Transmission and reflection times for scattering of wave packets off tunneling barriers

E. H. Hauge*
Elektronikklaboratoriet ved Norges Tekniske Høgskole, Universitetet i Trondheim, N-7034 Trondheim-NTH, Norway

J. P. Falck
Institutt for Teoretisk Fysikk, Norges Tekniske Høgskole, Universitetet i Trondheim, N-7034 Trondheim-NTH, Norway

T. A. Fjeldly
Institutt for Fysikalsk Elektronikk, Norges Tekniske Høgskole, Universitetet i Trondheim, N-7034 Trondheim-NTH, Norway
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The proper basis for the calculation of transmission and reflection times for wave packets scattered off arbitrary tunneling structures in one dimension is considered. With packets narrow in wave-number space, we demonstrate that the classic phase times are indeed correct to lowest order. Explicit, general expressions for the leading correction terms for finite wave packets are given. The physics associated with these corrections is discussed. We also consider the dwell time, as it is currently defined, and derive a general relation between this dwell time and the phase times. This relation shows when the dwell time can and cannot be used. Finally, we discuss wave packets transmitted from narrow resonances, and derive an explicit, exact formula for the tunneling time with resonance transmission from a symmetric double barrier. Comparison with earlier approximate results is made.

I. INTRODUCTION

Advances in molecular-beam-epitaxy (MBE) technology have opened up new possibilities for the design of semiconductor structures with linear dimensions in the nanometer range.[1] On the one hand, this will certainly have far-reaching consequences for tomorrow's devices. A pointer in this direction is, for example, the successful transistor operation of a double-barrier tunneling structure, recently achieved by Capasso *et al.*[2] On the other hand, the need for a better fundamental understanding of quantum transport theory has become urgent. The semiclassical approach, which has been so successful up until now, needs, as a minimal measure, important modifications. Possibly, a new start is necessary to build a reliable kinetic theory, applicable to the nanometer regime.

We shall be concerned with minimalism here. What is certainly needed as elemental input in any new kinetic theory, is the time for the completion of a basic event like tunneling through a static potential barrier. It is surprising that even a question of such fundamental simplicity has been controversial in recent years. Not that old answers do not exist. More than 30 years ago[3,4] the energy derivative of the scattering phase shifts was proposed as representing the time needed for events of this nature. The relevance of this "phase time" for the motion of wave packets has been questioned, however, and several counterproposals exist.[5-10] Direct numerical studies[11-14] of moving wave packets tend to favor[12] the phase time over its competition, except, perhaps, at low energies.

Different expressions for the tunneling time could, of course, be relevant under different circumstances. For example, Büttiker and Landauer[9] introduce a traversal time which emerges from a study of tunneling through a time-modulated barrier. The relevance of this traversal time for reactive scattering has been discussed by Pollak.[15] In the present paper only static potentials will be considered. Even for this simplest case different tunneling times could apply, depending on the form of the potential and the shape of the impinging wave packet. In fact, the result in the time domain of the scattering of an *arbitrary* wave packet can surely *not* be described by a single transmission and reflection time, in general. In order to make precise statements possible, the form of the packet must be sharply characterized. For example, Stevens[8] has studied wave packets with a well-defined front in real space. Such packets have a wide distribution in wave-number space (k space).

In this paper we shall be concerned with a different class of wave packets for which transmission and reflection times can be given a precise meaning. We restrict ourselves to packets *narrow* in wave-number space. In a sense, we take one step back from the stationary case, for which the wave packet degenerates into a δ function in k space. This brings time into the problem, and in our opinion, time delays can only be studied *reliably* by calculations on truly time-dependent problems. Plausible time interpretations of calculations on stationary states can be misleading. An example is the Larmor clock interpretation of stationary scattering problems studied by Baz,[6] Rybachenko,[7] and by Büttiker.[10] Related experiments are reported by Guéret *et al.*[16] In a separate publication[17] we show that a time-dependent calculation of the case studied in Ref. 10 reveals how to set this clock correctly. When properly set, the Larmor clock gives, to lowest order, times in perfect agreement with those found in the present paper.

After the recapitulation of some basic material in Sec. II, we analytically study the motion of wave packets narrow in k space in Secs. III and IV. The natural identification of the position as the "center of gravity" of the packet is used. To lowest order, the classic phase times for transmission and reflection are shown to describe the asymptotic motion. In addition, correction terms to leading order in the width $\sigma=\langle \Delta k^2\rangle^{1/2}$ are derived. These new correction terms have an interesting structure, and the physics underlying them will be discussed.

In Sec. V we derive a general relationship between the "dwell time", as it is currently defined,[10,18] and the phase times for transmission and reflection. This connection, which is reminiscent of relations discussed in the original paper by Smith,[5] clarifies the status of the dwell time. Results by Büttiker[10] on tunneling through a single barrier serve as an illustration at this point, and are quoted in the Appendix. The relation derived in Sec. V demonstrates that the dwell time *cannot*, in general, be interpreted as the average time a particle spends in a barrier.

In view of its current importance, we reconsider the double barrier structure in Sec. VI. The arguments of Sec. III for the validity of the phase time do not immediately apply in the context of a narrow resonance. The status of the phase time for resonant tunneling is clarified in Sec. VI A. In Sec. VI B the phase time at resonance is calculated exactly for symmetric double barriers. Earlier approximate results by Ricco and Azbel[18] for the strongly localized case are (with minor modifications) rederived and extended. Nonlinear Coulomb and finite temperature effects,[18–22] which are certainly important in practice, are not considered here. We close with some concluding remarks in Sec. VII.

II. BASICS

A. The stationary scattering problem

Most of the results in this paper are easily generalized to three dimensions. However, already the one-dimensional case contains the essence of the problem and is, in addition, of particular interest in connection with "vertical" electron transport in submicrometer devices. We shall consequently confine ourselves to the one-dimensional case here.

Consider a scattering process as shown in Fig. 1. In the stationary case the incoming particles are represented by a plane wave e^{ikx} of unit amplitude. The (effective) mass is m and the energy is $E=\hbar^2k^2/2m$. The particles are scattered by a potential $V(x)$ localized in the x interval (a,b). Some are elastically reflected and some are transmitted with energy $\tilde{E}=E+\Delta E=\hbar^2\tilde{k}^2/2m$.

The stationary wave function has the form

$$\psi_k(x)=\begin{cases} e^{ikx}+B(k)e^{-ikx}, & x\le a\\ \chi(x;k), & a<x<b\\ A(k)e^{i\tilde{k}x}, & x\ge b\ .\end{cases} \tag{2.1}$$

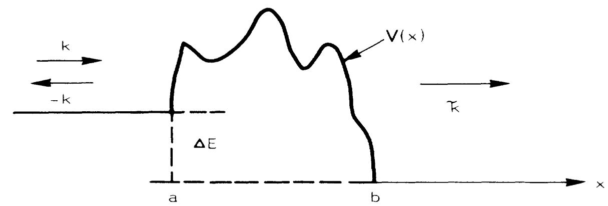

FIG. 1. Sketch of the potential $V(x)$. The potential is constant for $x<a$, arbitrary in the interval (a,b), and constant again for $x>b$. The difference between the constant energies is ΔE. The wave numbers are $\pm k$ for $x<a$ and $\tilde{k}$ for $x>b$.

We shall *assume* that the solution to the stationary problem is known for all energies, i.e., we shall consider the transmission and reflection amplitudes

$$A(k)=|A(k)|e^{i\alpha(k)},\quad B(k)=|B(k)|e^{i\beta(k)}\ , \tag{2.2}$$

and the wave function $\chi(x;k)$, in the scattering region, as known functions of k. Analytic solutions exist in simple cases,[23] and $A(k)$, $B(k)$, and $\chi(x;k)$ can, in principle, be found by a numerical solution of the time-independent Schrödinger equation for arbitrary $V(x)$.

Time-dependent solutions of the Schrödinger equation, such as those describing the evolution of a wave packet impinging on $V(x)$, can be constructed as linear combinations of the solutions (2.1).

B. The initial wave packet

We shall be interested in what happens when a wave packet, $\psi(x,t)$, with a narrow distribution of wave numbers k, is scattered off the potential, $V(x)$. For conceptual simplicity, assume that the initial wave packet, as given by $\psi(x,0)$, is confined to a finite x interval to the left of $x=a$. Beyond this, we shall characterize the initial packet by a few of its lowest moments only. We define the Fourier transform as

$$\phi(k)=\int dx\, e^{-ikx}\psi(x,0)=|\phi(k)|e^{i\xi(k)}\ . \tag{2.3}$$

The probability distribution over wave numbers is then $|\phi(k)|^2/2\pi$, with mean and variance given as

$$\begin{aligned} k_c=\langle k\rangle &= \int \frac{dk}{2\pi}k\,|\phi(k)|^2\ ,\\ \sigma^2=\langle(\Delta k)^2\rangle &= \int \frac{dk}{2\pi}(k-k_c)^2|\phi(k)|^2\ . \end{aligned} \tag{2.4}$$

We shall also need the average in x space and the cross correlation between x and k, expressed by $\xi(k)$ close to the mean value k_c of the narrow packet. Simple calculations show that [with $\xi'(k)\equiv d\xi/dk$, etc.]

$$\begin{aligned} \langle x(0)\rangle &= -\langle \xi'(k)\rangle = -\xi'(k_c)-\tfrac{1}{2}\xi'''(k_c)\sigma^2+\cdots\ ,\\ \langle \Delta k\,\Delta x(0)\rangle &= -\langle (k-k_c)\xi'(k)\rangle = -\xi''(k_c)\sigma^2+\cdots\ . \end{aligned} \tag{2.5}$$

Here the correlation function $\langle \Delta k\,\Delta x(0)\rangle$ is understood as the expectation value of the symmetrized product. The mean-square deviation in x space also depends on

$\xi''(k_c)$:

$$\langle \Delta x(0)^2 \rangle = \int \frac{dk}{2\pi}(|\phi|')^2 + [\xi''(k_c)]^2\sigma^2 + \cdots , \quad (2.6)$$

but we shall not use it in what follows, except for the requirement that $\langle x(0) \rangle$ must be sufficiently large and negative to accommodate $\langle [\Delta x(0)]^2 \rangle^{1/2}$ to the left of $x=a$.

III. TRANSMISSION TIME FOR THE CASE $\Delta E = 0$

In this section we consider the asymptotic behavior for long times of the transmitted part of a narrow (in k space) wave packet, scattered elastically off the potential $V(x)$. In particular, we shall focus on the mean position $\langle x(t) \rangle_T$ of the transmitted packet. The asymptotics of $\langle x(t) \rangle_T$ provides a natural basis on which velocity shifts, and space and time delays can be defined.[24] In Sec. IV we extend the results to the reflected packet, and to the case $\Delta E \neq 0$.

The time-dependent transmitted part of the wave function $\psi_T(x,t)$ can be constructed as a linear superposition of the stationary solutions (2.1) for $x > b$, with weights determined by the Fourier transform of the initial wave packet (2.3):

$$\psi_T(x,t) = \int \frac{dk}{2\pi}\phi(k)A(k)e^{ikx - iEt/\hbar} , \quad (3.1)$$

with $E = \hbar^2 k^2/2m$. The *unnormalized* probability distribution is the absolute square $P_T(x,t) = |\psi_T(x,t)|^2$:

$$P_T(x,t) = \int\int \frac{dk\,dk'}{(2\pi)^2}\phi(k)\phi^*(k')A(k)A^*(k')\exp\{i[(k-k')x - \hbar(k^2-k'^2)t/2m]\}$$
$$= \int\int \frac{dQ\,dq}{(2\pi)^2} e^{iqx - i\hbar qQt/m}\phi(Q+\tfrac{1}{2}q)\phi^*(Q-\tfrac{1}{2}q)A(Q+\tfrac{1}{2}q)A^*(Q-\tfrac{1}{2}q) , \quad (3.2)$$

in which we introduced

$$q = k - k', \quad Q = \tfrac{1}{2}(k+k') . \quad (3.3)$$

The normalization

$$N(t) = \int_b^\infty dx\, P_T(x,t) \quad (3.4)$$

clearly depends on time. For large times, however, $N(t)$ approaches a constant N. The reason for this is simply that, for large t, the transmitted packet will be well separated from the scattering region (a,b). The error made in replacing b by $(-\infty)$ as the lower limit of the x integral (3.4), then becomes negligible. As a result, integration over x gives $2\pi\delta(q)$, and one finds

$$N = \int \frac{dQ}{2\pi}|\phi(Q)|^2|A(Q)|^2 . \quad (3.5)$$

In a similar way, the asymptotics of the time-dependent average position $\langle x(t) \rangle_T$ of the transmitted wave packet can be calculated

$$\langle x(t) \rangle_T \simeq \frac{1}{N}\int_{-\infty}^\infty dx\, xP_T(x,t) , \quad (3.6)$$

where, based on the same reasoning as above, the lower limit b in the x integrals of both numerator and denominator has been replaced by $(-\infty)$. Use of (3.2), (2.2), and (2.3) gives

$$\langle x(t) \rangle_T \simeq \frac{-i}{N}\int_{-\infty}^\infty dx \int\int \frac{dQ\,dq}{(2\pi)^2}\left[\frac{d}{dq}e^{iqx}\right]$$
$$\times \exp\{i[-\hbar qQt/m + \xi(Q+\tfrac{1}{2}q) - \xi(Q-\tfrac{1}{2}q)$$
$$+\alpha(Q+\tfrac{1}{2}q) - \alpha(Q-\tfrac{1}{2}q)]\}\,|\phi(Q+\tfrac{1}{2}q)\phi(Q-\tfrac{1}{2}q)|\,|A(Q+\tfrac{1}{2}q)A(Q-\tfrac{1}{2}q)| . \quad (3.7)$$

Partial integration with respect to q (no boundary terms) and integration over x again gives $2\pi\delta(q)$. Consequently, the q derivatives of the two functions that are absolute values, vanish by symmetry. Introducing the transmission probability at Q, $T(Q) = |A(Q)|^2$, one is then left with (when $Q \to k$)

$$\langle x(t) \rangle_T \simeq \frac{1}{N}\int \frac{dk}{2\pi}|\phi(k)|^2 T(k)\left[\frac{\hbar k}{m}t - \xi'(k) - \alpha'(k)\right]$$
$$= \frac{\hbar}{m}\frac{\langle T(k)k \rangle}{\langle T(k) \rangle}t + \frac{\langle T(k)(-\xi'(k)) \rangle}{\langle T(k) \rangle}$$
$$- \frac{\langle T(k)\alpha'(k) \rangle}{\langle T(k) \rangle} , \quad (3.8)$$

where averages without subscript are, as always, taken with respect to the initial wave packet. Use of (2.5) gives the alternative form

$$\langle x(t) \rangle_T - \langle x(0) \rangle \simeq \frac{\hbar}{m}\frac{\langle T(k)k \rangle}{\langle T(k) \rangle}t$$
$$- \frac{\langle T(k)\alpha'(k) \rangle}{\langle T(k) \rangle} + \frac{\langle \Delta T(k)\Delta x(0) \rangle}{\langle T(k) \rangle} . \quad (3.9)$$

In $\langle \Delta T(k)\Delta x(0) \rangle$, as in $\langle \Delta k\, \Delta x(0) \rangle$ of (2.5), the symmetrized product is understood.

The assumption that $|\phi(k)|^2/2\pi$ is a sharply peaked probability distribution is *not* part of the derivation of (3.8) and (3.9). Those equation can therefore be used, also when $T(k)$ has resonances, sharp with respect to the incident wave packet. We shall return to this case in Sec. VI. In what follows, we assume that $|\phi(k)|^2/2\pi$ is peaked around k_c, and that the other functions in (3.9) vary slowly on the scale, σ of (2.4), set by the k distribution. To $O(\sigma^2)$, a simple calculation based on (3.9) gives

$$\langle x(t)\rangle_T-\langle x(0)\rangle \simeq \frac{\hbar k_c}{m}\left[1+\frac{T'\sigma^2}{Tk_c}\right]t-\alpha'\left[1+\frac{\alpha'''\sigma^2}{2\alpha'}+\frac{T'\alpha''\sigma^2}{T\alpha'}-\frac{T'}{T}\frac{\langle \Delta k\,\Delta x(0)\rangle}{\alpha'}\right]+o(\sigma^2)\,, \tag{3.10}$$

where, for example, $T'=dT(k_c)/dk$, and $o(\sigma^2)$ denotes terms smaller than $O(\sigma^2)$. Equation (3.10) is the basic result of this section.

With the motion of a *free* packet,

$$\langle x(t)\rangle_0-\langle x(0)\rangle=\hbar k_c t/m \tag{3.11}$$

as a reference, we now consider the various terms in (3.10). First note that when *all* correction terms are neglected, (3.10) reduces to

$$\langle x(t)\rangle_T-\langle x(0)\rangle \simeq \hbar k_c t/m-\alpha'(k_c)+O(\sigma^2)\,, \tag{3.12}$$

which demonstrates that, to lowest order, the spatial delay Δx_T, and the corresponding temporal delay $\Delta\tau_T$, of the transmitted packet read

$$\Delta x_T(k)=\alpha'(k),\quad \Delta\tau_T(k)=\frac{m}{\hbar k}\alpha'(k)=\hbar\frac{d\alpha}{dE} \tag{3.13}$$

(where the subscript c on k has been dropped). The corresponding *total* transmission time τ_T is

$$\tau_T(k)=\frac{m(b-a)}{\hbar k}+\frac{m}{\hbar k}\alpha'(k)\,. \tag{3.14}$$

This is in complete agreement with classic statements.[3,4]

Next, (3.10) shows that, when corrections of $O(\sigma^2)$ are included, the *speed* of the transmitted packet is slightly shifted with respect to the initial one, $\hbar k_c/m$. This can be understood as follows:[10] If the "barrier" $V(x)$ is more transparent for higher energies (around k_c), $T'>0$. In that case, the barrier preferably transmits the faster parts of the initial packet, and preferably reflects the slower ones. As a result, the average speed of the transmitted packet is shifted upwards. The converse is also possible: If k_c is just above a transmission resonance of $V(x)$, one has $T'<0$, and the transmitted packet is slowed down.

Due to the shift in average speed, some caution must be exercised in the definition of spatial and temporal delays. (Such caution is particularly important when results of numerical "experiments" are to be interpreted.) With reference to Fig. 2, the solid lines show the path of the initially free wave packet, and the asymptotic trajectory of the transmitted packet. The dashed lines are the corresponding linear extrapolations. From (3.10) it is clear that the natural definition of the spatial delay is

$$\Delta x_T=\langle x(0)\rangle-\langle x(0)\rangle_T\,, \tag{3.15}$$

where $\langle x(0)\rangle_T$ should be interpreted as the backward extrapolation. Its geometrical meaning is shown in Fig. 2.

The first correction to $\alpha'(k_c)$ in the spatial delay of (3.10) is $\frac{1}{2}\alpha'''(k_c)\sigma^2$. This correction can have either sign and is merely an expression of the fact that the incoming packet samples a range of phase shifts. The second correction is somewhat more subtle. If $T'>0$ and $\alpha''>0$, the barrier is more transparent for higher energies (around k_c) and the delay ($\sim\alpha'$) increases with energy. The combined result is a positive correction to the delay. Since T' and α'' tend to have the same sign (except at resonances, where they both vanish) this correction generally adds to the delay.

The third correction to the delay is proportional to the cross correlation, in the initial packet, between velocity and position. If this correlation is positive, the front part of the packet tends to move faster. If, in addition, $T'>0$, fast particles are preferably transmitted and, intuitively, the combined result should be a reduction of the delay. This agrees with the corresponding negative sign in (3.10). Either factor $\langle \Delta k\,\Delta x(0)\rangle$ or T' can be negative, however [i.e., $\langle T(k)\Delta x(0)\rangle$ of (3.9) can have either sign] so this correction can increase as well as decrease the delay.

Let us pause here to consider an apparent paradox. From (2.5) one has that $\langle \Delta k\Delta x(0)\rangle=-\sigma^2\xi''(k_c)$. But as time passes, the phase of the Fourier transform, $\phi(k)$, will change as $\xi(k)\rightarrow\xi(k)-\hbar k^2 t/2m$. This will increase the cross correlation by $\sigma^2\hbar t/m$. For a wave packet, having a given form when it impinges upon $V(x)$, the third correction in (3.10) to the spatial delay therefore depends on the choice of the zero point in time. This paradox is only apparent, however. The term propor-

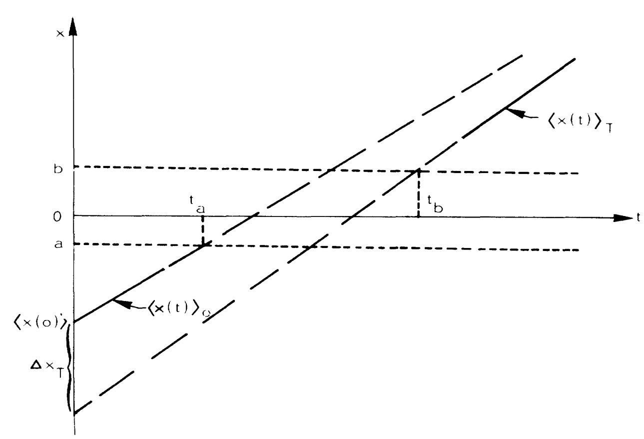

FIG. 2. The average motion of a free packet $\langle x(t)\rangle_0$ for $t<t_a$, and of a transmitted packet $\langle x(t)\rangle_T$ for $t>t_b$ are shown as solid lines. The dashed lines are the corresponding linear extrapolations.

tional to t in (3.10) will clearly *also* be affected by a shift in time, and the corresponding constant correction of $O(\sigma^2)$ precisely cancels the change in the correlation term. That this is so can be seen from the first version of (3.8), where a shift $t \to t - t_0$ will result in $\xi'(k) \to \xi'(k;t_0) = \xi'(k) - \hbar k t_0/m$. For a given wave impinging on the scattering region, the space delay, including all corrections, is therefore well defined.

From the space delay, (3.15) of (3.10), we now want to calculate time delays. The definition (3.15) of Δx_T is unambiguous. This is also true for the zeroth-order time delay (3.13), where the velocity after transmission coincides with the initial velocity. However, when the speed after transmission has been shifted, there is an ambiguity in the definition of time delays. Such delays can only be defined relative to free motion with velocity $\hbar k_c/m$ *before*, and the shifted velocity of (3.10) *after* transmission. *Where* in the x interval (a,b) the velocity of this reference motion changes, is a matter of choice. This arbitrariness carries over to the definition of the time delay.

There is no arbitrariness associated with the *total* transmission time τ_T, however. We define it as $\tau_T = t_b - t_a$. Here t_b is defined as the time when the transmitted wave packet by backward extrapolation is located at the far end, $x = b$, of the scattering region. The free packet at $x = a$ defines t_a similarly:

$$\langle x(t_b)\rangle_T \equiv b, \quad \langle x(t_a)\rangle_0 \equiv a \ . \tag{3.16}$$

Use of (3.10) and (3.11) gives, when $\tilde{k}_c$ and $\tilde{\alpha}'$ is a shorthand notation which includes the corrections of (3.10),

$$\begin{aligned}\tau_T &= \frac{m}{\hbar}\left[\frac{-a}{k_c} + \frac{b}{\tilde{k}_c} + \frac{\tilde{k}_c - k_c}{\tilde{k}_c k_c}\langle x(0)\rangle + \frac{\tilde{\alpha}'}{\tilde{k}_c}\right] \\ &= \frac{m}{\hbar}\left[\frac{-a}{k_c} + \frac{b}{\tilde{k}_c}\right] + \frac{m\alpha'}{\hbar k_c}\left[1 + \frac{\alpha'''\sigma^2}{2\alpha'} + \frac{T'\alpha''\sigma^2}{T\alpha'} - \frac{T'\sigma^2}{Tk_c} + \frac{T'}{T\alpha' k_c}[\sigma^2\langle x(0)\rangle - k_c\langle \Delta k\,\Delta x(0)\rangle]\right] + o(\sigma^2) \ .\end{aligned} \tag{3.17}$$

From the definitions (3.16) it is clear that t_a, t_b, and $\tau_T = t_b - t_a$ are invariant with respect to a shift of the origin of the x axis. Some of the separate terms in (3.17) are not, however. With the origin located between a and b, the term $(m/\hbar)[(-a)/k_c + b/\tilde{k}_c]$ in (3.17) can be interpreted as the *reference* transmission time: From $x = a$ (<0) to $x = 0$ the reference velocity is $\hbar k_c/m$, and from 0 to b it is $\hbar\tilde{k}_c/m$. Clearly, the corresponding delay $\Delta\tau_T$, defined by

$$\tau_T = \frac{m}{\hbar}\left[\frac{-a}{k_c} + \frac{b}{\tilde{k}_c}\right] + \Delta\tau_T \ , \tag{3.18}$$

also depends on the choice of the origin of x [through $\langle x(0)\rangle$]. In the context of (3.17), the simplest choice is to let the origin coincide with the left end point of the scattering region, i.e., to put $a = 0$. Other alternatives may be more convenient under different circumstances.

We shall not reiterate the discussion of the various terms in (3.17). They were already considered in the context of (3.10). Two remarks are, nevertheless, in order. The first one concerns the delay time $\Delta\tau_T$. In the square bracket $[\cdots]$, of the second form of (3.17), the two terms are individually sensitive to a shift, $t \to t - t_0$, corresponding to the apparent paradox discussed above. The sum is invariant, however, since by (2.4) and (2.5)

$$[\cdots] = -\langle(\Delta k)^2\rangle\langle\xi'(k)\rangle + \langle k\rangle\langle\Delta k\,\xi'(k)\rangle \ . \tag{3.19}$$

A shift in time corresponds to the addition to $\xi'(k)$ of a term linear in k. In the combination (3.19), such terms clearly vanish. A shift, $x \to x - x_0$, on the other hand, adds a constant to $\xi'(k)$. This affects the first but not the second term in (3.19). Although $\Delta\tau_T$ is invariant with respect to $t \to t - t_0$, it is *not* invariant with respect to $x \to x - x_0$.

The second remark concerns the correction to the delay as a function of $\langle x(0)\rangle$. Keep the cross correlation in the initial packet constant, and move $\langle x(0)\rangle$ to the left. With $T' > 0$, this will reduce the delay by an arbitrary amount. Consequently, the "correction" term can be made to dominate over $m\alpha'/\hbar k_c$. The underlying physics is clear: A large and negative $\langle x(0)\rangle$ allows strong cross correlations to develop before the packet reaches the scattering region.

IV. EXTENSIONS

A. The reflected packet

For $x \le a$, the linear superposition analogous to (3.1) reads, from (2.1)

$$\psi_<(x,t) = \int \frac{dk}{2\pi}\phi(k)[e^{ikx} + B(k)e^{-ikx}]e^{-iEt/\hbar} \ . \tag{4.1}$$

The existence of two terms in $\psi_<$ gives four terms in $|\psi_<|^2$. The first of these describes the wave packet moving towards the scattering region. Then there are two interference terms, and, finally, the fourth term describes the reflected part of the packet. The first three terms cannot survive indefinitely so that, asymptotically, we are left with the reflected packet. This is described by an unnormalized probability distribution, analogous to (3.2)

$$\begin{aligned}P_R(x,t) = \int\int \frac{dQ\,dq}{(2\pi)^2} e^{-iqx - i\hbar qQt/m} \\ \times\phi(Q+\tfrac{1}{2}q)\phi^*(Q-\tfrac{1}{2}q)B(Q+\tfrac{1}{2}q) \\ \times B^*(Q-\tfrac{1}{2}q) \ .\end{aligned} \tag{4.2}$$

The only changes from (3.2) to (4.2) are $x \to -x$ and $A(k) \to B(k)$. When $R(k) = |B(k)|^2$ denotes the reflection probability, we can therefore immediately write down the result analogous to (3.10)

$$\langle -x(t)\rangle_R - \langle x(0)\rangle \simeq \frac{\hbar k_c}{m}\left[1+\frac{R'\sigma^2}{Rk_c}\right]t - \beta'\left[1+\frac{\beta'''\sigma^2}{2\beta'}+\frac{R'\beta''\sigma^2}{R\beta'}-\frac{R'}{R}\frac{\langle \Delta k\,\Delta x(0)\rangle}{\beta'}\right]+o(\sigma^2) . \quad (4.3)$$

In Fig. 3 the spatial delay for reflection Δx_R is defined in analogy with Δx_T of Fig. 2 and (3.14). This delay has a meaning only with respect to a free packet, perfectly reflected at some chosen reference point. In Fig. 3, and in our calculations, this point is $x=0$. Since the position of $x=0$ is arbitrary, we turn instead to the total reflection time, uniquely given as $\tau_R = t_{aR} - t_a$. Here, we define t_{aR} and t_a by

$$\langle x(t_{aR})\rangle_R = a, \quad \langle x(t_a)\rangle_0 = a . \quad (4.4)$$

Neglecting terms of $O(\sigma^2)$, one finds from (4.3) and (3.11)

$$\tau_R(k) = \frac{m}{\hbar k}[-2a + \beta'(k)] \quad (4.5)$$

(where subscript c has been dropped). A shift, $x \to x - x_0$, of the x axis results in a shift, $\beta \to \beta - 2kx_0$, of the phase [see (2.1)]. The combination (4.5) is, consequently, invariant. However, unlike $\Delta\tau_T$, the reflection delay $\Delta\tau_R$ depends on the choice of origin already to zeroth order. With the simple choice $a=0$, $\Delta\tau_R = \tau_R$.

Inclusion of corrections to $O(\sigma^2)$ gives

$$\tau_R = \frac{m}{\hbar}\left[\frac{-a}{k_c}+\frac{-a}{\tilde{k}_c}+\frac{\tilde{k}_c - k_c}{\tilde{k}_c k_c}\langle x(0)\rangle + \frac{\tilde{\beta}'}{\tilde{k}_c}\right], \quad (4.6)$$

where $\tilde{k}_c$ and $\tilde{\beta}'$ now include the correction terms of (4.3). Equation (4.6) is completely analogous to (3.17). The discussion of (4.3) and (4.6) parallels that of (3.10) and (3.17). We shall not repeat it here. Note, however, that $R' = -T'$.

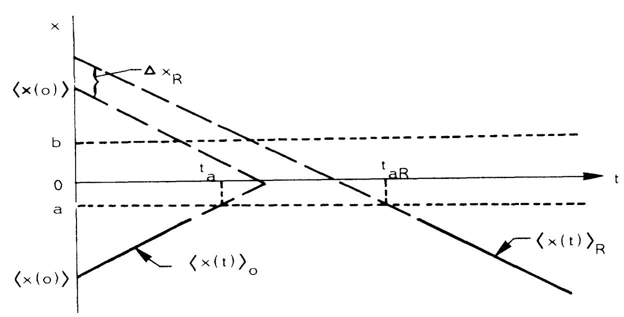

FIG. 3. The average motion of a free packet $\langle x(t)\rangle_0$ for $t < t_a$, and of a reflected packet $\langle x(t)\rangle_R$ for $t > t_{aR}$ are shown as solid lines. The dashed lines are the corresponding linear extrapolations. The mirror image of the free motion around $x=0$ is also dashed.

B. The transmitted packet when $\Delta E \neq 0$

When one generalizes to the case shown in Fig. 1, with $\Delta E \neq 0$, there is no (formal) change as far as the reflected packet is concerned. However, the calculations for the transmitted packet must be modified. With $\Delta E = \hbar^2 k_s^2/2m$ defining the constant k_s, one has

$$\tilde{k}^2 = k^2 + k_s^2 , \quad (4.7)$$

and the transmitted wave function now reads ($x \geq b$),

$$\psi_T(x,t) = \int \frac{dk}{2\pi}\phi(k)A(k)e^{i\tilde{k}x - i\tilde{E}t/\hbar} . \quad (4.8)$$

In analogy with (3.3) we introduce

$$\tilde{q} = \tilde{k} - \tilde{k}', \quad \tilde{Q} = \tfrac{1}{2}(\tilde{k} + \tilde{k}') \quad (4.9)$$

in the double integral defining $P_T(x,t)$. Note that, by (4.9) and (4.7)

$$\tilde{q}\tilde{Q} = qQ . \quad (4.10)$$

With $\phi(k)$ and $A(k)$ still considered as functions of k, (3.2) generalizes to

$$P_T(x,t) = \int\int \frac{dQ\,dq}{(2\pi)^2} e^{iqQx/\tilde{Q} - i\hbar qQt/m} \times \phi(Q+\tfrac{1}{2}q)\phi^*(Q-\tfrac{1}{2}q) \times A(Q+\tfrac{1}{2}q)A^*(Q-\tfrac{1}{2}q) , \quad (4.11)$$

where (4.10) has been used. The steps of Sec. III can now be repeated. The only new feature is additional factors $\tilde{Q}/Q$ in the $\delta(q)$ function, and in the differentiation to form $\langle x(t)\rangle_T$. With the modified definition $T(k) = (\tilde{k}/k)|A(k)|^2$, Eq. (3.8) now becomes

$$\langle x(t)\rangle_T \simeq \langle T(k)\rangle^{-1}\left[\frac{\hbar}{m}\langle T(k)\tilde{k}\rangle t + \left\langle T(k)\left[-\frac{\tilde{k}}{k}\xi'(k)\right]\right\rangle - \left\langle T(k)\frac{\tilde{k}}{k}\alpha'(k)\right\rangle\right] . \quad (4.12)$$

Although (4.12), like (3.8), can be expanded to $O(\sigma^2)$, we shall be content with stating the zeroth-order result here

$$\langle x(t)\rangle_T \simeq \frac{\hbar\tilde{k}_c}{m}t+\frac{\tilde{k}_c}{k_c}\langle x(0)\rangle-\frac{\tilde{k}_c}{k_c}\alpha'(k_c)+O(\sigma^2)\ . \tag{4.13}$$

The spatial delay is defined as in (3.15), and (4.13) gives (when subscript c is dropped)

$$\Delta x_T=\frac{\tilde{k}}{k}\alpha'(k)-\left[\frac{\tilde{k}}{k}-1\right]\langle x(0)\rangle\ . \tag{4.14}$$

The associated total transmission time, $\tau_T=t_b-t_a$, is

$$\tau_T(k)=\frac{m}{\hbar}\left[\frac{-a}{k}+\frac{b}{\tilde{k}}+\frac{\alpha'(k)}{k}\right]\ . \tag{4.15}$$

The analogy with (3.17) is evident. That both Δx_T and τ_T are invariant with respect to the shift $x \to x-x_0$, follows from the corresponding transformation $\alpha\to\alpha+(\tilde{k}-k)x_0$. In the present case, the delay $\Delta\tau_T$ depends on the reference chosen, already to leading order.

C. An alternative

In this paper we have identified the positions of the transmitted and reflected wave packets with their mean values $\langle x(t)\rangle_T$ and $\langle x(t)\rangle_R$. Although this is, in our opinion, *the* proper identification from a fundamental point of view, alternatives exist. For example, in numerical studies[11–14] of moving wave packets, a popular choice is the location of the *maximum* of $P_T(x,t)$ or $P_R(x,t)$. With this alternative definition one can (at least with packets of "reasonable" shape) repeat the arguments of Sec. III, with some technical modifications. We shall not pause to give the details here. The outcome is that, to lowest order, the classic result (3.13) on the delay is rederived. So is the structure of the correction terms discussed in Sec. III. However, the detailed *coefficients* of these corrections differ, in general, from those found in Sec. III. The exception is the (initial) Gaussian packet: In that case even the coefficients of the correction terms come out the same.

V. THE DWELL TIME

It is interesting to consider the dwell time, to be defined below, in conjunction with the phase times rederived and extended in Secs. I–IV. It was introduced by Smith[5] in 1960, in connection with collision theory in three dimensions. The dwell time used in recent papers[10,12,18] is not identical to the somewhat subtler concept introduced by Smith, however. In this section we shall derive, for the one-dimensional case, an exact relation (reminiscent of one found in Ref. 5) between the phase times τ_T and τ_R and the dwell time τ_d, as it is currently understood. This connection clarifies the status of τ_d, and shows when it can and cannot be used. For simplicity, we restrict the derivation to the case $\Delta E=0$, indicating the generalization to $\Delta E\neq 0$ at the end.

Consider the version of the situation shown in Fig. 1 in which $\Delta E=0$. Integrate the continuity equation across the scattering region (a,b) for an arbitrary time-dependent state $\psi(x,t)$. The result is

$$\frac{d}{dt}\int_a^b dx\,|\psi(x,t)|^2+j(b,t)-j(a,t)=0\ , \tag{5.1}$$

where $j(x,t)$ is the time-dependent current

$$j(x,t)=\frac{\hbar}{2im}\left[\psi^*(x,t)\frac{d}{dx}\psi(x,t)-\psi(x,t)\frac{d}{dx}\psi^*(x,t)\right]\ . \tag{5.2}$$

Since, in the case of interest to us, the wave packet was entirely to the left of $x=a$ initially, (5.1) can be integrated twice to give

$$I_1+I_2\equiv\int_{-\infty}^{\infty}dt\int_a^b dx\,|\psi(x,t)|^2+\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'[j(b,t')-j(a,t')]=0\ . \tag{5.3}$$

This equation serves as the basis for our derivation of the relation between τ_T, τ_R, and τ_d. Strictly speaking, the time integrals should start at $t=0$ not at $t=-\infty$. We can, however, imagine the wave packet moved backwards in time from its position at $t=0$. During this motion, the overlap with the x interval (a,b) will be (essentially) zero. (Remember that we are considering wave packets confined to $x<a$ at $t=0$, and with a spread of velocities small with respect to the average $\sigma \ll k_c$.) The range added to the time integrals therefore does not contribute in (5.3). The time integral in I_1 (and thus in I_2) clearly converges, since the integrand only lives during a finite time interval.

Use the Fourier decomposition of Sec. III but now with $\chi(x;k)$ of (2.1) as the stationary solution, to write

$$I_1=\int_{-\infty}^{\infty}dt\int_a^b dx\int\int\frac{dQ\,dq}{(2\pi)^2}e^{-i\hbar qQt/m}\phi(Q+\tfrac{1}{2}q)\phi^*(Q-\tfrac{1}{2}q)\chi(x;Q+\tfrac{1}{2}q)\chi^*(x;Q-\tfrac{1}{2}q)\ . \tag{5.4}$$

Integration over t gives $(2\pi m/\hbar Q)\delta(q)$, which, after integration over q (with $Q\to k$) yields

$$I_1=\int\frac{dk}{2\pi}|\phi(k)|^2\frac{m}{\hbar k}\int_a^b dx\,|\chi(x;k)|^2\equiv\int\frac{dk}{2\pi}|\phi(k)|^2\tau_d(k)\ . \tag{5.5}$$

This equation gives the now standard definition of the dwell time $\tau_d(k)$, for a given k, i.e., for the stationary situation. This dwell time is simply the particle density $|\chi(x;k)|^2$ integrated over the scattering region (assumed well defined), and divided by the incoming current $(\hbar k/m)1$. (The integral I_1 can be considered as an average dwell time for the given wave packet.) If all particles are transmitted, $\tau_d(k)$ clearly measures the average time spent in the scattering region. With both transmission and reflection present, the interpretation of τ_d becomes less clear, as we shall see.

Insertion of (2.1) with $\tilde{k}=k$ into (5.2) and (5.3) gives for the second integral

$$I_2=\frac{\hbar}{2m}\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'\int\int\frac{dQ\,dq}{(2\pi)^2}e^{-i\hbar qQt'/m}\phi(Q+\tfrac{1}{2}q)\phi^*(Q-\tfrac{1}{2}q)$$
$$\times\{2Q[A(Q+\tfrac{1}{2}q)A^*(Q-\tfrac{1}{2}q)e^{iqb}+B(Q+\tfrac{1}{2}q)B^*(Q-\tfrac{1}{2}q)e^{-iqa}-e^{iqa}]$$
$$+q[B(Q+\tfrac{1}{2}q)e^{-2iQa}-B^*(Q-\tfrac{1}{2}q)e^{2iQa}]\}\ . \tag{5.6}$$

When the stationary boundary term at $t'=-\infty$ is neglected, the t' integration brings down a factor $(-i\hbar qQ/m)^{-1}$. (The way our problem has been set up warrants neglect of this boundary term. Formally, one could justify it by adding a weak damping on the integrands for negative times, and letting the damping go to zero at the end of the calculation.) Subsequent integration over t gives $(2\pi m/\hbar Q)\delta(q)$ so that

$$I_2=i\int\frac{dQ}{2\pi}\int dq\frac{m}{\hbar Q}\delta(q)\phi(Q+\tfrac{1}{2}q)\phi^*(Q-\tfrac{1}{2}q)$$
$$\times\left[\frac{1}{q}[\,|A(Q+\tfrac{1}{2}q)A(Q-\tfrac{1}{2}q)|\,e^{iqb+i\alpha(Q+q/2)-i\alpha(Q-q/2)}\right.$$
$$+|B(Q+\tfrac{1}{2}q)B(Q-\tfrac{1}{2}q)|\,e^{-iqa+i\beta(Q+q/2)-i\beta(Q-q/2)}-e^{iqa}]$$
$$\left.+\frac{1}{2Q}[\,|B(Q+\tfrac{1}{2}q)|\,e^{i\beta(Q+q/2)-2iQa}-|B(Q-\tfrac{1}{2}q)|\,e^{-i\beta(Q-q/2)+2iQa}]\right]\ . \tag{5.7}$$

The zeroth-order term (in a power series in q) in the first square bracket of (5.7) vanishes, since $|A(k)|^2+|B(k)|^2=1$. Due to $\delta(q)$, the first-order term in the first square bracket and the zeroth order in the second one, are the only survivors of the q integration, and one finds (with $Q\rightarrow k$)

$$I_2=-\int\frac{dk}{2\pi}|\phi(k)|^2\frac{m}{\hbar k}\left[|A(k)|^2[b-a+\alpha'(k)]+|B(k)|^2[-2a+\beta'(k)]+\frac{1}{k}|B(k)|\sin[\beta(k)-2ka]\right]\ . \tag{5.8}$$

Here we recognize $(m/\hbar k)[b-a+\alpha'(k)]$ as the total transmission time $\tau_T(k)$ of (3.14). Similarly, $(m/\hbar k)[-2a+\beta'(k)]$ is the total reflection time $\tau_R(k)$ of (4.5). When we use that $|\phi(k)|^2$ is essentially arbitrary, and introduce the transmission and reflection probabilities, (5.3), (5.5), and (5.8) finally yield the relation sought

$$\tau_d(k)=T(k)\tau_T(k)+R(k)\tau_R(k)$$
$$+\frac{m}{\hbar k^2}\sqrt{R(k)}\sin[\beta(k)-2ka]\ . \tag{5.9}$$

Before commenting on the significance of (5.9), we note that its form remains *precisely* the same in the case $\Delta E\neq 0$, provided that $T(k)$ is given its appropriate interpretation as

$$T(k)=(\tilde{k}/k)|A(k)|^2=1-R(k)=1-|B(k)|^2\ ,$$

and that $\tau_T(k)$ is defined as in (4.15).

Several comments on our result (5.9) are in order: (i) As anticipated, with perfect transmission ($T=1$, $R=0$), the dwell time τ_d coincides with the phase time τ_T. (ii) The third term on the right of (5.9) can be written as $(\hbar/2E)\sqrt{R}\,\sin(\beta-2ka)$. This form emphasizes its role as a quantum interference term. It vanishes in the classical limit of high energies. (iii) To the extent that the interference term can be neglected, τ_d has the physical interpretation of a weighted average of the phase times for the two scattering channels existing here.[5] In particular, at a *resonance*, where τ_T and τ_R may become very large, the interference term is negligible. (iv) For small energies, however, and not too large τ_T and τ_R, the interference term is very important. Typically[10] τ_T and $\tau_R\sim k^{-1}$ as $k\rightarrow 0$, whereas $\tau_d\sim k$. The difference is due to the interference term which cancels the leading behavior in τ_T and τ_R. For small k, the dwell time has no physical meaning in the present context. (v) To calculate *physical* dwell times for transmitted and reflected particles separately, one would have to identify those with separate pieces of the total wave function in the scattering region. Such a splitting of the wave function is incompatible with the principles of quantum mechanics. (vi) We have put (5.9) to the nontrivial test set by reflection from, and tunneling through, a square barrier. The dwell and phase times calculated explicitly for that problem are in perfect agreement with (5.9). Details are found in the Appendix. (vii) As it stands, with (a,b) given as the (strictly localized) scattering region, all terms in (5.9) are uniquely defined. If, on the other hand, (a,b) is more liberally interpreted as *any* given interval which *includes* the scattering region, the quantities in (5.9) change with (a,b). The phase times increase linearly with a and b when (a,b) is thus expanded. The interference term, however, oscillates with a. This is a clear demonstration that the dwell time does *not*, in general, have the physical meaning of the average time spent in the interval (a,b). Note that for any given k, a can then be chosen such that the interference term vanishes. For a wave packet with a continuum of k values, however, this is not possible. (viii) The dwell time introduced by Smith[5] is a somewhat subtler concept than that discussed here. The freedom mentioned under the previous point, in combination with a limiting procedure, allows the definition of a dwell time for which a relation of the type (5.9), but without the interference term, can be proved. This more refined dwell time is not well adapted for applications in the transport theory of solids.

VI. RESONANT TRANSMISSION THROUGH A DOUBLE BARRIER

A. General considerations

In view of its current importance,[1] we shall, in this section, consider resonant tunneling through a double barrier. Most of the arguments of Sec. III were based on the assumption that the transmission probability $T(k)$ varies slowly on a scale set by the width σ, of the wave packet. With sharp resonances, this condition may be overly restrictive. We shall therefore go back to (3.8) and (3.9) and consider the inverse situation.

Equation (3.9) can be written as

$$\langle x(t)\rangle_T-\langle x(0)\rangle \simeq \frac{\hbar}{m}\frac{\langle T(k)k\rangle}{\langle T(k)\rangle}t - \frac{\langle T(k)\alpha'(k)\rangle}{\langle T(k)\rangle}+\frac{\langle \Delta T(k)(-\Delta\xi')\rangle}{\langle T(k)\rangle}. \tag{6.1}$$

Assume now that $T(k)$ has a sharp resonance at k_r and that all other functions vary slowly on the scale set by the width of this resonance. To lowest order, the two first terms on the right of (6.1) give $[\hbar k_r t/m-\alpha'(k_r)]$. If this were all, the only difference from the zeroth-order version of (3.10) would be the trivial one that k_c has been replaced by k_r. The last term in (6.1) represents something new, however. It involves, in general, *all* moments of the initial wave packet. If we restrict ourselves to packets characterized by moments of no higher than second order, we can write

$$-\Delta\xi'(k)=\frac{\langle \Delta k\, \Delta x(0)\rangle}{\sigma^2}(k-k_c) \tag{6.2}$$

[where $\langle \Delta k\, \Delta x(0)\rangle=O(\sigma^2)$]. In this simplest case (6.1) becomes, with neglect of all corrections due to the finite width of the resonance,

$$\langle x(t)\rangle_T-\langle x(0)\rangle \simeq \frac{\hbar k_r}{m}t-\alpha'(k_r)+\frac{\langle \Delta k\, \Delta x(0)\rangle}{\sigma^2}(k_r-k_c)\ . \tag{6.3}$$

The physics of the cross correlation term is precisely the same as that discussed in Sec. III. What is new here is its appearance already to leading order.

By calculations completely analogous to those of Sec. III, one finds for the total transmission time

$$\tau_T=\frac{m}{\hbar}\left\{\frac{-a}{k_c}+\frac{b}{k_r}+\frac{\alpha'(k_r)}{k_r}+\frac{k_r-k_c}{\sigma^2 k_r k_c}[\sigma^2\langle x(0)\rangle-k_c\langle \Delta k\, \Delta x(0)\rangle]\right\}. \tag{6.4}$$

This result is very similar to (3.17) and the same remarks found there apply to (6.4). Note, in particular, that, depending on the sign of (k_r-k_c), a large and negative $\langle x(0)\rangle$ will substantially reduce or increase the delay as given by the phase $\alpha'(k_r)$. Note, also, that a discussion of the *reflected* wave packet along the lines of this section does not make sense.

An alternative approach to that presented above would be to replace the initial wave packet by one filtered through $T(k)$, i.e., to take $\phi(k)\sqrt{T(k)}$ as the Fourier transform of an "effective" initial packet. This procedure would turn (6.4) into the standard form (3.14), since k_c would, by construction, coincide with k_r. This highlights the fact that the role of the term correcting the phase time in (6.4) is merely to adjust the awkward reference motion *prior* to tunneling into the resonance structure.

B. Calculations

We now turn to an explicit calculation of τ_T at the resonances of a symmetric double barrier. As the starting point we use (6.4), and set $k_c=k_r$ (i.e., we neglect the correction from the initially free motion). Approximate results (based on the dwell time) for the case of strong localization (i.e., high and/or wide barriers) have been given previously by Ricco and Azbel.[18] Our exact result reduces (with minor, but interesting modifications) to theirs, in the appropriate limit. It is not clear, however, that this limit is the relevant one for applications, since the corresponding delay time becomes uncomfortably long, and neglected Coulomb and finite temperature effects[18–22] then become significant.

The situation is shown in Fig. 4. A well of width w is located between two equal barriers, each of width b and height V_0. In the well there is a finite number (labeled $n=1,2,\ldots$) of quasieigenstates (resonances) which, in this symmetric case, correspond to k values where $T(k)=1$. We only highlight the essential steps in the calculation of τ_T below, since the procedure is standard.[23,3,18] The complex transmission amplitude is found to be

$$\begin{aligned}A(k)&=e^{-2ikb}/D(k)\ ,\\ D(k)&=\cosh^2(\kappa b)+\tfrac{1}{4}\sinh^2(\kappa b)[\sigma^2\cos(2kw)-\delta^2]\\ &\quad+i\sinh(\kappa b)[\delta\cosh(\kappa b)+\tfrac{1}{4}\sigma^2\sinh(\kappa b)\sin(2kw)]\ ,\end{aligned} \tag{6.5}$$

where

$$\begin{aligned}&E=\frac{\hbar^2k^2}{2m},\quad V_0=\frac{\hbar^2k_0^2}{2m},\quad \kappa^2=k_0^2-k^2\ ,\\ &\sigma=\frac{\kappa}{k}+\frac{k}{\kappa},\quad \delta=\frac{\kappa}{k}-\frac{k}{\kappa},\quad \sigma^2=\delta^2+4=\frac{k_0^4}{k^2\kappa^2}\ .\end{aligned} \tag{6.6}$$

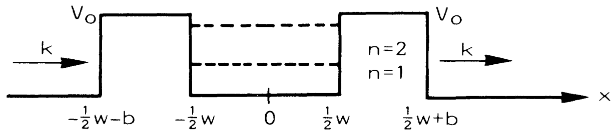

FIG. 4. A symmetric double barrier. The height of the barriers is V_0, their width b, and the distance between them is w. Two resonances are shown as dotted lines.

The resonance condition can be expressed in various ways. A useful one, which can also be applied to the asymmetric case, is

$$\frac{d}{dw}|D|^2=0\ . \tag{6.7}$$

A straightforward calculation based on (6.5) shows that (6.7) implies

$$\tan(2kw)=\frac{\delta\tanh(\kappa b)}{1-\frac{1}{4}\delta^2\coth(\kappa b)}\ , \tag{6.8}$$

The extremal condition (6.7) is satisfied both at resonances and when the transmission probability $T(k)=|D(k)|^{-2}$ has a minimum. Resonances correspond to those solutions of (6.8) at which

$$\cot(kw)=-\frac{\delta}{2}\tanh(\kappa b)\ . \tag{6.9}$$

A graphical solution of (6.9) is shown in Fig. 5, for the special choice $k_0w=8$, $k_0b=3$. There are three resonances.

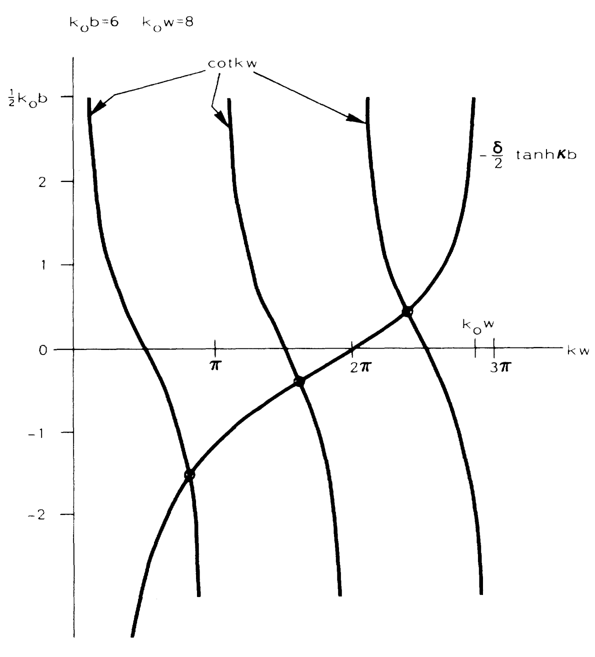

FIG. 5. Graphical solution of the resonance condition (6.9) for the special choice of $k_0w=8$ and $k_0b=6$. There are three tunneling resonances in this case.

When (6.9) is satisfied, $D(k)$ takes the form

$$D_{\rm res}=\frac{1-\frac{1}{4}\delta^2\tanh^2(\kappa b)+i\delta\tanh(\kappa b)}{1+\frac{1}{4}\delta^2\tanh^2(\kappa b)}\ . \tag{6.10}$$

Clearly, $T_{\rm res}=|D_{\rm res}|^{-2}=1$. Furthermore, the phase of $D=|D|e^{i\gamma}$ is, at resonance, given by

$$\tan\gamma_{\rm res}=\frac{\delta\tanh(\kappa b)}{1-\frac{1}{4}\delta^2\tanh^2(\kappa b)}=\tan(2kw)\ . \tag{6.11}$$

The proper solution of (6.11) is

$$\gamma_n=2k_nw-(2n-1)\pi\ , \tag{6.12}$$

where $n=1,2,\ldots$ labels the resonances from the lowest one up. Equation (6.10) can then be written

$$D_n=-\cos(2k_nw)-i\sin(2k_nw)\ . \tag{6.13}$$

Expansion of $D(k)$ of (6.5) to first order in $\Delta k=k-k_n$ at the nth resonance, gives an expression of the form

$$D(k)=-\cos(2k_nw)-i\sin(2k_nw)+(\xi_n+i\eta_n)\Delta k\ \ldots\ . \tag{6.14}$$

From this, the phase derivative follows as

$$\gamma'(k_n)=-\eta_n\cos(2k_nw)+\xi_n\sin(2k_nw)\ . \tag{6.15}$$

Tedious, but straightforward, algebra is necessary to calculate ξ_n and η_n. The result for the transmission time τ_{Tn} at the nth resonance is, finally

$$\begin{aligned}\tau_{Tn}&=\frac{m}{\hbar k_n}[2b+w-2b-\gamma'(k_n)]\\&=\frac{m}{\hbar k_n}\left\{\sigma^2\sinh^2(\kappa b)\left[\tfrac{1}{2}w+\frac{1}{\kappa}\coth(\kappa b)\right]\right.\\&\qquad\left.+w+b\left[1-\left[\frac{k}{\kappa}\right]^2\right]\right\}_n\ .\end{aligned} \tag{6.16}$$

The above calculation was based on the phase derivative. Since $T_n=1$ at resonances in the symmetric case, the same expression for τ_{Tn} should result if one would base the calculation of τ_{Tn} on the formula for the dwell time (5.5). We have checked this explicitly, and the agreement with (6.16) is perfect.

For the case of strong localization, $\kappa b\gg 1$, (6.16) yields

$$\begin{aligned}\tau_{Tn}&\simeq\frac{m}{\hbar k_n}\left[\frac{\sigma^2}{4}e^{2\kappa b}\left[\tfrac{1}{2}w+\frac{1}{\kappa}\right]\right]_n\\&=\frac{m}{\hbar k_n}\left[\frac{4}{T^{(1)}}\left[\tfrac{1}{2}w+\frac{1}{\kappa}\right]\right]_n\ ,\end{aligned} \tag{6.17}$$

where $T^{(1)}\simeq(16/\sigma^2)e^{-2\kappa b}$ is the transmission coefficient for a single barrier. Equation (6.17) agrees with the result of Ricco and Azbel,[18] except for the prefactor 4 and the factor $\frac{1}{2}$ in front of w. The overall prefactor was not taken seriously in Ref. 18, but the extra factor $\frac{1}{2}$ is more interesting. It reflects the fact that, at resonance, the wave function in the well is closely sinusoidal, rather than having a constant absolute value. With asymmetric barriers, where $T_n < 1$ in general, the discussion in Sec. V shows that a dwell time calculation, as in Ref. 18, can yield an approximate answer, but never the exact one.

VII. CONCLUDING REMARKS

This paper contains three principal results. The first one is the demonstration, in Secs. III and IV, that the classic phase times are indeed the relevant physical times when the motion of wave packets, narrow in k space, is to be discussed to leading order. As an integral part of this demonstration, new correction terms of $O(\sigma^2)$ have been derived, and their physical content discussed. These correction terms give quantitative meaning to the condition that the wave packets should be narrow in k space. The scattering off barriers of packets with a wide k distribution cannot, in general, be characterized by simple concepts like delay times. An exception is discussed in Sec. VI A. See also Ref. 8.

The second major result is the derivation, in Sec. V, of the identity (5.9), relating the dwell time, as it is currently used, to the phase times for transmission and reflection. The corresponding discussion shows that the dwell time is physically meaningful essentially only to the extent that it coincides with the relevant phase time. It is true that some numerical results[12] in the literature might be said to favor the dwell time over the phase time at small energies. This, we claim, must be due to numerical difficulties. The results of Secs. III and IV show that, for small energies, the packet has to be extremely narrow ($\sigma \ll k_c$) for meaningful results to be obtained. This puts the numerics under severe strain. Other arguments in favor of the dwell time have been based on calculations of stationary scattering of electrons, including spin, by a potential barrier with an infinitesimal magnetic field.[6,7,10] Although we do not challenge the calculations as such, we disagree with their interpretation. When the time dependence is explicitly handled, one finds, to lowest order, that a properly set Larmor clock shows the phase time.[17]

The third new result is an explicit exact formula for the transmission time, at resonance, through a symmetric double barrier. Under the provisos made explicit in Sec. VI A, the phase time can be used to characterize the delay of transmitted wave packets, even at narrow resonances. Our explicit formula will, hopefully, be of use in the discussion of resonant transmission, when the barriers singly are not too opaque. (An extension to asymmetric double barriers can be made without major difficulties.[25]) Needless to say, the validity of the formula is restricted by the assumptions basic to the model.

Note added in proof After this manuscript was submitted we became aware of recent related work by J. R. Barker,[26] His conclusions on the relevance of phase times are similar to ours. We differ, however, on the relation (tested in our Appendix) between the dwell time and the phase times.

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APPENDIX

The (elastic) transmission and reflection by a single energy barrier of width b and height V_0 has been considered in detail by Büttiker.[10] We sketch some of the results here, using the notation introduced in (6.6). The transmission and reflection amplitudes are, when the barrier fills the x interval $(0,b)$

$$A(k)=\frac{e^{-ikb}}{\cosh(\kappa b)+\frac{i}{2}\delta\sinh(\kappa b)}\ ,$$
$$B(k)=-\frac{i}{2}\sigma\sinh(\kappa b)e^{ikb}A(k)\ . \tag{A1}$$

This gives the corresponding phases as

$$\alpha(k)=-kb-\tan^{-1}[\tfrac{1}{2}\delta\tanh(\kappa b)]\ ,$$
$$\beta(k)=-\frac{\pi}{2}-\tan^{-1}[\tfrac{1}{2}\delta\tanh(\kappa b)]\ . \tag{A2}$$

The phase times are

$$\tau_T=\frac{m}{\hbar k}[b+\alpha'(k)]$$
$$=\frac{m}{\hbar k}\beta'(k)=\tau_R=\frac{m}{\hbar k\kappa}\frac{2\kappa bk^2(\kappa^2-k^2)+k_0^4\sinh(2\kappa b)}{4k^2\kappa^2+k_0^4\sinh^2(\kappa b)}\ . \tag{A3}$$

From (A1)–(A3) and the identity (5.9) with $a=0$, one calculates the dwell time as

$$\tau_d=\frac{mk}{\hbar\kappa}\frac{2\kappa b(\kappa^2-k^2)+k_0^2\sinh(2\kappa b)}{4k^2\kappa^2+k_0^4\sinh^2(\kappa b)} \tag{A4}$$

in complete agreement with that found by direct integration of the wave function through the barrier.

Note that (i) whereas $\tau_T=\tau_R\simeq(2m/\hbar\kappa k)\coth(\kappa b)\sim k^{-1}$ for small k, $\tau_d\sim k$. For small k, the interference term in (5.9) is very important, and τ_d becomes physically meaningless. (ii) For finite $\hbar/E$, the interference term in (5.9) (with $a=0$) can only be made to vanish by having $\sin\beta=0$. In the case of a single barrier (A2) shows this to be possible only for $\delta\to\infty$, i.e., only when the barrier becomes infinitely high. In that case, there is obviously no difference between quantum and classical reflection.

*Permanent address: Institutt for Teoretisk Fysikk, Norges Tekniske Høgskole, Universitetet i Trondheim, N-7034 Trondheim-NTH, Norway.

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