Systematic approach to define and classify quantum transmission and reflection times

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A systematic procedure to define and/or classify local transmission and reflection times for the passage of a quantum particle through a static potential barrier is described. Previously defined times and new quantities arise as particular cases of the general formalism. Generalizations for multidimensional and multichannel scattering systems are presented. The one-dimensional results are applied in detail to the rectangular potential. Other nonlocal approaches based on the current density are also examined, and the "Hartman effect" is quantitatively characterized for wave packets.

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I. INTRODUCTION

There is an ongoing debate to define the times characterizing the passage of a quantum particle through a given spatial region; in particular, when different outgoing channels are involved. Most of the recent research has dealt with tunneling through one-dimensional potential barriers, where the different "channels" are associated with transmission and reflection (see the recent reviews [1–5]). We shall limit for simplicity the main part of the present paper to one dimension, although the general case will also be examined.

The question "how much time has the transmitted particle spent in a given interval $[a,b]$" has a simple answer in classical mechanics, but in quantum mechanics complications arise essentially because "being at $[a,b]$" and "being transmitted" correspond to noncommuting operators.

Let us consider, along the x axis, a one-dimensional static potential barrier vanishingly small outside the interval $[x_1,x_2]$, not necessarily equal to $[a,b]$. At $t=0$ a particle is prepared in the state $|\psi(0)\rangle$, far apart from the left of the barrier, and with a negligible negative momentum component. (This boundary condition is implicitly assumed throughout the paper for wave packets. See [6] for a discussion of the consequences of having negative momenta.) This wave packet will evolve after the collision into transmitted and reflected parts.

At time t, the probability to find the particle in $[a,b]$ is $\langle D\rangle=\int_a^b|\langle x|\psi(t)\rangle|^2dx$, where D is the projector selecting the part of the wave function inside the interval $[a,b]$,

$$D\equiv D(a,b)\equiv\int_a^b|x\rangle\langle x|dx\ , \tag{1}$$

and the total average time the particle spends in $[a,b]$, usually called dwell or sojourn time, will be the integral over time, from $-\infty$ to $+\infty$, of that probability

$$\tau_D(a,b)\equiv\int_{-\infty}^{\infty}\langle\psi(t)|D(a,b)|\psi(t)\rangle dt\ . \tag{2}$$

The restriction to positive momenta in the initial wave function allows us to extend to $-\infty$ the lower integration limit. (From now on the integrals over time will always go from $-\infty$ to ∞.) The resulting quantity, $\tau_D(a,b)$, refers to all particles prepared in the state $|\psi(0)\rangle$, regardless of whether each one passes or is reflected from the barrier.

The problem appears when one tries to define a quantity describing the average duration of the passage of *transmitted* particles through the barrier (the discussion for reflected particles is parallel to this one). With the statement "the particle will be transmitted in the future" a new projector operator can be associated [7–9],

$$P\equiv\int_0^{\infty}|p^{(-)}\rangle\langle p^{(-)}|dp\ . \tag{3}$$

The states $|p^{(-)}\rangle$ are solutions of the Lippmann-Schwinger equation. They are to be distinguished from the more usual states $|p^{(+)}\rangle$,

$$|p^{(\pm)}\rangle=|p\rangle+\lim_{\varepsilon\to+0}\frac{1}{E\pm i\varepsilon-H}V|p\rangle\ . \tag{4}$$

Both of them are eigenstates of H with energy $E=p^2/(2m)$. [The normalization used throughout the paper is $\langle p^{(\pm)}|p'^{(\pm)}\rangle=\langle p|p'\rangle=\delta(p-p')$.] Here the full Hamiltonian H is separated into the kinetic energy term H_0 and the potential V, $H=H_0+V$. The plane wave $|p\rangle$ is common to both states. The second summand of $|p^{(+)}\rangle$ in (4) implies outgoing boundary conditions at asymptotic distances, while the second summand of $|p^{(-)}\rangle$ has the opposite, ingoing behavior. $|p^{(+)}\rangle$ and $|p^{(-)}\rangle$ are frequently expressed as $|p^{(\pm)}\rangle=\Omega_\pm|p\rangle$, where $\Omega_\pm=\lim_{t\to\mp\infty}e^{iHt/\hbar}e^{-iH_0t/\hbar}$ are Möller operators. However, the infinite time limit does not exist when $\Omega_\pm$ act on plane waves, so the use of a convergence factor to give (4) is to be understood implicitly in these expressions [10].

When acting on an arbitrary square integrable state, P selects the part of the wave function that will have positive momentum in the infinite future, and its time-independent average value is the transmittance, i.e., the probability of finding the particle transmitted in the infinite future, $T=\langle P\rangle$. The complementary projector of P, $Q\equiv\int_{-\infty}^{0}|p^{(-)}\rangle\langle p^{(-)}|dp$, selects the part of the incident wave function that will be finally reflected, having negative momentum in the infinite future, $\langle Q\rangle=R=1-T$.

Classically, the following procedures are equivalent:

(1) Make a measurement to ascertain that the particle will pass the barrier, and then check whether the particle is in $[a,b]$ or not; and (2) make first a measurement of position to detect the particle inside or outside the interval $[a,b]$, and then check whether it is finally transmitted.

Quantally both ways of proceeding are not equivalent and the ordering of P and D matters. In fact quantum mechanics does not provide a unique way to construct Hermitian operators for couples of noncommuting observables. Not even the common symmetrization rule is unambiguous in this case because the two operators involved are projection operators, see Sec. II, below. Several attitudes are then possible. (a) "Even though the basic theory does not seem to give a direct definite answer, one knows that classically the value of some observables depends ultimately on the time spent in the interaction region, and expects a similar result in quantum mechanics. The theoretical and experimental effort should then be devoted to identify the proper combinations of P and D leading to quantities with dimensions of time that determine the values of these observables (possibly different combinations for different observables)." (b) "The question is meaningless. Look for a different type of observable (find a new question) that does not involve P and D simultaneously." (c) "Maybe the usual interpretation of quantum mechanics is wrong. Let us use a different classical-like interpretation giving the particle a position and a momentum simultaneously."

The first attitude has led to successful applications in many fields of quantum mechanics. A well-known example is the generalized use of "symmetrized" operators combining two Hermitian but noncommuting operators; for example, in kinetic theory. However, the second attitude can cause no harm if it is positively used, i.e., if alternative quantities are found that provide information on the temporal characterization of the particle's behavior. The third attitude ([11] and references therein, [7,12–14]) may be interesting to explore, but we will not deal with it here, if only because there is still much to be learned from the other two.

The purpose of this paper is twofold: First, in the spirit of attitude (a), different combinations of P and D operators are systematically examined. Times previously defined by different authors are particular cases of the formalism, but also new times arise. Part of this program has already been carried out [7–9]. However, this work presents the ideas and results in a compact way, generalizes the treatment, and completes the derivations and physical discussion, including model calculations. Considering that the number of publications in the field is growing at a good pace and that it is not always easy to relate or compare the different proposals, we approach the topic with the intent to provide a unifying, referential framework.

Second, following the attitude (b), without necessarily accepting the first statement in it, we explore times that renounce from the start to combine P and D, and do not try to answer the question posed at the beginning of this introduction. Again, care has been exercised in comparing and relating previous works.

A final warning: This is not a comprehensive review paper, and in spite of addressing a remarkable number of approaches connected with our theory, not all of them, some of importance, can be dealt with following the treatments below.

Sections II and III present possible definitions of transmission and reflection times for wave packets and stationary waves, respectively; Sec. IV generalizes the previous results to multichannel scattering; Sec. V discusses general properties of the defined times; Sec. VI studies the case of a collision of a plane wave against a rectangular barrier; Sec. VII deals with the definition of times not related to operators P and D, but to distributions of times for the passage or arrival of particles. Relations to stationary phase time delays are established and the "Hartmann effect" is discussed; Sec. VIII finally summarizes the main results and conclusions.

II. TIME-DEPENDENT SCATTERING

There is no unique prescription for obtaining an operator associated with the product of two classical magnitudes with quantum counterparts that do not commute. In many cases the symmetrization rule is applied, but ultimately one should resort to experience to check if a given choice is appropriate. We shall first show how not even the application of the symmetrization rule leads to unique results in our case. Symmetrizing the product PD and using $P+Q=1$,

$$(PD)_{\text{symm}}=\frac{[P,D]_+}{2}=\frac{PD+DP}{2}=PDP+\frac{PDQ+QDP}{2} . \tag{5}$$

However, since P and D are projectors, $PD=PPD$, and the symmetrization of the last expression gives, taking all possible combinations of the three operators,

$$(PPD)_{\text{symm}}=\frac{PDP+PD+DP}{3}=PDP+\frac{PDQ+QDP}{3} . \tag{6}$$

Moreover, DPD is also symmetrical, in a different sense.

We are interested in studying systematically the times obtained by means of different combinations and orderings of P and D. In principle, an infinite number of times could be written, but only some of them will be considered. Two criteria have guided our selection: First, simplicity. Simple symmetrical combinations can be physically interpreted in terms of conditional probabilities that involve the events "being at time t in a given space interval $[a,b]$" and "passing the barrier potential in the future," see Sec. II E. Second, the obtainment of times proposed by other authors. In fact the two criteria overlap in several cases.

The discussion is organized into various "resolutions," i.e., particular ways of partitioning the D operator. In general we shall only give explicit expressions for times associated with transmission (subscript T). The corresponding reflection times are obtained from them by substituting T by R, and P by Q.

A. Resolution 1: Partial dwell times and interference contributions

Let us *first* select with P the part of $|\psi(t)\rangle$ that will be transmitted in the infinite future and *then* calculate the corresponding dwell time, using D. This procedure gives the quantity

$$\tau_T^{\rm PDP} \equiv \frac{1}{T}\int \langle P\psi(t)|D|P\psi(t)\rangle dt \ . \qquad (7)$$

The prefactor $T^{-1}=\langle\psi(t)|P|\psi(t)\rangle^{-1}$ naturally arises to normalize to unity the state $P|\psi(t)\rangle$.

As noted by Landauer [3], and others [15,16], the component $\langle x|P|\psi(0)\rangle$ is in general nonzero *on both sides of the barrier,* even if the initial packet $\langle x|\psi(0)\rangle$ is entirely on the left. The left and right parts of the projected state $\langle x|P|\psi(t)\rangle$ approach the collision region to evolve asymptotically into a unique wave with positive momentum on the right of the barrier.

This argument seems to complicate the physical interpretation of τ_T^{PDP} and the implementation of experiments capable of creating such peculiar states. However, it is a remarkable fact that in some circumstances (at least when they agree with the anticommutator times described below), they do have a physical content in connection with spin precession in weak magnetic fields, see the final summary.

An interesting relation between the dwell time and the two times τ_T^{PDP} and τ_R^{QDQ} is obtained by using the identity $P+Q=\mathbb{1}$ twice, to resolve D as

$$D=PDP+QDQ+PDQ+QDP \ , \qquad (8)$$

which introduces new terms as an effect of the interference between the "to be transmitted" and "to be reflected" parts of the wave packet. One can then define the complex quantity

$$\tau_{\rm int} \equiv \int \langle\psi(t)|PDQ|\psi(t)\rangle dt \ , \qquad (9)$$

such that

$$\tau_D = T\tau_T^{PDP} + R\tau_R^{QDQ} + 2{\rm Re}[\tau_{\rm int}] \ . \qquad (10)$$

This equation shows the classical structure of sum over magnitudes corresponding to mutually exclusive events (transmission and reflection), plus an interference term purely quantum in origin. The interference occurs because before measurement a particle cannot be labeled as "to be transmitted" or "to be reflected;" it is assigned to a state that combines both possibilities in the form of amplitudes rather than probabilities. For symmetric barriers the interference term vanishes when the intervals $[x_1,x_2]$ and $[a,b]$ are equal [17].

B. Resolution 2: The particle is localized first

One can proceed the other way around, *first* selecting the part of the wave function in $[a,b]$ at some instant t, by means of D, and *then* calculating the transmission probability, using P. Integration over time from $-\infty$ to $+\infty$ defines

$$\tau_T^{DPD} \equiv \frac{1}{T}\int \langle\psi(t)|DPD|\psi(t)\rangle dt \ , \qquad (11)$$

which, with τ_R^{DQD}, fulfills the relation

$$\tau_D = T\tau_T^{DPD} + R\tau_R^{DQD} \ , \qquad (12)$$

without any interference term, as can be seen from the resolution

$$D=DPD+DQD \ . \qquad (13)$$

C. Resolution 3: Complex "times"

D can also be decomposed as the sum of two non-Hermitian operators,

$$D=PD+QD \ . \qquad (14)$$

This resolution allows us to define the complex "times"

$$\tau_T^{PD} \equiv \frac{1}{T}\int \langle\psi(t)|PD|\psi(t)\rangle dt \ , \qquad (15)$$

for transmission, and τ_R^{QD} for reflection. Clearly, $\tau_D = T\tau_T^{PD} + R\tau_R^{QD}$.

These quantities are related to the ones defined before. Using $P+Q=\mathbb{1}$ in the definition (15) of τ_T^{PD}, the equality

$$\tau_T^{PD} = \tau_T^{PDP} + \frac{1}{T}\tau_{\rm int} \qquad (16)$$

can be easily established. An analogous relation exists for reflection,

$$\tau_R^{QD} = \tau_R^{QDQ} + \frac{1}{R}\tau_{\rm int}^* \ . \qquad (17)$$

The moduli of the complex "times" are the Büttiker-Landauer times [18,19].

D. Resolution 4: Hermitian and anti-Hermitian operators

Any operator can be decomposed into Hermitian and anti-Hermitian parts. For a couple of noncommuting Hermitian operators, the Hermitian part is one-half of the anticommutator. This Hermitian combination is standardly regarded as the quantum operator associated with the product of two noncommuting quantities in many applications. One more useful resolution of D is obtained by decomposing each of the operators PD and QD in (14), as the sum of two contributions: one-half of the commutator of P (or Q) and D, and one-half of the corresponding anticommutator,

$$D = \tfrac{1}{2}[P,D]_+ + \frac{1}{2i} i[P,D]_- + \tfrac{1}{2}[Q,D]_+ + \frac{1}{2i} i[Q,D]_- \ . \qquad (18)$$

Accordingly, the times

$$\tau_T^{[P,D]_+/2} \equiv \frac{1}{T}\int \left\langle \psi(t) \left| \frac{[P,D]_+}{2} \right| \psi(t) \right\rangle dt \ ,$$

$$\tau_T^{[P,D]_-/2i} \equiv \frac{1}{T}\int \left\langle \psi(t) \left| \frac{[P,D]_-}{2i} \right| \psi(t) \right\rangle dt \qquad (19)$$

can be introduced for transmission. They are, respectively, the real and imaginary parts of τ_T^{PD}.

E. Probability theory

It is worth viewing the above results in the light of probability theory [9]. The probabilities for the basic events, "being at $[a,b]$" and "passing eventually the barrier," are

$$p(D)\equiv\langle D\rangle=\langle\psi(t)|D|\psi(t)\rangle\ , \tag{20}$$

$$p(P)\equiv\langle P\rangle=\langle\psi(t)|P|\psi(t)\rangle=T\ . \tag{21}$$

Conditional probabilities can also be defined as

$$p(D|P)\equiv\frac{\langle\psi(t)|PDP|\psi(t)\rangle}{T}\ , \tag{22}$$

$$p(P|D)\equiv\frac{\langle\psi(t)|DPD|\psi(t)\rangle}{\langle D\rangle}\ . \tag{23}$$

The "joint probability" for being at $[a,b]$ and passing eventually the barrier, would be given, according to the axioms of probability theory, by $p(P|D)p(D)=p(D|P)p(P)$, but the two sides of this equation are here different, as occurs in general for noncommuting operators. No joint probability can be constructed in quantum mechanics for two noncommuting observables. This however, should not be understood as an argument against any other probability. In fact it is common practice in quantum mechanics to make use of the conditional probabilities, and of course, the "marginal" probabilities dealing with a single observable are constantly applied.

One can view τ_T^{DPD} and τ_T^{PDP} on the basis of probability theory as

$$\tau_T^{DPD}\equiv\frac{1}{p(P)}\int p(D)p(P|D)dt\ , \tag{24}$$

$$\tau_T^{PDP}\equiv\int p(D|P)dt\ . \tag{25}$$

For a classical ensemble of particles, the right-hand side (rhs) of (24) is equal to the rhs of (25), and to the classical average traversal time.

III. TIME-INDEPENDENT SCATTERING

The decompositions presented in Sec. II for wave packets can be used for non-normalizable states in the stationary regime, now assuming a plane wave of fixed momentum $p>0$ impinging on the potential barrier from the left. For this time-independent process, the dwell time defined for the space interval $[a,b]$ takes the form

$$\tau_D(p)\equiv\frac{1}{J_I}\langle p^{(+)}|D|p^{(+)}\rangle\ . \tag{26}$$

For Dirac δ-normalized functions, the incoming current density of the plane wave is $J_I=p/(hm)$.

The quantities referring to stationary scattering will be denoted by the same symbols used for wave packets, but with the additional argument (p). Particular care should be exercised to distinguish the wave-packet transmittance T, the stationary transmission coefficient $T(p)$, and the stationary transmission probability $|T(p)|^2$.

Again, $\tau_D(p)$ does not distinguish transmission and reflection but refers to the whole wave function, $|p^{(+)}\rangle$. We can proceed as before, acting on $|p^{(+)}\rangle$ with P and Q, to define for the stationary case the times

$$\tau_U^{\eta}(p)\equiv\frac{1}{J_I|U(p)|^2}\langle p^{(+)}|\eta|p^{(+)}\rangle\ . \tag{27}$$

Here, for $U=T$, η can be any of the operators in the previous section that combine P and D, such as PDP, DPD, PD, $[P,D]_+/2$, or $[P,D]_-/2i$, and similarly for $U=R$, with Q instead of P.

Resolution (8) serves to define $\tau_T^{PDP}(p)$ and $\tau_R^{QDQ}(p)$, and the interference term is now

$$\tau_{\rm int}(p)\equiv\frac{1}{J_I}\langle p^{(+)}|PDQ|p^{(+)}\rangle\ , \tag{28}$$

so the equivalent of relation (10) in the stationary case reads

$$\tau_D(p)=|T(p)|^2\tau_T^{PDP}(p)+|R(p)|^2\tau_R^{QDQ}(p)+2{\rm Re}[\tau_{\rm int}(p)]\ . \tag{29}$$

A relation analogous to (16) between τ_T^{PD}, τ_T^{PDP}, and $\tau_{\rm int}$ is also valid for a given momentum p in the stationary regime, as well as the corresponding equation for reflection magnitudes.

The different times are actually computed by using the expressions given in the Appendix, which show how the operators P and Q act on the states $|p^{(+)}\rangle$. We shall apply these expressions in Sec. VII for the rectangular potential.

Let us now examine the relation to the nonstationary case. Taking into account that the integral $\int_{-\infty}^{\infty}|p^{(+)}\rangle\langle p^{(+)}|dp$ leaves unchanged any scattering state $|\psi(t)\rangle$, i.e., in this space it acts as the identity operator, Eq. (7) can be written in the form

$$\tau_T^{PDP}=\frac{1}{T}\int\int\int\langle\psi(t)|p^{(+)}\rangle\langle p^{(+)}|PDP|p'^{(+)}\rangle\times\langle p'^{(+)}|\psi(t)\rangle dt\,dp\,dp'\ , \tag{30}$$

where the integrals go from $-\infty$ to ∞.

Since the Hamiltonian is time independent,

$$\tau_T^{PDP}=\frac{1}{T}\int\int\int\langle\psi(0)|\exp(iHt/\hbar)|p^{(+)}\rangle\times\langle p^{(+)}|PDP|p'^{(+)}\rangle\times\langle\psi(0)|\exp(iHt/\hbar)|p'^{(+)}\rangle^*\times dt\,dp\,dp'\ . \tag{31}$$

Acting with $\exp(iHt/\hbar)$ to the right, and integrating over time, a Dirac δ in the difference of the two momentum coordinates comes out,

$$\tau_T^{PDP} = \frac{1}{T}\int\int \delta(|p|-|p'|)\frac{mh}{|p|}\langle\psi(0)|p^{(+)}\rangle\langle p^{(+)}|PDP|p'^{(+)}\rangle\langle\psi(0)|p'^{(+)}\rangle^* dp\, dp'$$
$$= \frac{1}{T}\int_0^\infty |T(p)|^2 f(p)\tau_T^{PDP}(p)dp \ , \tag{32}$$

where $\tau_T^{PDP}(p)$ is defined by Eq. (27). To obtain the second equality, $|\langle p^{(+)}|\psi(0)\rangle|^2$ has been identified with the initial (asymptotic) momentum probability distribution $f(p)$.

Following the same steps for the other quantities introduced in Sec. II, one can generally write

$$\tau_U^\eta = \frac{1}{U}\int_0^\infty |U(p)|^2 f(p)\tau_U^\eta(p)dp \ , \tag{33}$$

where U is equal to T or R, and η is any of the combinations of P and D or of Q and D, respectively.

If all probabilities implicit in (33) were classical [$f(p)$, $|U(p)|^2$, and U], the result would amount to average the times for definite initial momentum over the probability density for finding a given initial momentum subject to the condition of being finally transmitted or reflected. Since they are not, however, this interpretation of $U^{-1}|U(p)|^2 f(p)$ as a conditional probability density is not rigorous or valid, although it may be of heuristic value, especially in the classical limit.

The case of the dwell time is slightly different, because it does not refer to transmission or reflection, but to both processes altogether. The relation between the quantity τ_D and the function $\tau_D(p)$ can be obtained in the same way as before [20],

$$\tau_D = \int_0^\infty \tau_D(p)f(p)dp \ . \tag{34}$$

Note that even when the case $\tau_D(p)=\tau_T^{PDP}(p)$ occurs (see Sec. VI for an example), the difference between Eq. (33) and Eq. (34) gives rise to different results for τ_D and τ_T^{PDP}, especially if $f(p)$ is concentrated over a region in which $T(p)$ changes appreciably.

IV. MULTICHANNEL SCATTERING

Interest in separating the dwell time into components, and in general of describing the temporal aspects of collision processes, is not limited to one-dimensional systems. For general applications in molecular and nuclear physics, or electronic transport in semiconductors, it is important to extend the previous discussion to multidimensional and multichannel scattering. This can be readily done within the present framework by using the appropriate scattering operators in each case. The basic idea is common for all systems, independently of their complexity: The total wave function can be resolved into independent components that will evolve into a particular "channel" i in the distant future. The decomposition is done by means of orthogonal projectors,

$$R_i R_j = R_i \delta_{ij} \ , \tag{35}$$

that commute with H (defining subdynamics [21]), and whose sum is the unity operator *in the space of scattering states.* A particular region of the coordinates, usually corresponding to the interaction region, where the wave function vanishes before and after collision, is selected with a projection operator D. Then the different times arise by decomposing the dwell time

$$\tau_D = \int \langle\psi(t)|D|\psi(t)\rangle dt \tag{36}$$

in terms of the resolutions of D:

$$D = \sum_i\sum_j R_i D R_j$$
$$= \sum_i R_i D \tag{37}$$
$$= D\left[\sum_i R_i\right]D$$
$$= \sum_j \tfrac{1}{2}(R_j D + D R_j) + i\frac{1}{2i}(R_j D - D R_j) \ , \tag{38}$$

which generalize the times and resolutions discussed in Secs. II and III.

The word "channel" is here used in a broad sense that includes cases where no internal states or different asymptotic Hamiltonians exist (e.g., in the one-dimensional system examined previously). To fix ideas let us discuss the construction of R_i in several typical cases.

In three-dimensional elastic scattering one may separate the Hilbert space of asymptotic states into subspaces defined by solid angles i. The asymptotic projectors

$$F_i = \int_i |\mathbf{p}\rangle\langle\mathbf{p}|d\mathbf{p} \ , \tag{39}$$

where the integral is restricted to vectors pointing into the solid angle i, serve to define the R_i's as

$$R_i = \Omega_- F_i \Omega_-^\dagger \ . \tag{40}$$

For inelastic scattering the channels are generally defined by the internal states, $\{|\phi_i^{\rm int}\rangle\}$, for example, of a diatomic molecule colliding with a structureless atom. The projectors then select the part of the total wave function that will end up in the internal state $|\phi_i^{\rm int}\rangle$:

$$R_i = \Omega_-|\phi_i^{\rm int}\rangle\langle\phi_i^{\rm int}|\Omega_-^\dagger \ . \tag{41}$$

Finally, the more complicated case of reactive scattering can also be handled. Associating the channels i with the possible asymptotic Hamiltonians $\{H_{0i}\}$, the channel Möller operators are defined as

$$\Omega_{i\pm} = \lim_{t\to\mp\infty} e^{iHt/\hbar}e^{-iH_{0i}t/\hbar} \ . \tag{42}$$

The projectors

$$R_i = \Omega_{i-}\Omega_{i-}^\dagger \tag{43}$$

commute with H (they are the basis of the Jauch resolution of the total wave function [22,23]), and fulfill the required conditions of orthogonality, Eq. (35), and completeness for scattering states.

In a generic case, the flexibility of the formalism enables us to tailor the R_i projectors for particular needs. One may be interested in defining projectors that select one asymptotic Hamiltonian *and* sets of internal states, for example. In the following we shall return to the simple one-dimensional case.

V. GENERAL PROPERTIES OF THE DIFFERENT TIMES

Using the projectors described in the previous sections, we can easily discuss and compare some of the general properties of the different times, valid for all shapes of the potential barrier and of the incident wave packet.

A. Additivity

The explicit expression of each time in terms of the operator D enable us to check whether or not a particular temporal magnitude associated with the space interval $[a,b]$ equals the sum of the corresponding quantities for $[a,c]$ and $[c,b]$, with $a \le c \le b$. Using $D(a,b)=D(a,c)+D(c,b)$ in Eq. (2), one can immediately verify the additivity of the dwell time, i.e., that $\tau_D(a,b)=\tau_D(a,c)+\tau_D(c,b)$. The same happens for all times that can be written with only one D operator: τ_T^{PDP}, τ_T^{PD}, $\tau_T^{[P,D]_+/2}$, $\tau_T^{[P,D]_-/2i}$, the corresponding reflection times, and $\tau_{\rm int}$. On the contrary, neither the Büttiker-Landauer times (the moduli of τ_T^{PD} for transmission and of τ_R^{QD} for reflection) nor τ_T^{DPD} (and τ_R^{DQD}) are additive. These quantities are not linear in D.

B. Real-complex

The condition of being a real or a complex quantity depends on the hermiticity of the basic operators. Hermitian operators, such as D, PDP, DPD, and $[P,D]_+/2$, lead to real times. In fact, all times except τ_T^{PD}, τ_R^{QD} and $\tau_{\rm int}$ are real numbers.

C. Positivity

With respect to the sign of each time, the dwell time is positively semidefined because it is the integral of a probability density, and the same can be said of τ_T^{PDP}, τ_T^{DPD}, and of the corresponding quantities for reflection. Also, trivially, Büttiker-Landauer times are always nonnegative.

The question is meaningless for complex numbers, such as τ_T^{PD}, and the answer depends on the particular shape of the barrier in the case of the real and imaginary parts of τ_T^{PD} and τ_R^{QD}. The rectangular barrier is examined in the next section.

D. Mutually exclusive events

Another point of interest, discussed repeatedly in previous papers [1,3,9,24], is the use of the "classically minded" relation

$$\tau_D = T\tau_T + R\tau_R \tag{44}$$

as a criterion of accepting or rejecting the quantities τ_T and τ_R, provided by a given theory, as actual traversal times for transmitted and reflected particles, respectively. In this section we will restrict ourselves to pointing out which of the above definitions verifies relation (44), by taking into account the resolution of the D operator used for the particular time.

τ_T^{PDP} and τ_R^{QDQ} verify Eq. (10) instead of (44), with an additional interference term $\tau_{\rm int}$ [9]. From Eq. (13) and definitions of τ_T^{DPD} and τ_R^{DQD}, it follows that these times relate themselves by means of an equation of the form of (44). The same is true for τ_T^{PD} and τ_R^{QD}, and for $\tau_T^{[P,D]_+/2}$ and $\tau_R^{[Q,D]_+/2}$, whereas the imaginary parts of τ_T^{PD} and τ_R^{QD} verify

$$T\tau_T^{[P,D]_-/2i} + R\tau_R^{[Q,D]_-/2i} = 0 \; . \tag{45}$$

Finally, Büttiker-Landauer times $|\tau_T^{PD}|$ and $|\tau_R^{QD}|$ do not add to give the dwell time once they are weighted with T and R, respectively.

VI. RECTANGULAR POTENTIAL

We will use here the rectangular barrier to illustrate the behavior of the new times defined in Secs. II and III in comparison to other already existing proposals. The scattering states $|p^{(+)}\rangle$ in coordinate representation are given by

$$\langle x|p^{(+)}\rangle = \frac{1}{\sqrt{h}} \begin{cases} \exp(ikx)+B\exp(-ikx) & \text{if } x \le 0 \; , \\ C_+\exp(ik'x)+C_-\exp(-ik'x) & \text{if } 0 \le x \le d \; , \\ A\exp(ikx) & \text{if } d \le x \; , \end{cases} \tag{46}$$

where $p=\hbar k \equiv \sqrt{2mE}$ and $p'=\hbar k' \equiv \sqrt{2m(E-V_0)}$. The coefficients have the form

$$\begin{aligned} A &\equiv T(p) = 4kk'\exp[-ik(x_2-x_1)]/F(k,k') \; , \\ B &\equiv R(p) = 2i(k'^2-k^2)\exp[2ikx_1]\sin[k'(x_2-x_1)]/F(k,k') \; , \\ C_+ &= 2k(k'+k)\exp[i(kx_1-k'x_2)]/F(k,k') \; , \\ C_- &= 2k(k'-k)\exp[i(kx_1+k'x_2)]/F(k,k') \; , \end{aligned} \tag{47}$$

with

$$F(k,k')=(k'+k)^2\exp[-ik'(x_2-x_1)]-(k'-k)^2\exp[ik'(x_2-x_1)] .$$

($x_1=0$ and $x_2=d$ are the barrier edges.)

Similarly, the states $|p^{(-)}\rangle$ are

$$\langle x|p^{(-)}\rangle=\frac{1}{\sqrt{h}}\begin{cases}\hat{A}\exp(ikx) & \text{if } x\le 0 ,\\ \hat{C}_+\exp(ik'x)+\hat{C}_-\exp(-ik'x) & \text{if } 0\le x\le d ,\\ \exp(ikx)+\hat{B}\exp(-ikx) & \text{if } d\le x ,\end{cases} \tag{48}$$

where the new coefficients, $\hat{A}$, $\hat{B}$, $\hat{C}_+$, and $\hat{C}_-$, are obtained from A, B, C_+, and C_-, respectively, by interchanging x_1 and x_2 in their expressions.

Substituting the state $|p^{(+)}\rangle$ in Eq. (26), we note that the dwell time takes the form

$$\tau_D(p)=\left[\frac{mk}{\hbar k'}\right]\frac{2k'(b-a)(k'^2+k^2)+(k'^2-k^2)\{\sin[2k'(d-a)]-\sin[2k'(d-b)]\}}{(k'^2-k^2)^2\sin^2(k'd)+4k^2k'^2} , \tag{49}$$

when $0\le a\le b\le d$. (If a and b are chosen to be 0 and d, respectively, the result of Ref. [19] is recovered.)

In this section the condition $x_1=0\le a\le b\le d=x_2$ is assumed in all expressions. Note that for $E<V_0$, k' becomes purely imaginary, $k'=i\kappa\equiv\sqrt{2m(E-V_0)}/\hbar$.

A. $\tau_T^{PDP}(p)$

The dwell time for the part of the incident plane wave that "will be transmitted in the future," $\tau_T^{PDP}(p)$, is

$$\tau_T^{PDP}(p)=\frac{1}{J_I}\langle p^{(-)}|D|p^{(-)}\rangle \tag{50}$$

$$=\left[\frac{mk}{\hbar k'}\right]\frac{2k'(b-a)(k'^2+k^2)+(k'^2-k^2)[\sin(2k'b)-\sin(2k'a)]}{(k'^2-k^2)^2\sin^2(k'd)+4k^2k'^2} . \tag{51}$$

We shall comment upon some particular cases: As k goes to zero these times also tend to zero; for $V_0=0$, the classical result $m(b-a)/p$ is obtained; when $a=0$ and $b=d$, $\tau_T^{PDP}(p)$ equals the dwell time of Eq. (49). Also, if $a=0$, $b=d$, and $\kappa d\gg 1$ (opaque barriers), $\tau_D(p)=\tau_T^{PDP}(p)\approx\hbar k/\kappa V_0$.

The reflection time

$$\tau_R^{QDQ}(p)=\frac{1}{J_I}\langle(-p)^{(-)}|D|(-p)^{(-)}\rangle \tag{52}$$

equals the dwell time for *any* values of a and $b\ge a$, inside the barrier.

In Fig. 1, $\tau_D(p;[0,d/2])$ is compared to $\tau_T^{PDP}(p;[0,d/2])$ as a function of the incident momentum p for an interval $[0,d/2]$ inside the rectangular barrier. At large momentum above the barrier both results approximate the classical value $md/(2p)$. At energies $E<V_0$, $\tau_D(p;[0,d/2])$ is much larger than $\tau_T^{PDP}(p;[0,d/2])$. Since the transmittance is small in this energy regime, most of the $P|\psi\rangle$ state is on the right of the barrier, with very little overlap onto the left half of the barrier. On the contrary, the reflected part enters this left half of the barrier, contributing to the dwell time.

B. $\tau_T^{PD}(p)$

$\tau_T^{PD}(p)$ is readily obtained as

$$\tau_T^{PD}(p)=\frac{1}{T(p)J_I}\langle p^{(-)}|D|p^{(+)}\rangle=\frac{m}{4\hbar k'^2[(k'^2-k^2)^2\sin^2(k'd)+4k^2k'^2]}$$
$$\times\{[8kk'^2(b-a)(k'^2+k^2)+4kk'(k'^2-k^2)\cos(k'd)s(a,b)]$$
$$+i[2k'(b-a)(k'^2-k^2)^2\sin(2k'd)+2(k'^4-k^4)\sin(k'd)s(a,b)]\} , \tag{53}$$

whereas for reflection,

$$\tau_R^{QD}(p)=\frac{1}{R(p)J_I}\langle(-p)^{(-)}|D|p^{(+)}\rangle=[\tau_D(p)-|T(p)|^2\tau_T^{PD}(p)]/|R(p)|^2$$

$$=\frac{mk}{\hbar k'[(k'^2-k^2)^2\sin^2(k'd)+4k^2k'^2]}$$

$$\times\Bigg\{2k'(b-a)(k'^2+k^2)+\left[\frac{2k^2k'^2}{(k'^2-k^2)\sin^2(k'd)}+(k'^2-k^2)\right]\{\sin[2k'(d-a)]-\sin[2k'(d-b)]\}$$

$$+\frac{2k^2k'^2}{(k'^2-k^2)\sin^2(k'd)}\{\sin(2k'a)-\sin(2k'b)\}$$

$$-i\frac{2kk'}{(k'^2-k^2)\sin(k'd)}[2k'(b-a)(k'^2-k^2)\cos(k'd)+(k'^2+k^2)s(a,b)]\Bigg\}\ ,$$

with

$$s(a,b)=\sin(k'd-2k'a)-\sin(k'd-2k'b)\ . \quad (54)$$

C. $\tau_T^{[P,D]_+/2}(p)$ $\tau_T^{[P,D]_-/2i}(p)$

Times associated with the commutator or anticommutator of P or Q and D are simply found as the real or imaginary parts of the complex valued functions $\tau_T^{PD}(p)$ and $\tau_R^{QD}(p)$, following the resolution (18) of D.

Figure 2 shows (a) the real and imaginary parts of $\tau_T^{PD}(p)$, and (b) the real and imaginary parts of $\tau_R^{QD}(p)$. For large momentum, $\mathrm{Re}[\tau_T^{PD}(p)]$ recovers the classical result $m(b-a)/p$, whereas the other quantities in Fig. 2 go to zero. The quantities for reflection show the resonance peaks over the barrier as a consequence of the $1/|R(p)|^2$ prefactor in the expression analogous to Eq. (17) for the stationary case.

In the opaque barrier regime, $\kappa d \gg 1$, and for $a=0$, and $b=d$, $-\mathrm{Im}[\tau_T^{PD}(p)]$ (this quantity, with the minus sign, equals the Larmor time $\tau_{zT}(p)$, see the final summary) tends to $md/(\hbar\kappa)$. This is the time that a particle would spend moving with a momentum equal to the modulus of the imaginary factor $\sqrt{2m(E-V_0)}$.

D. $\tau_{\rm int}(p)$

The real and imaginary parts of $\tau_{\rm int}(p)$ can be obtained from the previous results, using the relations

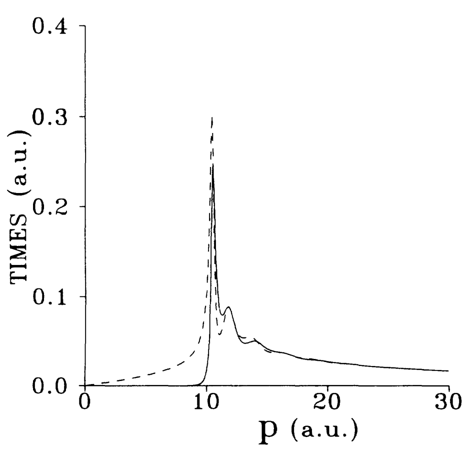

FIG. 1. Dwell time (dashed) and $\tau_T^{PDP}(p)$ (solid) as functions of the momentum of the incident particle, p, for an interval $[0,d/2]$. In atomic units, $V_0=50$, $x_1=0$, and $x_2=d=3\pi/10$. $m=\hbar=1$ in all figures.

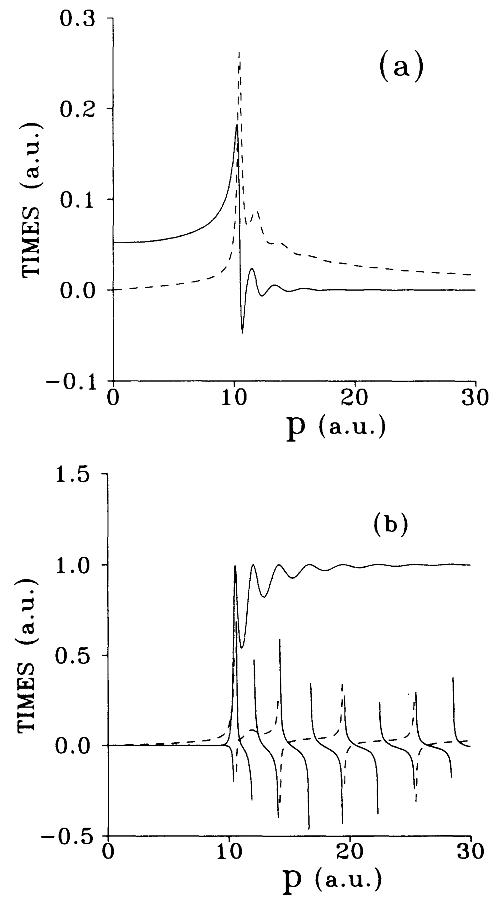

FIG. 2. (a) Real part of $\tau_T^{PD}(p)$ (dashed), and minus the imaginary part of $\tau_T^{PD}(p)$ (solid), vs p. Same conditions as Fig. 1. (b) Real part of $\tau_R^{QD}(p)$ (dashed), and minus the imaginary part of $\tau_R^{QD}(p)$ (solid) vs p. Same conditions as Fig. 1. The transmittance has been depicted for reference (dotted line).

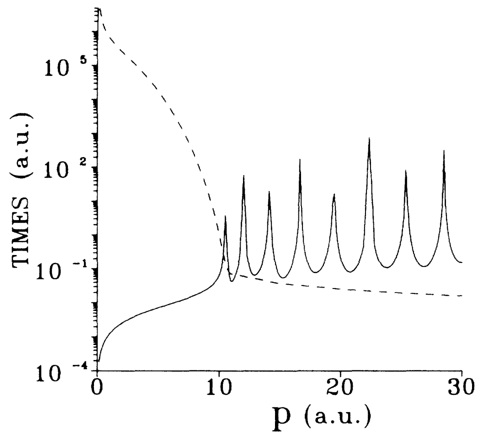

FIG. 3. $\tau_T^{DPD}(p)$ (dashed line), and $\tau_R^{QDQ}(p)$ (solid line) in logarithmic scale as functions of p, for the same interval and barrier of Figs. 1 and 2.

$$\mathrm{Re}[\tau_{\mathrm{int}}(p)]=\tfrac{1}{2}|T(p)|^2[\tau_R^{QDQ}(p)-\tau_T^{PDP}(p)] \tag{55}$$

and

$$\mathrm{Im}[\tau_{\mathrm{int}}(p)]=|T(p)|^2\mathrm{Im}[\tau_T^{PD}(p)]\ , \tag{56}$$

respectively. Equation (55) is valid for this case since $\tau_D(p)=\tau_R^{QDQ}(p)$.

E. $\tau_T^{DPD}(p)$

$\tau_T^{DPD}(p)$ can be obtained numerically with the expression

$$\tau_T^{DPD}(p)=\frac{1}{J_I|T(p)|^2}\langle p^{(+)}|DPD|p^{(+)}\rangle$$
$$=\frac{1}{J_I|T(p)|^2}\int_0^\infty |\langle p'^{(-)}|D|p^{(+)}\rangle|^2dp'\ . \tag{57}$$

($\langle p'^{(-)}|D|p^{(+)}\rangle$ has an analytic form for the rectangular barrier.) Its main features are shown in Fig. 3. $\tau_T^{DPD}(p)$ goes to the classical value $m(b-a)/p$ when p increases above the barrier and grows to infinity as momentum decreases under the potential, leading to large times for slow particles. $\tau_R^{DQD}(p)$ reveals the structure of resonances of the square barrier, giving infinite time for reflection when the particle completely passes to the right-hand side of the potential.

For the case $V_0=0$ an explicit expression can be found in terms of the sine integral: Contrary to $\tau_T^{PDP}(p)$, the classical value $m(b-a)/p$ is not recovered unless the dimensionless parameter $\hbar/[p(b-a)]$ goes to zero too. The first correction is given by

$$\tau_T^{DPD}(p;V_0=0)\approx\frac{m(b-a)}{p}\left[1+\frac{\hbar}{\pi p(b-a)}\right]\ . \tag{58}$$

VII. FLUXES, TIME DISTRIBUTIONS, "HARTMAN" EFFECT

A second viewpoint to overcome the difficulties for describing the temporal aspects of collisions consists on looking at the asymptotic properties of the flux, before or after the collision process. Some works, studying the mean value of the flux operator, have been recently presented in this direction [5,7,16,25–27]. This section discusses and compares the different approaches, and extends the analysis.

A. Average passage or arrival times

Consider again the wave packet impinging the barrier potential (between 0 and d) from the left, but now take the spatial interval $[a,b]$ well outside the barrier, so that the passage of the incident packet through a can be separated in time from the passage of the reflected packet through the same point. We shall denote as $t=t_c$ an arbitrary instant in the interval with vanishing flux at a between the passage of the incident and reflected waves.

The dwell time can be written as (see [7] for the precise conditions)

$$\tau_D=\int_{-\infty}^{\infty}[J(b,t')-J(a,t')]t'dt'\ , \tag{59}$$

$J(x,t)\equiv(\hbar/m)\mathrm{Im}[\psi^*(x,t)\partial\psi(x,t)/\partial x]$ being the current density at position x and time t. With this in mind, we defined traversal and reflection times as [7]

$$\tau_T=\langle t\rangle_b^{\mathrm{out}}-\langle t\rangle_a^{\mathrm{in}}\ ,$$
$$\tau_R=\langle t\rangle_a^{\mathrm{out}}-\langle t\rangle_a^{\mathrm{in}}\ , \tag{60}$$

so that the dwell time is decomposed as $\tau_D=T\tau_T+R\tau_R$. The average instants in (60) are given by

$$\langle t\rangle_b^{\mathrm{out}}=\frac{1}{T}\int_{-\infty}^{\infty}J(b,t')t'dt'\ ,$$
$$\langle t\rangle_a^{\mathrm{in}}=\int_{-\infty}^{t_c}J(a,t')t'dt'\ ,$$
$$\langle t\rangle_a^{\mathrm{out}}=\frac{1}{R}\int_{t_c}^{\infty}|J(a,t')|t'dt'\ . \tag{61}$$

$\langle t\rangle_b^{\mathrm{out}}$ was then understood as an average passage *instant* for the wave function leading the barrier region to the right at $x=b$. A similar interpretation was given to the quantities $\langle t\rangle_a^{\mathrm{in}}$ and $\langle t\rangle_a^{\mathrm{out}}$ to define the average *durations* of transmission or reflection as differences between "ingoing" and "outgoing" instants.

A formulation of time delays based also on time averages weighted by the current density at selected positions was introduced by Jaworsky and Wardlaw [26]. They concentrated on time delays with respect to free propagation rather than on the dwell time itself, and their delay times for transmission and reflection were evaluated with respect to some reference or departure time not necessarily coincident with our $\langle t\rangle_a^{\mathrm{in}}$. Similarly, Muga and Cruz [27] and Dumont and Marchioro [16] situate the incident packet around a at the instant $t=0$, and take this point as a reference to evaluate arrival times (only transmission is examined in these two papers). Our τ_T, Eq. (60), would be the same as these arrival times if we took the initial wave packet in such a way that $\langle t\rangle_a^{\rm in}$ were zero. In [16] the emphasis was on the semiclassical limit, while in [27] the dwell, arrival, and life times are compared for resonant scattering in a double barrier.

The average times for transmission and reflection introduced by Olkhovsky and Recami [5] have the same time-integral form as Eq. (61).

Note that in the ingoing average times at a, $\langle t\rangle_a^{\rm in}$, the effect of the noncommutability of P and D remains present, since one cannot separate before the barrier particles to be transmitted and particles to be reflected [7,28]. Independently of this fact, $\langle t\rangle_a^{\rm in}$ remains a significant and well-defined quantity that describes the average ingoing flux behavior at point a. In principle it is accessible experimentally by the time-of-flight technique.

These passage times or average times for transmission and reflection can be expressed in terms of the corresponding stationary phase time delays. The manipulations are similar to the ones carried out by Hauge, Falck, and Fjeldly [20], with different objectives. Olkhovsky and Recami found their expressions for very narrow packets (in momentum), but the following results are generally valid for Gaussian packets, and do not require that limitation.

We start with a wave packet

$$\psi(x,0)=\left[\frac{1}{2\pi\delta^2}\right]^{1/4}\exp\left[\frac{ip_cx}{\hbar}-\frac{(x-x_c)^2}{(4\delta^2)}\right] \tag{62}$$

centered around position x_c and momentum $p_c=\hbar k_c$. Its momentum representation is denoted as $\phi_0(p)$. The initial momentum distribution is $f(p)=|\phi_0(p)|^2$, a Gaussian distribution with variance $\sigma^2=[\hbar/(2\delta)]^2$. Then, far off the barrier one finds

$$\psi_T(x\gg x_2,t)=\frac{1}{\sqrt{h}}\int_0^\infty dp\,\phi_0(p)T(p)e^{i(px-Et)/\hbar} \tag{63}$$

for transmission and

$$\psi_R(x\ll x_1,t)=\frac{1}{\sqrt{h}}\int_0^\infty dp\,\phi_0(p)R(p)e^{-i(px+Et)/\hbar} \tag{64}$$

for reflection. There is in addition a term $\Psi_I(x\ll x_1,t)$, with the incident plane waves. Before collision, for the computation of $\langle t\rangle_a^{\rm in}$, the effect of Ψ_R and its interference with Ψ_I can be ignored. After collision, similarly, Ψ_I can be neglected for evaluating $\langle t\rangle_a^{\rm out}$, provided that a is an asymptotic position.

Substituting expressions (62), (63), and (64) in the time averages (61), making use of the Dirac δ, and using the notations $T(p)\equiv|T(p)|\exp[i\alpha(p)]$ and $R(p)\equiv|R(p)|\exp[i\beta(p)]$, one finds

$$\langle t\rangle_b^{\rm out}=\frac{1}{T}\int_0^\infty dp\,|\phi_0(p)|^2|T(p)|^2\frac{m}{p}\left[b-x_c+\hbar\frac{d\alpha(p)}{dp}\right] \tag{65}$$

and

$$\langle t\rangle_a^{\rm out}=\frac{1}{R}\int_0^\infty dp\,|\phi_0(p)|^2|R(p)|^2\frac{m}{p}\times\left[-a-x_c+\hbar\frac{d\beta(p)}{dp}\right], \tag{66}$$

which show again the simple structure found before between stationary and wave-packet results; see Eq. (32) or (33). The quantity $\tau_T^{\rm Ph}(p)\equiv m[b-x_c+\hbar\alpha'(p)]/p$ consists of the time a classical free particle with mass m and momentum p would spend from x_c to b, plus an amount $m\hbar\alpha'(p)/p$, the *stationary phase time delay*. [Similarly, the term in brackets in (66) is a time spent by a particle that travels freely from x_c to $x=0$, where its momentum is instantly reversed, plus a delay contribution. The integral gives an average for the reflection average *instant*.] Therefore, the average arrival time $\langle t\rangle_b^{\rm out}$ can be, loosely speaking, regarded as the average of the "phase times" $\tau_T^{\rm Ph}(p)$ over a pseudoconditional probability of, beginning at p, having been transmitted. Of course this is more a suggestive metaphor than a rigorous interpretation, and it is subject to the same reservations made after (33). Actually, the evaluation of the second moment provides extra terms without immediate semiclassical interpretation,

$$\langle t^2\rangle_b^{\rm out}=\int_0^\infty dp\,|\phi_0(p)|^2|T(p)|^2\left\{\frac{m[b-x_c+\hbar\alpha'(p)]}{p}\right\}^2+(m\hbar)^2\int_0^\infty\frac{dp}{p^2}\left\{\frac{3}{2p^2}|T(p)|^2|\phi_0(p)|^2-|T(p)|^2|\phi_0(p)|\frac{d^2|\phi_0(p)|}{dp^2}-|\phi_0(p)|^2|T(p)|\frac{d^2|T(p)|}{dp^2}-\frac{1}{2}\frac{d|\phi_0(p)|^2}{dp}\frac{d|T(p)|^2}{dp}\right\}. \tag{67}$$

Using ψ_I in (61), the expression

$$\langle t\rangle_a^{\rm in}=\int_0^\infty dp\,|\phi_0(p)|^2\frac{m(a-x_c)}{p} \tag{68}$$

is also obtained and related to the stationary plane waves.

Figure 4 shows $\langle t\rangle_a^{\rm out}$ versus p_0, the "height" of the barrier in momentum units, in comparison to $\tau_T^{[P,D]_+/2}$, τ_T^{PDP}, and τ_T^{DPD} for the wave packet of Eq. (62) centered at $x_c=-25$ and $p_c=10$, with $\delta=1$ (atomic units and $m=1$ are used throughout). $\langle t\rangle_a^{\rm out}$ is calculated at the right

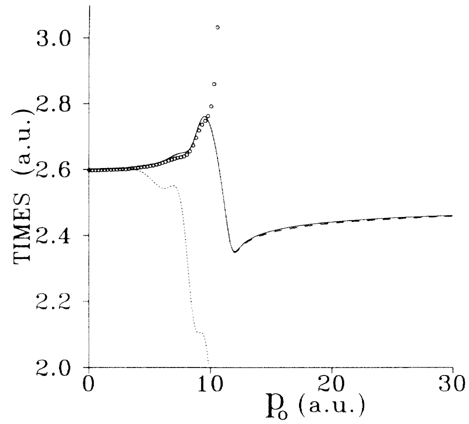

FIG. 4. $\langle t \rangle_d^{\text{out}}$ (solid line), $\text{Re}[\tau_T^{PD}]$ (dashed), τ_T^{PDP} (dotted), and τ_T^{DPD} (circles) as functions of p_0, the "height" of the rectangular barrier in momentum units. the incident wave packet of Eq. (62) has, in atomic units, $p_c=10$, $x_c=-25$ and $\delta=1$. The barrier is located between $x=0$ and $x=d=3\pi/10$ a.u.

edge of the barrier, at $x=d=4\pi/10$, and the spatial interval for the other three quantities is $[x_c,d]$. The times $\langle t \rangle_d^{\text{out}}$, $\tau_T^{[P,D]_+/2}$, and τ_T^{PDP} tend to the classical value when $p_0 \to 0$. Actually τ_T^{DPD} is also close to this value, see the discussion of this limit in Sec. VI C. The first two curves, $\langle t \rangle_d^{\text{out}}$ and $\tau_T^{[P,D]_+/2}$, are in good agreement for all p_0. For the energy range above the barrier they are indistinguishable in the scale of the figure. The agreement is due to the corresponding agreement of the stationary times. The relation between $\tau_T^{\text{Ph}}(p)$ and $\tau_T^{[P,D]_+/2}(p)$ has been discussed by several authors [1,19]: Their difference is only important at low momenta, and it is not significant in our case. In the tunneling region, at large p_0, there is a variety of behaviors.

(a) τ_T^{PDP} goes to zero because for large p_0 an important fraction of $P|\psi\rangle$ is initially on the right of the barrier, so that the overlap with the chosen spatial interval tends to vanish.

(b) τ_T^{DPD}, on the contrary, tends to infinity. By construction, this time is due to the "to be transmitted" part of the wave component $D|\psi\rangle$, Eq. (11). Figure 4 indicates that at large p_0 the barrier acts as a trap for this localized component.

(c) Finally, $\langle t \rangle_d^{\text{out}}$ and $\tau_T^{[P,D]_+/2}$ tend to a finite value. It can be identified as the classical time for a particle traveling between x_c and 0 with momentum p_c. To understand this value, let us separate the stationary phase time $\tau_T^{\text{Ph}}(p)$ as $-mx_c/p+m[d+\hbar\alpha'(p)]/p$. Since the second summand tends to zero as p_0 tends to infinity [29], the integral (65) is basically due to the first summand for large p_0. Also for large p_0, the overlap between $|T(p)|^2$ and $|\phi_0(p)|^2$ in the integrand of (65) is maximum very close to the peak of the Gaussian. The factor $-mx_c/p$ is approximately linear in the overlap region and can be taken out of the integral as its central value $-mx_c/p_c$, thus explaining the observed limiting value.

The case of an interval $[a,b]$ which allows to have interference between ingoing and reflected packets at $x=a$ is discussed in Refs. [5] and [7]. This situation does not correspond to an asymptotic measurement. The difference between the answer given by Olkhovsky and Recami [5] and ours [7] is important and perhaps not easily appreciated at first sight because of the similar notations used in both papers.

To distinguish between an incident and reflected packet Olkhovsky and Recami propose integration over the positive and negative parts, respectively, of the flux at $x=a$. They define the positive and negative parts as corresponding to positive and negative values for J. But if a is close enough to the barrier, the flux at a can be always positive and reflection would seem to not take place. Instead, the separation in [7] distinguishes two contributions, $J^+(a,t)$ and $J^-(a,t)$, from particles going to the right and to the left, respectively, even though the net flux is positive for all times. Our $J^+(a,t)$ nd $J^-(a,t)$ are nothing but the average values of the positive and negative (Hermitian) flux operators, respectively, whose form is better examined using the Weyl-Wigner equivalent representation (see, e.g., [13] and references therein). In particular, the positive flux is

$$J^+(x,t)=\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx' W(x',p,t)\frac{p}{m}\Theta(p)\delta(x-x') , \tag{69}$$

where Θ is the Heaviside function and W the Wigner function. The full current density is given by the same expression without the Heaviside function.

B. Arrival time distributions

The question may be posed whether the time $\langle t \rangle_b^{\text{out}}$ is indeed an average *arrival* time, and $J(b,t)/T$ a distribution of *arrival* times. In the present context the answer is yes, because asymptotically (if b is assumed to be large) the only flux is positive. To see this, one may use the representation of scattering theory in phase space formulated by Snider [30], and Muga and Snider [31]. Briefly, the *scattered* Wigner function can be separated into frequency components and their asymptotic form examined. But the asymptotic value of these components is zero for $p<0$ [32]. Moreover, the *incident* part of the Wigner function has only positive momenta, because of the initial boundary conditions, so no negative flux is possible at b. (In this phase-space representation there are no interference terms between the incident and the scattered parts of the Wigner function.)

C. "Hartman effect"

Relation (65) is suitable for examining the "Hartman effect" [29,33]. Hartman [29] studied the evolution of a wave packet with momentum distribution centered around p_c, colliding with a rectangular barrier of height $V_0>p_c^2/(2m)$, and width d. He found three regions according to the value of d (see also [34]). For large barrier widths (opaque barrier conditions), the stationary phase time associated with k, under the barrier, goes to a constant, $2m/(\hbar k\kappa)$, independent of d. When transmission is dominated by momentum components below the barrier, the transmitted wave packet seems to traverse the potential region in a time interval independent of d. This is the "Hartman effect."

However, if d is increased further, plane waves with momenta above the barrier height dominate the transmission, and classical behavior results, i.e., time grows linearly with d. See [35] for a quantitative description of this effect on the transmittance. Finally, for small barrier widths, Hartman defines a "thin barrier region" where the phase time depends generally on d.

Recently, Olkhovsky and Recami [5] studied this effect using Eqs. (61). Basically, they reached the same conclusions as Hartman did. However, they started by taking an initial wave function only with momenta under the barrier height, and so they did not find the regime corresponding to quasiclassical behavior for very large d. Our purpose next is to quantitatively describe this transition.

Let us consider the initial Gaussian wave packet of Eq. (62), with the center at $x=x_c$ and spatial width δ. For an energy distribution peaked around $E_c < V_0$ the following results can be drawn (see Fig. 5):

(a) For $\kappa_c d \equiv \sqrt{2m(V_0-E_c)}d/\hbar \gg 1$, $\langle t\rangle_d^{\rm out}$ does not vary appreciably when d increases, thus showing Hartman effect. This corresponds to the flat area in Fig. 5.

(b) When d is sufficiently large, the components of the wave packet under the barrier are so strongly depressed by $|T(p)|^2$ that higher momenta start to dominate, and $\langle t\rangle_d^{\rm out}$ grows almost linearly, as one expects classically.

(c) As δ is increases, larger values of d are needed to pass from the first regime to the second one. An estimation of the value of d which gives the transition between Hartman effect and quasiclassical behavior can be obtained for each value of δ by equating the factor $|T(p)|^2|\phi_0(p)|^2$ for $p=p_c$ and for $p=p_r$, where p_r is the momentum of the first resonance above the barrier. This procedure leads to the relation

$$\delta=\frac{\hbar\sqrt{-\ln|T(p_c)|}}{|p_r-p_c|}\approx\frac{\hbar\sqrt{\kappa_c d}}{|p_r-p_c|}\ , \qquad (70)$$

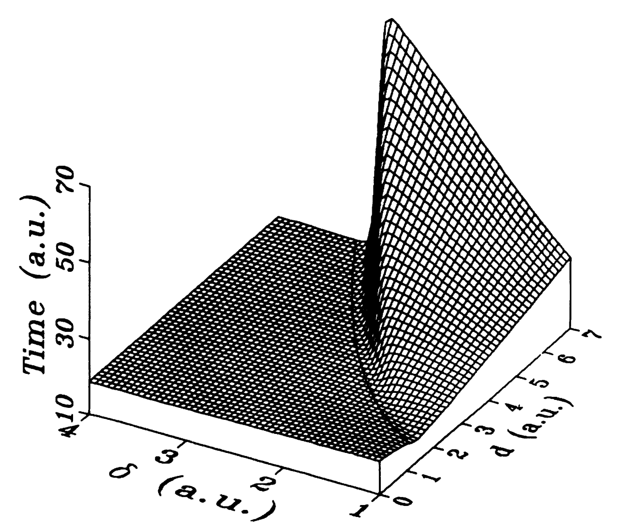

FIG. 5. $\langle t\rangle_d^{\rm out}$ as a function of δ and d, for the wave packet of Eq. (62). $p_c=8$, $x_c=-150$, and $V_0=50$ a.u. The barrier is located in the interval $[0,d]$.

between δ and d, which is also shown in Fig. 5, and that clearly separates quantum and quasiclassical behavior.

(d) For fixed δ, the transition is sharper at larger δ as a consequence of the narrower momentum distribution.

VIII. SUMMARY

We have presented a unifying, systematic theory of "local" interaction times that characterize the passage of a quantum-mechanical particle through a given spatial region. The presence of a potential barrier implies transmitted and reflected components of the wave function in the infinite future. The noncommutativity of the two basic operators P (associated with future transmission) and D (associated with the presence of the particle at the chosen spatial interval) makes the quantum characterization of the temporal aspects of the collision nontrivial. Indeed, finding a fundamental reason for choosing among the various combinations of noncommuting operators is still an open question in quantum mechanics.

The formalism described in Secs. II and III systematically combines P and D. It (a) contains some of the times previously used by other authors; (b) introduces alternative proposals; (c) serves to easily relate one to each other and to find their general properties; (d) allows to establish connections with probability theory concepts; (e) admits generalizations to arbitrarily complex cases, as shown in Sec. IV, because it is entirely based on scattering theory; (f) is equally suitable for stationary or wave-packet scattering; and (g) has been illustrated with a model calculation.

We shall briefly review some of the connections with previous results. Let us first recall, in the stationary case, the gedanken clock experiment which led to the local Larmor times (see, e.g., [19]): A beam of particles fully spin polarized in the y direction impinges on a barrier from the left in the x direction, in the presence of an infinitesimal uniform magnetic field $\mathbf{B}=B\theta(x-a)\theta(b-x)\hat{\mathbf{z}}$ covering the interval $[a,b]$.

We showed [8] that $\tau_T^{PD}(p)=\tau_{xT}(p)-i\tau_{zT}(p)$ and that $\tau_R^{QD}(p)=\tau_{xR}(p)-i\tau_{zR}(p)$, where $\tau_{xT,R}(p)$ are the Larmor times associated with spin precession in the x-y plane for transmitted (reflected) particles, and $\tau_{zT,R}(p)$ are the corresponding Larmor times for rotation in the y-z plane. These complex quantities were therefore identified with the complex "times" introduced by Leavens and Aers [36], or by Sokolovski and Baskin [37]. The moduli of $\tau_T^{PD}(p)$ and $\tau_R^{QD}(p)$ then equal Büttiker-Landauer times for transmission and reflection [18,19]. The "absorption times" were also shown to be equal to the Larmor clock times for spin rotation in successive steps [2,38,8]. While the previous connections were done within stationary scattering, the times examined for wave packets by Jaworsky and Wardlaw in relation to the Larmor clock [39] are also equivalent to the complex quantities τ_T^{PD} and τ_R^{QD} of Sec. III, as shown in [9].

Among the "new times" generated by the different combinations of noncommuting operators, it is easy to see, apart from trivial notational differences, that the transmission and reflection "conditional dwell times" recently given by the Tiggelen, Tip, and Lagendijk [17] are identical with the times τ_T^{PDP} and τ_R^{QDQ}. They were first proposed in [7], and then examined in their stationary and wave-packet versions [8,9].

Incidentally, all the times previously discussed, Larmor (or absorption) times, complex "times," Büttiker-Landauer times, and "conditional dwell times," are generalized in Sec. IV for multidimensional and multichannel scattering. For previous partial generalizations see [2,17,40].

In conclusion, the present formalism offers advantages to study, relate, generalize, or propose different local times. Of course, there is much work to be done from here. In particular, there remains the question of the usefulness and physical relevance, through its applications, of the different times.

Because of the noncommutativity of P and D, none of the times discussed fulfills all the conditions that one would impose on classical grounds (additivity, separability of the dwell time into transmission and reflection components, positivity, . . .). In fact this is a general result for times constructed with P and D. As an example, no combination of P's and D's with two or more D's can be additive. However, these "failures" are not necessarily a drawback in quantum mechanics, nor are they sufficient reason to reject these times as useful or descriptive of the progress of the collision. These times are to be useful through their connections with measurable quantities. Some of the times have been already related to auxiliary quantities, mainly through the Larmor clock and absorption of particles. But this type of connection has not been found for all proposals. By now only $\tau_T^{[P,D]_+/2}$ and $\tau_T^{[P,D]_-/2i}$ (and their combinations, such as the Büttiker-Landauer time and the complex "time") are clearly associated with other observables. Unfortunately, the sole definition of the times is not in general enough to grasp their possible physical associations, if any. As an example, a literal, direct operational interpretation of $\tau_T^{[P,D]_+/2}$ makes it, seemingly, a hopeless quantity to be really measured. Nevertheless, it is *directly connected to the Larmor precession*. As a second example, the *direct* measurement of τ_T^{DPD} by the procedure inspired by its definition in (24) appears also extremely cumbersome [41]. But in this case we ignore whether or not a connection exists between it and other observables that would allow it to be measured indirectly. It is however a candidate for further consideration because of its classical limit (in terms of joint probability distributions), its simplicity, and symmetry.

Some aspects of the temporal evolution of the collision can also be described without P and D operators. Thus, in addition to the systematic study of the times generated by means of combinations of P and D, other times, based on flux properties of the wave packet have been examined. We have (a) compared previous works; (b) justified the interpretation of the (normalized) flux at asymptotic positions as an arrival time distribution; (c) made explicit the connection with stationary phase times for the average and second moment; and (d) found an expression that delimits quantitatively the Hartman effect.

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APPENDIX: ACTION OF P AND Q ON THE SCATTERING STATES

The projection operator P transforms the state $|p^{(+)}\rangle$, with $p>0$, into $T(p)|p^{(-)}\rangle$. This result follows from the definition (3) of P and the relation

$$S_{p'p} \equiv \langle p'^{(-)}|p^{(+)}\rangle = \delta(p-p') - 2i\pi\delta(E_p - E_{p'})T_{p'p} \tag{71}$$

between the matrix elements in momentum representation of the scattering operator, $S_{p'p}$, and of the transition operator, $T_{p'p}$. [$T_{p'p}$ is to be distinguished from T or $T(p)$.]

After integration, one has

$$P|p^{(+)}\rangle = \left[1 - \frac{2\pi i m}{p}T_{pp}\right]|p^{(-)}\rangle = T(p)|p^{(-)}\rangle \ , \tag{72}$$

where the last equality follows from the first of the two relations [8]

$$T(p) = 1 - \frac{2mi\pi}{p}T_{pp} \ ,$$
$$R(p) = -\frac{2mi\pi}{p}T_{-pp} \ . \tag{73}$$

Similarly, the action of Q on $|p^{(+)}\rangle$ can be determined by means of Eq. (71) and a simple integration

$$Q|p^{(+)}\rangle = -\frac{2\pi i m}{p}T_{-pp}|(-p)^{(-)}\rangle = R(p)|(-p)^{(-)}\rangle \ . \tag{74}$$

In the last step, Eq. (73) has been used.

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