Arrival time in quantum mechanics

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A self-adjoint operator with dimensions of time is explicitly constructed, and it is shown that its complete and orthonormal set of eigenstates can be used to define consistently a probability distribution of the time of arrival at a spatial point. [S1050-2947(97)09210-X]

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I. INTRODUCTION

The role that time plays in quantum mechanics has always been controversial. This is in part a consequence of the rather singular status that time exhibits in nonrelativistic physics. In particular, time enters the Schrödinger equation as an external parameter and, accordingly, the quantum formalism is usually concerned with probability distributions of measurable quantities at a definite instant of time. However, one may also ask for the instant of time at which a certain property of a quantum system takes a given value. In this case time has the character of a dynamical variable: It depends on the initial state of the system and on its dynamical evolution, and appears as an intrinsic property of the physical system under study. Since such an instant of time is, in principle, a perfectly measurable quantity it seems natural to try to incorporate the concept of a time observable into the quantum formalism. However, this is not an easy task. The standard quantum formalism associates measurable quantities with self-adjoint operators acting on the Hilbert space of physical states, and postulates that the probability distribution of the outcomes of any well-designed measuring apparatus can be obtained in terms of the orthogonal spectral decomposition of the corresponding self-adjoint operator, with no explicit dependence on the particular properties of the measuring device. Therefore, the problem reduces, in principle, to finding a suitable quantum operator. This is usually accomplished via the correspondence principle, starting from the corresponding classical expressions and quantizing by using certain specific quantization rules. However, in doing so one frequently has to face the problem that in general there exists no unique way to obtain a quantum operator which reduces to a given known expression in the classical limit ($\hbar \to 0$).

Given the Hamiltonian $H(q,p)$ of a conservative classical system, expressed in terms of canonical variables (q,p), one can always make a canonical transformation to new canonical variables (H,T), where H is the Hamiltonian of the system and T its conjugate variable, which satisfies Hamilton's equation [1,2]

$$\frac{dT}{dt} = \{H,T\} = 1, \tag{1}$$

$\{H,T\}$ denoting the Poisson bracket of H and T. The important point is that the above equation clearly reflects that the canonical variable T is nothing but the interval of time. Thus the next step would be to take advantage of this desirable fact and translate the above formulation to the quantum framework. This can be easily accomplished by means of the *canonical quantization method* [3], which basically states that the classical formulation remains formally valid in the quantum domain with the substitution of Poisson brackets by commutators, $\{H,T\} \to 1/i\hbar[\hat{H},\hat{T}]$, and interpreting the dynamical variables as self-adjoint operators in the Heisenberg picture. Then, based on the correspondence principle and the canonical quantization method, one is led to look for a self-adjoint time operator conjugate to the Hamiltonian,

$$[\hat{H},\hat{T}] = i\hbar. \tag{2}$$

As can be easily verified, this commutation relation also holds true in the Schrödinger picture, and has the additional desirable consequence that it implies the uncertainty relation

$$\Delta H \Delta T \geqslant 1/2|[\hat{H},\hat{T}]|, \tag{3}$$

with ΔH and ΔT being the usual root-mean-square deviations of the corresponding dynamical variables. Unfortunately no such time operator exists. As remarked by Pauli, the existence of a self-adjoint operator satisfying the above commutation relation is incompatible with the semibounded character of the Hamiltonian spectrum [4].

The lack of a proper time observable has a number of consequences [5]. In particular, the time-energy uncertainty relation has remained unclear over the time. This is so basically because, contrary to what happens with the well-known position-momentum uncertainty relation, there exists no unique way to put in a quantitative setting what is really meant by the time spread ΔT. In fact the consequences derived from incorrect application of the time-energy uncertainty relation have led to a great deal of confusion.

Another related problem which remains controversial at present is that concerned with the formal definition of traversal and tunneling times [6,7]. This subtle question has received considerable attention in recent years [8–15], motivated in part by the possible applications of tunneling in semiconductor technology. However, the simplest problem involving time as a dynamical variable is that concerned with the time of arrival of a free particle at a given spatial point. Such a time constitutes a well-defined concept which at a classical level can be extracted from the formalism by simply inverting the corresponding equations of motion. Moreover it is a perfectly measurable quantity whose probability distribution can, in principle, be experimentally determined within any desirable precision. However, the standard quantum theory of measurement does not provide any formulation which allows one to infer such a probability distribution. In fact, some time ago Allcock [16] argued against such a possibility. This author claimed that it is not possible to construct any operationally meaningful and apparatus-independent probability formula. Even though more recently a number of works addressing this question from a more optimistic perspective have appeared [9,17–22], the problem is yet far from being resolved, and additional investigation on this fundamental question is worthwhile.

In this paper we analyze the possibility of defining a probability distribution for the arrival time of a quantum particle at a definite spatial point. Specifically, we are interested in searching for an apparatus-independent theoretical prediction for the probability distribution of arrival times at a given spatial point, as a certain function of the initial state of the system. Our results turn out to be similar to those previously obtained by Kijowski [17]. However, the approach by Kijowski was based on the definition of a nonconventional wave function which evolves on a family of $x=\text{const}$ planes (instead of evolving in time according to the Schrödinger equation), and whose relation to the conventional wave function is unclear [23,24]. Our approach, conversely, is entirely developed within the formalism of standard quantum mechanics.

We begin considering in detail the case of a free quantum particle, and then we study the more interesting case of a quantum particle scattered by a potential barrier. For simplicity we shall restrict ourselves to one spatial dimension. For our purpose, it proves to be useful first to analyze in some detail the reason for the nonexistence of a self-adjoint time operator in quantum mechanics.

II. NONEXISTENCE OF A TIME OPERATOR IN QUANTUM MECHANICS

As stated above, according to Pauli's argument, because of the semibounded character of the energy spectrum, there exists no self-adjoint operator conjugate to the Hamiltonian, i.e., satisfying the commutation relation (2). The same negative conclusion was found by Allcock [16] using a somewhat different argument based on the time-translation property of the arrival time concept.

If $\{|T\rangle\}$ denotes a set of measurement eigenstates for the arrival time at a given spatial point of a particle in the quantum state $|\psi\rangle$, then, according to the standard quantum formalism, the probability amplitude for the arrival time at the instant $t=T$ would be given by $\psi(T)=\langle T|\psi\rangle$. If one translates the state of the system forward through time by an amount τ, i.e., $|\psi\rangle\rightarrow|\psi'\rangle=\exp(-i\hat{H}\tau/\hbar)|\psi\rangle$, then it seems natural to expect the probability amplitude to transform according to $\psi(T)\rightarrow\psi'(T)=\psi(T+\tau)$. Since this transformation property must be true for any state vector $|\psi\rangle$, it follows that the measurement eigenstates $\{|T\rangle\}$ must satisfy

$$|T+\tau\rangle=e^{i\hat{H}\tau/\hbar}|T\rangle, \tag{4}$$

which reflects the fact that, under a translation backward in time by an amount τ, any measurement eigenstate corresponding to arrival time at the instant $t=T$ transforms into another measurement eigenstate, corresponding to an arrival time $t=T+\tau$. Based on general grounds, Allcock showed that measurement eigenstates with such a desirable property cannot be orthogonal, which implies that it is not possible to construct the corresponding self-adjoint arrival-time operator. It is not difficult to see that this negative conclusion can be traced back again to the semi-infinite nature of the Hamiltonian spectrum. To this end let us consider the following three statements.

(i) There exists a self-adjoint operator $\hat{T}$ conjugate to the Hamiltonian $\hat{H}$, i.e., satisfying $[\hat{H},\hat{T}]=i\hbar$.

(ii) There exists a self-adjoint operator $\hat{T}$, whose (orthonormal and complete) set of eigenstates $\{|T\rangle\}$ transforms under time-translations as $e^{i\hat{H}\tau/\hbar}|T\rangle=|T+\tau\rangle$.

(iii) There exists a self-adjoint operator $\hat{T}$ which generates unitary energy translations, i.e., such that for any energy eigenstate $|E\rangle$ and any parameter ε with dimensions of energy, it holds that

$$e^{i\hat{T}\varepsilon/\hbar}|E\rangle=|E-\varepsilon\rangle, \tag{5}$$

where the operator $\hat{T}$ is assumed to be defined onto the whole Hilbert space spanned by the Hamiltonian eigenstates.

It is not difficult to see that these statements are in fact equivalent. Indeed, if (i) is true, then, by induction, one has

$$[\hat{H}^n,\hat{T}]=in\hbar\hat{H}^{n-1}, \quad n\geqslant 1, \tag{6}$$

where $\hat{H}^0\equiv\mathbf{1}$. Of course the validity of Eq. (6) rests on the reasonable assumption that the Hamiltonian is well behaved enough so as to guarantee the existence of all its higher integer powers. Since it also holds that $[\hat{H}^n,\hat{T}]=0$ for $n=0$, then, multiplying Eq. (6) by $(i\tau/\hbar)^n/n!$ (τ being an arbitrary parameter with dimensions of time) and summing from $n=0$ to $n=\infty$, one finds

$$[e^{i\hat{H}\tau/\hbar},\hat{T}]=-\tau e^{i\hat{H}\tau/\hbar}. \tag{7}$$

If $\{|T\rangle\}$ denotes a complete and orthonormal set of eigenstates of $\hat{T}$, then, according to Eq. (7), it holds that

$$\hat{T}e^{i\hat{H}\tau/\hbar}|T\rangle=(T+\tau)e^{i\hat{H}\tau/\hbar}|T\rangle, \tag{8}$$

which after suitable choice of normalization and phase leads to statement (ii). Conversely, if (ii) is true for any eigenstate $|T\rangle$ and any parameter τ, then one can repeat the same steps backward to reach (i).

On the other hand, it can be readily seen that statement (i) also implies statement (iii). Indeed, if (i) holds, one has by induction that

$$[\hat{H},\hat{T}^n]=in\hbar\hat{T}^{n-1}, \quad n\geqslant 0 \tag{9}$$

($\hat{T}^0\equiv\mathbf{1}$), which implies that, for any parameter ε with dimensions of energy,

$$[\hat{H},e^{i\hat{T}\varepsilon/\hbar}]=-\varepsilon e^{i\hat{T}\varepsilon/\hbar}. \tag{10}$$

Therefore, according to Eq. (10) any energy eigenstate $|E\rangle$ verifies

$$\hat{H}e^{i\hat{\mathcal{T}}\varepsilon/\hbar}|E\rangle=(E-\varepsilon)e^{i\hat{\mathcal{T}}\varepsilon/\hbar}|E\rangle, \tag{11}$$

from which after proper normalization follows (iii). An analogous reasoning can be repeated from (iii) to (i), which shows the equivalence among the above three statements.

Since (iii) is obviously incompatible with a semibounded Hamiltonian spectrum, it follows that it is not possible to find a self-adjoint arrival time operator satisfying the desirable conditions (i) or (ii).

III. SELF-ADJOINT OPERATOR WITH DIMENSIONS OF TIME

We start by considering the simplest conceivable arrival time problem, namely, a one-dimensional free particle moving along the x axis toward a detector. In looking for a probability distribution of the time of arrival it is most convenient to work in the energy representation $\{|E,\alpha\rangle;E\geqslant 0, \alpha=+,-\}$ defined by the eigenvalue equations

$$\hat{H}_0|E,\pm\rangle=E|E,\pm\rangle, \tag{12}$$

$$\hat{P}|E,\pm\rangle=\pm\sqrt{2mE}|E,\pm\rangle \tag{13}$$

where $\hat{H}_0=\hat{P}^2/2m$ is the Hamiltonian of the free particle, and $\hat{P}$ its momentum operator. The orthonormal and complete set of energy eigenstates $\{|E,\alpha\rangle\}$, which satisfy

$$\sum_{\alpha=\pm}\int_0^\infty dE|E,\alpha\rangle\langle E,\alpha|=\mathbf{1}, \tag{14}$$

$$\langle E,\alpha|E',\alpha'\rangle=\delta_{\alpha\alpha'}\delta(E-E') \tag{15}$$

can be expressed in terms of the usual momentum representation by means of the relation

$$|E,\pm\rangle=(m/2E)^{1/4}|p=\pm\sqrt{2mE}\rangle, \tag{16}$$

where the momentum eigenstates $\{|p\rangle\}$ are normalized as

$$\int_{-\infty}^{+\infty}dp|p\rangle\langle p|=\mathbf{1}, \tag{17}$$

$$\langle p|p'\rangle=\delta(p-p'). \tag{18}$$

As stated above, the impossibility of finding a time-of-arrival operator can always be traced back to the bounded character of the Hamiltonian spectrum. To circumvent such a difficulty we shall instead look for a self-adjoint operator $\hat{\mathcal{T}}$ with dimensions of time, conjugate to a conveniently defined self-adjoint operator $\hat{\mathcal{H}}$, with dimensions of energy and a nonbounded spectrum,

$$[\hat{\mathcal{H}},\hat{\mathcal{T}}]=i\hbar. \tag{19}$$

Of course this is a somewhat arbitrary procedure, since the definition of $\hat{\mathcal{T}}$ depends in a fundamental way on the arbitrary choice one makes for the operator $\hat{\mathcal{H}}$. Moreover, as long as $\hat{\mathcal{H}}$ differs from the Hamiltonian of the system, the corresponding operator $\hat{\mathcal{T}}$ could not be associated to the actual physical time. Therefore, the fundamental question remains of verifying whether it is possible to give a proper physical interpretation to the selected $\hat{\mathcal{T}}$ operator in terms of measurement results, i.e., whether it is possible to define an algorithm which enables us to connect the probability distribution of measurement results with the set of eigenvalues and eigenstates of the operator $\hat{\mathcal{T}}$. At this point we shall postpone this essential question and simply consider the procedure just outlined to be worth exploring.

We now introduce projectors, $\Theta(\pm\hat{P})$, onto the subspaces generated by plane waves with positive and/or negative momenta,

$$\Theta(\pm\hat{P})=\int_0^\infty dp|\pm p\rangle\langle\pm p|, \tag{20}$$

and define the self-adjoint operator

$$\mathrm{sgn}(\hat{P})\equiv\Theta(\hat{P})-\Theta(-\hat{P}). \tag{21}$$

Obviously, $\mathrm{sgn}(\hat{P})$ commutes with the Hamiltonian and satisfies the eigenvalue equation

$$\mathrm{sgn}(\hat{P})|E,\pm\rangle=\pm|E,\pm\rangle. \tag{22}$$

This operator allows us to define a simple self-adjoint operator with dimensions of energy,

$$\hat{\mathcal{H}}\equiv\mathrm{sgn}(\hat{P})\hat{H}_0, \tag{23}$$

which exhibits a nonbounded spectrum,

$$\hat{\mathcal{H}}|E,\pm\rangle=\pm E|E,\pm\rangle \quad (E\geqslant 0). \tag{24}$$

Notice that this is, in a sense, the simplest choice, since the restrictions of $\hat{\mathcal{H}}$ to the subspaces spanned by plane waves with positive and/or negative momentum coincide with plus and/or minus the corresponding restrictions of the Hamiltonian $\hat{H}_0$. Specifically,

$$\Theta(\pm\hat{P})\hat{\mathcal{H}}\Theta(\pm\hat{P})=\pm\Theta(\pm\hat{P})\hat{H}_0\Theta(\pm\hat{P}). \tag{25}$$

Introducing for the energy eigenstates the notation

$$|\varepsilon\rangle=\begin{cases}|+E\rangle\equiv|E,+\rangle & \text{if } \varepsilon\geqslant 0,\\ |-E\rangle\equiv|E,-\rangle & \text{if } \varepsilon<0,\end{cases} \tag{26}$$

the above results can be rewritten in terms of the complete and orthonormal set of states $\{|\varepsilon\rangle;\varepsilon\in(-\infty,+\infty)\}$ satisfying the eigenvalue equations

$$\hat{\mathcal{H}}|\varepsilon\rangle=\varepsilon|\varepsilon\rangle, \tag{27}$$

$$\hat{P}|\varepsilon\rangle=\mathrm{sgn}(\varepsilon)\sqrt{2m|\varepsilon|}|\varepsilon\rangle, \tag{28}$$

$$\hat{H}_0|\varepsilon\rangle=|\varepsilon||\varepsilon\rangle. \tag{29}$$

Now searching for a self-adjoint operator $\hat{\mathcal{T}}$ conjugate to $\hat{\mathcal{H}}$ is a straightforward matter. To this end let us introduce the states $|\tau\rangle$ defined in the $\{|\varepsilon\rangle\}$ basis as

$$|\tau\rangle = h^{-1/2}\int_{-\infty}^{+\infty} d\varepsilon\, e^{i\varepsilon\tau/\hbar}|\varepsilon\rangle. \tag{30}$$

These states also constitute a complete and orthonormal set. Indeed,

$$\langle\tau|\tau'\rangle = \int_{-\infty}^{+\infty} d\varepsilon \langle\tau|\varepsilon\rangle\langle\varepsilon|\tau'\rangle = h^{-1}\int_{-\infty}^{+\infty} d\varepsilon\, e^{-i\varepsilon(\tau-\tau')/\hbar} = \delta(\tau-\tau'), \tag{31}$$

$$\int_{-\infty}^{+\infty} d\tau |\tau\rangle\langle\tau| = h^{-1}\int_{-\infty}^{+\infty} d\tau \int_{-\infty}^{+\infty} d\varepsilon \times \int_{-\infty}^{+\infty} d\varepsilon'\, e^{i(\varepsilon-\varepsilon')\tau/\hbar}|\varepsilon\rangle\langle\varepsilon'| = \int_{-\infty}^{+\infty} d\varepsilon |\varepsilon\rangle\langle\varepsilon| = \mathbf{1}. \tag{32}$$

We can therefore define a self-adjoint operator, with eigenstates and eigenvalues given by $|\tau\rangle$ and τ, respectively, in terms of its spectral decomposition

$$\hat{\mathcal{T}} = \int_{-\infty}^{+\infty} d\tau\, \tau |\tau\rangle\langle\tau|. \tag{33}$$

The operator so defined has dimensions of time and automatically satisfies the commutation relation (19). However, there exists no guarantee that it will be useful in the time-of-arrival problem. In fact, $\hat{\mathcal{T}}$ turns out to be invariant under time reversal, and consequently the variable τ cannot be identified with the physical time t. This can be most easily seen in the momentum representation

$$\langle p|\tau\rangle = (|p|/mh)^{1/2} e^{i\,\mathrm{sgn}(p)(p^2/2m)\tau/\hbar}. \tag{34}$$

Let $\hat{\mathcal{R}}$ denote the time-reversal operator; then we have

$$\hat{\mathcal{R}}|\tau\rangle = \int_{-\infty}^{+\infty} dp |-p\rangle\langle p|\tau\rangle^* = \int_{-\infty}^{+\infty} dp |-p\rangle\langle -p|\tau\rangle = |\tau\rangle, \tag{35}$$

so that, according to Eq. (33), it holds that $\hat{\mathcal{R}}\hat{\mathcal{T}}\hat{\mathcal{R}}^\dagger = \hat{\mathcal{T}}$. Moreover,

$$|\tau+\tau'\rangle = e^{i\hat{\mathcal{H}}\tau'/\hbar}|\tau\rangle \neq e^{i\hat{H}_0\tau'/\hbar}|\tau\rangle, \tag{36}$$

and the states $\{|\tau\rangle\}$ do not exhibit the desirable time-translation property (4) either.

In spite of these facts, it is possible to give a physical interpretation to the operator $\hat{\mathcal{T}}$. As we shall see below, one can consistently define a probability distribution of arrival times in terms of the eigenvalues and eigenstates of this operator. To this end it is convenient to decompose $|\tau\rangle$ to a superposition of negative- and positive-momentum contributions,

$$|\tau\rangle = h^{-1/2}\int_0^\infty dE\, e^{-iE\tau/\hbar}|E,-\rangle + h^{-1/2}\int_0^\infty dE\, e^{iE\tau/\hbar}|E,+\rangle. \tag{37}$$

Defining new states

$$|t,\pm\rangle \equiv h^{-1/2}\int_0^\infty dE\, e^{iEt/\hbar}|E,\pm\rangle, \tag{38}$$

we see that $|\tau\rangle$ can be written in the form

$$|\tau\rangle = |t=-\tau,-\rangle + |t=+\tau,+\rangle. \tag{39}$$

The important point is that $|\tau\rangle$ has been decomposed in terms of states $\{|t,\pm\rangle\}$ which do satisfy the time-translation property (4),

$$|t+\tau',\pm\rangle = e^{i\hat{H}_0\tau'/\hbar}|t,\pm\rangle, \tag{40}$$

and transform under time reversal as

$$\hat{\mathcal{R}}|t,\pm\rangle = |-t,\mp\rangle, \tag{41}$$

so that the variable t, unlike τ, could, in principle, be associated with physical time.

Note that even though the states $\{|t,\pm\rangle\}$ constitute a complete set

$$\sum_{\alpha=\pm}\int_{-\infty}^{+\infty} dt |t,\alpha\rangle\langle t,\alpha| = \mathbf{1}, \tag{42}$$

they are not orthogonal,

$$\langle t,\alpha|t',\alpha'\rangle = \sum_{\beta=\pm}\int_0^\infty dE \langle t,\alpha|E,\beta\rangle\langle E,\beta|t',\alpha'\rangle = \frac{\delta_{\alpha\alpha'}}{h}\int_0^\infty dE\, e^{-iE(t-t')/\hbar} = \tfrac{1}{2}\delta_{\alpha\alpha'}\left\{\delta(t-t') - P.P.\frac{i}{\pi(t-t')}\right\}. \tag{43}$$

For this reason, the states $\{|t,\pm\rangle\}$ cannot be used to construct a self-adjoint operator.

IV. MEAN ARRIVAL TIME

One of the most controversial aspects of quantum mechanics is that concerning the connection between the theoretical formulation and the corresponding measurement results. In its space-time representation, quantum mechanics becomes a continuous wave theory, whereas measuring devices usually deal with individual particles. The quantum formalism tells us how to obtain the probability distribution of the measurement results in terms of projections of the state vector onto appropriate subspaces of the Hilbert space. While in the standard interpretation it is commonly assumed that probability distributions refer to individual particles, their experimental verification requires an ensemble. Quantities defined in the ensemble may offer practical guidance not only in the interpretation of quantum measurement theory, but also in the search for the quantum counterpart of a classical physical variable. In this sense, the mean arrival time may be useful in looking for a probability distribution of arrival times.

Consider a classical statistical ensemble of particles of mass m, directed along a well-defined direction, and characterized by the phase-space distribution function $f(x,p,t)$. The average time of arrival at a spatial point x_0 is given by

$$\langle t_{x_0}\rangle = \frac{\int_{-\infty}^{+\infty} dt\, t\, J(x_0,t)}{\int_{-\infty}^{+\infty} dt\, J(x_0,t)}, \qquad (44)$$

where $J(x_0,t)$ represents the average current at x_0,

$$J(x_0,t) = \int\int f(x,p,t)\frac{p}{m}\delta(x-x_0)dx\,dp, \qquad (45)$$

and plays the role of an unnormalized probability distribution of arrival times. It seems natural to make use of the correspondence principle in order to translate the expression for the classical average time of arrival, Eq. (44), to the quantum formalism. This can be accomplished by substituting $J(x_0,t)$ by the expectation value of the current operator

$$\hat{J}(X) = \frac{1}{2m}(\hat{P}|X\rangle\langle X| + |X\rangle\langle X|\hat{P}). \qquad (46)$$

Such a quantum definition for the average time of arrival has been widely used in recent years [9,18–20]. However, unlike its classical counterpart, even for wave packets directed along a well-defined spatial direction, the quantum probability current is not positive definite. For this reason, it cannot be considered as a probability distribution of individual arrival times, and the validity of the above expressions in a quantum context is questionable. In fact, strictly speaking, $\hat{J}(X)$ is an operator-valued distribution (the operator analog of a generalized function), and, as pointed out by Goldrich and Wigner [25], there exist quantum quantities, such as $\hat{J}(X)$, whose expectation values do not correspond to averages of individual measurements (eigenvalues), but represent a measurable property of the ensemble as a whole.

In spite of the general inadequacy of $\hat{J}(X)$ to describe the probability distribution of arrival times, when quantum backflow contributions become negligible the quantum current becomes positive and admits a probability interpretation [18]. Such a situation occurs, at large times, for freely moving packets containing only positive momenta, and it also occurs under the standard asymptotic conditions of scattering theory. In fact, Eq. (44) can be operationally justified in the quantum case by using a *perfect absorber*, i.e., a complex potential that absorbs the incoming wave in an arbitrary small spatial region, without reflection or transmission [20]. According to such an operational model, which simulates the detection of incoming particles by a destructive procedure, the average time given by Eq. (44) coincides with the average time of absorption (detection) within any desirable precision. Thus, any properly defined arrival time probability distribution should be compatible with Eq. (44).

V. PROBABILITY DISTRIBUTION OF ARRIVAL TIMES: FREE PARTICLE

We shall restrict ourselves to the case of a free particle moving along a well-defined direction toward a detector situated at the point $x=X$. Specifically, we assume that the ingoing asymptote of the actual state of the particle corresponds, in the position representation, to a wave packet which is either a linear superposition of positive plane waves or a linear superposition of negative plane waves,

$$|\psi_{\pm,\mathrm{in}}\rangle \equiv \Theta(\pm\hat{P})|\psi_{\pm,\mathrm{in}}\rangle. \qquad (47)$$

Under these circumstances, the in asymptote becomes indistinguishable from the actual state $|\psi_\pm(t=0)\rangle$, so that we shall not discriminate between them from now on. Note that as a consequence of the commutation between the time-evolution operator $e^{-i\hat{H}_0 t/\hbar}$ and the projectors $\Theta(\pm\hat{P})$, at any time t it also holds that

$$|\psi_\pm(t)\rangle \equiv \Theta(\pm\hat{P})|\psi_\pm(t)\rangle. \qquad (48)$$

As stated in Sec. IV, the mean arrival time at a point X is given by

$$\langle t_X\rangle_\pm = \frac{\int_{-\infty}^{+\infty} d\tau\, \tau \langle\psi_\pm(\tau)|\hat{J}(X)|\psi_\pm(\tau)\rangle}{\int_{-\infty}^{+\infty} d\tau \langle\psi_\pm(\tau)|\hat{J}(X)|\psi_\pm(\tau)\rangle}, \qquad (49)$$

where $\hat{J}(X)$ is the current operator in the Schrödinger picture, given in Eq. (46), and $\langle\psi_\pm(\tau)|\hat{J}(X)|\psi_\pm(\tau)\rangle$ is the probability current at the instant of time $t\equiv\tau$ in the (Schrödinger) state $|\psi_\pm(\tau)\rangle$.

In the free case, we have

$$\int_{-\infty}^{+\infty} d\tau \langle\psi_\pm(\tau)|\hat{J}(X)|\psi_\pm(\tau)\rangle = \pm 1, \qquad (50)$$

so that the mean arrival time $\langle t_X\rangle_\pm$ can be expressed as the expectation value

$$\langle t_X\rangle_\pm \equiv \pm\langle\psi_\pm|\hat{\mathcal{J}}_\pm(X)|\psi_\pm\rangle, \qquad (51)$$

where $|\psi_\pm\rangle$ denotes the state of the particle in the Heisenberg picture, i.e.,

$$|\psi_\pm\rangle = e^{i\hat{H}_0\tau/\hbar}|\psi_\pm(\tau)\rangle = |\psi_\pm(0)\rangle, \qquad (52)$$

and we have introduced the operator

$$\hat{\mathcal{J}}_\pm(X) \equiv \int_{-\infty}^{+\infty} d\tau\, \tau\, \Theta(\pm\hat{P})\hat{J}_{\mathrm{H}}(X,\tau)\Theta(\pm\hat{P}), \qquad (53)$$

where $\hat{J}_{\mathrm{H}}(X,\tau)$ is the Heisenberg current operator,

$$\hat{J}_{\mathrm{H}}(X,\tau) = e^{i\hat{H}_0\tau/\hbar}\hat{J}(X)e^{-i\hat{H}_0\tau/\hbar}. \qquad (54)$$

For later convenience use has been made in the above equations of the identity $|\psi_\pm(0)\rangle \equiv \Theta(\pm\hat{P})|\psi_\pm(0)\rangle$.

Inserting twice the resolution of unity, Eq. (14), and using

$$\Theta(\pm\hat{P})|E,\alpha\rangle=\delta_{\alpha,\pm}|E,\alpha\rangle, \tag{55}$$

$\hat{\mathcal{J}}_{\pm}(X)$ takes the form

$$\hat{\mathcal{J}}_{\pm}(X)=\int_{-\infty}^{+\infty}d\tau\,\tau\int_0^{\infty}dE\int_0^{\infty}dE'\,e^{i(E-E')\tau/\hbar}|E,\pm\rangle \times\langle E,\pm|\hat{J}(X)|E',\pm\rangle\langle E',\pm|. \tag{56}$$

Substituting expression (46) for $\hat{J}(X)$, using Eq. (13), and taking into account that, according to Eq. (16),

$$\langle X|E,\pm\rangle=h^{-1/2}(m/2E)^{1/4}e^{\pm i\sqrt{2mE}X/\hbar}, \tag{57}$$

the matrix element in the integrand of Eq. (56) can be rewritten in the form

$$\langle E,\pm|\hat{J}(X)|E',\pm\rangle =\pm\frac{1}{2h}\left\{\left(\frac{E}{E'}\right)^{1/4}+\left(\frac{E'}{E}\right)^{1/4}\right\}e^{\mp i(\sqrt{2mE}-\sqrt{2mE'})X/\hbar}. \tag{58}$$

After insertion of Eq. (58) into Eq. (56), the operator $\hat{\mathcal{J}}_{\pm}(X)$ reads

$$\hat{\mathcal{J}}_{\pm}(X)=e^{-i\hat{P}X/\hbar}\hat{\mathcal{J}}_{\pm}(X=0)e^{+i\hat{P}X/\hbar}, \tag{59}$$

where we have again taken advantage of Eq. (13) to write

$$e^{i\hat{P}X/\hbar}|E,\pm\rangle=e^{\pm i\sqrt{2mE}X/\hbar}|E,\pm\rangle, \tag{60}$$

and $\hat{\mathcal{J}}_{\pm}(X=0)$, which is the operator involved in the determination of the mean arrival time at the point $X=0$, is given by

$$\hat{\mathcal{J}}_{\pm}(0)=\pm\int_{-\infty}^{+\infty}d\tau\,\tau\int_0^{\infty}dE\int_0^{\infty}dE'\,\frac{1}{2h}\left\{\left(\frac{E}{E'}\right)^{1/4}+\left(\frac{E'}{E}\right)^{1/4}\right\} \times e^{i(E-E')\tau/\hbar}|E,\pm\rangle\langle E',\pm|. \tag{61}$$

In order to guarantee that the integrand is well behaved over the whole interval of integration, we shall restrict ourselves to physical states satisfying the boundary conditions

$$\lim_{E\to\infty}E^{1/4}\langle E,\pm|\psi_{\pm}\rangle=0,$$

$$\lim_{E\to 0}E^{-1/4}\langle E,\pm|\psi_{\pm}\rangle=0, \tag{62}$$

which, in the more familiar momentum representation, take the form

$$\lim_{p\to\pm\infty}\langle p|\psi_{\pm}\rangle=0,\qquad \lim_{p\to 0}p^{-1}\langle p|\psi_{\pm}\rangle=0. \tag{63}$$

Put another way, we shall restrict ourselves to normalizable wave packets, which are superpositions of either positive or negative plane waves, and which vanish faster than p as p approaches zero.

The integral in the τ variable, in Eq. (61), can be readily performed to obtain

$$\hat{\mathcal{J}}_{\pm}(0)=\mp\frac{i\hbar}{2}\int_0^{\infty}dE\int_0^{\infty}dE'\left(\frac{\partial}{\partial E}\delta(E-E')\right) \times\left\{\left(\frac{E}{E'}\right)^{1/4}+\left(\frac{E'}{E}\right)^{1/4}\right\}|E,\pm\rangle\langle E',\pm|. \tag{64}$$

To proceed further, it is convenient to consider the matrix elements of $\hat{\mathcal{J}}_{\pm}(0)$ between arbitrary states $|\Phi\rangle$, $|\Psi\rangle$ satisfying the boundary conditions (62). Using the derivative of the Dirac δ in the integrand of (64) to perform one of the two energy integrals, one arrives at

$$\langle\Phi|\hat{\mathcal{J}}_{\pm}(0)|\Psi\rangle=\pm i\hbar\int_0^{\infty}dE\langle E,\pm|\Psi\rangle\frac{\partial}{\partial E}\langle\Phi|E,\pm\rangle. \tag{65}$$

On the other hand, using the resolution of the unity, Eq. (32), and taking into account that

$$\pm i\hbar\frac{\partial}{\partial E}\langle\tau|E,\pm\rangle=\tau\langle\tau|E,\pm\rangle, \tag{66}$$

one can obtain a useful alternative expression for the energy derivative in the integrand of Eq. (65), in terms of the self-adjoint ''time'' operator defined in Eq. (33). Indeed,

$$\pm i\hbar\frac{\partial}{\partial E}\langle\Phi|E,\pm\rangle=\pm i\hbar\int_{-\infty}^{+\infty}d\tau\langle\Phi|\tau\rangle\frac{\partial}{\partial E}\langle\tau|E,\pm\rangle =\int_{-\infty}^{+\infty}d\tau\,\tau\langle\Phi|\tau\rangle\langle\tau|E,\pm\rangle=\langle\Phi|\hat{\mathcal{T}}|E,\pm\rangle. \tag{67}$$

Therefore,

$$\langle\Phi|\hat{\mathcal{J}}_{\pm}(0)|\Psi\rangle=\int_0^{\infty}dE\langle\Phi|\hat{\mathcal{T}}|E,\pm\rangle\langle E,\pm|\Psi\rangle. \tag{68}$$

Taking $|\Phi\rangle=|\Psi\rangle=e^{+i\hat{P}X/\hbar}|\psi_{\pm}\rangle$, we have

$$\langle t_X\rangle_{\pm}\equiv\pm\langle\psi_{\pm}|e^{-i\hat{P}X/\hbar}\hat{\mathcal{J}}_{\pm}(0)e^{+i\hat{P}X/\hbar}|\psi_{\pm}\rangle= \pm\int_0^{\infty}dE\langle\psi_{\pm}|e^{-i\hat{P}X/\hbar}\hat{\mathcal{T}}|E,\pm\rangle\langle E,\pm|e^{+i\hat{P}X/\hbar}|\psi_{\pm}\rangle. \tag{69}$$

Using the identity

$$|E,\pm\rangle\langle E,\pm|\equiv\Theta(\pm\hat{P})\sum_{\alpha=\pm}|E,\alpha\rangle\langle E,\alpha|, \tag{70}$$

as well as Eq. (14), and taking into account that $\Theta(\pm\hat{P})e^{+i\hat{P}X/\hbar}|\psi_{\pm}\rangle=e^{+i\hat{P}X/\hbar}|\psi_{\pm}\rangle$, we finally find

$$\langle t_X\rangle_{\pm}=\pm\langle\psi_{\pm}|e^{-i\hat{P}X/\hbar}\hat{\mathcal{T}}e^{+i\hat{P}X/\hbar}|\psi_{\pm}\rangle. \tag{71}$$

Accordingly, the self-adjoint operator involved in the determination of the mean arrival time at an arbitrary point X, is given by the spatial translation of the operator $\hat{\mathcal{T}}$ previously defined,

$$\hat{\mathcal{T}}(X)=e^{-i\hat{P}X/\hbar}\hat{\mathcal{T}}e^{+i\hat{P}X/\hbar}, \tag{72}$$

and its spectral resolution reads

$$\hat{\mathcal{T}}(X)=\int_{-\infty}^{+\infty}d\tau\,\tau|\tau;X\rangle\langle\tau;X|, \tag{73}$$

where

$$|\tau;X\rangle=e^{-i\hat{P}X/\hbar}|\tau\rangle$$
$$=h^{-1/2}\int_{-\infty}^{+\infty}d\varepsilon\, e^{i(\varepsilon\tau-\mathrm{sgn}(\varepsilon)\sqrt{2m|\varepsilon|}X)/\hbar}|\varepsilon\rangle. \tag{74}$$

Since the states $\{|\tau;X\rangle\}$ are generated from the complete and orthonormal set $\{|\tau\rangle\}$ via a unitary transformation, they also constitute, for a given X, a complete and orthonormal set.

Introducing the complete but nonorthogonal set of shifted states $\{|t,\pm;X\rangle\}$, defined as the spatial translation of the set $\{|t,\pm\rangle\}$,

$$|t,\pm;X\rangle\equiv e^{-i\hat{P}X/\hbar}|t,\pm\rangle$$
$$=h^{-1/2}\int_{0}^{+\infty}dE\, e^{i(Et\mp\sqrt{2mE}X)/\hbar}|E,\pm\rangle, \tag{75}$$

the states $|\tau;X\rangle$ can be decomposed as a superposition of negative- and positive-momentum contributions, in the form

$$|\tau;X\rangle=|t=-\tau,-;X\rangle+|t=+\tau,+;X\rangle. \tag{76}$$

Inserting now the spectral resolution of $\hat{\mathcal{T}}(X)$, Eq. (73), into Eq. (71), one can express the mean arrival time at the spatial position X, in the form

$$\langle t_X\rangle_{\pm}=\int_{-\infty}^{+\infty}d\tau(\pm\tau)|\langle\tau;X|\psi_{\pm}\rangle|^2, \tag{77}$$

so that

$$\langle t_X\rangle_{+}=\int_{-\infty}^{+\infty}d\tau\,\tau|\langle t=+\tau,+;X|\psi_{+}\rangle|^2, \tag{78}$$

$$\langle t_X\rangle_{-}=\int_{-\infty}^{+\infty}d\tau(-\tau)|\langle t=-\tau,-;X|\psi_{-}\rangle|^2. \tag{79}$$

On the other hand, taking into account the resolution of the unity,

$$\sum_{\alpha=\pm}\int_{-\infty}^{+\infty}dt|t,\alpha;X\rangle\langle t,\alpha;X|=\mathbf{1}, \tag{80}$$

we have

$$1=\langle\psi_{\pm}|\psi_{\pm}\rangle=\int_{-\infty}^{+\infty}dt|\langle t,\pm;X|\psi_{\pm}\rangle|^2, \tag{81}$$

which, for a free particle, coincides with the total probability of arriving at the point X at any instant.

Therefore, the quantities $|\langle\tau;X|\psi_{\pm}\rangle|^2$ enter the above equations as a probability density, and lead to an expression for the mean arrival time having the correct semiclassical limit in terms of the probability current. However, unlike the latter, it is definite positive. Accordingly, for a free particle in the Heisenberg state $|\psi_{+}\rangle$, one can interpret consistently $\langle\tau;X|\psi_{+}\rangle=\langle t=+\tau,+;X|\psi_{+}\rangle$ as the probability amplitude of arriving at the spatial point X from the left, at the instant $t=\tau$. Similarly, for a free particle in the Heisenberg state $|\psi_{-}\rangle$, the scalar product $\langle-\tau;X|\psi_{-}\rangle=\langle t=+\tau,-;X|\psi_{-}\rangle$ can be interpreted as the probability amplitude of arriving at X from the right, at the instant $t=\tau$.

VI. PROBABILITY DISTRIBUTION OF ARRIVAL TIMES. POTENTIAL BARRIER

Consider the passage of particles incident from the left over a one-dimensional potential barrier $V(x)$. As usual, we assume that far away from the scattering center, $V(x)$ vanishes sufficiently fast as to guarantee the validity of the standard scattering theory formalism. Under the conditions we are interested in, the ingoing asymptote, $|\psi_{\rm in}\rangle$, of the actual state of the particle satisfies

$$|\psi_{\rm in}\rangle\equiv\Theta(\hat{P})|\psi_{\rm in}\rangle. \tag{82}$$

The Møller operators $\hat{\Omega}_{\pm}$, which play a central role in scattering theory, are defined as

$$\hat{\Omega}_{\pm}=\lim_{t\to\mp\infty}e^{i\hat{H}t/\hbar}e^{-i\hat{H}_0t/\hbar}, \tag{83}$$

where $\hat{H}_0=\hat{P}^2/2m$, and $\hat{H}=\hat{H}_0+V(\hat{X})$ is the Hamiltonian governing the dynamical evolution of the system. These operators have the importance that they map the asymptotic states onto the corresponding scattering states. Specifically, the actual state of the particle, $|\psi(t=0)\rangle$, is related to its in and out asymptotes, $|\psi_{\rm in}\rangle$ and $|\psi_{\rm out}\rangle$, by means of

$$|\psi(t=0)\rangle=\hat{\Omega}_{+}|\psi_{\rm in}\rangle=\hat{\Omega}_{-}|\psi_{\rm out}\rangle. \tag{84}$$

Making use of the intertwining relations for the Møller operators [26],

$$\hat{\Omega}_{\pm}^{\dagger}\hat{H}\hat{\Omega}_{\pm}=\hat{H}_0, \tag{85}$$

the mean arrival time at a spatial point X, on the right of the barrier and asymptotically far from the interaction region is given by

$$\langle t_X\rangle=\frac{\int_{-\infty}^{+\infty}d\tau\,\tau\langle\psi(\tau)|\hat{J}(X)|\psi(\tau)\rangle}{\int_{-\infty}^{+\infty}d\tau\langle\psi(\tau)|\hat{J}(X)|\psi(\tau)\rangle}, \tag{86}$$

where now we have

$$\langle\psi(\tau)|\hat{J}(X)|\psi(\tau)\rangle=\langle\psi_{\rm in}|e^{i\hat{H}_0\tau/\hbar}\hat{\Omega}_{+}^{\dagger}\hat{J}(X)\hat{\Omega}_{+}e^{-i\hat{H}_0\tau/\hbar}|\psi_{\rm in}\rangle. \tag{87}$$

Inserting twice the resolution of unity, Eq. (17), and taking advantage of Eq. (82) to write $\langle p|\psi_{\rm in}\rangle=\Theta(p)\langle p|\psi_{\rm in}\rangle$, one obtains

$$\langle \psi(\tau)|\hat{J}(X)|\psi(\tau)\rangle = \int_0^\infty dp' \int_0^\infty dp\, e^{iE_{p'}\tau/\hbar} e^{-iE_p\tau/\hbar}\langle\psi_{\rm in}|p'\rangle \times\langle p'|\hat{\Omega}_+^\dagger \hat{J}(X)\hat{\Omega}_+|p\rangle\langle p|\psi_{\rm in}\rangle, \quad (88)$$

where $E_p = p^2/2m$.

The state $|p+\rangle \equiv \hat{\Omega}_+|p\rangle$, which is the solution of the Lippmann-Schwinger equation corresponding to an ingoing plane wave $|p\rangle$, satisfies the eigenvalue equation $\hat{H}|p+\rangle = E_p|p+\rangle$ with the boundary conditions

$$x\to-\infty:\quad \langle x|p+\rangle \sim \langle x|p\rangle + R(p)\langle x|-p\rangle, \quad (89)$$

$$x\to+\infty:\quad \langle x|p+\rangle \sim T(p)\langle x|p\rangle, \quad (90)$$

$R(p)$ and $T(p)$ being the reflection and transmission coefficients, respectively. Thus, for spatial points X on the right and asymptotically far from the interaction center one has

$$\langle p'+|\hat{J}(X)|p+\rangle = T^*(p')T(p)\langle p'|\hat{J}(X)|p\rangle, \quad (91)$$

where use has been made of Eqs. (46) and (90). Substituting in Eq. (88), we obtain

$$\langle \psi(\tau)|\hat{J}(X)|\psi(\tau)\rangle = \int_0^\infty dp' \int_0^\infty dp\, T^*(p')\langle\psi_{\rm in}|p'\rangle \times\langle p'|e^{i\hat{H}_0\tau/\hbar}\hat{J}(X)e^{-i\hat{H}_0\tau/\hbar}|p\rangle \times\langle p|\psi_{\rm in}\rangle T(p). \quad (92)$$

Taking Eq. (92) into account, the τ integral in the denominator of (86) can be readily carried out to obtain a Dirac's delta,

$$\delta(E_{p'}-E_p) = \frac{m}{|p|}\delta(p'-p) + \frac{m}{|p|}\delta(p'+p), \quad (93)$$

and this can in turn be used to obtain finally,

$$\int_{-\infty}^{+\infty} d\tau \langle\psi(\tau)|\hat{J}(X)|\psi(\tau)\rangle = \int_0^\infty dp|T(p)|^2|\langle p|\psi_{\rm in}\rangle|^2, \quad (94)$$

which is nothing but the transmittance. Defining the (unnormalized) freely evolving transmitted state $|\psi_{\rm tr}\rangle$ as

$$|\psi_{\rm tr}\rangle \equiv \int_0^\infty dp\, T(p)\langle p|\psi_{\rm in}\rangle|p\rangle, \quad (95)$$

and using Eq. (92), the mean arrival time (86) takes the form

$$\langle t_X\rangle = \frac{1}{\langle\psi_{\rm tr}|\psi_{\rm tr}\rangle}\langle\psi_{\rm tr}|\int_{-\infty}^{+\infty} d\tau\, \tau\Theta(\hat{P})\hat{J}_{\rm I}(X,\tau)\Theta(\hat{P})|\psi_{\rm tr}\rangle, \quad (96)$$

where we have taken advantage of Eq. (82), and $\hat{J}_{\rm I}(X,\tau)$ denotes the current operator in the interaction picture,

$$\hat{J}_{\rm I}(X,\tau) \equiv e^{i\hat{H}_0\tau/\hbar}\hat{J}(X)e^{-i\hat{H}_0\tau/\hbar}. \quad (97)$$

A comparison between Eqs. (97) and (54) shows that the current operator in the interaction picture coincides with the *free* current operator in the Heisenberg picture. This is the important point which allows us to rewrite $\langle t_X\rangle$ in terms of the freely evolving operator $\hat{\mathcal{J}}_+(X)$ of Eq. (53) and, consequently, exploit the formalism developed in the previous section for the free case, to obtain finally,

$$\langle t_X\rangle = \frac{\langle\psi_{\rm tr}|\hat{\mathcal{J}}_+(X)|\psi_{\rm tr}\rangle}{\langle\psi_{\rm tr}|\psi_{tr}\rangle} = \frac{\langle\psi_{\rm tr}|\hat{\mathcal{T}}(X)|\psi_{\rm tr}\rangle}{\langle\psi_{\rm tr}|\psi_{\rm tr}\rangle}. \quad (98)$$

Inserting the expression for the self-adjoint operator $\hat{\mathcal{T}}(X)$, given in Eqs. (73) and (74), the mean arrival time at a spatial point X behind the barrier and asymptotically far from the interaction center takes the suggestive form

$$\langle t_X\rangle = \frac{1}{\langle\psi_{\rm tr}|\psi_{\rm tr}\rangle}\int_{-\infty}^{+\infty} d\tau\, \tau|\langle\tau;X|\psi_{\rm tr}\rangle|^2. \quad (99)$$

Furthermore, taking into account that, for a given X, the states $\{|\tau;X\rangle\}$ constitute a complete and orthonormal set, we find that the integral

$$\int_{-\infty}^{+\infty} d\tau|\langle\tau;X|\psi_{\rm tr}\rangle|^2 = \langle\psi_{\rm tr}|\psi_{\rm tr}\rangle = \int_0^\infty dp|T(p)|^2|\langle p|\psi_{\rm in}\rangle|^2 \quad (100)$$

coincides with the transmittance, which is nothing but the total probability of arriving at an asymptotic point behind the barrier. Therefore, we can consistently interpret $\langle\tau;X|\psi_{\rm tr}\rangle = \langle t=\tau,+;X|\psi_{\rm tr}\rangle$ as the (unnormalized) probability amplitude of arriving at the asymptotic point X, behind the barrier, at the instant $t=\tau$.

The above results can be expressed in terms of the ingoing asymptote $|\psi_{\rm in}\rangle$ by using the scattering operator $\hat{S} \equiv \hat{\Omega}_-^\dagger\hat{\Omega}_+$, which relates the in and out asymptotes $|\psi_{\rm out}\rangle = \hat{S}|\psi_{\rm in}\rangle$. Indeed, it is shown in the Appendix that the freely evolving transmitted state $|\psi_{\rm tr}\rangle$ can be written as

$$|\psi_{\rm tr}\rangle = \Theta(\hat{P})\hat{S}|\psi_{\rm in}\rangle, \quad (101)$$

so that the (unnormalized) probability density of arriving at an asymptotic point X, behind the barrier, at the instant $t=\tau$ reads

$$|\langle\tau;X|\Theta(\hat{P})\hat{S}|\psi_{\rm in}\rangle|^2 = |\langle t=\tau,+;X|\hat{S}|\psi_{\rm in}\rangle|^2. \quad (102)$$

Finally, it should be noted that when the wave packet corresponding to the actual scattering state at $t=0$ (which is assumed to be a linear superposition of only positive plane waves) does not overlap with the potential barrier, then it becomes physically indistinguishable from the asymptotic ingoing wave packet, and the above equations hold true with the substitution $|\psi_{\rm in}\rangle \to |\psi(t=0)\rangle$.

VII. TIME-ENERGY UNCERTAINTY RELATION

Giving a precise meaning to the well-known time-energy uncertainty relation seems to be a reasonable requirement for any quantum formulation of the time-of-arrival concept. As already stated, the commutation relation $[\hat{H},\hat{T}]=i\hbar$ automatically leads to the uncertainty relation (3). Although, it has not been possible to develop a quantum formulation of the arrival-time concept based on such a commutation relation, there is still room for a time-energy uncertainty relation, because even though the existence of a commutation relation is a sufficient condition for the existence of an uncertainty relation, it is by no means a necessary condition.

It should be noted that the self-adjoint operator $\hat{\mathcal{T}}(X)$ defined by Eqs. (72)–(74) is conjugate to the operator $\hat{\mathcal{H}}$. Specifically,

$$[\hat{\mathcal{H}},\hat{\mathcal{T}}(X)]=e^{-i\hat{P}X/\hbar}[\hat{\mathcal{H}},\hat{\mathcal{T}}]e^{+i\hat{P}X/\hbar}=i\hbar. \tag{103}$$

Introducing a probability amplitude for the time of arrival in terms of the eigenvalues and eigenstates of a self-adjoint operator satisfying the above commutation relation has as an important consequence the existence of a time-energy uncertainty relation. To see this, let us consider the problem studied in Sec.VI, namely, the arrival time of a quantum particle at a detector located behind a potential barrier and asymptotically far from the interaction center. [The free case is nothing but a particular case of the latter corresponding to $T(p)\to 1$, which implies $|\psi_{\rm tr}\rangle\to|\psi_{\rm in}\rangle$.]

Because of Eq. (103), it automatically holds that

$$\Delta\mathcal{H}\Delta\mathcal{T}_X\geq\hbar/2, \tag{104}$$

where $\Delta\mathcal{H}$ and $\Delta\mathcal{T}_X$ are the root-mean-square deviations of the corresponding observables, i.e., $(\Delta\mathcal{H})^2\equiv\langle\hat{\mathcal{H}}^2\rangle-\langle\hat{\mathcal{H}}\rangle^2$, and $(\Delta\mathcal{T}_X)^2\equiv\langle\hat{\mathcal{T}}^2(X)\rangle-\langle\hat{\mathcal{T}}(X)\rangle^2$, with $\langle\hat{\mathcal{A}}\rangle\equiv\langle\psi_{\rm tr}|\hat{\mathcal{A}}|\psi_{\rm tr}\rangle/\langle\psi_{\rm tr}|\psi_{\rm tr}\rangle$. However, from Eqs. (23) and (95) it follows that

$$\hat{\mathcal{H}}|\psi_{\rm tr}\rangle=\hat{H}_0|\psi_{\rm tr}\rangle, \tag{105}$$

and hence $\Delta\mathcal{H}$ coincides with the statistical spread of the energy of particles arriving at the detector,

$$(\Delta\mathcal{H})^2=\langle\hat{H}_0^2\rangle-\langle\hat{H}_0\rangle^2\equiv(\Delta E)^2. \tag{106}$$

On the other hand, according to Eqs. (73) and (98) we have

$$\begin{aligned}(\Delta\mathcal{T}_X)^2&=\langle[\hat{\mathcal{T}}(X)-\langle t_X\rangle]^2\rangle\\&=\frac{1}{\langle\psi_{\rm tr}|\psi_{\rm tr}\rangle}\int_{-\infty}^{+\infty}d\tau(\tau-\langle t_X\rangle)^2|\langle\tau;X|\psi_{\rm tr}\rangle|^2\\&\equiv(\Delta t_X)^2,\end{aligned} \tag{107}$$

and since $|\langle\tau;X|\psi_{\rm tr}\rangle|^2/\langle\psi_{\rm tr}|\psi_{\rm tr}\rangle$ is the probability distribution of the arrival time of particles at the detector, the above equation shows that $\Delta\mathcal{T}_X$ is nothing but the corresponding statistical deviation Δt_X. Therefore, the statistical spreads of the energy, ΔE, and time of arrival, Δt_X, of particles reaching the detector satisfy the time-energy uncertainty relation

$$\Delta E\Delta t_X\geq\hbar/2. \tag{108}$$

VIII. CONCLUSION

Despite its fundamental nature, the quantum formulation of the time-of-arrival concept is a problem which remains open nowadays. This question has the additional interest that probability distributions of arrival times are, in principle, experimentally accessible via the time-of-flight technique. Moreover, a quantum formulation of such a problem may provide a useful tool for a better understanding of the tunneling time problem as well as its possible technological applications.

The main difficulty in defining a quantum time operator lies in the nonexistence, in general, of a self-adjoint operator conjugate to the Hamiltonian, a problem which can be always traced back to the semibounded nature of the energy spectrum. In turn, the lack of a self-adjoint time operator implies the lack of a properly and unambiguously defined probability distribution of arrival times.

Although it has been shown that under certain circumstances of physical interest, the probability current becomes positive and admits a proper interpretation as an unnormalized probability distribution of the time of arrival [18–20], it cannot be considered as a fully satisfactory solution of the problem, for it is not positive definite as it should be.

In searching for a probability distribution defined through a quantum time operator one has to circumvent the problem stated above. There are two possibilities. If one decides that any proper time operator must be strictly conjugate to the Hamiltonian, then one has to abandon the idea of finding a self-adjoint operator. (Even though such a property is a hallmark of any observable in the standard quantum formalism, it is not strictly necessary for a consistent formulation of probability distributions of measurements results [27,28].) If, conversely, one imposes self-adjointness as a desirable requirement for any observable, then one necessarily has to abandon the requirement that such an operator be conjugate to the Hamiltonian. In the present paper we have adopted the latter view. We have explicitly constructed a self-adjoint operator $\hat{\mathcal{H}}$ with dimensions of energy, and a nonbounded spectrum. Such an operator is essentially the energy of the particle with the sign of its momentum. The nonbounded character of its spectrum enables us to introduce a self-adjoint operator with dimensions of time, $\hat{\mathcal{T}}$, by demanding it to be conjugate to $\hat{\mathcal{H}}$. Since the latter is essentially the Hamiltonian, except for sign, one expects the self-adjoint operator $\hat{\mathcal{T}}$ so defined to be physically meaningful and relevant to the arrival time problem. Indeed, we have shown that it is possible to define consistently a probability distribution of arrival times at a spatial point, in terms of the eigenvalues and eigenstates of such an operator. This probability distribution, which is a function of the initial state of the system, does not depend on the particular design of the measuring device, and has the additional desirable consequence that it leads to a precisely defined time-energy uncertainty relation.

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APPENDIX A: TRANSMITTED STATE AS A FUNCTION OF THE INGOING ASYMPTOTE

In this appendix we show that the freely evolving transmitted state $|\psi_{\rm tr}\rangle$ can be written in terms of the ingoing asymptote $|\psi_{\rm in}\rangle$ in the form [Eq. (101)]

$$|\psi_{\rm tr}\rangle=\Theta(\hat{P})|\psi_{\rm out}\rangle=\Theta(\hat{P})\hat{S}|\psi_{\rm in}\rangle, \qquad (A1)$$

where $\hat{S}$ denotes the scattering operator, relating the ingoing and outgoing asymptotes,

$$|\psi_{\rm out}\rangle=\hat{S}|\psi_{\rm in}\rangle=\int_{-\infty}^{+\infty}dp'\int_{-\infty}^{+\infty}dp|p'\rangle\langle p'|\hat{S}|p\rangle\langle p|\psi_{\rm in}\rangle. \qquad (A2)$$

Taking into account that the matrix elements of the scattering operator can be written in terms of the *on-the-energy-shell* $\hat{\mathsf{T}}$ *matrix* as [26]

$$\langle p'|\hat{S}|p\rangle=\delta(p-p')-2\pi i\,\delta(E_p-E_{p'})\langle p'|\hat{\mathsf{T}}(E_p+i0)|p\rangle, \qquad (A3)$$

Eq. (A2) reads

$$\begin{aligned}|\psi_{\rm out}\rangle&=\hat{S}|\psi_{\rm in}\rangle\\ &=\int_0^\infty dp[1-2\pi im/p\langle p|\hat{\mathsf{T}}(E_p+i0)|p\rangle]\langle p|\psi_{\rm in}\rangle|p\rangle\\ &\quad+\int_0^\infty dp[-2\pi im/p\langle -p|\hat{\mathsf{T}}(E_p+i0)|p\rangle]\\ &\quad\times\langle p|\psi_{\rm in}\rangle|-p\rangle. \end{aligned}\qquad (A4)$$

On the other hand, from the Lippmann-Schwinger equation for $|p+\rangle$, it follows that the wave function $\langle x|p+\rangle$ can be written as

$$\begin{aligned}\langle x|p+\rangle=\langle x|p\rangle+\int dx'\langle x|(E_p+i0-\hat{H}_0)^{-1}|x'\rangle\\ \times\langle x'|\hat{\mathsf{T}}(E_p+i0)|p\rangle.\end{aligned}\qquad (A5)$$

Substituting in the above equation the expression for the Green's function (which can be easily obtained by inserting the resolution of unity in terms of momentum eigenstates and evaluating the resulting integral by contour integration in the complex plane),

$$\langle x|(E_p+i0-\hat{H}_0)^{-1}|x'\rangle=-\frac{im}{\hbar|p|}e^{i|p||x-x'|/\hbar}, \qquad (A6)$$

one obtains, for $p>0$ and $x\to+\infty$,

$$\begin{aligned}\langle x|p+\rangle&\sim\langle x|p\rangle-2\pi im/p\langle x|p\rangle\int dx'\langle p|x'\rangle\\ &\quad\times\langle x'|\hat{\mathsf{T}}(E_p+i0)|p\rangle\\ &=[1-2\pi im/p\langle p|\hat{\mathsf{T}}(E_p+i0)|p\rangle]\langle x|p\rangle.\end{aligned}\qquad (A7)$$

A comparison with Eq. (90) yields

$$T(p)=[1-2\pi im/p\langle p|\hat{\mathsf{T}}(E_p+i0)|p\rangle]. \qquad (A8)$$

Similarly, for $p>0$ and $x\to-\infty$, Eq. (A5) leads to

$$\begin{aligned}\langle x|p+\rangle&\sim\langle x|p\rangle-2\pi im/p\langle x|-p\rangle\int dx'\langle -p|x'\rangle\\ &\quad\times\langle x'|\hat{\mathsf{T}}(E_p+i0)|p\rangle\\ &=\langle x|p\rangle+[-2\pi im/p\langle -p|\hat{\mathsf{T}}(E_p+i0)|p\rangle]\\ &\quad\times\langle x|p-\rangle,\end{aligned}\qquad (A9)$$

and comparing with Eq. (89) we find

$$R(p)=[-2\pi im/p\langle -p|\hat{\mathsf{T}}(E_p+i0)|p\rangle]. \qquad (A10)$$

Substituting Eqs. (A8) and (A10) in (A4) we finally arrive at

$$\begin{aligned}|\psi_{\rm out}\rangle&=\hat{S}|\psi_{\rm in}\rangle\\ &=\int_0^\infty dp\,T(p)\langle p|\psi_{\rm in}\rangle|p\rangle+\int_0^\infty dp\,R(p)\langle p|\psi_{\rm in}\rangle|-p\rangle,\end{aligned}\qquad (A11)$$

from which follows Eq. (A1).

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