, $\beta(r) \equiv |r^2-1|/(1+r^2)$, and

$$\alpha(r,qL) \equiv \sin^{-1}(\{(r^2+1)[\sin(2qL)]/2r\}/\{1+[(r^2-1)(\sin 2qL)/2r]^2\}^{1/2}) \ .$$

The traversal time for tunneling ($E<V_0$) is obtained by simply replacing q by $i\bar{q}$ [where $\bar{q} \equiv \sqrt{2m(V_0-E)}/\hbar$] in (30a) and (30b).

III. DISCUSSION

We have shown in Sec. II that the concept of quantum traversal time can be formulated within a framework that does not depart radically from the classical physical picture. This constitutes the fundamental conceptual dissimilarity with respect to previous approaches. Nevertheless, a comparative analysis of previous results and ours is in order. To make a connection with the stationary-phase method and our definition (29), we begin by recalling that the time delay in a scattering event may be considered intuitively to be the difference ($\Delta\tau_s$) between the time spent by the colliding particle in the interaction region and the time it would have spent in the same region had it moved freely.[5,22] One of the most essential features of this time delay is its strong energy dependence in the vicinity of resonances. So, we find that at the resonance $qL=N\pi$ (for which the barrier is transparent) the time delay is given by

$$\Delta\tau_s^{\text{res}} = (2mL^2/\pi\hbar N)F[(\pi/2);\beta(N\pi/kL)] - (m/\hbar k)L \ .$$

Due to the presence of the first term, no agreement can be established with the result found via the stationary-phase method. The energy sensitivity in the latter approach arises in the evolution of the colliding particle through the phase shift of the wave packet (relative to the incident one), whereas in ours it comes about through both the *local* stationary wave-packet phase and the local probability amplitude, which are related to the particle current and stochastic velocities, respectively. Since the two velocities v and u satisfy a system of coupled Eqs. (2) and (3), they are not independent of each other. That can also be seen in Eqs. (8) and (9), for the stationary-regime case. The stochastic velocity can be interpreted as a manifestation of the mechanism responsible for the interaction between the particle and the quantum medium through which it moves. In the hydrodynamical formulation of the Schrödinger equation, this interaction is represented by Bohm's quantum potential.[43,49]

For an opaque rectangular barrier, however, the stationary-phase method yields a time delay that is *in-*

dependent of the barrier width.[4,35] This result depends strongly on the form of the wave packet, and is sound if the wave packet is characterized by a narrow momentum distribution. If a wave packet with a wide momentum distribution strikes a barrier, the transmitted wave packet will exhibit a distribution displaced to higher momenta (since the high-energy components of the wave-packet tunnel more easily that the low-energy ones). Thus, the transmitted wave packet moves faster and the reflected wave packet moves slower than the incident one.[24,29] Such a wave packet has an envelope which can rise and fall only slowly and thus the position of the maximum may be difficult to measure accurately. In fact, Stevens[7] has illustrated magnificently this strong dependence on the wave-packet form. In contrast, an important facet of our traversal-time definition is that, while working in the configuration space, we avoid the restricted condition on the initial momentum-distribution width. In the Smith kinetic approach (as also advanced by others)[8,12,13,15,16,20,21,23] the time delay for an opaque barrier is *independent* of the barrier width. As remarked by Büttiker and Landauer,[2,3,6] this approach does not distinguish between particles, which at the end of their stay in the interaction region have been reflected, and those that were transmitted. This yields the average dwell time of a particle in the barrier, and not the traversal time, if most particles are reflected. In our approach, the traversal time is defined in terms of both the *stationary* forward and backward particle velocities, which compound the traversal motion. The overall additional significance of our reasoning is that it is possible to determine the quantum traversal time through a barrier for particles corresponding to a wave function for a stationary state of energy E and still maintain a conceptual reciprocity between the classical and quantum definitions. Furthermore, it is essential to point out the fact that we find a real traversal-time expression, contrasting with the complex-time expressions proposed in Refs. 1 and 5.

For the thin-barrier tunneling problem, we find that the traversal time is given by

$$\tau_t = (m/\hbar k)L \quad (L \to 0)$$

whereas, for the opaque-barrier case,

$$\tau_t = (m/\hbar \bar{q})L \quad (L \to \infty)\ .$$

Hence, for both limiting cases above, τ_t is linearly proportional to L, in agreement with the results of Refs. 2, 3, 5, 6, 7, and 17, although our general expression for intermediate values of L differs from that obtained in these works.

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