

Space-time properties of free-motion time-of-arrival eigenfunctions

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The properties of the time-of-arrival operator for free motion introduced by Aharonov and Bohm [Phys. Rev. **122**, 1649 (1961)] and of its self-adjoint variants are studied. The domains of applicability of the different approaches are clarified. It is shown that the arrival time of the eigenfunctions is not sharply defined. However, strongly peaked real-space (normalized) wave packets constructed with narrow Gaussian envelopes centered on one of the eigenfunctions provide an arbitrarily sharp arrival time. [S1050-2947(98)05612-1]

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I. INTRODUCTION

The extension of the classical *arrival-time* concept to quantum mechanics is problematic because of the absence of trajectories in the standard interpretation of the quantum formalism. The question is important since the detection of particles in time-of-flight and coincidence experiments is quite common and quantum mechanics should be able to predict and interpret the statistics of the arrivals. A recent review discusses the main theoretical approaches and open questions [1].

The customary way to specify a dynamical variable in quantum mechanics is to define the corresponding operator, but Pauli showed that a self-adjoint time operator conjugate to the Hamiltonian \hat{H} cannot be constructed if the spectrum of \hat{H} is bounded from below [2]; see also [3–5]. There are, however, several ways to circumvent this objection and quantize the classical arrival time, at least in simple cases such as free motion. Aharonov and Bohm introduced the operator [6]

$$\hat{T} = -m \left(\hat{q} \frac{1}{\hat{p}} - \frac{\hbar}{2i} \frac{1}{\hat{p}^2} \right) = -\frac{m}{2} \left(\hat{q} \frac{1}{\hat{p}} + \frac{1}{\hat{p}} \hat{q} \right) \quad (1)$$

by symmetrizing the classical expression for the time of arrival at $X=0$ for a particle with position q and momentum p at time $t=0$. The same result is obtained by using the quantization rules of Weyl, Rivier, or Born-Jordan [7], but this coincidence does not justify Eq. (1) since, *a priori*, no rule is more fundamental than any other rule. They simply provide a number of quantum generalizations of a classical quantity; one (or some) of these can be selected by requiring either agreement with a particular experimental procedure or that certain desirable conditions be satisfied, such as properties obeyed by the classical counterpart. It is thus essential to carefully examine the behavior of a given operator and of its eigenfunctions to ascertain their ultimate physical content. Paul and others have examined the mathematical properties of \hat{T} as a linear operator in Hilbert space [8–10,4]. In Sec. II we shall first review these properties. Then the relations between \hat{T} and positive operator value measures, or its self-adjoint variants, are examined and the important question of the domains of applicability of the theories associated with

the different operators is clarified. In Sec. III less abstract aspects are studied, such as the functional form of the eigenfunctions in the coordinate representation and their time dependence. Finally, the behavior of normalized wave packets “peaked” around one of the eigenfunctions is discussed in Sec. IV.

II. TIME OPERATORS

\hat{T} is not a self-adjoint operator, but it is in a sense the next best thing, namely, a maximal symmetric operator [10–12]. This means that it is Hermitian (or “symmetric” in the mathematical literature), but it does not admit a self-adjoint extension. Indeed, one way to circumvent Pauli’s argument is to relax the standard requirement and admit Hermitian but non-self-adjoint operators as representations of physical properties. By imposing Hermiticity and square integrability of the states in its range, its domain $D(\hat{T})$ is given by the set of states with momentum representation obeying [8]

$$\lim_{p \rightarrow 0} \frac{\phi(p)}{p^{3/2}} \rightarrow 0. \quad (2)$$

The eigenvalue equation in momentum representation $\langle p | \hat{T} | \psi \rangle = T \langle p | \psi \rangle$,

$$-mi\hbar \left(\frac{1}{p} \frac{d}{dp} - \frac{1}{2p^2} \right) \langle p | \psi \rangle = T \langle p | \psi \rangle, \quad (3)$$

is solved (for $p \neq 0$) by

$$\langle p | T, \alpha \rangle = (|p|/mh)^{1/2} e^{ip^2 T/(2m\hbar)} \Theta(\alpha p), \quad (4)$$

where $\alpha = \pm$ and Θ is the Heaviside step distribution. These are “weak eigenfunctions” [4] that satisfy $\langle T, \alpha | (\hat{T} - T) | \phi \rangle = 0$, for all $\phi \in D(\hat{T})$. These (improper) eigenfunctions have the appropriate transformation behavior for a state arriving at time T ,

$$e^{-i\hat{H}t/\hbar} | T, \alpha \rangle = | T - t, \alpha \rangle, \quad (5)$$

namely, if the original state had already evolved for a time t then it would arrive at $T - t$ instead; however, they are not

square integrable functions so they do not define physically realizable state vectors in the Hilbert space $\mathcal{H} = L^2$. The constant factor in Eq. (4) is chosen to satisfy the resolution of the identity

$$1_{\text{op}} = \sum_{\alpha} \int_{-\infty}^{\infty} dT |T, \alpha\rangle \langle T, \alpha|. \quad (6)$$

In the physical interpretation of this expression, one assumes that all particles arrive sooner or later. Notice the inclusion of negative times. In an experimental context, all measured arrival times are positive if the single-particle state $\psi(t)$ of interest is prepared at the instant $t=0$. However, as discussed in considerable detail by Grot *et al.* [13], the theoretical analysis is much simpler if one considers a different problem in which it is imagined that the state is prepared at $t = -\infty$ in the state that (in the absence of an interaction) evolves to the actually prepared state $\psi(t=0)$ and the arrival time distribution includes both negative and positive arrival times. This is very useful from the mathematical point of view [e.g., see Eq. (6) or Eqs. (15) and (22) below.]

The eigenfunctions $|T, \alpha\rangle$ are complete, but they are not orthogonal,

$$\langle T', \alpha' | T, \alpha \rangle = \frac{\delta_{\alpha, \alpha'}}{2} \left[\delta(T - T') + \frac{i}{\pi} \text{P} \left(\frac{1}{T - T'} \right) \right]. \quad (7)$$

The nonorthogonality of the eigenstates has been associated with the intrinsically ‘‘unsharp’’ character of this ‘‘observable’’ by the proponents of the ‘‘operational approach to quantum mechanics’’ [11]. Giannitrapani in particular [4], points out that the states $|T, \alpha\rangle$ provide a ‘‘positive operator value measure’’ (POVM) for the arrival time. This means that for an interval of time $[T_1, T_2]$ the positive, bounded operator

$$\hat{B}(T_2, T_1) = \sum_{\alpha} \int_{T_1}^{T_2} |T, \alpha\rangle \langle T, \alpha| \quad (8)$$

can be constructed. This is not a projector, but one does not necessarily require projectors in order to introduce probabilities in quantum mechanics [11,14]. By taking the trace with the normalized physical density operator $\hat{\rho}$, the function

$$P(T_2, T_1) = \text{tr}[\hat{B}(T_2, T_1)\hat{\rho}] \quad (9)$$

fulfills in principle the conditions of a probability for arrival between T_1 and T_2 : It is positive, additive for disjoint sets, and, using Eq. (6), tends to 1 as $T_1 \rightarrow -\infty$ and $T_2 \rightarrow \infty$. In particular, an arrival time distribution (for a pure state ψ at time t) is defined by

$$\Pi(T; \psi(t)) = \sum_{\alpha} |\langle T, \alpha | \psi(t) \rangle|^2. \quad (10)$$

According to Eq. (5), the POVM satisfies the ‘‘covariance condition’’

$$e^{-i\hat{H}t/\hbar} \hat{B}(T_2, T_1) e^{i\hat{H}t/\hbar} = \hat{B}(T_2 - t, T_1 - t). \quad (11)$$

and this means in particular that

$$\Pi(T; \psi(0)) = \Pi(T - t; \psi(t)). \quad (12)$$

In words, the probability for arriving at T is equal to the probability for arriving at $T - t$ when the original state has evolved a time t . This is a basic physical requirement that any candidate for an arrival time distribution should obey. This is of course also true in classical mechanics.

The time-of-arrival operator \hat{T} is the ‘‘first moment’’ of the POVM. For any ϕ and $\psi \in D(\hat{T})$,

$$\begin{aligned} \langle \phi | \hat{B}^{(1)} | \psi \rangle &\equiv \int T \langle \phi | \hat{B}(dT) | \psi \rangle = \langle \phi | \hat{T} | \psi \rangle \\ &= \sum_{\alpha} \int_{-\infty}^{\infty} dT \langle \phi | T, \alpha \rangle T \langle T, \alpha | \psi \rangle. \end{aligned} \quad (13)$$

There are in principle other POVMs compatible with Eqs. (11) and (13), but Eq. (8) has the following unique feature: Its second moment operator obeys, for states in $D(\hat{T})$,

$$\Delta(\psi) \equiv \int T^2 \langle \psi | \hat{B}(dT) | \psi \rangle - \langle \hat{T} \psi | \hat{T} \psi \rangle = 0, \quad (14)$$

which is by no means an obvious relation since the eigenvectors of \hat{T} are not orthogonal. [An equation like Eq. (14) would be satisfied trivially by a self-adjoint operator since in that case the moments of the distribution of the observable are obtained as the expectation values of the powers of the operator.] $\Delta(\psi)$ is called the variance form [10]. In classical mechanics the true arrival time distribution makes the analogous quantity minimal, so this property has also been invoked to select a proper quantum distribution [15,10].

Another condition satisfied by $\Pi(T)$ is that, for the state ψ_1 defined by $\langle p | \psi_1 \rangle = \langle p | \psi \rangle^*$,

$$\Pi(T, \psi(0)) = \Pi(-T, \psi_1(0)), \quad (15)$$

which follows immediately from the symmetry property

$$\langle p | T, \alpha \rangle^* = \langle p | -T, \alpha \rangle. \quad (16)$$

Equation (15) is also a classically motivated relation that must hold when the arrival point is $X=0$ [15,10]. (If only covariance and minimum variance were imposed the arrival point would not be specified.)

The distribution of arrival times (10) was obtained by Kijowski [15] and was later rederived, studied, or generalized by several authors [10,16,13,5,17,18]. Werner in particular [10], for states with positive momenta justified the uniqueness of Eq. (10) subject to the conditions (12), (14), and (15). Grot, Rovelli, and Tate [13] introduced a regularized self-adjoint operator and considered the full expression (10) for possible application to more general states having both positive and negative momenta but vanishing in the proximity of $p=0$. Delgado and Muga [5], for states with purely positive or negative momenta, arrive at the distribution using a different self-adjoint operator. We shall next discuss these two proposals for self-adjoint arrival time operators.

Self-adjoint variants of \hat{T}

Grot, Rovelli, and Tate [13] trace the nonorthogonality of the eigenfunctions to the singularity at $p=0$, and produce a ‘regularized’ self-adjoint time operator \hat{T}_ε with eigenfunctions that differ from Eq. (4) only in a small momentum region around $p=0$,

$$\langle p|T_\pm\rangle_\varepsilon = \Theta(\pm p)[hm f_\varepsilon(p)]^{-1/2} \exp\left(\frac{iT}{m\hbar} \int_{\pm\varepsilon}^p \frac{dp'}{f_\varepsilon(p')}\right), \quad (17)$$

where ε is a small positive number,

$$f_\varepsilon = \begin{cases} 1/p, & |p| > \varepsilon \\ \varepsilon^{-2}p, & |p| < \varepsilon. \end{cases} \quad (18)$$

The integral in Eq. (17), which plays the role of the energy when divided by m , becomes

$$\int_{\pm\varepsilon}^p \frac{dp'}{f_\varepsilon(p')} = \begin{cases} (p^2 - \varepsilon^2)/2, & |p| > \varepsilon \\ \varepsilon^2 \ln(|p|/\varepsilon), & |p| < \varepsilon, \end{cases} \quad (19)$$

so that the regularization amounts to changing the energy spectrum in the region around $p=0$ by introducing negative energies. In this manner Pauli’s objection is avoided. While Grot, Rovelli, and Tate modify the eigenfunctions (and therefore the time operator) in the proximity of $p=0$, Paul discussed a similar idea [8], namely, to modify the physical state vector wave functions infinitesimally around this point so that \hat{T} can be applied to them. He concluded, however, that such modifications were not physically meaningful since these infinitesimal changes may lead, for example, to arbitrary values of the expectation value of the square of \hat{T} , $\langle \hat{T}^2 \rangle$. Note that the small p region is responsible for the long time asymptotic behavior of the arrival time distribution (see Appendix A) and therefore any infinitesimal change there affects drastically quantities such as $\langle \hat{T}^n \rangle$, even though it will affect only infinitesimally other expectation values, for example, $\langle \hat{q}^n \rangle$, or $\langle \hat{p}^n \rangle$, with $n=1,2,3,\dots$ [8]. Paul’s observation is correct, but we shall argue in Sec. V that the consequences are not necessarily as negative as he thought.

A second proposal that was already pointed out by Kijowski (Sec. 8 of [15]) and has been developed further by Delgado and Muga [5] is to take the two pieces of \hat{T} ,

$$\hat{T} = \hat{T}\Theta(\hat{p}) + \hat{T}\Theta(-\hat{p}), \quad (20)$$

the first acting on the positive momentum subspace and the second acting on the negative momentum subspace, and combine them with a negative sign instead,

$$\hat{T}_- = \hat{T}\Theta(\hat{p}) - \hat{T}\Theta(-\hat{p}). \quad (21)$$

This operator is self-adjoint and has eigenvectors $|T\rangle$ formed by the combination

$$|T\rangle \equiv |T+\rangle + |-T-\rangle. \quad (22)$$

This time operator avoids Pauli’s argument in a different manner. It is not conjugate to \hat{H} but to an operator \hat{H}

$= \text{sgn}(\hat{p})\hat{H}$ related to \hat{H} by the change of the sign for negative momenta. Technically, because \hat{T} is a maximal symmetric operator, \hat{T}_- cannot be its self-adjoint extension and only gives the same result as \hat{T} when acting on the subspace of positive momenta (there is a change of sign for the negative momentum subspace).

So one can in principle construct self-adjoint variants of \hat{T} . However, what do they mean and what information can we extract from them? Unfortunately, neither the states $|T_\pm\rangle_\varepsilon$ nor the states $|T\rangle$ transform according to Eq. (5). Equivalently, none of the self-adjoint operators discussed satisfies the covariance condition and the arrival-time distributions computed with them do not in general satisfy the basic physical requirement (12). To avoid this problem, in both approaches the domains of *physical applicability* of the self-adjoint operators have to be restricted with respect to the mathematical domains. For the approach by Grot, Rovelli, and Tate the domain should be restricted to states with momentum support outside the regularization region around $p=0$ ($-\varepsilon, \varepsilon$), so that in fact the arrival time distribution is again given by Eq. (10). Similarly, the approach associated with \hat{T}_- is only physically meaningful for states with purely positive/negative momenta and the corresponding distributions are therefore contained in Eq. (10). In summary, the apparent advantage of these two proposals is misleading since in practice they are only applicable when their results are equivalent to the ones provided by the POVM related to the Aharonov-Bohm operator. In fact, the limitations on the domains of applicability of these two approaches are quite severe. The arrivals at a screen or detector will occur for all states in \mathcal{H} and not just for a special set of states. A complete theory should provide the arrival-time distribution in all cases. The important point is that the distribution associated with the POVM applies for all states in \mathcal{H} (irrespective of their behavior at $p=0$), so it is in this sense a more complete approach. This is perfectly compatible with $D(\hat{T}) \neq \mathcal{H}$ since the time operator is only one of its moments. Let us recall that a probability distribution exists independently of the existence of its moments. In fact, in classical mechanics ensembles with nonzero probability at $p=0$ have no finite average arrival time, but the distribution is nevertheless well defined. In this respect only the POVM approach provides a correct classical limit.

In summary, the distribution $\Pi(T)$ is satisfactory in many ways. There is, however, an important point that has not been considered yet. How do the eigenfunctions of \hat{T} behave? Do they really represent states that arrive at a given time for a given position? The meaning of these eigenfunctions, although central, has not been sufficiently discussed. In particular, they have always been studied in the momentum representation without paying attention to its coordinate representation and time dependence. These aspects are examined in Sec. III. Before doing so, it is noted that, because of the symmetry (16), the coordinate representations of the time evolved states $|T_t \pm\rangle \equiv \exp(-i\hat{H}t/\hbar)|T_\pm\rangle$ are related by

$$\langle x|T_t-\rangle = \langle -x|T_t+\rangle, \quad (23)$$

so that it is enough to study one of the cases. Further simplification comes from the fact that, as a consequence of Eq. (5), studying the time dependence of one of the states, say $|T'_i+\rangle$, from $t=0$ to the nominal arrival time $t=T'$, is equivalent to considering the sequence of eigenstates $|T+\rangle$ from $T=T'$ to $T=0$. The space-time analysis that we shall carry out in the next section should be taken with some precaution because these are not square integrable states. As occurs with the continuum stationary states used in scattering theory, their physical interpretation requires the construction of normalizable wave packets peaked at one of them.

III. COORDINATE REPRESENTATION

The coordinate representation of the wave function (4) is given by the integral

$$\langle x|T+\rangle = \int_0^\infty \langle x|p\rangle \left(\frac{p}{m\hbar}\right)^{1/2} e^{ip^2T/2m\hbar} dp, \quad (24)$$

where δ -function normalization $\langle x|p\rangle = h^{-1/2} \exp(ipx/\hbar)$ is used for the plane waves. Let us assume for the time being that $T > 0$. The original path of integration is very inefficient numerically because of the rapid oscillations of the exponentials. The easiest way to calculate the integral is to deform the contour in the complex p plane along the imaginary axis from the origin up to the intersection with the steepest descent path defined by

$$p_I = mx/T + p_R \quad (25)$$

(p_R and p_I are, respectively, the real and imaginary parts of p) and then to follow this steepest descent path rightward to infinity in the first quadrant. The saddle is on the real axis at $-mx/T$. Two cases have to be distinguished. For $x > 0$ the path does not cross the saddle and the value of the integral is small. In this case the origin is the only relevant critical point. Use of Watson's lemma [19] for large x and small T provides the leading term

$$\langle x|T+\rangle \sim \frac{h^{1/2} e^{3i\pi/4}}{x^{3/2} \pi^{5/2} m^{1/2}}, \quad x \rightarrow \infty. \quad (26)$$

Note that this asymptotic behavior is independent of T . However, for $x < 0$ the saddle becomes the dominant critical point. Retaining the leading term [19],

$$\langle x|T+\rangle \sim \frac{(m|x|/\hbar)^{1/2}}{T} e^{i\pi/4} e^{-ix^2m/2\hbar T}, \quad x \rightarrow -\infty. \quad (27)$$

In the first case $\langle x|T+\rangle$ decreases as $x^{-3/2}$, whereas in the second one it increases as $|x|^{1/2}$ asymptotically. In fact, the integral can be expressed exactly in terms of parabolic cylinder functions, but the approximate critical point treatment just outlined is worthwhile since it allows a simple rationalization of the exact results. By means of the change of variable

$$s = \alpha p, \quad (28)$$

where

$$\alpha = -\left[\frac{T}{m\hbar}\right]^{1/2} e^{-i\pi/4}, \quad (29)$$

Eq. (24) becomes

$$\frac{1}{hm^{1/2}(\alpha^{1/2})^3} \int_C ds s^{1/2} e^{-s^2/2 + zs}, \quad (30)$$

where all square roots are calculated with a branch cut on the negative real axis and

$$z = x e^{-i\pi/4} \left(\frac{m}{\hbar T}\right)^{1/2}. \quad (31)$$

The integration path C in Eq. (30) goes now from 0 to ∞ along the bisector of the second quadrant in the complex s plane. Note that z is the saddle point of $\exp(w) \equiv \exp(-s^2/2 + sz)$. It lies on the bisector of the second/fourth quadrant for positive/negative x . The steepest descent paths from it are parallel to the real axis and C lies on the border between the "hill" and "valley" [$w_R \equiv \text{Re}(w) = 0$]. It can, however, be deformed into a line just above the branch cut since there is no contribution at infinity. As the integrand across the branch cut simply changes sign, Eq. (30) is one-half of the loop integral around the cut. In this fashion one of the integral forms of the parabolic cylinder function $D_{-3/2}(z)$ can be recognized [20],

$$\langle x|T+\rangle = \frac{\Gamma(3/2)}{hm^{1/2}(\alpha^{1/2})^3} e^{z^2/4} D_{-3/2}(z). \quad (32)$$

The asymptotic behavior for large $|z|$ (see [21]) is in agreement with the expressions (26) and (27). The corresponding results for the case $T < 0$ are simply obtained by using the symmetry

$$\langle x|T+\rangle^* = \langle -x|-T+\rangle. \quad (33)$$

The asymptotic behavior for negative and positive x (growing and decaying, respectively) changes abruptly at $T=0$. Since $|T+\rangle$ does not represent a physical state vector, the discontinuity at $T=0$ is not problematic, but indicates again that a literal physical interpretation of these states is not allowed. We shall see later that normalized wave packets formed with these states do not present this singularity.

There is a region close to $x=0$ that cannot be described by the asymptotic formulas for a large argument. In that region, however, the parabolic cylinder function can be expressed by means of a power series [20]

$$D_{-3/2}(z) = \frac{\Gamma(-1/4)}{\pi^{1/2} 2^{5/4}} - \frac{\Gamma(1/4)}{\pi^{1/2} 2^{3/4}} z + O(z^2). \quad (34)$$

Combining Eqs. (34) and (32), explicit expressions for $\langle x=0|T+\rangle$ and for its "flux" $J(x=0)$ can be obtained [22]. In particular,

$$J(x=0) = \frac{[\Gamma(3/2)\Gamma(-1/4)]^2}{(2\pi)^3 T^2 2^{3/2}}. \quad (35)$$

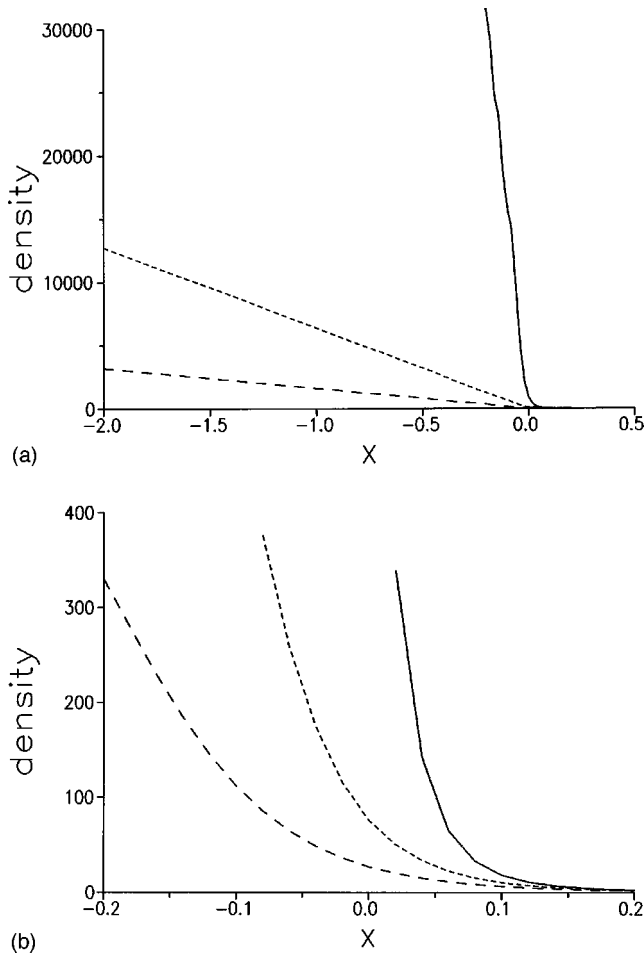


FIG. 1. (a) $|\langle x|T+\rangle|^2$ versus x for $T=0.01$ (long-dashed line), 0.005 (short-dashed line), and 0.001 (solid line) and $m=1$. All quantities are in a.u. (b) Same as (a), but for a smaller x interval.

For $T>0$, neither the wave function $\langle x|T+\rangle$ nor the flux are zero at $x=0$. Both the “density” $|\langle x=0|T+\rangle|^2$ and $J(x=0)$ grow monotonically as $T\rightarrow 0$. Figures 1(a) and 1(b) illustrate all the dependences discussed. $|\langle x|T+\rangle|^2$ is depicted for a series of decreasing times $T>0$ as a function of x for two different scales: between $x=-2$ and $x=0.2$ [Fig. 1(a)] and between $x=-0.2$ and $x=0.2$ [Fig. 1(b)] (atomic units are used in all numerical examples). In the larger scale the density of the eigenstate is essentially a straight line, pivoting at $x=0$, that approaches the vertical as $T\rightarrow 0$. The finer scale, however, shows that the arrival is not sharply defined. Even though, in a loose sense, “most of the wave” $\langle x|T+\rangle$ passes from $x<0$ to $x>0$ at $T=0$, there is a tail at $x>0$ present for an arbitrary T . Since these states are not normalized to one it is not possible to quantify the fraction of particles that can be found to the right of $x=0$ before $T=0$.

One might think that the eigenstates of the self-adjoint operators, which are orthogonal, could avoid this type of unsharpness [23], but they do not. For arbitrary values of ϵ we have numerically checked (see Appendix B) that there is a nonvanishing density $|\langle x|T+\rangle_\epsilon|^2$ at $x>0$ for fixed T . Similarly, the states $\langle x|T\rangle$ are also nonzero on the right-hand side. Using their defining equations (22), (23), and (33), one finds

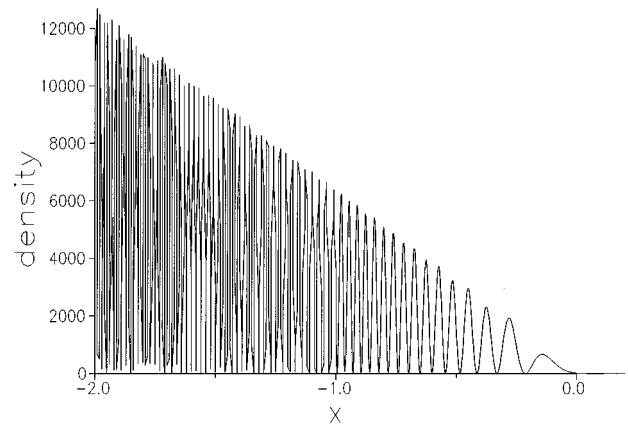


FIG. 2. $|\langle x|T\rangle|^2$ versus x for $T=0.01$ and $m=1$.

$$\langle x|T\rangle = 2 \operatorname{Re}\langle x|T+\rangle. \quad (36)$$

[It is to be noted that the corresponding time evolved state does not take this form. Instead, $\langle x|T_t\rangle \equiv \langle x|e^{-iHt/\hbar}|T\rangle = \langle x|(T-t)\rangle + \langle x|(T+t)\rangle^*$.] Figure 2 represents the square of this quantity for a relatively large spatial interval (the small but nonzero density for $x>0$ is not seen in this scale). The figure corresponding to the imaginary part is very similar. Note the increasingly rapid oscillation as $x\rightarrow -\infty$. Cancellation of these oscillations occurs in linear combinations of the states $\langle x|T\rangle$ or $\langle x|T+\rangle$ over a nonzero band leading to localization in a region closer to the origin; see Fig. 3 and the discussion in the following section. There is a helpful classical association to understand the oscillatory pattern: High-velocity particles (fast oscillations) have to start at longer distances and low-velocity particles (slow oscillations) at shorter distances if they all have to arrive at $X=0$ simultaneously.

IV. COORDINATE AND TIME DEPENDENCE OF THE NORMALIZED QUASIEIGENSTATES

We shall here construct normalized wave packets by using a Gaussian distribution of the states $\langle x|T'_t+\rangle$ peaked at $T'_t=T$ [24],

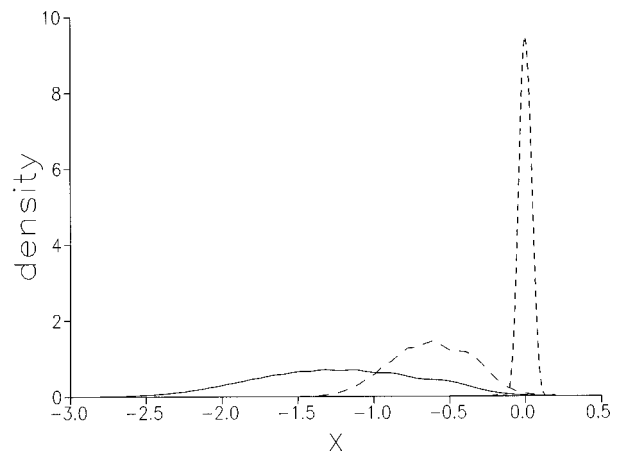


FIG. 3. Probability density of normalized quasieigenstates [see Eq. (37)] for $T=0.04$, $m=1$, $\Delta T=0.002$, $t=0$ (solid line), $t=0.02$ (long-dashed line), and $t=0.04$ (short-dashed line).

$$\langle x|\Psi(t;T,\Delta T)\rangle = N \int_{-\infty}^{\infty} e^{-(T-T')^2/2(\Delta T)^2} \langle x|T'_t+\rangle dT'. \quad (37)$$

Carrying out the Gaussian integral over T' and then determining the normalization constant N by evaluation of $\int_{-\infty}^{\infty} dx |\langle x|\Psi(t;T,\Delta T)\rangle|^2$ gives the normalized wave packet

$$\begin{aligned} \langle x|\Psi(t;T,\Delta T)\rangle &= \frac{2\pi^{1/4}(\Delta T)^{1/2}}{hm^{1/2}} \int_0^{\infty} p^{1/2} e^{ipx/\hbar} \\ &\times e^{i(T-t)p^2/2m\hbar} e^{-(\Delta T)^2 p^4/8m^2\hbar^2} dp. \end{aligned} \quad (38)$$

This integral is readily evaluated numerically because of the exponential dependence on $-p^4$. The momentum representation is given explicitly by

$$\begin{aligned} \langle p|\Psi(t;T,\Delta T)\rangle &= \frac{2\pi^{1/4}(\Delta T)^{1/2}}{(hm)^{1/2}} p^{1/2} e^{i(T-t)p^2/(2m\hbar)} e^{-(\Delta T)^2 p^4/(8m^2\hbar^2)} \Theta(p). \end{aligned} \quad (39)$$

As $\Delta T \rightarrow 0$ these states are orthogonal and satisfy the eigenvalue equation to any desired degree of accuracy:

$$\begin{aligned} \langle \Psi(t;T',\Delta T)|\Psi(t;T,\Delta T)\rangle &= w \left(\frac{T-T'}{2\Delta T} \right) = \begin{cases} 1 & \text{if } T=T' \\ \sim O\left(\frac{\Delta T}{T-T'}\right) & \text{as } \frac{\Delta T}{T-T'} \rightarrow 0, \end{cases} \quad (40) \\ \langle p|\hat{T}|\Psi(0;T,\Delta T)\rangle &= T \langle p|\Psi(0;T,\Delta T)\rangle + O(\Delta T)^{5/2}, \end{aligned} \quad (41)$$

where $w(z) = \exp(-z^2) \operatorname{erfc}(-iz)$ is the “ w function” [20]. The moments $\langle \hat{p}^n \rangle$ of the momentum distribution can be obtained from Eq. (39),

$$\langle \hat{p}^n \rangle = \Gamma\left(\frac{n+2}{4}\right) \pi^{-(1+n)/2} \left(\frac{\Delta T}{hm}\right)^{-n/2}. \quad (42)$$

Both the average energy $\langle E \rangle \equiv \langle \hat{p}^2 \rangle / 2m = h/2\pi^{3/2} \Delta T$ and $\Delta E = [2^{-1} - \pi^{-1}]^{1/2} \hbar / \Delta T$ diverge as ΔT goes to zero.

Similarly, from Eq. (38) one finds

$$\langle \hat{x} \rangle = -\frac{\Gamma(3/4)}{\pi} \left(\frac{h}{m\Delta T}\right)^{1/2} (T-t), \quad (43)$$

whereas higher moments diverge. (A finite “width” can, however, be defined as the half-width at half height.) The average velocity $\langle \hat{p}/m \rangle$, which is also the velocity of the centroid $\langle \hat{x} \rangle$, is given by $\Gamma(3/4)[h/\Delta T m \pi^2]^{1/2}$. The behavior of these states is arbitrarily close to what one could desire for an ideal arrival time eigenvector: They are normalized and there is no discontinuity at $t=T$; for a fixed ΔT , they still obey a transformation law of the form (5); the wave travels towards the origin with constant velocity and the average position crosses the origin at time $t=T$, which is also the time when the spatial width of the wave packet attains its

minimum value. Of course a certain unsharpness remains: From Eq. (38) one finds $\langle -x|\Psi(2T-t;T,\Delta T)\rangle = \langle \Psi(t;T,\Delta T)|x \rangle$, so the probability density has inversion symmetry in (x,t) with respect to the space time “origin” $(0,T)$. In particular, for $t=T$, half the norm is to the right of $x=0$ independently of ΔT . (The question of the existence of quantum states where the particle stays strictly on one side of X before T and on the other side after T is addressed in Appendix C.) However, the wave packet density and flux are more and more peaked at the space-time point $(x=0, t=T)$ as $\Delta T \rightarrow 0$, so that the passage of probability from left to right is sharp to any desired accuracy,

$$|\langle x=0|\Psi(t=T;T,\Delta T)\rangle|^2 = \left(\frac{m}{h\Delta T}\right)^{1/2} \frac{\Gamma(3/8)^2}{\pi 2^{5/4}}, \quad (44)$$

$$J(x=0, t=T) = \frac{\Gamma(3/8)\Gamma(5/8)}{\Delta T \pi^{3/2} 2^{3/4}}. \quad (45)$$

The normalized wave packets constructed with the eigenfunctions (17) have been examined in [25], where it is reported that this arbitrarily sharp accuracy is not found in that case.

V. DISCUSSION

Given the importance of the timed detection of particles at screens or in time-of-flight experiments, finding a theoretical description of the arrival times seems imperative. Apparatus-dependent results are available, for example, via modeling the detection with complex absorbing potentials or other measurement models [26–28], but it is reasonable to inquire if an intrinsic, apparatus-independent distribution can be naturally defined by means of the usual operator approach to quantum mechanics. We have seen in Secs. II and III that the POVM and the corresponding distribution $\Pi(T)$ associated with the time operator \hat{T} provide a rather satisfactory answer from the point of view of the properties satisfied: covariance with respect to time translations, minimum variance, appropriate symmetries, physically correct domain of applicability, and sharp space-time behavior of the normalized quasi-eigenstates.

One of the objections by Paul to \hat{T} , which is also a shortcoming of the theories based on self-adjoint operators, namely, the restrictive domain of the time operator(s) (which does not include, for example, states such as minimum uncertainty product Gaussians), is overcome by the POVM theory. An important point is to consider the primary object as the POVM (or, equivalently, the resolution of the identity or the arrival time distribution) rather than the operator. In this manner, the domain of applicability of the theory is \mathcal{H} and the classical limit is correct. Moreover, in this light the other problem indicated by Paul, namely, the extreme sensitivity of the expectation values of powers of \hat{T} to small perturbations, is relatively unimportant. It is a fact that some quantities are very sensitive to certain small perturbations and we are simply dealing with one of them. The moments in the classical case would also suffer from such a sensitivity. The moral is that one should not pay as much attention to the moments of a time-of-arrival distribution (highly unstable

with respect to small perturbations or changes in the apparatus resolution and possibly divergent) but to general features of the distribution (peaks, global form, or width at half height, for example). A consequence is that an uncertainty principle in terms of $\langle \hat{T}^2 \rangle$ is not of much use since this quantity will generally diverge. If it does not, it will be too unstable with respect to small perturbations. It is preferable to express the uncertainty principle in terms of other measurements of width, such as the half-width at half height.

Apart from the positive features of $\Pi(T)$, it is also fair to point out several unclear points or open questions. For example, it is necessary to generalize the treatment to higher dimensions or to scattering problems. The connection between $\Pi(T)$ and measurements (especially in nonclassical cases) is also pending; see [27]. We can, however, advance as a preliminary analysis two important features of a hypothetical measurement of $\Pi(T)$. The resolution of identity (6) implies the structure of $\Pi(T)$,

$$\Pi(T) = |\langle T+ | \psi_+ \rangle|^2 + |\langle T- | \psi_- \rangle|^2, \quad (46)$$

where $|\psi_{\pm}\rangle = \Theta(\pm \hat{p})|\psi\rangle$. This implies ignoring the ‘‘interference terms’’ $|\psi_-\rangle\langle\psi_+|$ and $|\psi_+\rangle\langle\psi_-|$, so that in a hypothetical operational procedure to measure $\Pi(T)$, only the diagonal terms of the density operator contribute,

$$\hat{\rho} \rightarrow |\psi_+\rangle\langle\psi_+| + |\psi_-\rangle\langle\psi_-|. \quad (47)$$

Apart from the fact that the practical implementation of this diagonalization may be cumbersome, the neglect of interferences is not a desirable feature since many different quantum states would give the same distribution. A second problematic aspect is associated with the interpretation of $|\langle T+ | \psi_+ \rangle|^2$ as the contribution to $\Pi(T)$ from particles arriving from the left and of $|\langle T- | \psi_- \rangle|^2$ as the contribution from those arriving from the right. This is particularly evident when the *backflow effect*

$$J \leq 0 \quad \text{for} \quad |\psi\rangle = |\psi_+\rangle, \quad (48)$$

$$J \geq 0 \quad \text{for} \quad |\psi\rangle = |\psi_-\rangle \quad (49)$$

occurs [29]. Then $\Pi(T)$ assigns zero probability to arrivals from the ‘‘anomalous side’’ (e.g., from the right when $|\psi\rangle = |\psi_+\rangle$). This implies that if $|\psi\rangle = |\psi_+\rangle$ or $|\psi\rangle = |\psi_-\rangle$ then either particles should be found to arrive either only from the left or only from the right, respectively, even during the time interval when J has the ‘‘wrong sign,’’ or the theory is appropriate when the ‘‘screen’’ is ‘‘one sided,’’ failing to detect any particles arriving from the anomalous side. Now consider the corresponding implication for the general state $|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle$ with both $|\psi_+\rangle$ and $|\psi_-\rangle$ nonzero. One possibility is that the interference terms do not in fact contribute to the intrinsic arrival time distribution. The other is that the distribution (46) is only appropriate when the apparatus measures the sign of the momentum of each incident particle, thus collapsing the wave function of that particle to either $|\psi_+\rangle$ or $|\psi_-\rangle$ and then switches on the appropriate one-sided detecting screen.

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APPENDIX A: LARGE- T BEHAVIOR OF $\Pi(T)$

Let us consider the asymptotic, large- T behavior of $\langle T+ | \psi \rangle$,

$$\langle T+ | \psi \rangle = \frac{1}{(m\hbar)^{1/2}} \int_0^\infty p^{1/2} e^{-ip^2 T/(2m\hbar)} \langle p | \psi \rangle dp. \quad (A1)$$

Assuming that $\langle p | \psi \rangle$ can be analytically continued into the fourth quadrant in the complex p plane we deform the integral contour into the ray $p = \gamma e^{-i\pi/4}$ ($0 \leq \gamma < \infty$). With the change $g = \gamma^2/2m\hbar$ the integral takes the form

$$\langle T+ | \psi \rangle = \frac{(m\hbar)^{1/4}}{2\pi^{3/4}} e^{-i\pi^{3/8}} \int_0^\infty dg e^{-gt} \psi(g) g^{1/4}, \quad (A2)$$

where the origin appears as the critical point. If, as $g \rightarrow 0$, $\psi(g) \sim cg^u$ (where u is not necessarily an integer), use of Watson’s lemma provides the dominant term

$$\langle T+ | \psi \rangle \sim e^{-i\pi^{3/8}} \frac{c(m\hbar)^{1/4}}{2\pi^{3/4}} \frac{\Gamma(u+5/4)}{T^{u+5/4}}. \quad (A3)$$

APPENDIX B: COORDINATE REPRESENTATION OF $|T+\rangle_\epsilon$

The integral over p for the coordinate representation $\langle x | T+ \rangle_\epsilon$ can be separated into two parts, from 0 to ϵ , I_1 , and from ϵ to ∞ , I_2 . The second one can be obtained numerically with the treatment of Sec. III by deforming the contour and using the steepest descent path from the saddle. I_1 can be expressed as

$$I_1 = \frac{\epsilon^{1-iT\epsilon^2/m\hbar}}{hm^{1/2}} \int_0^\epsilon e^{ixp/\hbar} p^{(iT\epsilon^2/m\hbar-1/2)} dp. \quad (B1)$$

With the change of variable $u = -ixp/\hbar$ the incomplete γ function is recognized,

$$I_1 = \frac{\epsilon^{3/2}}{hm^{1/2}} \left(\frac{x\epsilon}{i\hbar} \right)^{-A} \gamma(A, -ix\epsilon/\hbar) \quad (B2)$$

$$= \frac{\epsilon^{3/2}}{hm^{1/2}} \sum_{n=0}^\infty \frac{(ix\epsilon/\hbar)^n}{n!(A+n)}, \quad (B3)$$

where $A = iT\epsilon^2/m\hbar + 1/2$. It is easy to calculate an upper bound on the $p \leq \epsilon$ contribution, $I_1(x, t; T)$, to $\langle x | T_t+ \rangle$. The change of variable $p = \epsilon u$ gives

$$I_1(x, t; T) = \frac{\epsilon^{3/2}}{hm^{1/2}} \int_0^1 \frac{du}{u^{1/2}} \exp \left[i \left(\frac{\epsilon x u}{\hbar} - \frac{\epsilon^2 t u^2}{2m\hbar} + \frac{\epsilon^2 T}{\hbar m} \ln u \right) \right]. \quad (B4)$$

Hence both the real and imaginary parts of $I_1(x,t;T)$ are bounded in an absolute value by

$$\frac{\epsilon^{3/2}}{hm^{1/2}} \int_0^1 \frac{du}{u^{1/2}} = \frac{2\epsilon^{3/2}}{hm^{1/2}} \quad (\text{B5})$$

and $|I_1(x,t;T)| \leq (2\epsilon)^{3/2}/hm^{1/2}$, independently of x , t , and T .

APPENDIX C: STRICTLY SHARP ARRIVAL STATES

Are there quantum-mechanical states where the particle stays strictly on one side of X before T and on the other side after T ? We have seen, by examining the coordinate representation of the eigenstates of different time operators, that none of the proposals (fulfilling either the covariance condition or the self-adjointness condition) satisfies strictly this requirement. Is this an inherent limitation of standard quantum mechanics? We shall argue that there are no quantum states, pure or mixed, that satisfy fully this condition. To this end let us use the equivalent phase-space Weyl-Wigner formalism. Its advantage for free motion dynamics is that the evolution kernel and dynamical equation of motion are equal in classical and quantum mechanics [30]. Therefore, a Liouville theorem applies, so that each phase-space point carries its own ‘‘probabilistic weight’’ (that can be negative in the quantum case), so that in the intermediate calculations one

may think and operate classically, the only difference being in the domains of states allowed in both mechanics and the interpretation of the formalism [30,31]. The Wigner distribution $f(q,p)$ in the position-momentum phase space represents a valid quantum-mechanical state if the associated density operator $\hat{\rho}$ is positive; see, e.g., [32]. Necessary conditions may be found for $f(q,p)$ itself, such as

$$|f(q,p)| \leq 2/h, \quad (\text{C1})$$

$$h \int f(q,p) dq dp \leq 1. \quad (\text{C2})$$

What kind of ensemble of classical particles, having negative positions at time $t=0$, would arrive at the same time T at a point $X=0$? Since momentum is conserved, it is necessarily a coordinated motion where faster particles start moving further away and slower particles start closer to $X=0$ so that they all arrive at the same time. The phase-space density that satisfies these requisites is

$$f_T(x_0,p;t=0) = g(x_0)\Theta(-x_0)\delta(x_0+pT/m), \quad (\text{C3})$$

with $g(x_0) \geq 0$. However, this distribution is too singular to satisfy Eq. (C1) or (C2).

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