

## Generalized reflection time for one-dimensional structures

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A generalized reflection time which follows directly from the Schrödinger equation without approximation is obtained. By the Winger-Eisenbud approach, this reflection time is conceptually well defined and can be applied to arbitrary continuous potentials including both quantum tunneling and quantum reflection issue. A simple explanation for the quantum reflection phenomenon is proposed and the explicit expression of the difference between the quantum reflection time and the classical reflection time is also derived.

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Since numerous theoretical predictions seem to contradict each other, the tunneling time issue is replete with controversy [1–4]. Among them, two principal frameworks are the Büttiker-Landauer traversal time and the Wigner-Eisenbud time (the group delay or phase time). The recent advance in experimental techniques has made the direct measurements of this quantity increasingly accessible to laboratory experiments. There already exist various experiments done with “single photons,” light pulses, etc.; some of them even show apparent superluminality [5–9]. However, these experiments have severed to add fuel to the current debate over tunneling time. In a very recent experiment, the measured upper limit on the tunneling delay of an electron in strong field ionization of a helium atom is much shorter than the prediction of the Büttiker-Landauer traversal time [9]. In an effort to resolve the Hartman effect, Winful proposed that the Wigner phase time is well defined but should be reinterpreted as a lifetime [3,4]. In this Brief Report, we explore the related issue of the quantum-mechanical reflection time in the general case of arbitrary continuous structures and derive a generalized expression of reflection time directly from the time-independent Schrödinger equation via the Wigner-Eisenbud approach. Since it is well established that, for a symmetric potential, the Wigner phase times for tunneling and for reflection are identical quantities [3], the proposed expression is also the expression of the tunneling time in these cases.

Moreover, the recent explosive growth of experiments on cold atoms near surfaces illustrates the importance of this proposed reflection time. Experiments have already confirmed that a particle can be reflected in the classically allowed region [10,11]; such an effect is referred to as quantum reflection. Previous theoretical work formulated by Friedrich and co-workers was based on the globally accurate wave functions constructed by matching the exact or highly accurate wave functions in the quantal regions to the WKB wave functions in the semiclassical regions and concentrated mainly on the long-range attractive potential tails. They pointed out that the quantum reflected wave is always delayed when compared to the classical particle accelerated in the same attractive potential [12,13]. When the reflection time proposed in this Brief Report is extended to study this issue, a clear physical picture of the quantum reflection effect is presented; furthermore, we obtain the explicit expression of the time gain (delay) that the quantum reflected wave experiences with respect to the classical particle under the influence of the same attractive potential.

We start with the time-independent Schrödinger equation with position-dependent effective mass  $m(x)$ ,

$$\left[ -\frac{d}{dx} \frac{\hbar^2}{2m(x)} \frac{d}{dx} + V(x) \right] \psi(x) = E\psi(x), \quad (1)$$

and, equivalently, the Riccati equation is given as

$$\frac{1}{m(x)} \frac{d}{dx} q(x) = - \left[ q(x)^2 + \left( \frac{\kappa(x)}{m(x)} \right)^2 \right], \quad (2)$$

where

$$\kappa(x) = \frac{p(x)}{\hbar} = \frac{\sqrt{2m(x)(E - V(x))}}{\hbar}, \quad (3)$$

$$q(x) = m(x)^{-1} \psi(x)^{-1} \frac{d\psi(x)}{dx}. \quad (4)$$

Here, the relation between the term  $q(x)$  and the quantum-mechanical wave impedance  $Z(x)$  takes a simple form  $Z(x) = \hbar q(x)/i$  [14], and  $p(x)$  denotes the momentum. Defining  $\varphi(x) = -\arctan[m(x)q(x)/\kappa(x)]$ , it follows that

$$\frac{d\varphi(x)}{dx} = \kappa + \frac{q(\kappa' m - m' k)}{\kappa^2 + m^2 q^2}. \quad (5)$$

Here, we denote differentiations with respect to  $x$  by primes. Integrating Eq. (5) over the interval  $a < x < b$ , one obtains

$$\int_a^b d\varphi(x) = \int_a^b \left( \kappa + \frac{q(\kappa' m - m' k)}{\kappa^2 + m^2 q^2} \right) dx = n\pi + \varphi(b) - \varphi(a), \quad (6)$$

where  $n$  is related to the number of nodes of  $\kappa(x)\psi(x)$  in this interval. So far, no specific potential profile has been introduced; thus, Eq. (6) is general. In our previous works [15,16], the term  $q(\kappa' m - m' k)/(\kappa^2 + m^2 q^2)$  ( $-q\kappa'/q'$  when  $m'=0$ ) was referred to as the wave number of the scattered subwaves. Since this term has the same momentum dimension as  $\kappa$ , we represent it by  $\Delta\kappa$  from now on for the sake of clarity.

For an arbitrary point  $s$  in the classically allowed region where  $E \geq V(s)$ , the potential can always be considered as constant in a sufficiently small neighborhood of  $s$ ; thus, it is always possible to write the wave function in this neighbor-

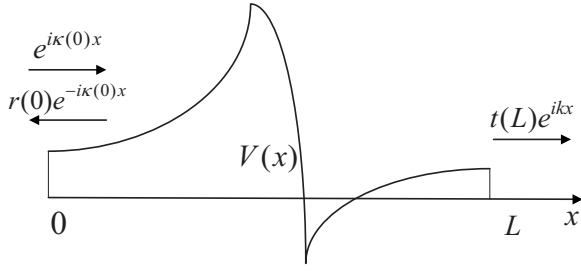


FIG. 1. Potential profile of an arbitrary continuous potential  $V(x)$ . The plane-wave components of the electron wave function are also indicated.

hood as a superposition of incoming and outgoing waves,

$$\psi(x) \propto \exp[i\kappa(x-s)] + r(s)\exp[-i\kappa(x-s)], \quad (7)$$

where  $r(s)$  is the reflection coefficient at the point  $s$ . (The reflection coefficient is defined with respect to plane waves incident from the left throughout this Brief Report.) Substituting Eq. (7) in Eq. (4), we obtain the relation

$$r(s) = \frac{\kappa(s) + im(s)q(s)}{\kappa(s) - im(s)q(s)} = \exp[-i2\varphi(s)]. \quad (8)$$

We next rewrite Eq. (6) in the form

$$\exp[-2i\varphi(a)] = \exp\left(-2i\varphi(b) + 2i \int_a^b (\kappa + \Delta\kappa) dx\right). \quad (9)$$

From the above two equations, it follows that

$$r(a) = r(b)\exp\left(2i \int_a^b (\kappa + \Delta\kappa) dx\right). \quad (10)$$

Since the case of steplike varying potentials has already been discussed in detail, let us consider an arbitrary continuous potential that has its support on the interval  $[0, L]$  as shown in Fig. 1 and an electron incident from  $x=0$  with particle energy  $E = \hbar^2 k^2 / (2m_0)$ . Without loss of generality, we set  $m(x) = m_0$  for  $x > L$ .

Then in view of Eq. (10), one has

$$r(0) = r(L)\exp\left(2i \int_0^L (\kappa + \Delta\kappa) dx\right), \quad (11)$$

where  $r(L)$  in Eq. (11) is simply given by

$$r(L) = \frac{m_0\kappa(L) - m(L)k}{m_0\kappa(L) + m(L)k}. \quad (12)$$

Equation (11) is a general expression of the reflection coefficient. Note that the time-independent Schrödinger equation and the Helmholtz equation are identical in form; therefore, Eq. (11) can also be applied to electromagnetic waves. It is well established that, for a wave packet whose momenta are restricted to a narrow range, the time delay for scattering processes can be calculated by following the peak of the wave packet via the method of the stationary phase, i.e., this time delay depends only on the energy derivative of the phase shift  $\phi_r$  of the reflection coefficient [1–3]. Thus, the Wigner phase time  $\tau_r$  for the reflected wave packet is

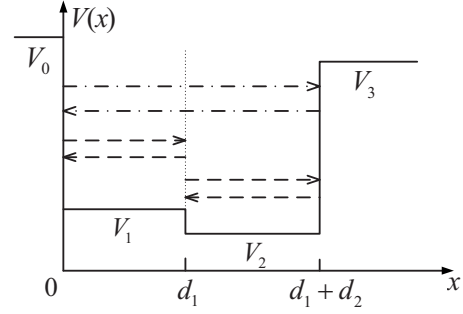


FIG. 2. The stepped potential well.

$$\tau_r = \hbar \frac{\partial \phi_r}{\partial E}. \quad (13)$$

As was pointed out in Ref. [3]—after reviewing the key experiments on optical, microwave, and acoustic tunneling times—that “the group delay (phase time) indeed describes the time at which the transmitted pulse peaks at the exit.” It is from this point of view that the Wigner phase time is well established. Finally, substituting Eq. (11) into Eq. (13), we obtain the generalized expression of reflection time,

$$\tau_r(0) = \tau_r(L) + 2\hbar \operatorname{Re}\left(\frac{\partial}{\partial E} \int_0^L (\kappa + \Delta\kappa) dx\right), \quad (14)$$

where  $\tau_r(L)$  can be obtained via Eqs. (12) and (13).

Why do we refer to the term  $\Delta\kappa$  as the wave number of the scattered subwaves? In order to make this clearer, let us consider a simple stepped potential well as shown in Fig. 2 with constant mass  $m_0$ . The eigenfunction of the bound states corresponding to the eigenvalues  $V_3 > E > V_1$  can be written as

$$\psi(x) = \begin{cases} A_0 \exp(\alpha_0 x), & x < 0 \\ A_1 \exp(i\kappa_1 x) + B_1 \exp(-i\kappa_1 x), & 0 < x < d_1 \\ A_2 \exp(i\kappa_2 x) + B_2 \exp(-i\kappa_2 x), & d_1 < x < d_1 + d_2 \\ A_3 \exp(-\alpha_3 x), & x > d_1 + d_2, \end{cases} \quad (15)$$

where  $\hbar\kappa_i = \sqrt{2m_0(E - V_i)}$  ( $i=1, 2$ ) and  $\hbar\alpha_j = \sqrt{2m_0(V_j - E)}$  ( $j=0, 3$ ). Requiring the wave function  $\psi(x)$  and its first derivative  $\psi'(x)$  to be continuous, one obtains

$$\exp[i2(\kappa_1 d_1 + \kappa_2 d_2 - \varphi_{10} - \varphi_{23})] + r_{12} \exp[i2(\kappa_1 d_1 - \varphi_{10})] + r_{21} \exp[i2(\kappa_2 d_2 - \varphi_{23})] = 1, \quad (16)$$

where  $\varphi_{10} = \arctan(\alpha_0 / \kappa_1)$  and  $\varphi_{23} = \arctan(\alpha_3 / \kappa_2)$  denote the half-phase shift at the boundaries of the well and  $r_{12}, r_{21}$  are given by  $r_{12} = -r_{21} = (\kappa_1 - \kappa_2) / (\kappa_1 + \kappa_2)$ . It is clear that the first term on the left-hand side of Eq. (16) (shown in Fig. 2 as dashed-dotted line) represents the waves only reflected at turning points  $x=0$  and  $x=d_1+d_2$ , while the second and third terms (shown in Fig. 2 as dashed lines) represent the waves reflected at nonturning point  $x=d_1$ . By purely algebraic methods, Eq. (16) can be recast into [16]

$$(\kappa_1 d_1 + \kappa_2 d_2) + \phi = n\pi + \varphi_{10} + \varphi_{23}. \quad (17)$$

Comparing Eqs. (6) and (17), it is obvious that the term  $\phi$ , which is the simplest form of  $\int \Delta\kappa dx$ , denotes the phase contribution picked up by the scattered subwaves that result from the interface between the potentials  $V_1$  and  $V_2$ . From the above simple example, it is evident that when generalized to arbitrary continuous potentials, the wave number  $\Delta\kappa$  represents the wave number of the scattered subwaves that originate inherently from the inhomogeneity of the fields.

For the quantum reflection issue, i.e., the particle travels in a classically allowed region where there is no classical turning point; as a result the momentum  $p = \hbar\kappa$  is always positive, so does the integral of  $\kappa(x)$ . This gives

$$\left| \exp\left(i2 \int_0^L \kappa dx\right) \right| \equiv 1, \quad (18)$$

which means that this integral has no effect on the reflection probability  $R = rr^*$ ; the waves with wave number  $\kappa$  can only affect the phase of reflection coefficient. In view of Eq. (11), the modulus of the reflection coefficient  $|r|$  can be written as

$$|r(0)| = \left| r(L) \exp\left(i2 \int_0^L \Delta\kappa dx\right) \right|. \quad (19)$$

The above simple expression indicates that quantum reflection is resulted from the reflection of the scattered subwaves. It is convenient to rewrite the expression of reflection time (14) as

$$\tau_r(0) - \tau_r(L) = \tau_{cl}|_0^L + \Delta\tau|_0^L, \quad (20)$$

where we have introduced the notations

$$\tau_{cl}|_0^L = 2 \operatorname{Re} \left( \int_0^L \frac{\partial p(x)}{\partial E} dx \right), \quad (21)$$

$$\Delta\tau|_0^L = 2\hbar \operatorname{Re} \left( \frac{\partial}{\partial E} \int_0^L \Delta\kappa dx \right). \quad (22)$$

In classical allowed regions, one has  $\partial p(x)/\partial E = m(x)/p(x) = 1/v(x)$ . Here, the term  $v(x)$  denotes the exact velocity of a classical particle with the same effective mass  $m(x)$  and momentum  $p(x)$ ; then Eq. (21) reduces to

$$\tau_{cl}|_0^L = 2 \int_0^L \frac{1}{v(x)} dx. \quad (23)$$

Therefore  $\tau_{cl}|_0^L$  corresponds to the time that a classical particle takes to travel in the same potential and to be reflected at the boundary, i.e.,  $\tau_{cl}$  is rather similar to the classical concept of reflection time. Furthermore, the term  $\Delta\tau$  given by Eq. (22) is completely determined by  $\Delta\kappa$ ; it is a property of the entire wave function made up of transmitted and reflected components. As mentioned before,  $\Delta\kappa$  represents the wave number of the scattered subwaves that can be reflected at nonturning points; in contrast, classical particles can only be reflected at turning points. In a word, this term  $\Delta\tau$  is in fact displaying the wavelike behavior of the reflected electron,

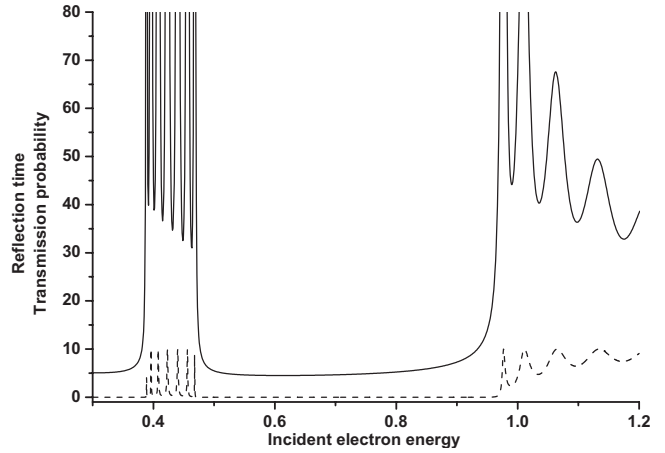


FIG. 3. The electron reflection time (solid line) follows the resonant behavior of transmission probability  $10T$  (dashed line) as a function of incident electron energy for the superlattice structure given by Eq. (26).

while the term  $\tau_{cl}$  manifests the particlelike behavior of the reflected electron.

Simply put, quantum reflection is the reflection of the scattered subwaves and Eq. (22) is exactly the expression of the time delay or the time advance of the quantum reflected wave when compared to a classical particle traveling in the same potential and reflected at the boundary. It should be noted that, in a null potential with constant mass, where the wave function is of the simple form  $\psi(x) \propto A \exp(ikx)$ ,  $\Delta\tau$  is nonzero. Instead, in this case  $\Delta\tau$  is equal to  $-\tau_{cl}$ ; this could be easily understood for the fact that since the null potential is a reflectionless potential, the total reflection time given by Eq. (20) will be equal to zero automatically. For arbitrary continuous structures, the key point in the calculation of the reflection time via Eq. (14) is  $q(x)$ . Analytical wave functions are already known for all the shape invariant potentials and other solved potentials, so one can obtain their  $q(x)$  analytically. Otherwise, one needs to solve the Riccati equation (2) numerically or apply the ATM method. An arbitrary continuous potential can always be approximated as a succession of steplike varying regions, and each region is represented by a transfer matrix

$$M_i = \begin{bmatrix} \cos(\kappa_i \hbar) & -(m_i/\kappa_i) \sin(\kappa_i \hbar) \\ \kappa_i/m_i \sin(\kappa_i \hbar) & \cos(\kappa_i \hbar) \end{bmatrix}, \quad (24)$$

where  $\hbar\kappa_i = \sqrt{2m_i(E - V_i)}$  and  $V_i, m_i$  stands for the potential energy and the effective mass in the  $i$ th region. Using the condition that the wave function and its first derivative are continuous at the boundary between two neighboring regions, the matrix equation is given as

$$\begin{bmatrix} \psi(0) \\ \psi'(0)/m_0 \end{bmatrix} = \prod M_i \begin{bmatrix} \psi(L) \\ \psi'(L)/m_L \end{bmatrix}. \quad (25)$$

From Eq. (25), one can easily obtain  $q(x)$ .

For the first example, we consider a simple superlattice structure given by

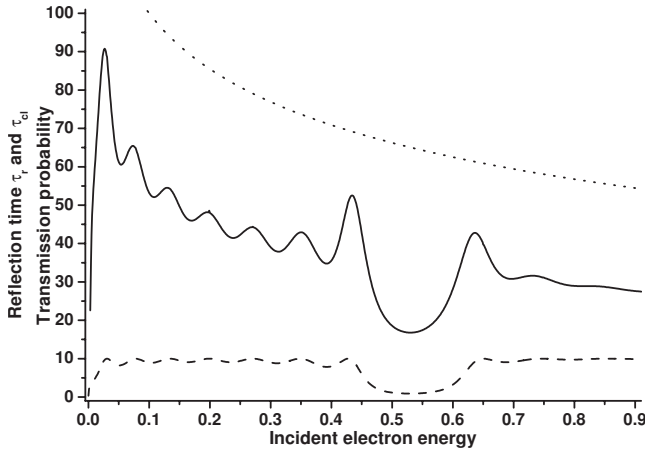


FIG. 4. Reflection time  $\tau_r$  (solid line), classical reflection time  $\tau_{cl}$  (dotted line), and transmission probability  $10T$  (dashed line) as functions of incident electron energy.

$$V(x) = \frac{1}{2} - \frac{1}{2}\cos(2\pi x), \quad -4 < x < 4. \quad (26)$$

Atomic units are used for all the illustrated examples, i.e., we set  $\hbar = 2m = 1$ . The transmission probability and the reflection time for this structure are calculated and shown in Fig. 3.

It is worth pointing out that the reflection time given by Eq. (14) for this superlattice is rather similar to the tunneling time calculated in Ref. [17] for a similar structure (see Fig. 2 in Ref. [17]). This example demonstrates that Eq. (14) can be applied to calculate the tunneling time for all the symmetric structures.

For a second illustration, it is interesting to compare the generalized reflection time  $\tau_r$  and the classical reflection time  $\tau_{cl}$  given by Eq. (23) for a quantum reflection problem. Let us consider a simple attractive potential

$$V(x) = -\frac{1}{2} + \frac{1}{2}\cos(2\pi x), \quad -5 < x < 5. \quad (27)$$

Figure 4 shows the calculated results. It is clear that the quantum reflected wave is faster when compared to the correspondent classical particle, which indicates that the term  $\Delta\tau$  is negative in this case.

In conclusion, we derived directly from the Schrödinger equation a simple formula [Eq. (14)] of the generalized reflection time. In a conceptually well-defined manner, this reflection time can be applied to arbitrary one-dimensional continuous structures.

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