Time delay in tunneling: Transmission and reflection time delays

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The problem of time delay in one-dimensional quantum-mechanical scattering by a potential barrier is studied in the framework of time-dependent scattering theory. It is shown how the concept of sojourn time can be used to define three separate time delays: the time delay for transmission through the barrier, the time delay for reflection, and the total time delay (i.e., averaged over transmission and reflection). In addition to the anticipated dependence on the S matrix and its energy derivative, the time delays depend on certain parameters which can be interpreted as describing positions of detectors in a *gedanken*-experiment measurement. The problem of defining separate time delays for transmission and reflection appears to be rooted in the foundations of quantum theory and its interpretation.

I. INTRODUCTION

The majority of theoretical studies of scattering processes is concerned with a stationary description of scattering in terms of cross sections, but the collision process itself is always understood in terms of time-dependent dynamics. Experimentally, the temporal aspects of scattering are readily accessible only in collisions involving long-lived intermediate states. In general, interaction or collision times cannot be measured directly at present but instead must be inferred in a qualitative fashion from the characteristics of other quantities such as the scattering angle distribution (differential cross section), internal and translational energy distributions, or various polarizations. The temporal aspects of scattering are important in understanding the behavior of many of the quantities traditionally measured in scattering experiments and in the selection of appropriate theoretical collision models. These considerations motivate both experimental and theoretical interest in the time of duration of a collision, a particularly useful definition of which is the time delay.

Interest in the study of time delay is also stimulated by its role in other areas.[1] Topics include the principle of causality,[2] the partitioning of scattering amplitudes or the S matrix into direct and fluctuating parts,[3] the manifestations and characteristics of chaos in the time delay,[4] the interpretation of virial coefficients,[5] and more direct experimental measurements of collision times.[6]

The theory of time delay in classical mechanical scattering[7] is, at least conceptually, a straightforward matter due to the fact that the arrival and the departure times of a classical particle are well defined and meaningful. This is unfortunately not the case with quantum theory. It is well known that there does not exist a generally accepted and unambiguous formula for the time of arrival of a quantum particle at a detector.[8] This quantity, although evidently experimentally accessible, does not have a self-adjoint operator as its quantum-theory counterpart. All theoretical approaches to time delay must somehow circumvent this problem. An elegant and efficient way to do this is by employing the concept of sojourn time of a particle in a spatial region.[9] This approach has received considerable theoretical attention and is well founded mathematically (two-body and many-body problems have been thoroughly investigated[10,11]). However, so far the concept of sojourn time has been successfully applied to deal only with the so-called total time delay, i.e., the time delay averaged over all angles in two-body scattering or over all angles and all channels in multichannel scattering. We find it most desirable to show that the concept of sojourn time does in fact provide a unified base for the general theory of time delays, including angle-dependent time delay in two-body scattering and state-to-state time delay in multichannel scattering. Other approaches to the treatment of time delay are summarized and classified in Ref. 1.

In the present paper we study a one-dimensional scattering by a potential barrier. In this case one can speak about three separate time delays: the time delay for particles transmitted through the barrier, the time delay for reflected particles, and the total time delay, i.e., appropriately averaged over the transmitted and reflected particles. We show how all these time delays can be defined using the concept of sojourn time. We think the solution points the way to application of the sojourn-time concept to the more complex problems of the angular and the state-to-state time delays mentioned above. At the same time, the study is also of some independent interest in view of considerable theoretical efforts devoted in recent years to the definition of the time a particle needs to tunnel through a potential barrier.[12–19]

No practical applications are included here since this was deemed to be incompatible with the goal and spirit of the paper. Our time-delay expressions can nevertheless be easily evaluated for any solvable model. Naturally, the practical significance of the results would be best assessed by application to models whose form and parameters are suggested by physical considerations.

II. SCATTERING THEORY PRELIMINARIES

We consider a one-dimensional quantum-mechanical system with Hilbert space $\mathcal{H}=L^2(\mathbb{R})$ and the Hamiltonian $H=-\frac{1}{2}(d^2/dx^2)+V(x)$. The potential $V(x)$ (further called also the potential barrier) is assumed to have finite range, i.e., there is an $R_0>0$ such that $V(x)=0$ for $|x|\geq R_0$. This restriction is made in order to facilitate mathematical treatment. It by no means provides a necessary condition for the validity of our main results of Secs. IV and V, which, no doubt, remain true for a much wider class of potentials. H_0 denotes the free Hamiltonian, $H_0=-\frac{1}{2}(d^2/dx^2)$ and $\mathcal{H}_b\subseteq L^2(\mathbb{R})$ is the subspace of all bound states of H (possibly $\mathcal{H}_b=\{0\}$). We put $\hbar=1$ throughout.

The Møller operators

$$\Omega_{\pm}=s-\lim_{t\mp\infty}\exp(itH)\exp(-itH_0) \tag{2.1}$$

are assumed to map $\mathcal{H}=L^2(\mathbb{R})$ isometrically onto the orthogonal complement $\mathcal{H}_b^{\perp}$ of $\mathcal{H}_b$. In particular, every state vector $\Psi\in\mathcal{H}_b^{\perp}$ represents a scattering state, i.e., possesses in- and out-asymptotes Ψ^- and Ψ^+, $\Omega_{\pm}\Psi^{\mp}=\Psi$,

$$\lim_{t\pm\infty}\|\exp(-itH)\Psi-\exp(-itH_0)\Psi^{\pm}\|=0\ . \tag{2.2}$$

Ψ^+ and Ψ^- are related by the scattering operator $S=\Omega_-^{\dagger}\Omega_+$, $\Psi^+=S\Psi^-$, which is a unitary operator from $L^2(\mathbb{R})$ onto $L^2(\mathbb{R})$.

It will be most convenient to work in the (two-valued) energy representation employing the Hilbert space $L^2((0,\infty),\mathbb{C}^2)$ which consists of pairs $F=(f_1,f_2)$ of square integrable functions defined on the continuous-spectrum energy range $(0,\infty)$. [The meaning of f_1 and f_2 is made clear in Eq. (2.4) and below.] The scalar product of $F=(f_1,f_2)$ and $G=(g_1,g_2)$ is given by

$$\langle F\mid G\rangle=\int_0^{\infty}[f_1^*(E)g_1(E)+f_2^*(E)g_2(E)]dE\ . \tag{2.3}$$

The unitary correspondence $U:L^2(\mathbb{R})\rightarrow L^2((0,\infty),\mathbb{C}^2)$ between the usual position representation and our energy representation reads

$$(U\Psi)(E)=(2E)^{-1/4}(\hat{\Psi}(\sqrt{2E}),\hat{\Psi}(-\sqrt{2E})),\quad E>0 \tag{2.4}$$

where $\hat{\Psi}$ denotes the Fourier transform (momentum representation) of Ψ. Correspondingly,

$$\begin{aligned}(U^{-1}(\Phi_1,\Phi_2))(x)&=(2\pi)^{-1/2}\left[\int_0^{\infty}dk\,\sqrt{k}\,\exp(ikx)\Phi_1(k^2/2)+\int_{-\infty}^0 dk\sqrt{-k}\,\exp(ikx)\Phi_2(k^2/2)\right]\\&=\int_0^{\infty}dE\,\varepsilon_{1E}(x)\Phi_1(E)+\int_0^{\infty}dE\,\varepsilon_{2E}(x)\Phi_2(E)\ ,\end{aligned} \tag{2.5}$$

where

$$\begin{aligned}\varepsilon_{1E}(x)&=(2\pi)^{-1/2}(2E)^{-1/4}\exp(ix\sqrt{2E})\ ,\\ \varepsilon_{2E}(x)&=(2\pi)^{-1/2}(2E)^{-1/4}\exp(-ix\sqrt{2E})\end{aligned} \tag{2.6}$$

are the two linearly independent continuous-spectrum eigenfunctions of the free Hamiltonian, normalized so that

$$\int_{-\infty}^{\infty}dx\,\varepsilon_{iE}^*(x)\varepsilon_{jE'}(x)=\delta_{ij}\delta(E-E')\ . \tag{2.7}$$

In the above energy representation, the free Hamiltonian acts simply as multiplication by E. The momentum operator p takes the form

$$(p(\Phi_1,\Phi_2))(E)=\sqrt{2E}\,(\Phi_1(E),\ -\Phi_2(E))\ . \tag{2.8}$$

The scattering operator S, as an operator commuting with H_0, acts on the energy representation wave function (Φ_1,Φ_2) as follows:

$$(S(\Phi_1,\Phi_2))(E)=(S_{11}(E)\Phi_1(E)+S_{12}(E)\Phi_2(E),\ S_{21}(E)\Phi_1(E)+S_{22}(E)\Phi_2(E))\ , \tag{2.9}$$

where for each $E>0$, $S_{ij}(E)$ is a two-dimensional unitary matrix. We will assume that the functions $S_{ij}(E)$ are sufficiently smooth functions of E.

The state vectors of the form $(\Phi_1,0),(0,\Phi_2)\in L^2((0,\infty),\mathbb{C}^2)$ describe states (wave packets) with positive and negative momentum, respectively, cf. (2.5) and (2.6). If the actual state of the system at time $t=0$ has an in-asymptote of the form (in the energy representation) $\Psi^-=(\Phi_1,0)$, then this means that the particle (wave packet) approaches the potential barrier from the left before colliding with it. Long after the collision, the time evolution is essentially the free time evolution determined by the asymptotic out state Ψ^+,

$$\Psi^+(E)=(S_{11}(E)\Phi_1(E),\ S_{21}(E)\Phi_1(E))\ . \tag{2.10}$$

This is a superposition of states corresponding to the particle moving to the right and to the left, i.e., corresponding to the transmitted and reflected particle, respectively. The probabilities of transmission and reflection are

$$\int_0^\infty dE\ |S_{11}(E)|^2\,|\Phi_1(E)|^2 \tag{2.11}$$

and

$$\int_0^\infty dE\ |S_{21}(E)|^2\,|\Phi_1(E)|^2\ , \tag{2.12}$$

respectively (for $\int_0^\infty dE\ |\Phi_1(E)|^2=1$).

The stationary scattering states are solutions of the differential equations

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right]\varepsilon'_E(x)=E\varepsilon'_E(x)\ , \tag{2.13}$$

where $E>0$. Since our potential has finite range R_0, we have

$$\varepsilon'_E(x)=\begin{cases}A\exp(i\sqrt{2E}x)+B\exp(-i\sqrt{2E}x) & \text{for } x\le -R_0 \quad (2.14)\\ C\exp(i\sqrt{2E}x)+D\exp(-i\sqrt{2E}x) & \text{for } x\ge R_0\ . \quad (2.15)\end{cases}$$

The coefficients A,B,C,D are related by the matrix $S(E)=[S_{ij}(E)]$:

$$\begin{bmatrix}C\\B\end{bmatrix}=S(E)\begin{bmatrix}A\\D\end{bmatrix}\ . \tag{2.16}$$

For each $E>0$ two linearly independent solutions $\tilde{\varepsilon}_{1E}$ and $\tilde{\varepsilon}_{2E}$ of (2.13) can be chosen so that $\tilde{\varepsilon}_{iE}=\Omega_+\varepsilon_{iE}$, or more correctly, so that

$$\int_0^\infty dE\ \varepsilon_{1E}(x)\Phi_1(E)+\int_0^\infty dE\ \varepsilon_{2E}(x)\Phi_2(E) \xrightarrow{\Omega_+} \int_0^\infty dE\,\tilde{\varepsilon}_{1E}(x)\Phi_1(E)+\int_0^\infty dE\,\tilde{\varepsilon}_{2E}(x)\Phi_2(E)\ . \tag{2.17}$$

$\tilde{\varepsilon}_{1E}$ and $\tilde{\varepsilon}_{2E}$ are normalized in the same way as ε_{1E} and ε_{2E}, cf. (2.7). Asymptotically,

$$\tilde{\varepsilon}_{1E}(x)=\begin{cases}\varepsilon_{1E}(x)+S_{21}(E)\varepsilon_{2E}(x) & \text{for } x\le -R_0 \quad (2.18)\\ S_{11}(E)\varepsilon_{1E}(x) & \text{for } x\ge R_0\ , \quad (2.19)\end{cases}$$

$$\tilde{\varepsilon}_{2E}(x)=\begin{cases}S_{22}(E)\varepsilon_{2E}(x) & \text{for } x\le -R_0 \quad (2.20)\\ \varepsilon_{2E}(x)+S_{12}(E)\varepsilon_{1E}(x) & \text{for } x\ge R_0\ . \quad (2.21)\end{cases}$$

Equation (2.17) means that each scattering state can be expanded in a continuous superposition of $\tilde{\varepsilon}_{1E}$ and $\tilde{\varepsilon}_{2E}$. The two orthogonal components

$$\int_0^\infty dE\,\tilde{\varepsilon}_{1E}(x)\Phi_1(E)$$

and

$$\int_0^\infty dE\,\tilde{\varepsilon}_{2E}(x)\Phi_2(E)$$

correspond to the particle approaching the barrier from the left and from the right, respectively.

III. THE CONCEPT OF THE TIME DELAY

Imagine an experiment in which a source of particles is located (e.g.) on the left of our potential barrier in the region where the influence of the potential is negligible. For simplicity, let the source be ideal in that each particle leaving it is in the same pure quantum state. The beam of particles directed towards the barrier is partly reflected and partly transmitted. The intensities of the transmitted and reflected beams are proportional to the transmission and reflection probabilities (2.11) and (2.12), respectively. These probabilities provide the basic "stationary" description of the experiment.

One can also be interested in some temporal correlations present in the experiment. We can imagine that the source of particles is equipped with a shutter controlled by the observer, and that during the time interval (t',t'') when the shutter is kept open only one particle emerges. The instant t' or t'' provides the observer with a reference time, a "departure" time. The particle after colliding with the barrier is picked up by detectors located at points a and b ($a<b$) on opposite sides of the barrier in the region where the potential is negligible. We measure the arrival times of the particle at a (reflection) or at b (transmission). Repeating the experiment many times, each time we come out with a transit time for the particle defined as the difference between the arrival time and the departure time. Finally, we can calculate mean transit times: τ_{tr} for transmitted particles and τ_r for reflected ones. When we perform the same experiment without the presence of the barrier, i.e., for free particles, we obtain a mean free transit time τ_f. Note that in the latter experiment all the particles are picked up by detector b. The differences

$$\Delta\tau_{\text{tr}}=\tau_{\text{tr}}-\tau_f,\quad \Delta\tau_r=\tau_r-\tau_f \tag{3.1}$$

define the (experimental) transmission time delay and the reflection time delay, respectively. When P_{tr} denotes the transmission probability and P_r the reflection probability, $P_{\text{tr}}+P_r=1$, then the weighted sum

$$\Delta\tau=P_{\text{tr}}\,\Delta\tau_{\text{tr}}+P_r\,\Delta\tau_r=(P_{\text{tr}}\tau_{\text{tr}}+P_r\tau_r)-\tau_f \tag{3.2}$$

gives us the mean total time delay for particles incident from the left of the barrier—a global quantity which does not distinguish between the case of transmisson and reflection (note that $P_{\text{tr}}\tau_{\text{tr}}+P_r\tau_r$ is just the mean transit time from the source to the detectors a,b treated as a single detecting device).

The quantities $\Delta\tau_{\rm tr}, \Delta\tau_r, \Delta\tau$ are free from inevitable ambiguities present in the definition of the departure time (these ambiguities cancel out in the process of subtraction). However, $\Delta\tau_{\rm tr}, \Delta\tau_r, \Delta\tau$ do, in general, depend on the positions of the detectors. We will come back to this point after deriving theoretical expressions for our time delays.

IV. THE TOTAL TIME DELAY

The mean sojourn time of our particle in a spatial interval (a,b) during a time interval (t_1,t_2) reads

$$\tau((a,b),t_1,t_2;\Psi)=\int_{t_1}^{t_2}dt\int_a^b dx\ |\Psi_t(x)|^2\ , \tag{4.1}$$

where $\Psi_t=\exp(-itH)\Psi$. The corresponding quantity for the freely evolving particle will be denoted by $\tau_0((a,b),t_1,t_2;\Psi)$, i.e.,

$$\tau_0((a,b),t_1,t_2;\Psi)=\int_{t_1}^{t_2}dt\int_a^b dx\ |\Psi_{0t}(x)|^2\ , \tag{4.2}$$

where $\Psi_{0t}=\exp(-itH_0)\Psi$. In (4.1) and (4.2), $-\infty\le a<b\le\infty$, $-\infty\le t_1<t_2\le\infty$, and the sojourn times can be, in general, infinite. When $t_1=-\infty$, $t_2=\infty$, we speak about the mean total sojourn times.

In the following, Ψ will always denote the state vector at time $t=0$ of our particle interacting with the potential barrier. Ψ^- will be the corresponding in-asymptote, i.e., $\Omega_+\Psi^-=\Psi$. We shall write (Φ_1,Φ_2) for the energy representation of Ψ^-, i.e., $\Psi^-=U^{-1}(\Phi_1,\Phi_2)$, cf. (2.5).

In analogy with two-body scattering[10] the definition of the total time delay goes as follows. We take a long interval (a,b) containing the barrier and compare the sojourn time $\tau((a,b),-\infty,\infty;\Psi)$ of our particle in (a,b) with the corresponding sojourn time $\tau_0((a,b),-\infty,\infty;\Psi^-)$ of the free particle. The difference

$$\Delta\tau_{a,b}(\Psi)=\tau((a,b,),-\infty,\infty;\Psi)-\tau_0((a,b),-\infty,\infty;\Psi^-) \tag{4.3}$$

is the mean excess time spent by our particle in (a,b) while interacting with the barrier; it is the time delay and depends on the interval (a,b). In terms of the *gedanken* experiment described in Sec. III, $\Delta\tau_{a,b}(\Psi)$ pertains to the arrangement with detectors placed at a and b.

In the analogous two-body problem a sphere of radius R and center coinciding with the center of mass of the colliding objects plays the role of the interval (a,b). The limit $R\to\infty$ is eventually taken to eliminate the R dependence of the time delay. This limit procedure seems to be natural and goes without further comment in theoretical treatments. However, for a one-dimensional potential barrier, especially when it is not symmetric, it is not clear how to choose an analogous-limit procedure. One can of course take $a=-r$, $b=r$, $r\to\infty$, but more generally one can also choose $a=-r+c$, $b=r+c$, $r\to\infty$, where c is an arbitrary constant. As we will see below, for each c the limit $\lim_{r\to\infty}\Delta\tau_{c-r,c+r}(\Psi)$ exists and depends in a definite way on c. This indicates that the time delay cannot be unambiguously defined by means of a $r\to\infty$ limit without some convention regarding the definition of a center of the barrier. This problem seems to have been overlooked so far.

In Appendix A we derive asymptotic expressions (A7) and (A15) for $\tau_0((a,b),-\infty,\infty;\Psi)$ and $\tau((a,b),-\infty,\infty;\Psi)$ as $a\to-\infty$, $b\to\infty$. Substituting them into (4.3) one obtains, after some simple algebra,

$$\begin{aligned}\Delta\tau_{a,b}(\Psi)=&\int_0^\infty dE(2E)^{-1/2}\{b[\,|S_{11}(E)\Phi_1(E)+S_{12}(E)\Phi_2(E)|^2-|\Phi_1(E)|^2]\\&\qquad-a[\,|S_{21}(E)\Phi_1(E)+S_{22}(E)\Phi_2(E)|^2-|\Phi_2(E)|^2]\}\\&+\int_0^\infty dE\sum_{i,j=1}\Phi_i^*(E)Q_{ij}(E)\Phi_j(E)\ ,\end{aligned} \tag{4.4}$$

where $Q(E)=-iS^\dagger(E)[\partial S(E)/\partial E]$, or

$$Q_{ij}(E)=-i\sum_{k=1}^{z}S_{ki}^*(E)\frac{\partial S_{kj}(E)}{\partial E}\ , \tag{4.5}$$

is the lifetime matrix $Q(E)$ first introduced by Smith[20] in the general context of multichannel scattering.

It can be seen that $\Delta\tau_{a,b}(\Psi)$ is explicitly dependent on a and b. Substituting $a=c-r$, $b=c+r$, and taking the (now trivial) limit $r\to\infty$ yields the c-dependent quantity

$$\begin{aligned}\Delta\tau_c(\Psi)=c\int_0^\infty dE(2E)^{-1/2}[\,&|S_{11}(E)\Phi_1(E)+S_{12}(E)\Phi_2(E)|^2-|\Phi_1(E)|^2\\&-|S_{21}(E)\Phi_1(E)+S_{22}(E)\Phi_2(E)|^2+|\Phi_2(E)|^2]+\int_0^\infty dE\sum_{i,j=1}^{2}\Phi_i^*(E)Q_{ij}(E)\Phi_j(E)\ .\end{aligned} \tag{4.6}$$

If the potential barrier were symmetric with respect to a certain point α, then it would seem natural to choose the origin of the coordinate system at α and choose $c=0$. In that case one is left only with the term involving the Q matrix and recovers the traditionally accepted expression for the total time delay. However, when the potential has no symmetry then there does not exist any natural choice of either the origin of the x axis or of the point c.[21]

V. THE TRANSMISSION AND REFLECTION TIME DELAYS

The concepts of transmission and reflection time delays are meaningful only when in the remote past the particle approaches the barrier either from the left or from the right, i.e., when the actual state Ψ at time $t=0$ has an in-asymptote of the form $\Psi^-=U^{-1}(\Phi_1,0)$ or $\Psi^-=U^{-1}(0,\Phi_2)$, cf. (2.5). Without any loss of generality we treat here only the case of the particle approaching the barrier from the left, i.e., $\Psi^-=U^{-1}(\Phi_1,0)$.

The sojourn time $\tau((a,b),t_1,t_2;\Psi)$ does not distinguish between transmission and reflection. Consider, however, the sojourn time

$$\tau((b,\infty),t_1,t_2;\Psi)=\int_{t_1}^{t_2}dt\int_b^\infty dx\ |\Psi_t(x)|^2 . \quad (5.1)$$

We assume b to be very large, $b\to\infty$. Since the particle approaches the barrier from the left, it can be present in (b,∞) only as the transmitted particle. Therefore, $P_{\text{tr}}^{-1}(\Psi)\tau((b,\infty),t_1,t_2;\Psi)$, with $P_{\text{tr}}(\Psi)$ being the transmission probability (2.11), can be interpreted as the mean time spent by the transmitted particle in the region (b,∞) during the time interval (t_1,t_2). When $t_1\to-\infty$, $t_2\to\infty$, we expect $\tau((b,\infty),t_1,t_2;\Psi)$ to have the asymptotics

$$P_{\text{tr}}^{-1}(\Psi)\tau((b,\infty),t_1,t_2;\Psi)\approx t_2-\gamma_b(\Psi) . \quad (5.2)$$

Classically one would interpret the constant term $\gamma_b(\Psi)$ as the mean arrival time at b of the transmitted particles.

Consider also the corresponding free sojourn time

$$\tau_0((b,\infty),t_1,t_2;\Psi^-)=\int_{t_1}^{t_2}dt\int_b^\infty dx\ |\Psi_{0t}^-(x)|^2 . \quad (5.3)$$

We expect that

$$\tau_0((b,\infty),t_1,t_2;\Psi^-)\approx t_2-\gamma_{0b}(\Psi^-) , \quad (5.4)$$

as $t_1\to-\infty$, $t_2\to\infty$. The asymptotic expressions (5.2) and (5.4) do indeed hold true as is shown in Appendix A, cf. (A9) and (A18). Therefore the limit

$$\Delta\tau_{\text{tr},b}(\Psi)=\lim_{\substack{t_1\to-\infty\\ t_2\to\infty}}\tau_0((b,\infty),t_1,t_2;\Psi^-)-P_{\text{tr}}^{-1}(\Psi)\tau((b,\infty),t_1,t_2;\Psi) \quad (5.5)$$

exists and can be interpreted as the difference between the mean arrival times at b of the transmitted and the free (reference) particles. We take it as the theoretical definition of the transmission time delay.

For $b\to\infty$, $\Delta\tau_{\text{tr},b}(\Psi)$ can be effectively evaluated via the asymptotics (A9) and (A18). One then obtains

$$\begin{aligned}\Delta\tau_{\text{tr},b}(\Psi)\approx{}& b\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2\left[\frac{|S_{11}(E)|^2}{P_{\text{tr}}(\Psi)}-1\right]\\&+\int_0^\infty dE\,\Phi_1^*(E)\left[-i\frac{\partial\Phi_1(E)}{\partial E}\right]\left[\frac{|S_{11}(E)|^2}{P_{\text{tr}}(\Psi)}-1\right]+P_{\text{tr}}^{-1}(\Psi)\int_0^\infty dE\ |\Phi_1(E)|^2S_{11}^*(E)\left[-i\frac{\partial S_{11}(E)}{\partial E}\right]\\&=b\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2\left[\frac{|S_{11}(E)|^2}{P_{\text{tr}}(\Psi)}-1\right]+\int_0^\infty dE\ |\Phi_1(E)|^2\frac{\partial\varphi_1(E)}{\partial E}\left[\frac{|S_{11}(E)|^2}{P_{\text{tr}}(\Psi)}-1\right]\\&+P_{\text{tr}}^{-1}(\Psi)\int_0^\infty dE\,|S_{11}(E)\Phi_1(E)|^2\,\text{Re}\left[-iS_{11}^{-1}(E)\frac{\partial S_{11}(E)}{\partial E}\right]\quad\text{as } b\to\infty ,\end{aligned} \quad (5.6)$$

where all terms on the right-hand side are real. Here by $\varphi_1(E)$ we denote the phase of $\Phi_1(E)$, i.e., $\Phi_1(E)=|\Phi_1(E)|\exp[i\varphi_1(E)]$.

Theoretical transmission and reflection time delays should satisfy Eq. (3.2) with P_{tr} and P_r given by (2.11) and (2.12), respectively. Therefore, the reflection time delay $\Delta\tau_{r,a,b}(\Psi)$ can now be found by using our formulas for $\Delta\tau_{a,b}(\Psi)$ and $\Delta\tau_{\text{tr},b}(\Psi)$, and unitarity of the S matrix. The result is

$$\Delta\tau_{r,a,b}(\Psi)\approx -a\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2\frac{|S_{21}(E)|^2}{P_r(\Psi)}-b\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2$$
$$+\int_0^\infty dE\,\Phi_1^*(E)\left[-i\frac{\partial\Phi_1(E)}{\partial E}\right]\left[\frac{|S_{21}(E)|^2}{P_r(\Psi)}-1\right]+P_r^{-1}(\Psi)\int_0^\infty dE\,|\Phi_1(E)|^2S_{21}^*(E)\left[-i\frac{\partial S_{21}(E)}{\partial E}\right]$$
$$=-aP_r^{-1}(\Psi)\int_0^\infty dE(2E)^{-1/2}|S_{21}(E)\Phi_1(E)|^2-b\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2$$
$$+\int_0^\infty dE\,|\Phi_1(E)|^2\frac{\partial\varphi_1(E)}{\partial E}\left[\frac{|S_{21}(E)|^2}{P_r(\Psi)}-1\right]$$
$$+P_r^{-1}(\Psi)\int_0^\infty dE\,|S_{21}(E)\Phi_1(E)|^2\,\mathrm{Re}\left[-iS_{21}^{-1}(E)\frac{\partial S_{21}(E)}{\partial E}\right]\quad\text{as } a\to-\infty \text{ and } b\to\infty\,, \tag{5.7}$$

where $P_r(\Psi)$ is the reflection probability (2.12).

VI. DISCUSSION

Using the concept of sojourn time we have derived theoretical expressions for the transmission time delay, the reflection time delay, and the total time delay as measured in the *gedanken* experiment of Sec. III. These expressions exhibit a simple linear dependence on the parameters a and b which can be interpreted as describing positions of the detectors. According to (5.6), (5.7), and (4.4) (with $I_2=0$—the particle incident from the left), we have

$$\Delta\tau_{\mathrm{tr},b+\beta}(\Psi)-\Delta\tau_{\mathrm{tr},b}(\Psi)\approx\beta\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2\left[\frac{|S_{11}(E)|^2}{P_{\mathrm{tr}}(\Psi)}-1\right]\quad\text{as } b\to\infty\,, \tag{6.1}$$

$$\Delta\tau_{r,a,b+\beta}(\Psi)-\Delta\tau_{r,a,b}(\Psi)\approx-\beta\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2\quad\text{as } a\to-\infty \text{ and } b\to\infty\,, \tag{6.2}$$

$$\Delta\tau_{a,b+\beta}(\Psi)-\Delta\tau_{a,b}(\Psi)\approx\beta\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)|^2[|S_{11}(E)|^2-1]\quad\text{as } a\to-\infty \text{ and } b\to\infty\,, \tag{6.3}$$

$$\Delta\tau_{r,a+\alpha,b}(\Psi)-\Delta\tau_{r,a,b}(\Psi)\approx-\alpha P_r^{-1}(\Psi)\int_0^\infty dE(2E)^{-1/2}|S_{21}(E)\Phi_1(E)|^2\quad\text{as } a\to-\infty \text{ and } b\to\infty\,, \tag{6.4}$$

$$\Delta\tau_{a+\alpha,b}(\Psi)-\Delta\tau_{a,b}(\Psi)\approx-\alpha\int_0^\infty dE(2E)^{-1/2}|S_{21}(E)\Phi_1(E)|^2\quad\text{as } a\to-\infty \text{ and } b\to\infty\,. \tag{6.5}$$

Note that $(2E)^{1/2}$ is the velocity outside the barrier, and that $|\Phi_1(E)|^2$, $P_{\mathrm{tr}}^{-1}(\Psi)|S_{11}(E)\Phi_1(E)|^2$, and $P_r^{-1}(\Psi)|S_{21}(E)\Phi_1(E)|^2$ are the energy distributions for the incoming, the transmitted, and the reflected particles, respectively. Therefore Eqs. (6.1)–(6.5) are what one would expect upon shifting detectors in our *gedanken* experiment. A shift in b changes the mean transit time (from the source to the detector) of the free (reference) particles by the amount

$$\beta\int_0^\infty dE\,(2E)^{-1/2}|\Phi_1(E)|^2\,,$$

and the transit time for transmitted particles by the amount

$$\beta P_{\mathrm{tr}}^{-1}(\Psi)\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)S_{11}(E)|^2\,.$$

The transit time for the reflected particles (detected at a) remains unaltered. This clearly yields (6.1) and (6.2); (6.3) then follows from (3.2). Analogously, a shift in a affects only the transit time for the reflected particles, the result being (6.4) and (6.5).

It is to be noted that the above dependence of the time delays on a and b follows from the choice of Ψ^- as our reference wave packet. Theoretically speaking there is nothing in our method which precludes any other choice. However, the same reference wave packet should be used to define all three of the time delays if Eq. (3.2) is to remain valid. This is consistent with our *gedanken*-experiment measurements, indicating that the choice of Ψ^- is the most natural one.

Expressions (4.4), (5.6), and (5.7) greatly simplify in the limit of wave packets with well-defined momentum, i.e., when $\Phi_1(E)$ vanishes outside a narrow interval $(E_0,E_0+\delta)$. Then, approximately

$$\Delta\tau_{\mathrm{tr},b}(\Psi)\approx\mathrm{Re}\left[-iS_{11}^{-1}(E_0)\frac{\partial S_{11}(E_0)}{\partial E}\right], \tag{6.6}$$

$$\Delta\tau_{r,a,b}(\Psi)\approx-(a+b)(2E_0)^{-1/2}+\mathrm{Re}\left[-iS_{21}^{-1}(E_0)\frac{\partial S_{21}(E_0)}{\partial E}\right], \tag{6.7}$$

$$\Delta\tau_{a,b}(\Psi)\approx-(a+b)|S_{21}(E_0)|^2(2E_0)^{-1/2}+Q_{11}(E_0)\,. \tag{6.8}$$

Equation (6.6) agrees with the Eisenbud definition of the "state-to-state" time delay.[20,22] The dependence of

$\Delta\tau_{\mathrm{tr},b}(\Psi)$ on b disappears since in the limit of well-defined momentum the transmitted and the incoming wave packets become indistinguishable. This is, however, not the case with $\Delta\tau_{r,a,b}(\Psi)$ and $\Delta\tau_{a,b}(\Psi)$. That they must remain dependent on a and b agrees with (6.2)–(6.5).

The dependence of the total time delay on a and b results in the impossibility of defining an absolute time delay which is independent of the choice of a "center" of the barrier.[23] We have discussed this point in Sec. IV.

Consider now the effect of a spatial shift of the barrier on our time delays. A shift ξ changes the potential from $V(x)$ to $V_\xi(x)=V(x-\xi)$, i.e.,

$$V_\xi=\exp(-i\xi p)V\exp(i\xi p)\ ,$$

where p is the momentum operator. Since

$$\exp(-i\xi p)H_0\exp(i\xi p)=H_0\ ,$$

we can write

$$H\to H_\xi=\exp(-i\xi p)H\exp(i\xi p)\ .$$

It follows from the definition of the S operator, cf. Sec. II, that

$$S\to S_\xi=\exp(-i\xi p)S\exp(i\xi p)\ .$$

In our energy representation the translation operator $\exp(i\xi p)$ has the matrix

$$\begin{bmatrix}\exp(i\xi\sqrt{2E}\,) & 0\\ 0 & \exp(-i\xi\sqrt{2E}\,)\end{bmatrix}. \qquad (6.9)$$

Hence, S_ξ has the matrix

$$\begin{bmatrix}S_{11}(E) & S_{12}(E)\exp(-i2\xi\sqrt{2E}\,)\\ S_{21}(E)\exp(i2\xi\sqrt{2E}\,) & S_{22}(E)\end{bmatrix}. \qquad (6.10)$$

Using Eqs. (5.6), (5.7), and (4.4) (with $\Phi_2=0$) we can now easily show that the time delays are affected by the shift as follows:

$$\Delta\tau_{\mathrm{tr},b}(\Psi)\to\Delta\tau_{\mathrm{tr},b}(\Psi)\ , \qquad (6.11)$$

$$\Delta\tau_{r,a,b}(\Psi)\to\Delta\tau_{r,a,b}(\Psi)+2\xi P_r^{-1}(\Psi)\int_0^\infty dE(2E)^{-1/2}\times|S_{21}(E)\Phi_1(E)|^2\ , \qquad (6.12)$$

$$\Delta\tau_{a,b}(\Psi)\to\Delta\tau_{a,b}(\Psi)+2\xi\int_0^\infty dE(2E)^{-1/2}\times|S_{21}(E)\Phi_1(E)|^2\ . \qquad (6.13)$$

[The shift ξ to which Eqs. (6.11)–(6.13) refer cannot be arbitrarily large. One should have $|\xi|\ll b-a$, because formulas (5.6), (5.7), and (4.4) are not exact but asymptotic formulas for the time delays as $a\to-\infty$, $b\to\infty$.] The results are, in fact, not quite trivial. In terms of our *gedanken* experiment (6.11) implies that the mean transit time (from the source to detector b) of the transmitted particles is independent of the location of the barrier. On the other hand, the mean transit time (from the source to detector a) of the reflected particles is, according to (6.12), changed by twice the mean time free particles with energy distribution $P_r^{-1}(\Psi)|S_{21}(E)\Phi_1(E)|^2$ need to travel the distance ξ. Classically that would suggest that the energy distribution of the transmitted or reflected particles is the same before and after the collision with the barrier. The point is that quantum mechanically there is no sense in speaking about transmitted or reflected particles before they are detected as such. Let us also note that the results (6.11)–(6.13) favor the ensemble interpretation of the wave function against the single-particle interpretation. If one assumes that the wave function describes a single particle, then the energy distribution before the collision is $|\Phi_1(E)|^2$ and after the collision,

$$P_{\mathrm{tr}}^{-1}(\Psi)|S_{11}(E)\Phi_1(E)|^2$$

when the particle is transmitted and

$$P_r^{-1}(\Psi)|S_{21}(E)\Phi_1(E)|^2$$

when it is reflected. This makes it difficult to understand the factor 2 in (6.12) or the invariance in (6.11). The above considerations indicate that the study of separate time delays for transmission and reflection is a nontrivial problem deeply rooted in the foundations of quantum theory and its interpretation.

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APPENDIX A: CALCULATION OF THE SOJOURN TIMES

1. The free sojourn time

Integration by parts applied to (4.2) yields

$$\tau_0((a,b),t_1,t_2;\Psi)=\int_{t_1}^{t_2}dt\,\frac{dt}{dt}\int_a^b dx\,|\Psi_{0t}(x)|^2=t\int_a^b dx\,|\Psi_{0t}(x)|^2\Big|_{t_1}^{t_2}-\int_{t_1}^{t_2}dt\,t\frac{d}{dt}\int_a^b dx\,|\Psi_{0t}(x)|^2$$
$$=t\int_a^b dx\,|\Psi_{0t}(x)|^2\Big|_{t_1}^{t_2}+\int_{t_1}^{t_2}dt\,t[J(b,\Psi_{0t})-J(a,\Psi_{0t})]\ , \qquad (A1)$$

where $J(x,\Psi_{0t})$ is the usual probability current,

$$J(x,\Psi_{0t})=(2i)^{-1}\left[\Psi_{0t}^*(x)\frac{\partial\Psi_{0t}(x)}{\partial x}-\Psi_{0t}(x)\frac{\partial\Psi_{0t}^*(x)}{\partial x}\right]. \tag{A2}$$

For $t_1\rightarrow-\infty$, $t_2\rightarrow\infty$ one can derive simple asymptotic expressions for $\tau_0((a,b),t_1,t_2;\Psi)$ in terms of the energy representation wave function (Φ_1,Φ_2), i.e., $\Psi=U^{-1}(\Phi_1,\Phi_2)$, cf. (2.5). Strictly speaking, our derivation is mathematically legitimate only for sufficiently well-behaved wave functions, e.g., when $\Phi_1,\Phi_2\in C_0^\infty((0,\infty))$ (infinitely differentiable with compact support). It rests upon some properties of the one-dimensional free motion which we find convenient to list and justify separately in Appendix B.

The first term on the right-hand side of (A1) can be evaluated using one of the formulas (B6)–(B10) of Appendix B. The asymptotics of the second will involve convergent integrals

$$\int_{-\infty}^{\infty} dt\, tJ(x,\Psi_{0t})$$

[cf. (B19) and (B20) of Appendix B]. They can be dealt with as follows. If $x=\pm\infty$, then $J(x,\Psi_{0t})=0$ [by (B19) and (B20)]. If $|x|<\infty$, then by (2.5):

$$J(x,\Psi_{0t})=(2\pi)^{-1}\,\mathrm{Re}\left[\int_0^\infty dE\exp(-itE)(2E)^{-1/4}[\Phi_{1x}(E)+\Phi_{2x}(E)]\right]^*\times\left[\int_0^\infty dE\exp(-itE)(2E)^{1/4}[\Phi_{1x}(E)-\Phi_{2x}(E)]\right], \tag{A3}$$

where we use the abbreviations

$$\Phi_{1x}(E)=\Phi_1(E)\exp(ix\sqrt{2E}),\quad \Phi_{2x}(E)=\Phi_2(E)\exp(-ix\sqrt{2E}). \tag{A4}$$

Then, by integrating by parts the second factor in (A3) we obtain

$$tJ(x,\Psi_{0t})=(2\pi)^{-1}\mathrm{Re}\left[\int_0^\infty dE\exp(-itE)(2E)^{-1/4}[\Phi_{1x}(E)+\Phi_{2x}(E)]\right]^*\times\left[\int_0^\infty dE\exp(-itE)(2E)^{1/4}\left[-i\frac{\partial\Phi_{1x}(E)}{\partial E}+i\frac{\partial\Phi_{2x}(E)}{\partial E}\right]-i2^{-7/4}\int_0^\infty dE\exp(-itE)E^{-3/4}[\Phi_{1x}(E)-\Phi_{2x}(E)]\right]. \tag{A5}$$

Finally, unitarity of the Fourier transform yields

$$\begin{aligned}\int_{-\infty}^{\infty} dt\, tJ(x,\Psi_{0t})&=\mathrm{Re}\left[\int_0^\infty dE[\Phi_{1x}(E)+\Phi_{2x}(E)]^*\left[-i\frac{\partial\Phi_{1x}(E)}{\partial E}+i\frac{\partial\Phi_{2x}(E)}{\partial E}\right]\right]\\&\quad-\mathrm{Re}\left[i\int_0^\infty dE[\Phi_{1x}(E)+\Phi_{2x}(E)]^*(4E)^{-1}[\Phi_{1x}(E)-\Phi_{2x}(E)]\right]\\&=\int_0^\infty dE\left[\Phi_1^*(E)\left[-i\frac{\partial\Phi_1(E)}{\partial E}\right]+\Phi_2^*(E)\left[i\frac{\partial\Phi_2(E)}{\partial E}\right]\right]\\&\quad+x\int_0^\infty dE(2E)^{-1/2}[|\Phi_1(E)|^2+|\Phi_2(E)|^2]\\&\quad+\mathrm{Re}\left[i\int_0^\infty dE(4E)^{-1}\Phi_1(E)^*\Phi_2(E)\exp(-2ix\sqrt{2E})\right].\end{aligned} \tag{A6}$$

We can now see that for $-\infty<a<b<\infty$ and our well-behaved wave function Ψ, the mean total sojourn time $\tau_0((a,b),-\infty,\infty;\Psi)$ is finite and reads

$$\begin{aligned}\tau_0((a,b),-\infty,\infty;\Psi)&=(b-a)\int_0^\infty dE(2E)^{-1/2}[|\Phi_1(E)|^2+|\Phi_2(E)|^2]\\&\quad+\mathrm{Re}\left[i\int_0^\infty dE(4E)^{-1}\Phi_1^*(E)\Phi_2(E)[\exp(-2ib\sqrt{2E})-\exp(-2ia\sqrt{2E})]\right].\end{aligned} \tag{A7}$$

Since $\sqrt{2E}$ is the velocity of our particle (the mass $m=1$), the first term is what one expects on classical grounds. The second term disappears whenever the direction of the momentum of the particle is specified (i.e., $\Phi_1=0$ or $\Phi_2=0$). Generally it expresses interference of the components of the wave function describing particles moving in opposite directions. By the Riemann-Lebesgue lemma this term always vanishes in the limit $a\rightarrow-\infty$, $b\rightarrow\infty$.

The asymptotic expressions for $\tau_0((-\infty,a),t_1,t_2;\Psi)$ and $\tau_0((b,\infty),t_1,t_2;\Psi)$ read

$$\tau_0((-\infty,a),t_1,t_2;\Psi)\approx t_2\int_0^\infty dE\ |\Phi_2(E)|^2-t_1\int_0^\infty dE\ |\Phi_1(E)|^2+\int_0^\infty dE\left[-i\Phi_1^*(E)\frac{\partial\Phi_1(E)}{\partial E}+i\Phi_2^*(E)\frac{\partial\Phi_2(E)}{\partial E}\right]$$
$$+a\int_0^\infty dE(2E)^{-1/2}[\,|\Phi_1(E)|^2+|\Phi_2(E)|^2]$$
$$+\mathrm{Re}\left[i\int_0^\infty dE(4E)^{-1}\Phi_1^*(E)\Phi_2(E)\exp(-2ia\sqrt{2E}\,)\right]\quad\text{as } t_1\to-\infty \text{ and } t_2\to\infty\ , \tag{A8}$$

$$\tau_0((b,\infty),t_1,t_2;\Psi)\approx t_2\int_0^\infty dE\,|\Phi_1(E)|^2-t_1\int_0^\infty dE\,|\Phi_2(E)|^2-\int_0^\infty dE\left[-i\Phi_1^*(E)\frac{\partial\Phi_1(E)}{\partial E}+i\Phi_2^*(E)\frac{\partial\Phi_2(E)}{\partial E}\right]$$
$$-b\int_0^\infty dE(2E)^{-1/2}[\,|\Phi_1(E)|^2+|\Phi_2(E)|^2]$$
$$-\mathrm{Re}\left[i\int_0^\infty dE(4E)^{-1}\Phi_1^*(E)\Phi_2(E)\exp(-2ib\sqrt{2E}\,)\right]\quad\text{as } t_1\to-\infty \text{ and } t_2\to\infty\ . \tag{A9}$$

Again, the final terms in (A8) and (A9) can be dropped in the limit $a\to-\infty$, $b\to\infty$.

2. The sojourn time for the interacting particle

To find an asymptotic expression for the sojourn time $\tau((a,b),-\infty,\infty;\Psi)$ $(-\infty<a<b<\infty)$ as $a\to-\infty$, $b\to\infty$ one starts with the analogue of Eq. (A1), i.e.,

$$\tau((a,b),-\infty,\infty;\Psi)=t\int_a^b dx\ |\Psi_t(x)|^2\int_{-\infty}^{\infty}+\int_{-\infty}^{\infty}dt\,t[J(b,\Psi_t)-J(a,\Psi_t)]$$
$$=t\left[1-\int_{-\infty}^{a}dx\ |\Psi_t(x)|^2-\int_b^\infty dx\ |\Psi_t(x)|^2\right]\Bigg|_{-\infty}^{\infty}+\int_{-\infty}^{\infty}dt\ t[J(b,\Psi_t)-J(a,\Psi_t)]\ . \tag{A10}$$

We expand Ψ_t in terms of the continuous-spectrum eigenfunctions $\mathfrak{E}_{1E}$ and $\mathfrak{E}_{2E}$, as in (2.17). (A10) involves $\Psi_t(x)$ only for $x\le a$ and $x\ge b$. Assuming that $a\le -R_0$, $b\ge R_0$ we can use the asymptotic expressions (2.18)–(2.21). This yields

$$\Psi_t(x)=\Psi_{0t}^{(1)}(x)\quad\text{for } x\le a\le -R_0\ , \tag{A11}$$
$$\Psi_t(x)=\Psi_{0t}^{(2)}(x)\quad\text{for } x\ge b\ge R_0\ , \tag{A12}$$

with $\Psi_{0t}^{(1)}=\exp(-itH_0)\Psi^{(1)}$, $\Psi_{0t}^{(2)}=\exp(-itH_0)\Psi^{(2)}$, and

$$\Psi^{(1)}(x)=\int_0^\infty dE\ \Phi_1(E)\varepsilon_{1E}(x)+\int_0^\infty dE[S_{21}(E)\Phi_1(E)+S_{22}(E)\Phi_2(E)]\varepsilon_{2E}(x)\ , \tag{A13}$$
$$\Psi^{(2)}(x)=\int_0^\infty dE[S_{11}(E)\Phi_1(E)+S_{12}(E)\Phi_2(E)]\varepsilon_{1E}(x)+\int_0^\infty dE\ \Phi_2(E)\varepsilon_{2E}(x) \tag{A14}$$

[(Φ_1,Φ_2) is the energy representation of Ψ^-]. Due to (A11) and (A12) we can use Eqs. (B7)–(B10) for the free particle to demonstrate that the first term on the right-hand side of (A10) vanishes. The second one can be easily evaluated using (A6), where the last term can be dropped in the limit $a\to-\infty$, $b\to\infty$. The resulting asymptotic expression for $\tau((a,b),-\infty,\infty;\Psi)$ reads

$$\tau((a,b),-\infty,\infty;\Psi)=-a\int_0^\infty dE(2E)^{-1/2}[\,|\Phi_1(E)|^2+|S_{21}(E)\Phi_1(E)+S_{22}(E)\Phi_2(E)|^2]$$
$$+b\int_0^\infty dE(2E)^{-1/2}[\,|\Phi_2(E)|^2+|S_{11}(E)\Phi_1(E)+S_{12}(E)\Phi_2(E)|^2]$$
$$+\int_0^\infty dE\sum_{i,j=1}^{2}\Phi_i^*(E)Q_{ij}(E)\Phi_j(E)\quad\text{as } a\to-\infty \text{ and } b\to\infty\ , \tag{A15}$$

where $Q(E)=-iS^\dagger(E)[\partial S(E)/\partial E]$ or

$$Q_{ij}(E)=-i\sum_{k=1}^{2}S_{ki}^*(E)\frac{\partial S_{kj}(E)}{\partial E}\ . \tag{A16}$$

The sojourn time $\tau((b,\infty),t_1,t_2;\Psi)$ can be treated in a similar fashion. Here we assume that $\Psi^-=U^{-1}(\Phi_1,0)$, since this is enough for our treatment of the transmission time delay in Sec. V. In place of Eq. (A10) we now have

$$\tau((b,\infty),t_1,t_2;\Psi)=t\int_b^\infty dx\ |\Psi_t(x)|^2\Big|_{t_1}^{t_2}-\int_{t_1}^{t_2}dt\ tJ(b,\Psi_t)\ . \tag{A17}$$

When $b \geq R_0$, we can use the asymptotic expressions (A12) and (A14) (with $\Phi_2=0$). Then (B9), (B10), and (A6) yield

$$\tau((b,\infty),t_1,t_2;\Psi)\approx t_2 P_{\rm tr}(\Psi)-\int_0^\infty dE\ |S_{11}(E)|^2\Phi_1^*(E)\left[-i\frac{\partial\Phi_1(E)}{\partial E}\right]$$
$$-b\int_0^\infty dE(2E)^{-1/2}|\Phi_1(E)S_{11}(E)|^2-\int_0^\infty dE\ |\Phi_1(E)|^2 S_{11}^*(E)\left[-i\frac{\partial S_{11}(E)}{\partial E}\right]$$
$$\text{as } t_1\to-\infty,\ t_2\to\infty,\text{ and } b\geq R_0\ , \quad \text{(A18)}$$

where $P_{\rm tr}(\Psi)$ is the transmission probability (2.11).

APPENDIX B: SOME PROPERTIES OF THE ONE-DIMENSIONAL FREE MOTION

Let Ψ be an initial state of the free particle and let $\Psi_{0t}=\exp(-itH_0)\Psi$. If (a,b) is a bounded interval, then

$$\lim_{t\to\pm\infty}\int_a^b dx\ |\Psi_{0t}(x)|^2=0\ . \quad \text{(B1)}$$

This is the well-known evanescence of the probability of finding the particle in (a,b). For semibounded intervals $(-\infty,a)$ and (b,∞) we have

$$\lim_{t\to-\infty}\int_{-\infty}^a dx\ |\Psi_{0t}(x)|^2=\int_0^\infty dp\ |\hat\Psi(p)|^2 =\int_0^\infty dE\ |\Phi_1(E)|^2\ , \quad \text{(B2)}$$

$$\lim_{t\to\infty}\int_{-\infty}^a dx\ |\Psi_{0t}(x)|^2=\int_{-\infty}^0 dp\ |\hat\Psi(p)|^2 =\int_0^\infty dE\ |\Phi_2(E)|^2\ , \quad \text{(B3)}$$

$$\lim_{t\to-\infty}\int_b^\infty dx\ |\Psi_{0t}(x)|^2=\int_{-\infty}^0 dp\ |\hat\Psi(p)|^2 =\int_0^\infty dE\ |\Phi_2(E)|^2\ , \quad \text{(B4)}$$

$$\lim_{t\to\infty}\int_b^\infty dx\ |\Psi_{0t}(x)|^2=\int_0^\infty dp\ |\hat\Psi(p)|^2 =\int_0^\infty dE\ |\Phi_1(E)|^2\ , \quad \text{(B5)}$$

where $\hat\Psi$ is the momentum representation of Ψ, and (Φ_1,Φ_2) is the energy representation of Ψ, $\Psi=U^{-1}(\Phi_1,\Phi_2)$, cf. (2.4) and (2.5). The intuitively transparent statements (B1)–(B5) can be easily proved using an asymptotic formula for $\exp(itH_0)$, cf. Ref. 24. However, we will need the stronger version of Eqs. (B1)–(B5):

$$t\int_a^b dx\ |\Psi_{0t}(x)|^2\approx 0 \quad \text{as } |t|\to\infty\ , \quad \text{(B6)}$$

$$t\int_{-\infty}^a dx\ |\Psi_{0t}(x)|^2\approx t\int_0^\infty dE\ |\Phi_1(E)|^2 \quad \text{as } t\to-\infty\ , \quad \text{(B7)}$$

$$t\int_{-\infty}^a dx\ |\Psi_{0t}(x)|^2\approx t\int_0^\infty dE\ |\Phi_2(E)|^2 \quad \text{as } t\to\infty\ , \quad \text{(B8)}$$

$$t\int_b^\infty dx\ |\Psi_{0t}(x)|^2\approx t\int_0^\infty dE\ |\Phi_2(E)|^2 \quad \text{as } t\to-\infty\ , \quad \text{(B9)}$$

$$t\int_b^\infty dx\ |\Psi_{0t}(x)|^2\approx t\int_0^\infty dE\ |\Phi_1(E)|^2 \quad \text{as } t\to\infty\ . \quad \text{(B10)}$$

Here the exact meaning of the symbol $\approx$ is that the difference of the right- and left-hand sides coverges to zero as t approaches $\pm\infty$ as indicated. Relations (B6)–(B10) hold true for sufficiently well-behaved wave functions; in particular, for $\Phi_1,\Phi_2\in C_0^\infty((0,\infty))$ [infinitely differentiable of compact support in $(0,\infty)$]. We proceed to the proof.

The freely evolving wave function Ψ_{0t} can be written in the form

$$\Psi_{0t}(x)=\int_0^\infty dE\exp(-itE)\varepsilon_{1E}(x)\Phi_1(E)+\int_0^\infty dE\exp(-itE)\varepsilon_{2E}(x)\Phi_2(E)$$
$$=(2\pi)^{-1/2}\int_{-\infty}^\infty dk\ \hat\Psi(k)\exp(ikx-itk^2/2)\ . \quad \text{(B11)}$$

We assume that $\Phi_1,\Phi_2\in C_0^\infty((0,\infty))$. Then by (2.4), $\hat\Psi\in C_0^\infty(\mathbb{R}\setminus\{0\})$.

When t and x are such that

$$kt-x\neq 0 \quad \text{(B12)}$$

for all $k\in\operatorname{supp}\hat\Psi$, then one can apply the following integration by parts to the last integral in (B11):

$$\Psi_{0t}(x)=(2\pi)^{-1/2}\int_{-\infty}^\infty dk\ \hat\Psi(k)\frac{i}{kt-x}\frac{d}{dk}\times\exp(ikx-itk^2/2)$$
$$=(2\pi)^{-1/2}\int_{-\infty}^\infty dk\exp(ikx-itk^2/2)(-i)\times\frac{d}{dk}\left[\frac{1}{kt-x}\hat\Psi(k)\right]\ . \quad \text{(B13)}$$

After the nth iteration of this procedure we clearly have

$$\Psi_{0t}(x)=(2\pi)^{-1/2}\int_{-\infty}^\infty dk\exp(ikx-itk^2/2)(-i)^n\times\left[\frac{d}{dk}\circ\frac{1}{kt-x}\right]^n\hat\Psi(k)\ , \quad \text{(B14)}$$

where $(d/dk)\circ[1/(kt-x)]$ is to be understood as the differential operator equal to

$$-\frac{t}{(kt-x)^2}+\frac{1}{kt-x}\frac{d}{dk}\ .$$

It is a matter of straightforward induction to prove that

$$\left[\frac{d}{dk}\circ\frac{1}{kt-x}\right]^n\hat{\Psi}(k)=\sum_{j=n}^{2n}(kt-x)^{-j}\sum_{s=0}^{j-n}t^s f_{sj}(k)\ , \tag{B15}$$

where all the functions f_{sj} are derivatives of various orders of the function $\hat{\Psi}$.

Let (a,b) be a bounded interval. There exists an $\varepsilon>0$ with $(-\varepsilon,\varepsilon)\cap\text{supp}\hat{\Psi}=\varnothing$. Take $T\geq 1$ with $\varepsilon|T|-\max(|a|,|b|)>0$. Then (B12) is satisfied for all $x\in(a,b)$, $|t|\geq T$, and all $k\in\text{supp}\hat{\Psi}$. Substituting (B15) into (B14) we obtain

$$\begin{aligned}|\Psi_{0t}(x)|&\leq(2\pi)^{-1/2}\int_{-\infty}^{\infty}dk\sum_{j=n}^{2n}\sum_{s=0}^{j-n}\frac{|t|^s}{|kt-x|^j}|f_{sj}(k)|\\&\leq(2\pi)^{-1/2}\sum_{j=n}^{2n}\sum_{s=0}^{j-n}\frac{|t|^{j-n}}{[\varepsilon|t|-\max(|a|,|b|)]^j}\int_{-\infty}^{\infty}dk\ |f_{sj}(k)|\end{aligned} \tag{B16}$$

for $|t|\geq T$ and all $x\in(a,b)$. Since n is arbitrary, this implies, in particular, (B6).

The proofs of relations (B7)–(B9) all follow the same pattern. Let us prove (B7), for example. We define

$$\Psi_{10t}(x)=\int_0^{\infty}dE\exp(-itE)\varepsilon_{1E}(x)\Phi_1(E)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}dk\ \hat{\Psi}_1(k)\exp(ikx-itk^2/2)\ , \tag{B17}$$

$$\Psi_{20t}(x)=\int_0^{\infty}dE\exp(-itE)\varepsilon_{2E}(x)\Phi_2(E)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}dk\ \hat{\Psi}_2(k)\exp(ikx-itk^2/2)\ . \tag{B18}$$

Here, $\hat{\Psi}_1\in C_0^{\infty}((0,\infty))$, $\hat{\Psi}_2\in C_0^{\infty}((-\infty,0))$; $\hat{\Psi}=\hat{\Psi}_1+\hat{\Psi}_2$, $\Psi_{0t}=\Psi_{10t}+\Psi_{20t}$.

For some $\varepsilon>0$ we have $(-\infty,\varepsilon)\cap\text{supp}\hat{\Psi}_1=\varnothing$. Thus if we take $T_1\geq 1$ with $-\varepsilon T_1-a<0$, then (B12) will be satisfied for all $t\leq -T_1$, $x\geq a$, and all $k\in\text{supp}\hat{\Psi}_1$. Substituting (B15) into (B14) we obtain

$$\begin{aligned}|\Psi_{10t}(x)|&=(2\pi)^{-1/2}\int_{-\infty}^{\infty}dk\sum_{j=n}^{2n}\sum_{s=0}^{j-n}\frac{|t|^s}{|kt-x|^{j-n}|kt-x|^{n/2}|kt-x|^{n/2}}|f_{sj}(k)|\\&\leq(2\pi)^{-1/2}\sum_{j=n}^{2n}\sum_{s=0}^{j-n}\frac{|t|^{j-n}}{(\varepsilon|t|+a)^{j-n}}\frac{1}{(\varepsilon|t|+a)^{n/2}}\frac{1}{(x+\varepsilon T_1)^{n/2}}\int_{-\infty}^{\infty}dk\ |f_{sj}(k)|\\&=O((1+|t|)^{-n/2}(1+|x|)^{-n/2})\end{aligned} \tag{B19}$$

for $t\leq -T_1$ and $x\geq a$. Note that in the same way one can show that the bound (B19) holds also for $t\geq T_1'$ and $x\leq a$.

Analogously,

$$|\Psi_{20t}(x)|=0((1+|t|)^{-n/2}(1+|x|)^{-n/2}) \tag{B20}$$

for $t\leq -T_2$ and $x\leq a$, or $t\geq T_2'$ and $x\geq a$.

To prove (B7) we write

$$\begin{aligned}\left|\int_{-\infty}^{a}dx\ |\Psi_{0t}(x)|^2-\int_0^{\infty}dE\ |\Phi_1(E)|^2\right|&=\left|\int_{-\infty}^{a}dx\ |\Psi_{10t}(x)+\Psi_{20t}(x)|^2-\int_{-\infty}^{\infty}dx\ |\Psi_{10t}(x)|^2\right|\\&\leq\int_a^{\infty}dx\ |\Psi_{10t}(x)|^2+\int_{-\infty}^{a}dx\ |\Psi_{20t}(x)|^2\\&\quad+2\left|\int_{-\infty}^{a}dx[\Psi_{10t}(x)]^*\Psi_{20t}(x)\right|\\&\leq\int_a^{\infty}dx\ |\Psi_{10t}(x)|^2+\int_{-\infty}^{a}dx\ |\Psi_{20t}(x)|^2\\&\quad+2\left[\int_{-\infty}^{a}dx\ |\Psi_{20t}(x)|^2\right]^{1/2}\left[\int_{-\infty}^{\infty}dx\ |\Psi_{10t}(x)|^2\right]^{1/2}.\end{aligned} \tag{B21}$$

Applying now inequalities (B19) and (B20) with $n\geq 3$ to majorize the right-hand side of (B21) we see immediately that (B7) holds true.

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