Time-of-arrival distribution for arbitrary potentials and Wigner's time-energy uncertainty relation

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A realization of the concept of ''crossing state'' invoked, but not implemented, by Wigner, allows advancement in two important aspects of the formalization of the time of arrival in quantum mechanics: (i) For free motion, we find that the limitations described by Aharonov *et al.* in Phys. Rev. A **57**, 4130 (1998) for the time-of-arrival uncertainty at low energies for certain measurement models are in fact already present in the intrinsic time-of-arrival distribution of Kijowski Π_K; (ii) we have also found a covariant generalization of this distribution for arbitrary potentials and positions.

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In spite of the emphasis of quantum theory on the concept of ''observable,'' the formalization of ''time observables'' is still a major open and challenging question. The ''arrival time'' has in particular received much attention in the last few years (see [1] for a recent review). Considering several candidates proposed for the time-of-arrival distribution in the simple free-motion, one-dimensional (1D) case, some of us have recently argued [2] in favor of a distribution originally proposed by Kijowski [3], Π_K, because it satisfies a number of desirable conditions.

This distribution can be associated with a positive operator valued measure (POVM) and obtained in terms of the eigenfunctions $|T,\alpha;X\rangle$ $(\alpha=\pm)$ of the time-of-arrival operator $\hat{T}$ introduced by Aharonov and Bohm [4]

$$\hat{T}=-\frac{m}{2}\left[(\hat{q}-X)\frac{1}{\hat{p}}+\frac{1}{\hat{p}}(\hat{q}-X)\right], \tag{1}$$

$$\Pi_K(T;X;\psi(t_r))=\sum_{\alpha}|\langle T,\alpha;X|\psi(t_r)\rangle|^2, \tag{2}$$

(we consider here the general 1D case with both positive and negative momenta as in [2,5,6]) where m is the mass, X is the arrival point, $\hat{q}$ and $\hat{p}$ are position and momentum operators, and

$$|T,\alpha;X\rangle=e^{i\hat{H}_0T/\hbar}(|\hat{p}|/m)^{1/2}\Theta(\alpha\hat{p})|X\rangle. \tag{3}$$

(The operator $|\hat{p}|^{1/2}$ is defined by its action on momentum plane waves, $|\hat{p}|^{1/2}|p\rangle=|p|^{1/2}|p\rangle$.) $\Pi_K(T;X;\psi(t_r))$ represents the probability density of arriving at X, at the instant $T+t_r$, i.e., an interval of time T after the reference instant t_r when the wave packet $\psi(t_r)$ is specified. [Typically one sets $t_r=0$ so that T is the ''nominal arrival time.'' In short notation, $\Pi_K(T)\equiv\Pi_K(T;X;\psi(t_r=0))$.] This distribution satisfies in particular the important *covariance condition* under time translations, $\Pi_K(T-t';X;\psi(t_r+t'))=\Pi_K(T;X;\psi(t_r))$. For other properties see [2,3,7].

In this paper we study two major aspects of this distribution that to our knowledge had not been addressed: (i) For states with positive or negative momenta we shall obtain the states of minimum time uncertainty (for given energy width), and find the same type of limitation pointed out by Aharonov *et al.* [8]; (ii) we shall also generalize Eq. (2) for arbitrary potentials.

To handle conveniently these two issues let us first elaborate on the form of Π_K. For $\alpha=+$ the contribution in Eq. (2) can be interpreted as a quantum version of the positive flux at the time $T+t_r$ due to right-moving particles. Similarly, for $\alpha=-$, one has a quantum version of minus the negative flux due to left-moving particles, again a positive quantity. Explicitly,

$$\Pi_{K,\alpha}(T)=\langle\psi(T)|(|\hat{p}|/m)^{1/2}\Theta(\alpha\hat{p})\delta(\hat{q}-X)\Theta(\alpha\hat{p})\times(|\hat{p}|/m)^{1/2}|\psi(T)\rangle, \tag{4}$$

where $\delta(\hat{q}-X)=|X\rangle\langle X|$. The positive operator in Eq. (4) corresponds to the classical dynamical variable

$$\delta(q-X)\frac{\alpha p}{m}\Theta(\alpha p), \tag{5}$$

whose average represents the modulus of the flux of particles of the classical ensemble that arrive at X *from one side* at a given time. This connection was pointed out by Delgado [9,10]. There are, of course, many possible quantizations of this quantity but the symmetrical one in Eq. (4) turns out to be the only one that satisfies the symmetry and minimum variance properties of Π_K.

It is useful to write the positive operator in Eq. (4) in the form $|u_\alpha\rangle\langle u_\alpha|$, where

$$|u_\alpha\rangle = |T=0,\alpha;X\rangle \tag{6}$$

is the ''crossing state.'' As emphasized in [2], its literal interpretation is problematic because it is not normalizable. Only normalized wave packets peaked around these states have properties as close as desired to the sharp crossing behavior expected on intuitive grounds.

Let us first discuss the point (i) related to the time-energy uncertainty principle. Since the Hamiltonian and the time operator (1) are conjugate variables a minimum uncertainty product can be established in the usual fashion [6]. However, Aharonov *et al.* have proposed, based on a series of models, a second limitation on the possible values of the time-of-arrival uncertainty: $\delta t\, E_k > \hbar$, where δt is the width of the ''pointer variable'' used to measure the arrival time, and E_k ''the typical initial kinetic energy of the particle'' [8]. It is to be stressed that this relation is based on measurement models for the arrival time where some extra (clock) degree of freedom is coupled continuously with the particle. We shall see that in fact the ''intrinsic'' distribution Π_K (there is no explicit recourse to additional pointer degrees of freedom to define Π_K) is consistent with the behavior that Aharonov *et al.* described for their models [8].

There are many other time-energy uncertainty relations [11], but here we shall be mainly interested in the version of Wigner [12], because his formalism is particularly suited for the time of arrival. In his original paper Wigner did not consider in detail any application and described a variational method to find the states of minimum uncertainty product, but did not actually obtain these states, except in two analytically solvable cases [12]. We shall extend Wigner's work in several directions by evaluating the states of minimum uncertainty product and applying the formalism to the arrival time. For completeness we shall next briefly summarize the main results obtained by Wigner in [12], and add a number of comments and observations relevant for our application.

He defines the basic amplitude as $\chi(t) = \langle u|\psi(t)\rangle$, where $|u\rangle$ is in principle any state vector. (Wigner's formalism encompasses many different time-energy uncertainty products, depending on the $|u\rangle$ chosen, each with its own physical interpretation.) Note that t is considered the independent variable of χ, and $|u\rangle$ is fixed. $|u\rangle$ is not necessarily a Hilbert space normalizable vector. It may also be, for example, a position or a time-of-arrival eigenvector provided the minimum uncertainty product state obtained is square integrable. $P(t) \equiv |\chi(t)|^2/\int_{-\infty}^{\infty}|\chi(t)|^2 dt$ plays the role of a normalized distribution for being found in $|u\rangle$ at time t. This is not a standard quantity in the ordinary formulation of quantum mechanics (which assigns probabilities only at fixed time t), but the interpretation is consistent with the ordinary formulation in the following way: Here ''being found'' implies operationally to perform measurements of $|u\rangle\langle u|$ at a given time t for the members of an ensemble prepared at $t' < t$ according to $\psi(t')$. This is repeated at different times but the ensemble is always prepared anew at t' with the same specifications. The distribution of positive counts as a function of time is proportional to $|\langle u|\psi(t)\rangle|^2$, and $P(t)$ is obtained when this distribution can be normalized (which is not always the case). [$P(t)$ does not correspond to a continuous measurement that modifies $\psi(t)$.] The moments of $P(t)$ are defined in the usual way, and in particular the *second moment with respect to* t_0 is defined as

$$\tau^2 \equiv \frac{\int_{-\infty}^{\infty}|\chi(t)|^2 (t-t_0)^2 dt}{\int_{-\infty}^{\infty}|\chi(t)|^2 dt}. \tag{7}$$

The information contained in $\chi(t)$ can also be encoded in its Fourier transform,

$$\eta(E) \equiv h^{-1/2}\int_{-\infty}^{\infty}\chi(t)e^{iEt/\hbar}dt. \tag{8}$$

The conjugate variable E has dimensions of energy, but $\eta(E)$ is not, in general, an energy amplitude in the conventional sense. η and the conventional energy amplitude of $\psi(t=0)$, can be related by expanding $\psi(t)$ in a basis of energy eigenstates $|E,\alpha\rangle$,

$$\eta(E) = h^{1/2}\sum_\alpha \langle u|E,\alpha\rangle\langle E,\alpha|\psi(0)\rangle\Theta(E). \tag{9}$$

In a general case α is an index to account for the possible degeneracy. In particular, for free motion, $\alpha = \pm$, and

$$|E,\alpha\rangle = \left(\frac{m}{2E}\right)^{1/4}|p = \alpha(2mE)^{1/2}\rangle. \tag{10}$$

Analogously to Eq. (7) the second energy moment *with respect to* E_0 is defined as

$$\epsilon^2 \equiv \frac{\int_0^{\infty}|\eta(E)|^2(E-E_0)^2 dE}{\int_0^{\infty}|\eta(E)|^2 dE}. \tag{11}$$

Neither t_0 nor E_0 should in general be identified with the average values of time and energy. They are instead reference parameters fixed beforehand to evaluate the moments. As a consequence, ϵ^2 and τ^2 should not in general be identified with the ''variances'' $(\Delta E)^2$ and $(\Delta t)^2$, which are the second moments with respect to the average values.

Since $\eta(E)$ and $\chi(t)$ are Fourier transforms of each other the uncertainty product $\epsilon\tau$ is greater than $\hbar/2$ (a peculiarity of time and energy with respect to position and momentum is that the equality is never satisfied [12]). In fact the bound increases substantially as E_0 decreases. Wigner sought the function $\eta(E)$ that renders τ to a minimum for fixed ϵ. In order to have a finite second moment τ^2, $\eta(E)$ must vanish at the origin $\eta(0)=0$, so η must vanish at both ends of integration $E=0,\infty$. Using partial integration and the notation $\eta_0 = \eta e^{-iEt_0/\hbar}$ (Wigner showed that the minimum of $\tau\epsilon$ must correspond to a real η_0), one finds that

$$\tau^2 = \frac{\hbar^2 \int_0^\infty |\partial \eta_0(E)/\partial E|^2 dE}{\int_0^\infty |\eta_0(E)|^2 dE}. \tag{12}$$

The product $\tau^2\epsilon^2$ subject to the constraint of fixed ϵ^2 is minimized by variational calculus. This leads, using Eqs. (11) and (12), to

$$-\hbar^2 \frac{\partial^2 \eta_0}{\partial E^2} + \frac{\lambda'}{\epsilon^2}(E-E_0)^2 \eta_0 = (\tau^2 + \lambda')\eta_0, \tag{13}$$

where λ' is a Lagrange multiplier. This equation is formally similar to the Schrödinger equation for the harmonic oscillator, except for the boundary condition at $E=0$, $\eta_0(0)=0$, and the subsidiary condition for ϵ, Eq. (11). The minimum τ is obtained from the lowest eigenvalue corresponding to the value of λ' where the subsidiary condition is satisfied. Fortunately the solution depends only on the ratio E_0/ϵ, namely, $\eta(E;E_0;\epsilon) = g(E/\epsilon;E_0/\epsilon)$, where g is the solution of Eq. (13) with $\epsilon=1$. Note also that, since $|\eta_0|^2 = |\eta|^2$, the value of t_0 does not play any role in the minimization process. [Physically the state $\chi_0(t)$ corresponding to $t_0=0$ is valid for any other time t_0 by a shift of the argument.] The minimization of τ for fixed E_0/ϵ requires a method to solve the differential equation (13) for many different values of λ', until $\epsilon^2=1$ is satisfied. In our calculation the successive values $\lambda'(n)$ have been obtained with a Newton-Raphson algorithm, and the lowest eigenstate and eigenvalue of Eq. (13) for each $\lambda'(n)$ are obtained with a very efficient ''relaxation method'' [13].

The only explicit case considered in the original paper by Wigner was $|u\rangle = |X\rangle$. The corresponding $P(t)$ provides a time distribution for the *presence* of the particle at X but not for its arrival. In an intriguing ''general observation,'' Wigner stated that, instead of asking for the probability that the particle be at a definite landmark in space, just at the time t, ''it would be more natural to ask . . . for the probability that the particle crosses the aforementioned landmark at the time t from the left, and also that it crosses the landmark, at a given time, from the right.'' But the paragraph ends with ''This point . . . interesting though it may be, will not be elaborated further.'' Precisely, it is our aim here to elaborate further on this question. Indeed the probabilities mentioned by Wigner can be obtained by means of the crossing states $|u_+\rangle$ and $|u_-\rangle$ discussed before, see Eq. (6). Specializing to states having only positive-negative momentum $\Pi_{K,\alpha}(t) = |\langle u_\alpha|\psi(t)\rangle|^2$ provides the arrival time distribution at t. Considering $\chi(t) = \langle u_\alpha|\psi(t)\rangle$, we see that Wigner's probability density is nothing but Kijowski's distribution $P(t) = \Pi_{K,\alpha}(t) = |\chi(t)|^2$. Moreover, the Fourier transform of $\chi(t)$ is in this case up to a phase factor the standard energy amplitude, $\eta(E) = \langle E,\alpha|\psi(0)\rangle \exp[iX(2mE)^{1/2}/\hbar]$, so that ϵ becomes the spread (around E_0) of the ordinary energy distribution.

For a given ratio E_0/ϵ there is a minimum value of $\tau\epsilon$. The family of states of minimal uncertainty $\eta(E;E_0;\epsilon)$ with

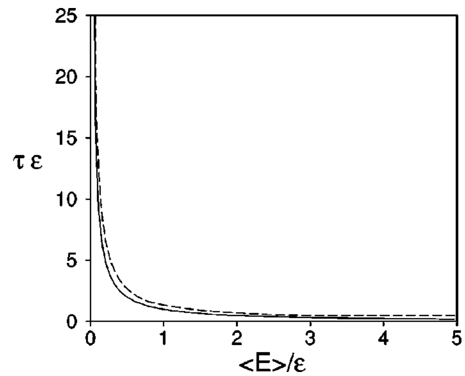

FIG. 1. $\epsilon\tau$ (in a.u., $\hbar=1$) vs $\langle E\rangle/\epsilon$ for the states of minimized uncertainty product (dashed line); $\epsilon/\langle E\rangle$ (solid line).

the same ratio E_0/ϵ have in common the same value of $\langle E\rangle/\epsilon$. Figure 1 shows $\tau\epsilon$ vs $\langle E\rangle/\epsilon$ for the states of minimized time-energy uncertainty product. For comparison we also show the curve $\epsilon/\langle E\rangle$. Clearly

$$\tau > \hbar/\langle E\rangle, \tag{14}$$

which has the same *form* as the relation proposed by Aharonov *et al.* based on measurement models [8]. However, τ is not due to the effect of any measuring apparatus, it is an intrinsic uncertainty associated with an intrinsic time-of-arrival distribution. It is not the coupling introduced in a measurement between the particle and other degrees of freedom that leads to this relation but the very quantum-mechanical nature of the particle alone and the lower bound of the energy.

To elaborate the figure, E_0/ϵ has been increased regularly from the minimum possible value -1. (For smaller values it is impossible to satisfy the subsidiary condition.) For each value the minimization of $\tau\epsilon$ is performed and the corresponding $\langle E\rangle/\epsilon$ is obtained. As $\langle E\rangle/\epsilon \to \infty$ the minimum uncertainty product tends to the (global) minimum $\hbar/2$, the same value found for position and momentum, because the effect of the lower bound of the energy tends to disappear in that limit, and $\eta(E)$ gets closer and closer to a Gaussian centered at E_0 with variance ϵ^2 [12]. However, in the opposite limit the lower bound at $E=0$ plays an important role. Indeed, $\langle E\rangle/\epsilon \to 0$ corresponds to the limit $E_0/\epsilon \to -1$, and the only way to satisfy the constraint is by strictly localizing $\eta(E)$ at $E=0$ ($\Delta E \to 0$), but this completely delocalizes the conjugate time variable, namely, $\tau \to \infty$. Thus, Eq. (14) appears as a consequence of the ordinary uncertainty principle, due to the tendency of the minimum uncertainty product states to have smaller variances for smaller energies. (The precise dependence for arbitrary values of E_0/ϵ has to be obtained numerically.)

The second question we shall address in this paper is the generalization of the free-motion distribution (2) for arbitrary potentials and positions (a previous attempt was only applicable to asymptotic positions where the motion is essentially free [14]). A generalization based on a quantization of classical expressions as in Eq. (1) is problematic: the classical expressions for the time of arrival will rarely be analytical, not all phase-space points lead to arrival, and the ordering problems may be formidable. The way out though, will be surprisingly simple in terms of crossing states.

There is in fact nothing that limits Eq. (5), and the corresponding operator in Eq. (4) to free motion. In particular, the classical motivation for considering $|u_\alpha\rangle$ a ''crossing state'' is equally valid when an arbitrary potential is present. The state (3) may be regarded as one that has evolved ''backwards'' with H_0 a time T from the crossing state $|u_\alpha\rangle$ so that it becomes $|u_\alpha\rangle$ precisely at the nominal arrival time T. In the same vein we construct for an arbitrary Hamiltonian H

$$|T,\alpha;X\rangle_H = e^{i\hat{H}T/\hbar}|u_\alpha\rangle, \tag{15}$$

so that at the nominal arrival time T, $|u_\alpha\rangle$ is recovered. The generalization of the arrival time distribution for arbitrary potentials is therefore

$$\Pi_H(T;X;\psi(t_r)) = \sum_\alpha |\langle u_\alpha|e^{-i\hat{H}T/\hbar}|\psi(t_r)\rangle|^2. \tag{16}$$

[As we have done for Π_K, it is convenient to use the short notations $\Pi_H(T)\equiv\Pi_H(T;X;\psi(t_r=0))$, or $\Pi_H(t)\equiv\Sigma_\alpha|\langle u_\alpha|\psi(t)\rangle|^2$.] It is evidently covariant under time translations as it should; in general it is not normalized, and it may be unnormalizable (its classical counterpart shares these properties). For example, it may be constant for stationary states, or periodic for oscillating coherent states in a harmonic potential, but it provides in any case relative information by comparison of two times. Consistent with this, the states $|T,\alpha;X\rangle_H$ do not form in general a complete basis. One important property for its interpretation is that its classical analog (the sum of the absolute values of positive and negative fluxes) takes into account any crossings (not only first, or last).

In order to have a better grasp of the meaning of our generalization, we portray in Fig. 2 several aspects of the collision, in a tunneling regime, of a Gaussian wave packet with a square barrier. In Fig. 2(a) we show the two components of Π_H ($\Pi_{H,+}$ and $\Pi_{H,-}$), and the current density J as functions of time t at a position in front of the barrier (i.e., on the incident side). J and $\Pi_{H,+}-\Pi_{H,-}$ are very close numerically, and the situation would be identical to the free case, were it not for the hump in $\Pi_{H,-}$ (in this hump $-\Pi_{H,-}$ and J are essentially coincident), which corresponds to the reflecting wave packet, traversing the reference point after the collision. In Fig. 2(b) we see the various distributions at the center of the barrier, in the interacting regime. There is a delay between the maxima of Π_+ and Π_-, due to the fact that Π_- is mostly associated with the reflection.

As to Fig. 2(c), corresponding to a position after the barrier, the maximum of Π_+ is brought forward when compared to the free case, in accordance with the well-known Hartmann effect [15]. Additionally, J, Π_+, and $\Pi_+-\Pi_-$ are indistinguishable in the scale of the figure. Well after the collision has occurred the wave is monochromatic over many periods, so the difference between $\Pi_+-\Pi_-$ and J tends to vanish. In this ''classical'' limit the different quantization orderings chosen for the momentum in the corresponding

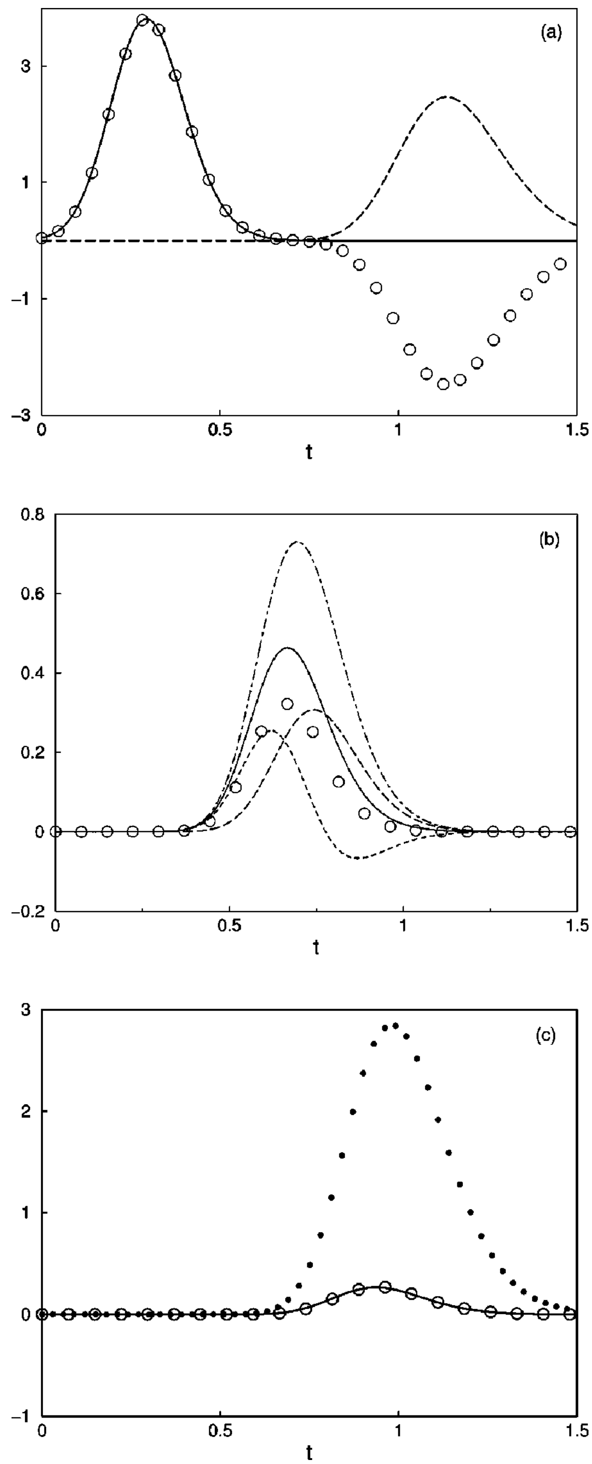

FIG. 2. (a) Current density (circles), Π_+ (solid line), and Π_- (long-dashed line) before the barrier ($X=8$) for a collision with a square barrier of energy 40 located between $x=12$ and 12.5 (all quantities in a.u.). The initial state ($t=0$) is a minimum position-momentum uncertainty product Gaussian with $\langle\hat{q}\rangle=\langle\hat{p}\rangle=5$, and $\langle(\hat{q}-5)^2\rangle=1$, for a particle of mass $m=1/2$. (b) Same as (a), but *at* the barrier $X=12{,}25$. Also depicted are $\Pi_++\Pi_-$ (dotted-dashed line), and $\Pi_+-\Pi_-$ (short-dashed line). (c) Same as (a), but *after* the barrier $X=15$. Π_- is negligible in this scale. Also depicted are Π_+ and J (indistinguishable) for free motion (dotted line).

operators is irrelevant (since in each expectation value $\hat{p}$ can be substituted by a number). As a consequence, the analysis performed with J that describes the asymptotic particle passage in terms of ''phase times'' is still valid for Π_H, see, e.g., [15,16], and J or Π_H may be very close to the absorption rate of ideal detectors, as shown in [17]. Contrast this to the quantum regime at the barrier, Fig. 2(b), where J and $\Pi_{H,+}-\Pi_{H,-}$ are clearly different. An interesting challenge is the actual measurement of these quantities in the barrier region. Testing experimentally the predicted values of $\Pi_{H,\pm}$ may be much more difficult there, since standard detectors are usually designed to compute only the first arrival, not several crossings. Moreover Π_H as Π_K [2] ignores the interference components of the density operator between positive and negative momenta. Thus, an experimental test for an arbitrary state should be able to effectively perform a collapse into positive and negative momentum components.

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