

# Quantum probability distribution of arrival times and probability current density

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This paper compares the proposal made in previous papers for a quantum probability distribution of the time of arrival at a certain point with the corresponding proposal based on the probability current density. Quantitative differences between the two formulations are examined analytically and numerically with the aim of establishing conditions under which the proposals might be tested by experiment. It is found that quantum regime conditions produce the biggest differences between the formulations which are otherwise near indistinguishable. These results indicate that in order to discriminate conclusively among the different alternatives, the corresponding experimental test should be performed in the quantum regime and with sufficiently high resolution so as to resolve small quantum effects. [S1050-2947(99)02602-5]

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## I. INTRODUCTION

The problem of incorporating the time-of-arrival concept in the theory of quantum measurement has remained controversial over the years, and even nowadays this question is open to debate [1–18]. In recent times this issue has acquired renewed interest in part due to the development of new experimental techniques for probing quantum systems in the time domain. For instance, by exciting an atomic system with a pulsed laser and measuring the subsequent flux of electrons ejected from autoionizing states, as a function of the time of arrival at the detector, one can gain important physical information which is not obtainable by probing the system in the more familiar energy domain [19]. On the other hand, the time domain is more related to the macroscopic phenomena and for this reason turns out to be particularly suitable for investigating quantum systems at the mesoscopic scale [20].

Another related issue that has stimulated considerable theoretical effort is that concerning the definition and characterization of tunneling times [21,22]. In connection with this problem, Dumont and Marchioro proposed the probability current density as a quantum definition for the (unnormalized) probability distribution of arrival times at an asymptotic point behind a one-dimensional potential barrier [7].

There exists additional motivation for trying to incorporate such a definition into the formalism of quantum mechanics. Indeed, the average current  $\langle J(X) \rangle$  of a classical statistical ensemble of particles propagating in one spatial dimension along a well-defined direction plays the role of a probability distribution of arrival times at  $X$ . A simple way for translating such a result into the framework of quantum mechanics consists in invoking the Weyl-Wigner quantization rule, which provides a prescription for constructing a quantum operator  $\hat{A}(\hat{X}, \hat{P})$  corresponding to a given classical dynamical variable  $A(x, p)$  [23,24],

$$\begin{aligned} A(x, p) &\rightarrow \hat{A}(\hat{X}, \hat{P}) \\ &= \frac{1}{4\pi^2} \int \int \int \int A(x, p) \\ &\quad \times e^{i[\theta(\hat{X}-x) + \tau(\hat{P}-p)]} dx dp d\theta d\tau. \end{aligned} \quad (1)$$

Furthermore, the operator so obtained has the nice property that its expectation value is given by the classical expression

$$\langle \hat{A}(\hat{X}, \hat{P}) \rangle = \int \int f_W(x, p) A(x, p) dx dp, \quad (2)$$

with the Wigner function  $f_W(x, p)$  playing the role of a quasiprobability distribution function in phase space.

The Weyl-Wigner quantization rule must be used with caution for it does not necessarily lead to the correct quantum operator. In the present context, one obtains that the Weyl-Wigner operator corresponding to the classical current  $J(X) = p/m \delta(x-X)$  is nothing but the usual current operator

$$\hat{J}(X) = \frac{1}{2m} (\hat{P} |X\rangle \langle X| + |X\rangle \langle X| \hat{P}). \quad (3)$$

However, unlike the classical case, because of the fact that  $\hat{J}(X)$  is not positive definite, its expectation value cannot be properly considered as a probability distribution of arrival times. It has been argued, nonetheless, that asymptotically far from a potential barrier the transmitted current becomes positive, and this circumstance justifies its interpretation as a probability distribution [7,9]. In this regard, McKinnon and Leavens [8,15] have also shown that within the framework of Bohmian mechanics it is possible to unambiguously define a probability distribution of the time of arrival in terms of the modulus of the probability current density. However, even though such a definition circumvents the problem mentioned above, in principle there is no justification for extrapolating it to the framework of standard quantum mechanics.

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A natural way for introducing time into the quantum framework as a physical variable consists in considering it as such already at the classical level (a fact that can be implemented by making a suitable canonical transformation) and then quantizing the corresponding formulation by using the canonical quantization method [25] in order to look for the desired probability distribution in terms of the spectral decomposition of an appropriate self-adjoint operator. In doing so, one arrives at a time operator defined as the operator canonically conjugate to the relevant Hamiltonian [12,26,27]. However, in general, no such a self-adjoint operator exists [1,3,12]. This is the technical reason that explains to a great extent the difficulty found for incorporating a time operator into the quantum formalism.

A reasonable way of circumventing this problem consists in looking instead for a self-adjoint operator with dimensions of time not strictly conjugate to the Hamiltonian. Even though there exist appreciable differences among them, the approaches of Kijowski [4], Grot *et al.* [10], as well as the one developed in Refs. [12] and [13] can be ascribed to this category. The first two approaches are concerned with the time of arrival of a free particle, and its supposed range of validity includes quantum states having, in the momentum representation, positive- and negative-momentum components, while the latter is also applicable (asymptotically) in the presence of a one-dimensional scattering potential and its range of validity is restricted to quantum states having either positive- or negative-momentum contributions. In this paper we shall focus on this latter approach. It should be remarked, however, that within their common range of applicability all of them provide the same theoretical prediction for the probability distribution of the time of arrival at a certain point.

Agreement with a conclusive experimental test is the ultimate requirement for establishing the validity of any theoretical proposal. However, discriminating experimentally among different alternatives is not always a straightforward matter. It may happen that under certain experimental conditions predictions corresponding to different proposals become indistinguishable in practice. This is the case in the present context when considering quantum states largely semiclassical in character. Indeed, in the semiclassical limit [13] the proposal for the probability distribution of arrival times based on the operator approach coincides with that based on the modulus of the probability current density, which is the result obtained by McKinnon and Leavens within Bohmian mechanics [8,15]. More generally, since in this limit the quantum current becomes necessarily positive, it follows that the predictions based on the operator approach become in fact indistinguishable from those based in general on the probability current density. Consequently, any experimental test performed under these particular conditions would be inconclusive. It is therefore worthwhile to investigate quantitatively to what extent appreciable differences among the competing proposals can be expected as well as to examine how such differences depend on the various controllable parameters. This is the main purpose of the present work [28]. More specifically, quantitative differences between the two formulations will be examined analytically and numerically (as a function of both the initial quantum state describing the particle and the parameters characterizing an intermediate potential barrier) with the aim of estab-

lishing conditions under which the proposals might be tested by experiment. To this end we shall begin by briefly reviewing the required formulation.

## II. PROBABILITY DISTRIBUTION OF ARRIVAL TIMES

Consider a quantum particle moving along the  $x$  axis toward a detector located at a certain asymptotic point  $X$  behind a one-dimensional scattering center  $V(\hat{X})$ . In looking for a probability distribution of the time of arrival for such a physical system, we introduced in previous papers [12,13] a self-adjoint operator with dimensions of time  $\hat{T}(X)$  defined in terms of its orthogonal spectral decomposition by

$$\hat{T}(X) = \int_{-\infty}^{+\infty} d\tau \tau |\tau; X\rangle \langle \tau; X|, \quad (4)$$

$$|\tau; X\rangle \equiv e^{i \operatorname{sgn}(\hat{P}) (\hat{P}^2/2m) \tau/\hbar} \sqrt{\frac{|\hat{P}|}{m}} |X\rangle. \quad (5)$$

The operators  $\operatorname{sgn}(\hat{P})$  and  $\sqrt{|\hat{P}|}$  are in turn given by the expressions

$$\sqrt{|\hat{P}|} \equiv \int_{-\infty}^{+\infty} dp \sqrt{|p|} |p\rangle \langle p|, \quad (6)$$

$$\operatorname{sgn}(\hat{P}) \equiv \int_0^{\infty} dp (|p\rangle \langle p| - |-p\rangle \langle -p|), \quad (7)$$

where the momentum eigenstates  $\{|p\rangle\}$  are assumed to be normalized as  $\langle p|p'\rangle = \delta(p-p')$ .

Note that the above equations define, in fact, a one-parameter family  $\{\hat{T}(X)\}$  of self-adjoint operators (labeled by the position  $X$  of the detector) which are canonically conjugate to the operator  $\hat{H} \equiv \operatorname{sgn}(\hat{P}) \hat{H}_0$ , with  $\hat{H}_0 \equiv \hat{P}^2/2m$  being the energy of the free particle.

Let  $\Theta(+\hat{P})$  [ $\Theta(-\hat{P})$ ] represent the projector onto the subspace spanned by plane waves with positive [negative] momenta,

$$\Theta(\pm\hat{P}) = \int_0^{\infty} dp |\pm p\rangle \langle \pm p|. \quad (8)$$

By taking advantage of the resolution of the unity  $\Theta(+\hat{P}) + \Theta(-\hat{P}) = \hat{1}$ , we can rewrite the eigenstates  $|\tau; X\rangle$  (which are manifestly symmetric under time reversal) in the form

$$\begin{aligned} |\tau; X\rangle &= \Theta(+\hat{P}) e^{i\hat{H}_0\tau/\hbar} \sqrt{\frac{|\hat{P}|}{m}} |X\rangle \\ &+ \Theta(-\hat{P}) e^{-i\hat{H}_0\tau/\hbar} \sqrt{\frac{|\hat{P}|}{m}} |X\rangle, \end{aligned} \quad (9)$$

which involves the state  $\sqrt{|\hat{P}|/m} |X\rangle$  translated (freely) both forward and backward in time by the amount  $\tau$ .

Substituting then Eq. (9) into Eq. (4), one obtains

$$\hat{\mathcal{T}}(X) = \Theta(+\hat{P}) \left[ \int_{-\infty}^{+\infty} d\tau \tau \hat{J}_1^{(+)}(X, \tau) \right] \Theta(+\hat{P}) \\ - \Theta(-\hat{P}) \left[ \int_{-\infty}^{+\infty} d\tau \tau \hat{J}_1^{(+)}(X, \tau) \right] \Theta(-\hat{P}), \quad (10)$$

where the positive-definite current  $\hat{J}_1^{(+)}(X, \tau)$  is a straightforward quantum version (in the interaction picture) of the modulus of the classical current  $|J(X)| = |p|/m \delta(x-X)$ ,

$$\hat{J}_1^{(+)}(X, \tau) = e^{i\hat{H}_0\tau/\hbar} \hat{J}^{(+)}(X) e^{-i\hat{H}_0\tau/\hbar}, \quad (11)$$

$$\hat{J}^{(+)}(X) \equiv \sqrt{\frac{|\hat{P}|}{m}} \delta(\hat{X} - X) \sqrt{\frac{|\hat{P}|}{m}}. \quad (12)$$

Even though  $\hat{\mathcal{T}}(X)$  is symmetric under time reversal, its restrictions to the subspaces spanned by either positive- or negative-momentum plane waves are not. This fact enables us to define a probability distribution of the time of arrival for quantum states belonging to either of such subspaces. To be specific, let us assume the particle under study to be incident from the left of the potential barrier, and let the state vector  $|\psi_{\text{in}}\rangle$  [which is assumed to satisfy the identity  $|\psi_{\text{in}}\rangle \equiv \Theta(\hat{P})|\psi_{\text{in}}\rangle$ ] represent the incoming asymptote of the actual scattering state of the particle at  $t=0$ . The mean arrival time at an asymptotic point  $X$  can then be defined consistently as [12,13]

$$\langle t_X \rangle = \frac{\langle \psi_{\text{tr}} | \hat{\mathcal{T}}(X) | \psi_{\text{tr}} \rangle}{\langle \psi_{\text{tr}} | \psi_{\text{tr}} \rangle} \\ = \frac{1}{\langle \psi_{\text{tr}} | \psi_{\text{tr}} \rangle} \int_{-\infty}^{+\infty} dt t \langle \psi_{\text{tr}} | \hat{J}_1^{(+)}(X, t) | \psi_{\text{tr}} \rangle, \quad (13)$$

where  $|\psi_{\text{tr}}\rangle$  is the projection of the outgoing asymptote (at  $t=0$ ) onto the channel of transmitted particles, i.e.,

$$|\psi_{\text{tr}}\rangle = \Theta(\hat{P})|\psi_{\text{out}}\rangle = \Theta(\hat{P})\hat{S}|\psi_{\text{in}}\rangle \\ = \int_0^{\infty} dp T(p) \langle p | \psi_{\text{in}} \rangle |p\rangle, \quad (14)$$

with  $\hat{S}$  and  $T(p)$  being, respectively, the scattering operator and the transmission coefficient characterizing the potential barrier.

It is worth noting the remarkable formal analogy between Eq. (13) and its corresponding classical counterpart. Indeed, the positive-definite current  $\langle \psi_{\text{tr}} | \hat{J}_1^{(+)}(X, t) | \psi_{\text{tr}} \rangle$  enters the expression for  $\langle t_X \rangle$  playing the role of an (unnormalized) probability distribution. We can thus define the probability distribution of the time of arrival at the asymptotic point  $X$  as

$$P_X(t) \equiv \frac{1}{\mathbb{T}} |\langle t; X | \psi_{\text{tr}} \rangle|^2 = \frac{1}{\mathbb{T}} \langle \psi_{\text{tr}}(t) | \hat{J}^{(+)}(X) | \psi_{\text{tr}}(t) \rangle, \quad (15)$$

where  $\mathbb{T} \equiv \langle \psi_{\text{tr}} | \psi_{\text{tr}} \rangle = \langle \psi_{\text{tr}}(t) | \psi_{\text{tr}}(t) \rangle$  is the transmittance and we have written the latter expression in the more familiar Schrödinger picture by introducing the (Schrödinger) freely evolving transmitted state

$$|\psi_{\text{tr}}(t)\rangle \equiv e^{-i\hat{H}_0 t/\hbar} |\psi_{\text{tr}}\rangle. \quad (16)$$

Equation (15) along with Eqs. (14) and (16) enable us to compute the desired probability distribution in terms of the ingoing asymptote  $|\psi_{\text{in}}\rangle$ . It is worth, however, obtaining an alternative formula in terms of the actual scattering state  $|\psi(t=0)\rangle$ . This can be accomplished by means of the Møller operators,

$$\hat{\Omega}_{\pm} \equiv \lim_{t \rightarrow \mp \infty} e^{i\hat{H}t/\hbar} e^{-i\hat{H}_0 t/\hbar}, \quad (17)$$

which map the ingoing and outgoing asymptotic states onto the corresponding scattering state

$$|\psi(t=0)\rangle = \hat{\Omega}_+ |\psi_{\text{in}}\rangle = \hat{\Omega}_- |\psi_{\text{out}}\rangle. \quad (18)$$

Using these relations and introducing the projector

$$\hat{\mathcal{P}} \equiv \hat{\Omega}_- \Theta(\hat{P}) \hat{\Omega}_-^\dagger \quad (19)$$

(which selects that part of a given state vector that will be transmitted), one finally obtains (Appendix A)

$$P_X(t) = \frac{1}{\mathbb{T}} \langle \psi(0) | \hat{\mathcal{P}} \hat{\Omega}_- \hat{J}_1^{(+)}(X, t) \hat{\Omega}_-^\dagger \hat{\mathcal{P}} | \psi(0) \rangle \\ = \frac{1}{\mathbb{T}} \langle \psi(t) | \hat{\mathcal{P}} \hat{\Omega}_- \hat{J}^{(+)}(X) \hat{\Omega}_-^\dagger \hat{\mathcal{P}} | \psi(t) \rangle, \quad (20)$$

where  $|\psi(t)\rangle \equiv e^{-i\hat{H}t/\hbar} |\psi(0)\rangle$  is the usual Schrödinger state vector. It is interesting to note that the above equation is merely the expectation value of the modulus of the current  $\hat{J}^{(+)}(X)$  in the quantum state  $1/\sqrt{\mathbb{T}} \hat{\Omega}_-^\dagger \hat{\mathcal{P}} |\psi(t)\rangle$ , which, in turn, is the normalized outgoing asymptote corresponding to that part of  $|\psi(t)\rangle$  that is going to be transmitted in the future.

In practice, whenever the actual scattering state at  $t=0$  does not overlap appreciably with the potential barrier, the state vectors  $|\psi_{\text{in}}\rangle$  and  $|\psi(0)\rangle$  become physically indistinguishable [29] and, consequently, one can legitimately use Eqs. (14)–(16) with the substitution  $|\psi_{\text{in}}\rangle \rightarrow |\psi(0)\rangle$ .

For our purposes it is convenient to write the expectation values of  $\hat{J}(X)$  and  $\hat{J}^{(+)}(X)$  as

$$\langle \psi_{\text{tr}}(t) | \hat{J}(X) | \psi_{\text{tr}}(t) \rangle = \frac{1}{mh} \frac{1}{2} (I^*[p]I[1] + \text{c.c.}), \quad (21)$$

$$\langle \psi_{\text{tr}}(t) | \hat{J}^{(+)}(X) | \psi_{\text{tr}}(t) \rangle = \frac{1}{mh} (I^*[\sqrt{p}]I[\sqrt{p}]), \quad (22)$$

where we have introduced the functional

$$I[f] \equiv \int_0^{\infty} dp T(p) f(p) \langle p | \psi_{\text{in}} \rangle e^{-i(p^2/2m)t/\hbar} e^{ipX/\hbar}. \quad (23)$$

Note finally that the free case is a particular case of the above formulation with the Møller operators  $\hat{\Omega}_{\pm}$  reducing to

the unit operator and, consequently,  $\hat{P} \rightarrow \Theta(\hat{P})$ . Since the scattering operator can be written as  $\hat{S} = \hat{\Omega}_-^\dagger \hat{\Omega}_+$ , it also follows that  $\hat{S} \rightarrow \hat{\mathbf{1}}$ , and hence, by virtue of Eq. (14),  $T(p) \rightarrow 1$  and  $|\psi_{\text{tr}}\rangle \rightarrow |\psi_{\text{in}}\rangle \rightarrow |\psi(0)\rangle$ . With these substitutions the above formulas are applicable to the study of the arrival time of a free particle at a point  $X$ .

### III. ANALYTICAL APPROXIMATION FOR THE EXPECTATION VALUE OF $\hat{J}^{(+)}(X)$

In this section we are interested in obtaining analytical expressions that permit us to compare the proposed probability distribution of the time of arrival  $\langle \psi_{\text{tr}}(t) | \hat{J}^{(+)}(X) | \psi_{\text{tr}}(t) \rangle$  with the standard probability current density  $\langle \psi_{\text{tr}}(t) | \hat{J}(X) | \psi_{\text{tr}}(t) \rangle$ . To this end we shall restrict ourselves to a free particle characterized, at  $t=0$ , by a minimum Gaussian wave packet with centroid  $x_0$ , having a negligible

contribution of negative-momentum components, and propagating with average momentum  $p_0 > 0$  along the  $x$  axis toward a detector located at a certain position  $X > x_0$ . Specifically,

$$\langle p | \psi(0) \rangle = [2\pi(\Delta p)^2]^{-1/4} \exp\left[-\left(\frac{p-p_0}{2\Delta p}\right)^2 - i\frac{px_0}{\hbar}\right], \quad (24)$$

where the momentum spread  $\Delta p \ll p_0$  is assumed to be sufficiently small so as to satisfy  $\langle p | \psi(0) \rangle \approx \Theta(p) \langle p | \psi(0) \rangle$  to a good approximation. As stated above, under these conditions  $T(p) \rightarrow 1$  and we may substitute  $|\psi_{\text{tr}}(t)\rangle \rightarrow |\psi(t)\rangle$  throughout the relevant formulas. The integrals involved in the definition of the probability current density [Eqs. (21) and (23)] can then be easily carried out to obtain the well-known formula

$$\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle = \frac{\sqrt{2/\pi}\Delta p}{m\hbar} \frac{\left(p_0 + 4\frac{(\Delta p)^4(X-x_0)}{m\hbar^2}t\right)}{\left(1 + 4\frac{(\Delta p)^4}{m^2\hbar^2}t^2\right)^{3/2}} \exp\left(-2\frac{(\Delta p)^2}{\hbar^2} \frac{\left[(X-x_0) - \frac{p_0}{m}t\right]^2}{1 + 4\frac{(\Delta p)^4}{m^2\hbar^2}t^2}\right). \quad (25)$$

As far as the probability distribution  $\langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle$  is concerned, some additional simplification is needed. We shall content ourselves with an analytical approximation valid up to order  $(\Delta p/p_0)^2$ . To this end, following Grot *et al.* [10], we expand the argument of the functional  $I[\sqrt{p}]$  entering Eq. (22) as a Taylor series about the average momentum  $p_0$ , i.e.,

$$\sqrt{p} = \sqrt{p_0} \left[ 1 + \frac{p-p_0}{2p_0} - \frac{1}{2} \left( \frac{p-p_0}{2p_0} \right)^2 + O\left( \frac{p-p_0}{p_0} \right)^3 \right]. \quad (26)$$

Substitution of this expansion into  $I[\sqrt{p}]$  leads to

$$I[\sqrt{p}] = \frac{1}{4}\sqrt{p_0} \left[ \frac{3}{2}I[1] + \frac{3}{p_0}I[p] - \frac{1}{2p_0^2}I[p^2] + O\left(\frac{\Delta p}{p_0}\right)^3 \right]. \quad (27)$$

The important point is that both  $I[p]$  and  $I[p^2]$  can be written in terms of  $I[1]$ , yielding an expression for  $\langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle$  that can be easily related to the probability current density given in Eq. (25). Indeed, substituting Eq. (24) in the integrand of  $I[1]$  and taking into account that  $\langle p | \psi(0) \rangle \approx 0$  for  $p < 0$ , one arrives at the Gaussian integral

$$I[1] = N \int_{-\infty}^{+\infty} dp e^{-\delta(p-\lambda)^2}, \quad (28)$$

where

$$\delta \equiv \frac{1}{4(\Delta p)^2} + i\frac{t}{2m\hbar}, \quad (29)$$

$$\lambda \equiv \frac{p_0 + 2i(\Delta p)^2(X-x_0)/\hbar}{1 + 2i(\Delta p)^2t/m\hbar}. \quad (30)$$

(The factor  $N$  is not relevant to our purposes and consequently is not given here.) Note that  $\text{Re}(\delta) > 0$ , as required for the integral to converge. As is well known, the integral of Eq. (28) is, in fact, independent of  $\lambda$ . Thus, by differentiating  $I[1]$  with respect to  $\lambda$  one can readily show that

$$I[p] = \lambda I[1]. \quad (31)$$

Likewise, a second differentiation with respect to  $\lambda$  leads to

$$I[p^2] = \left(\lambda^2 + \frac{1}{2\delta}\right) I[1]. \quad (32)$$

By inserting Eq. (31) into Eq. (21), one obtains

$$\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle = \frac{1}{m\hbar} \text{Re}(\lambda) |I[1]|^2. \quad (33)$$

Substitution of Eqs. (31) and (32) into Eq. (27) yields an expression for  $I[\sqrt{p}]$  depending only on  $I[1]$ . Inserting then the expression so obtained into Eq. (22) and using Eq. (33) to eliminate  $|I[1]|^2$  in favor of the probability current  $\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle$ , we arrive at

$$\begin{aligned} \langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle = & \frac{3}{16p_0^3 \text{Re}(\lambda)} \left\{ \frac{3}{4} p_0^4 + 3p_0^3 \text{Re}(\lambda) + 3p_0^2 |\lambda|^2 - \frac{1}{2} p_0^2 \text{Re} \left( \lambda^2 + \frac{1}{2\delta} \right) \right. \\ & \left. - p_0 \text{Re} \left[ \lambda \left( \lambda^2 + \frac{1}{2\delta} \right)^* \right] + \frac{1}{12} \left| \lambda^2 + \frac{1}{2\delta} \right|^2 + O \left( \frac{\Delta p}{p_0} \right)^3 \right\} \langle \psi(t) | \hat{J}(X) | \psi(t) \rangle. \end{aligned} \quad (34)$$

Of course, for this cumbersome expression to be useful some simplification is still required. Let  $t_0 = (X - x_0)m/p_0$  be the classical time of arrival at the detector located at  $X$ . Restricting ourselves to particles arriving in the time interval  $[0, 2t_0]$ , we have

$$t \leq 2t_0 \quad \Rightarrow \quad \frac{(\Delta p)^2 t}{m\hbar} \leq \rho \left( \frac{\Delta p}{p_0} \right), \quad (35)$$

where the parameter  $\rho$  denotes the distance between the centroid of the wave packet at  $t=0$  and the detector's position, in units of the spatial spread  $\Delta x = \hbar/2\Delta p$ , i.e.,  $(X - x_0) \equiv \rho \Delta x$ . The important point is that when  $\rho \sim O(1)$ , the term  $2(\Delta p)^2 t/m\hbar$  involved in the expressions of both  $1/\delta$  and  $\lambda$

[Eqs. (29) and (30)] becomes of order  $(\Delta p/p_0)$ . This fact enables us to approximate the various terms contributing to Eq. (34) as Taylor's expansions up to terms of order  $(\Delta p/p_0)^2$ . For instance, under the assumptions just stated we would have

$$\text{Re}(\lambda) = p_0 \left[ 1 + 4 \frac{(\Delta p)^4 (X - x_0) t}{mp_0 \hbar^2} - 4 \frac{(\Delta p)^4 t^2}{m^2 \hbar^2} + O \left( \frac{\Delta p}{p_0} \right)^3 \right], \quad (36)$$

with similar expansions for the rest of the terms entering the above expression for  $\langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle$ . The substitution of all of these expansions into Eq. (34) leads, after a rather lengthy calculation, to the final result

$$\langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle = \left[ 1 + \Lambda_0 - \Lambda_1 t + \Lambda_2 t^2 + O \left( \frac{\Delta p}{p_0} \right)^3 \right] \langle \psi(t) | \hat{J}(X) | \psi(t) \rangle, \quad (37)$$

where the coefficients  $\Lambda_0$ ,  $\Lambda_1$ , and  $\Lambda_2$  are defined as

$$\Lambda_0 \equiv -\frac{1}{2} \left( \frac{\Delta p}{p_0} \right)^2 + \frac{2(\Delta p)^4 (X - x_0)^2}{\hbar^2 p_0^2}, \quad (38)$$

$$\Lambda_1 \equiv 4 \frac{(\Delta p)^4 (X - x_0)}{mp_0 \hbar^2}, \quad (39)$$

$$\Lambda_2 \equiv 2 \frac{(\Delta p)^4}{m^2 \hbar^2}. \quad (40)$$

Equation (37) constitutes the main result of this section. When used along with Eq. (25), it enables us to obtain analytically the probability distribution  $\langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle$  up to order  $(\Delta p/p_0)^2$ . When the detector is located at a position  $X$  initially separated from the centroid  $x_0$  a distance of order  $\Delta x$ , its range of applicability extends over the time interval  $[0, 2t_0]$ . However, the validity of Eq. (37) is not restricted to this particular configuration. Indeed, it is not difficult to see that for any detector location  $X > x_0$  (i.e., any  $\rho > 0$ ), Eq. (37) remains true within the interval  $[0, \sigma t_0]$ , with  $\sigma \approx \min\{(2/\rho), (2/\rho)^2\}$ . For greater times the contribution from those terms neglected in the various expansions increases, so that they can no longer be considered to be of order  $(\Delta p/p_0)^3$  and Eq. (37) might fail as an approximation valid up to order  $(\Delta p/p_0)^2$ .

As is apparent from the above formulas, the difference between the expectation values of  $\hat{J}(X)$  and  $\hat{J}^{(+)}(X)$  turns

out to be of order  $(\Delta p/p_0)^2$ , so that, in the limit  $(\Delta p/p_0) \rightarrow 0$ , both of them coincide, a result that is in agreement with Ref. [10] and confirms the asymptotic analysis of Ref. [13]. A comparison between these two quantities is, however, most conveniently done in terms of their relative difference.

#### IV. RELATIVE DIFFERENCE

Given a Hamiltonian  $\hat{H} = \hat{H}_0 + V(\hat{X})$  and a state vector  $|\psi(0)\rangle$  having no contribution of negative-momentum components, and not overlapping appreciably with the potential barrier [so that one may legitimately substitute  $|\psi_{\text{in}}\rangle \rightarrow |\psi(0)\rangle$ ], the relative difference  $\Delta$  between the probability distribution  $\langle \psi_{\text{tr}}(t) | \hat{J}^{(+)}(X) | \psi_{\text{tr}}(t) \rangle$  and the corresponding probability current density  $\langle \psi_{\text{tr}}(t) | \hat{J}(X) | \psi_{\text{tr}}(t) \rangle$  can be written as [see Eq. (14)]

$$\Delta = 1 - \frac{\langle \psi(0) | \hat{S}^\dagger \Theta(\hat{P}) \hat{J}_1(X, t) \Theta(\hat{P}) \hat{S} | \psi(0) \rangle}{\langle \psi(0) | \hat{S}^\dagger \Theta(\hat{P}) \hat{J}_1^{(+)}(X, t) \Theta(\hat{P}) \hat{S} | \psi(0) \rangle}. \quad (41)$$

This quantity, which constitutes the basis for our subsequent analysis, is (for any  $t$ ) a state functional that enables us to quantify the differences we are interested in, as a function of the initial state  $|\psi(0)\rangle$ . To this end we shall consider an initial state vector of the form

$$|\psi(0)\rangle = \alpha(\beta |\psi_1\rangle + |\psi_2\rangle), \quad (42)$$

where  $\alpha$  is the normalization constant,

$$\alpha = (\beta^2 + 2\beta \operatorname{Re}\langle\psi_1|\psi_2\rangle + 1)^{-1/2}, \quad (43)$$

and  $\beta$  is an arbitrary real coefficient. On the other hand, for computational simplicity we shall choose  $\langle p|\psi_j\rangle$  ( $j=1,2$ ) to be minimum Gaussian wave packets centered at  $x_0$ , with momentum spread  $\Delta p$  and average momentum  $p_j$ , respectively,

$$\langle p|\psi_j\rangle = [2\pi(\Delta p)^2]^{-1/4} \exp\left[-\left(\frac{p-p_j}{2\Delta p}\right)^2 - i\frac{px_0}{\hbar}\right]. \quad (44)$$

Furthermore, we take  $p_2 \geq p_1 > 0$  and  $\Delta p \ll p_1$  in order to guarantee that  $|\psi(0)\rangle$  has no appreciable contribution of negative-momentum components.

The interest in choosing  $|\psi(0)\rangle$  this way comes from the fact that by varying the continuous parameters  $\beta$ ,  $p_1$ ,  $p_2$ ,  $\Delta p$ , and  $x_0$  we can easily explore different regions of the Hilbert space. Such an analysis will be the aim of the next section. For the time being, consider a free particle described at  $t=0$  by the state vector defined by Eqs. (42)–(44) with  $p_2 \rightarrow p_1 \equiv p_0$ . In this particular case,  $|\psi(0)\rangle \rightarrow |\psi_1\rangle$  and the initial state reduces to the simple minimum Gaussian wave packet considered in the preceding section [Eq. (24)]. Under these circumstances, an analytical expression can be derived for  $\Delta$ . By substituting Eq. (37) into Eq. (41), one finds (for  $0 \leq t \leq \sigma t_0$ )

$$\Delta = \Lambda_2(t-t_0)^2 - \frac{1}{2}\left(\frac{\Delta p}{p_0}\right)^2 + O\left(\frac{\Delta p}{p_0}\right)^3, \quad (45)$$

with  $\Lambda_2$  given in Eq. (40). Therefore, as a function of  $t$ , the relative difference  $\Delta$  is given by a parabola which reaches its minimum at the classical arrival time  $t_0 = (X-x_0)m/p_0$ . From Eq. (45) it follows that  $\Delta(t_0) < 0$ , and consequently

$$\langle\psi(t_0)|\hat{J}^{(+)}(X)|\psi(t_0)\rangle < \langle\psi(t_0)|\hat{J}(X)|\psi(t_0)\rangle, \quad (46)$$

so that the probability of arriving at  $t_0$  as predicted by the current  $\hat{J}(X)$  is always greater than that predicted by the modulus of the current  $\hat{J}^{(+)}(X)$ . More generally, it can be readily seen that for any  $t \geq 0$  within the symmetric interval  $[t_0 - m\Delta x/p_0, t_0 + m\Delta x/p_0]$  about  $t_0$ , it holds that

$$\langle\psi(t)|\hat{J}^{(+)}(X)|\psi(t)\rangle \leq \langle\psi(t)|\hat{J}(X)|\psi(t)\rangle, \quad (47)$$

where the equality is satisfied at the boundaries of the interval [up to terms of order  $(\Delta p/p_0)^2$ ].

## V. QUANTITATIVE ANALYSIS

### A. Free particle

We begin the analysis of the relative difference  $\Delta$  between the probability distribution  $\langle\psi_{\text{tr}}(t)|\hat{J}^{(+)}(X)|\psi_{\text{tr}}(t)\rangle$  and the probability current density  $\langle\psi_{\text{tr}}(t)|\hat{J}(X)|\psi_{\text{tr}}(t)\rangle$  by considering a free particle described at  $t=0$  by the minimum Gaussian wave packet defined in Eq. (24) [which, as already said, is nothing but a particular case of the state vector previously introduced in Eqs. (42)–(44)]. To be specific, we shall restrict our investigation to an electron with average

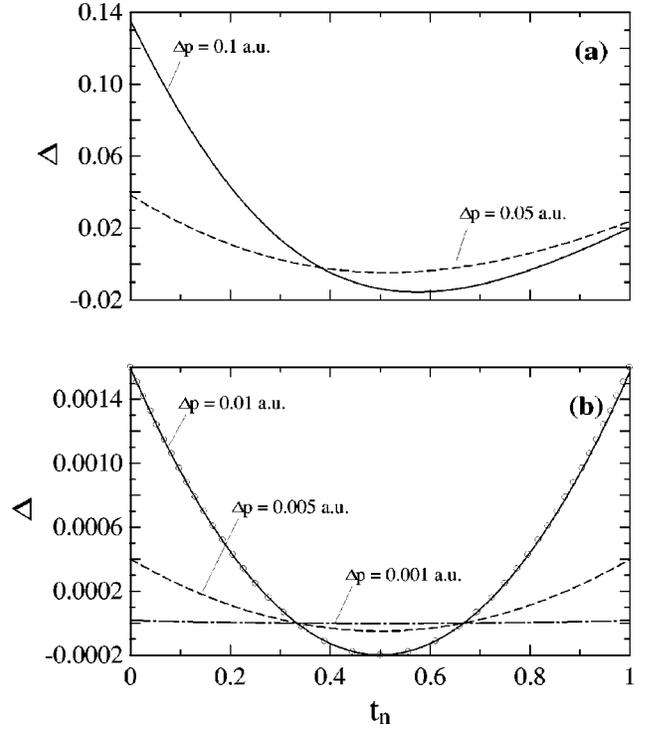


FIG. 1. Relative difference  $\Delta$  as a function of the (normalized) time of arrival  $t_n \equiv t/2t_0$  [where  $t_0$ , which depends on  $\Delta p$ , is the classical arrival time:  $t_0 \equiv (X-x_0)m/p_0 = 3m\hbar/2p_0\Delta p$ ]. The circles superimposed in the case  $\Delta p = 0.01$  a.u. correspond to the theoretical prediction of Eq. (45).

momentum  $p_0 = 0.5$  a.u., and place the detector at  $X = x_0 + 3\Delta x$ , where  $\Delta x = \hbar/2\Delta p$  is the spatial spread of  $|\psi(0)\rangle$ .

Figures 1(a) and 1(b) show the relative difference  $\Delta$ , as a function of the time of arrival, for several values of  $\Delta p$  ranging over two orders of magnitude. The detection interval has been chosen to be symmetric about the classical arrival time  $t_0$ , i.e.,  $t \in [0, 2t_0]$ . Moreover, for comparison purposes the final instant of time has been normalized to unity in all cases (i.e.,  $t \rightarrow t_n \equiv t/2t_0$ ), so that  $t_0$  lies always in the middle of the detection interval considered. It is worth remarking that the probability current density turns out to be positive in all of the cases studied.

Besides the results obtained from a direct numerical integration of the corresponding formulas, Fig. 1(b) also shows the behavior of  $\Delta$  as predicted by Eq. (45). (Only the theoretical values corresponding to  $\Delta p = 0.01$  a.u. have been explicitly plotted [circles in Fig. 1(b)] since for smaller  $\Delta p$  the agreement is even better.) As is apparent from this figure, within the range of validity of the theoretical prediction (that is, for  $(\Delta p/p_0) \ll 1$  and  $t \in [0, \sigma t_0]$ ) the agreement turns out to be excellent (as it should be). In fact, for any momentum uncertainty  $\Delta p \leq 0.01$  a.u., the relative difference between  $\langle\hat{J}^{(+)}(X)\rangle(t)$  and  $\langle\hat{J}(X)\rangle(t)$ , considered as a function of  $t$ , behaves as a parabola which cuts the horizontal axis at  $t_n = 1/3$  and  $t_n = 2/3$ , reaching its minimum value at the classical time  $t_n = 1/2$ . Furthermore, while within the interval  $[1/3, 2/3]$  the expectation value of  $\hat{J}(X)$  always dominates over the expectation value of  $\hat{J}^{(+)}(X)$ , just the opposite occurs outside such an interval.

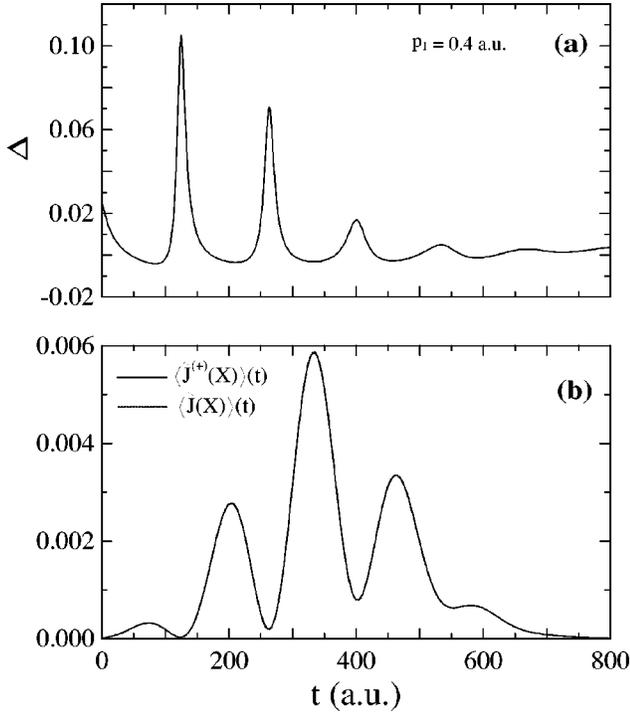


FIG. 2. (a) Relative difference  $\Delta$  as a function of the time of arrival  $t$ . (b) Expectation values (indistinguishable on the present scale) of  $\hat{J}^{(+)}(X)$  and  $\hat{J}(X)$  (in a.u.) as a function of  $t$ .

From Figs. 1(a) and 1(b), the rapid decrease of  $\Delta$  with the momentum spread is also apparent, which is a direct consequence of the fact that for  $\Delta p/p_0$  sufficiently small,  $\Delta$  is of order  $(\Delta p/p_0)^2$ . In this regard, note that for  $\Delta p \leq 0.01$  a.u. the relative difference is already less than 0.2% over all of the detection interval considered, and that figure would be even smaller if one focused attention on a time interval more localized about the most probable time of arrival  $t_0$ . This fact would render any attempt to discriminate between  $\langle \hat{J}^{(+)} \times (X) \rangle(t)$  and  $\langle \hat{J}(X) \rangle(t)$  almost impossible in practice. Such a negative conclusion should not be extrapolated, however. A minimum Gaussian wave packet represents a very special type of quantum state, for it exhibits the lowest possible uncertainty product  $\Delta x \Delta p$  and consequently is expected to be largely semiclassical in character. On the other hand, as can be inferred from an asymptotic analysis [13], in the semiclassical limit  $\hbar \rightarrow 0$  it holds that

$$\langle \psi(t) | \hat{J}^{(+)}(X) | \psi(t) \rangle \rightarrow \langle \psi(t) | \hat{J}(X) | \psi(t) \rangle, \quad (48)$$

so that the small value found for  $\Delta$  in the cases considered above is not surprising.

A simple way for generating initial states having a more genuine quantum character consists in allowing  $p_1$  to be different from  $p_2$  in Eqs. (42)–(44). In fact, a marked interference pattern can be induced in the probability current density (as well as in the corresponding position probability density) by simply increasing the distance (in momentum space) between  $p_1$  and  $p_2$  while keeping unchanged the remaining parameters.

Figures 2 and 3 show the results obtained by taking  $\beta = 2$ ,  $p_2 = 0.5$  a.u.,  $\Delta p = 0.01$  a.u., and allowing  $p_1$  to vary

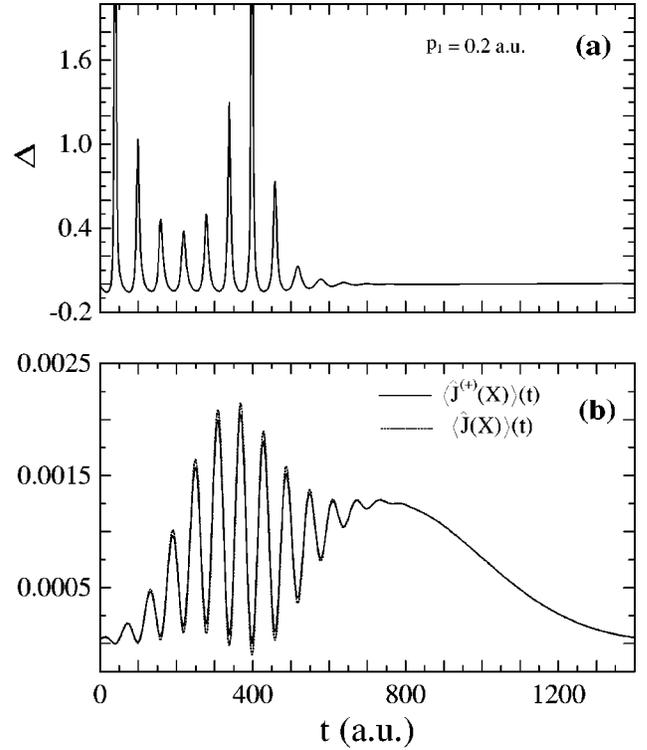


FIG. 3. (a) Relative difference  $\Delta$  as a function of the time of arrival  $t$ . (b) Expectation values of  $\hat{J}^{(+)}(X)$  and  $\hat{J}(X)$  (in a.u.) as a function of  $t$ .

between 0.4 and 0.2 a.u., respectively. The detector's position has been chosen as before (more precisely, we have taken  $X - x_0 = 3\hbar/2\Delta p$ ) and the detection interval (now expressed in atomic units) has been chosen in such a way that its final time  $t_f$  satisfies

$$\langle \psi(t_f) | \hat{J}^{(+)}(X) | \psi(t_f) \rangle \approx \langle \psi(0) | \hat{J}^{(+)}(X) | \psi(0) \rangle. \quad (49)$$

In Figs. 2(b) and 3(b) we have plotted the expectation values of both  $\hat{J}^{(+)}(X)$  and  $\hat{J}(X)$  corresponding, respectively, to  $p_1 = 0.4$  a.u. and  $p_1 = 0.2$  a.u. These curves can be considered as being obtained by means of a continuous deformation (induced by varying  $p_1$ ) starting from the initial Gaussian profile corresponding to  $p_1 = p_2 = 0.5$  a.u. Since a marked interference pattern is a hallmark of quantum behavior, it is evident that by decreasing  $p_1$  we are probing domains of the Hilbert space with increasing quantum character. As is apparent from these figures, while for  $p_1 = 0.4$  a.u. the probability current density remains positive over all of the time interval considered, the same does not occur for  $p_1 = 0.2$  a.u., and in this case  $\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle$  attains negative values in the neighborhood of  $t = 40$  a.u. and  $t = 400$  a.u.

The analysis of the corresponding relative differences, plotted in Figs. 2(a) and 3(a), reveals that now  $\Delta$  exhibits a series of maxima (clearly related to the interference pattern of the probability current density) where it can take values of order 10% (in the first case) or 100% (in the second one). [In fact, in this latter case the maxima which have been truncated in the figure correspond, respectively, to  $\Delta(39.1 \text{ a.u.}) = 31.96$  and  $\Delta(398.05 \text{ a.u.}) = 1011.58$ .] Therefore, the probability distributions of the time of arrival as predicted by

$\langle \hat{J}^{(+)}(X) \rangle(t)$  or  $\langle \hat{J}(X) \rangle(t)$  can be quite different in these cases. A comparison with the bound 0.2% obtained previously for  $p_1 = p_2 = 0.5$  a.u. [Fig. 1(b)] reflects the fact that the choice of the initial state plays an essential role in both the magnitude and the behavior of the relative discrepancy between  $\langle \hat{J}^{(+)}(X) \rangle(t)$  and  $\langle \hat{J}(X) \rangle(t)$ .

An interesting limiting situation, where quantum effects dominate the behavior of the probability current density, can be achieved by taking  $\Delta p \rightarrow 0$  and  $p_2/p_1 \gg \beta \gg 1$  in Eqs. (42)–(44). In this particular case, the initial state becomes a purely quantum state with no classical analog, consisting of the coherent superposition of two macroscopically distinguishable states in momentum space. Under these circumstances, the main contribution to  $\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle$  comes from the interference terms and one obtains, to leading order as  $\Delta p \rightarrow 0$  [13],

$$\begin{aligned} \langle \psi(t) | \hat{J}(X) | \psi(t) \rangle &\sim \frac{2\sqrt{2}\pi}{mh} \beta \alpha^2 \Delta p p_2 \\ &\times \cos[p_2^2 t / 2\hbar m - p_2(X - x_0) / \hbar] \\ &+ O((\Delta p)^2). \end{aligned} \quad (50)$$

This case is illustrated in Figs. 4(a) and 4(b), where we have specifically taken  $\beta = 100$ ,  $p_2 = 1$  a.u.,  $p_1 = 4 \times 10^{-3}$  a.u.,  $\Delta p = 5 \times 10^{-4}$  a.u., and  $X - x_0 = 3\hbar/2\Delta p$ . Also plotted in Fig. 4(b) is the modulus of the probability current density,  $|\langle \psi(t) | \hat{J}(X) | \psi(t) \rangle|$ , which is the proposal by McKinnon and Leavens [8] for the probability distribution of the time of arrival.

From a comparison between Figs. 4(a) and 4(b) it can be seen that the relative difference  $\Delta$  between  $\langle \hat{J}(X) \rangle(t)$  and  $\langle \hat{J}^{(+)}(X) \rangle(t)$  reaches a local maximum exactly when  $\langle \hat{J}(X) \rangle(t)$  reaches a local minimum, and in this case  $\Delta \gg 1$ , so that

$$\Delta \approx - \frac{\langle \hat{J}(X) \rangle(t)}{\langle \hat{J}^{(+)}(X) \rangle(t)} = \frac{|\langle \hat{J}(X) \rangle(t)|}{\langle \hat{J}^{(+)}(X) \rangle(t)}. \quad (51)$$

Consequently, the main effect produced by the replacement  $\langle \hat{J}(X) \rangle(t) \rightarrow |\langle \hat{J}(X) \rangle(t)|$  upon the corresponding relative difference would consist in a change of sign. A similar conclusion could be inferred from Fig. 3(a) for those instants of time where the probability current density becomes negative. The important consequence is that, from a quantitative setting, by replacing the probability current density by its modulus one in general does not achieve a better agreement with the probability distribution  $\langle \hat{J}^{(+)}(X) \rangle(t)$ .

### B. Potential barrier

The presence of a potential barrier might, in principle, induce some additional discrepancy between  $\langle \hat{J}(X) \rangle(t)$  and  $\langle \hat{J}^{(+)}(X) \rangle(t)$ . In order to examine whether this is the case, we shall consider next a quantum particle propagating toward a detector located at a certain asymptotic point  $X$  behind a one-dimensional potential barrier. It turns out to be most convenient restricting to initial states as simple as possible since in these cases the effect produced specifically by

the barrier can be more easily identified. Accordingly, we shall consider an electron characterized at  $t = 0$  by the Gaussian state given in Eq. (24), with  $p_0 = 0.5$  a.u. The potential barrier is assumed to occupy the segment  $[0, d]$  of the  $x$  axis, and its height  $V_0$  has been chosen in all cases so that  $p_B \equiv \sqrt{2mV_0} = 0.8$  a.u.

Our primary interest consists in investigating the behavior of the relative difference  $\Delta$  as a function of both the barrier's width  $d$  and the momentum spread  $\Delta p$ . To this end we have selected the centroid  $x_0$  of the initial wave packets in such a way that  $\langle x | \psi(0) \rangle$  does not overlap appreciably (in comparison with the transmittance  $\mathcal{T}$ ) with the interaction center. Specifically,  $x_0$  has been implicitly defined by

$$\int_0^\infty dx |\langle x | \psi(0) \rangle|^2 \approx 10^{-3} \mathcal{T} \quad (52)$$

and, consequently, is a function of both  $\Delta p$  and  $d$ . On the other hand, in order to guarantee the applicability of the formalism (which requires the particle to be asymptotically free), the detector has been assumed to be switched on at a certain instant  $t_i$  satisfying the condition that the probability of finding the particle within the interaction region is already negligible. More precisely, we have defined implicitly  $t_i$  by the condition

$$\int_{-\infty}^d dx |\langle x | \psi_u(t_i) \rangle|^2 \approx 10^{-3} \mathcal{T}. \quad (53)$$

The detector has also been assumed to be located at a certain position  $X$  behind the interaction center sufficiently far from the barrier's edge so as to satisfy the condition that when it is

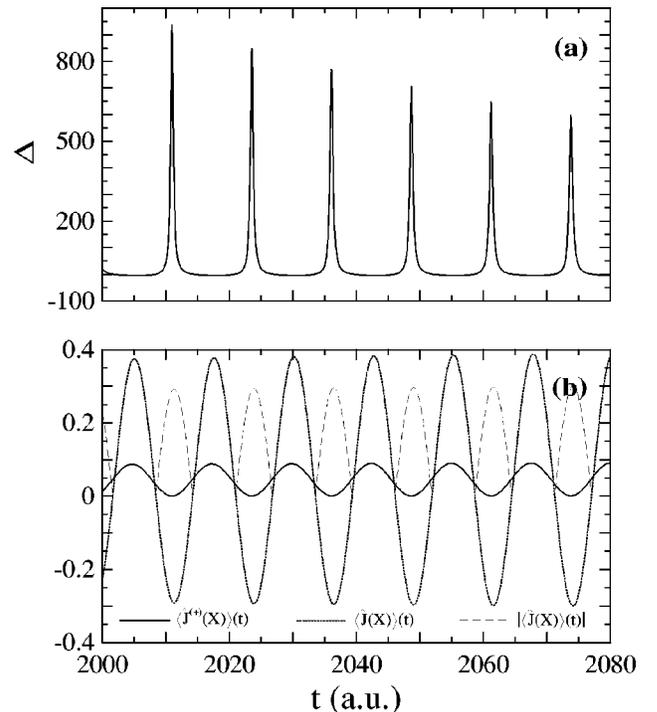


FIG. 4. (a) Relative difference  $\Delta$  between  $\langle \hat{J}^{(+)}(X) \rangle(t)$  and  $\langle \hat{J}(X) \rangle(t)$  as a function of the time of arrival  $t$ . (b)  $\langle \hat{J}^{(+)}(X) \rangle(t)$ ,  $\langle \hat{J}(X) \rangle(t)$ , and  $|\langle \hat{J}(X) \rangle(t)|$  (in  $10^{-6}$  a.u.) as a function of  $t$ .

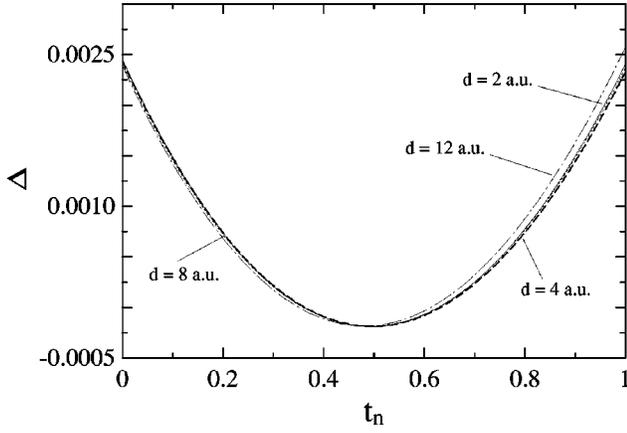


FIG. 5. Relative difference  $\Delta$  as a function of the (normalized) time of arrival  $t_n \equiv (t - t_i)/(t_f - t_i)$ , for  $\Delta p = 0.01$  a.u. and barrier widths  $d = 2, 4, 8,$  and  $12$  a.u.

switched on (at  $t = t_i$ ) the probability of finding (in the absence of detector) the transmitted particle within the region  $x \geq X$  is still negligible. That is,  $X$  has been obtained from the condition

$$\int_X^\infty dx |\langle x | \psi_{tr}(t_i) \rangle|^2 \approx 10^{-3} T. \quad (54)$$

Finally, it has been assumed that the detector is switched off at a certain instant  $t_f$  satisfying

$$\langle \psi_{tr}(t_f) | \hat{J}^{(+)}(X) | \psi_{tr}(t_f) \rangle \approx \langle \psi_{tr}(t_i) | \hat{J}^{(+)}(X) | \psi_{tr}(t_i) \rangle. \quad (55)$$

Combining Eqs. (53) and (54) we see that at  $t = t_i$ , i.e., when the detector is switched on, the transmitted particle can be found in the region between the barrier's edge and the detector's position with a probability of 99.8%, a fact that guarantees the applicability of the formulation developed in the preceding sections.

Figure 5 shows the relative difference  $\Delta$  obtained by taking  $\Delta p = 0.01$  a.u. and allowing the barrier width to vary between  $d = 2$  a.u. and  $d = 12$  a.u. The corresponding values for the parameters  $x_0$ ,  $t_i$ ,  $t_f$ , and  $X$  [obtained numerically from Eqs. (52)–(55)] are given in Table I. For comparison purposes, the time interval  $[t_i, t_f]$  has been renormalized to the interval  $[0, 1]$  by means of the mapping  $t \rightarrow t_n \equiv (t - t_i)/(t_f - t_i)$ . As is apparent from Fig. 5, the potential barrier seems to produce no special effect on  $\Delta$ . In fact, even though the transmitted state  $|\psi_{tr}(t)\rangle$  depends to a great extent on the barrier width  $d$ , the relative difference between the corresponding expectation values of  $\hat{J}(X)$  and  $\hat{J}^{(+)}(X)$  exhibits no appreciable dependence on this parameter. Furthermore,  $\Delta$  remains very small (of order 0.25%) in all cases.

Things are quite different, however, when the momentum spread increases. For  $\Delta p = 0.1$  a.u. (Figs. 6 and 7 and Table II), the relative difference not only takes greater values, but also exhibits a clear dependence on the barrier width. From Fig. 6(a) we see that for  $d = 8$  a.u.,  $\Delta$  manifests an oscillatory behavior which [from a comparison with Fig. 6(b)] can be straightforwardly related to the emergence of an incipient interference pattern in the corresponding probability current

TABLE I. Parameters corresponding to  $\Delta p = 0.01$  a.u. All values in atomic units.

$d$	$x_0$	$t_i$	$t_f$	$X$
2	-201.8	785	1550	379.0
4	-228.0	839	1600	382.0
8	-275.4	933	1700	386.5
12	-316.6	1014	1800	391.0

density. The appearance of such an interference pattern can in turn be traced back to the interference dynamically induced between tunneling and over-the-barrier contributions in the corresponding transmitted wave packet [30].

A similar behavior associated, however, with greater relative differences can be appreciated in Figs. 7(a) and 7(b), which show the results corresponding to a barrier width  $d = 10$  a.u. This particular case is interesting for still another reason. As is shown in the inset of Fig. 7(b), the probability current density takes in this case negative values in the neighborhood of the arrival time  $t = 373$  a.u. (though, admittedly, very small ones). This fact demonstrates that even for initial Gaussian wave packets having no appreciable contribution of negative-momentum components, the probability current density can take negative values at an asymptotic point  $X$  behind a one-dimensional potential barrier. This sole reason is sufficient to invalidate (even under such special circumstances) its interpretation as a probability distribution of arrival times. Of course, there still exists the possibility of considering instead the modulus of the probability current

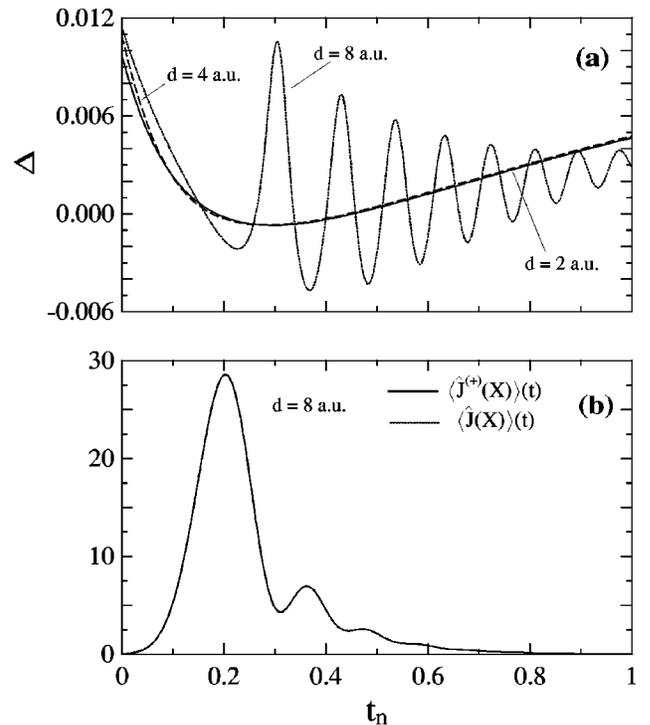


FIG. 6. (a) Relative difference  $\Delta$  as a function of the (normalized) time of arrival  $t_n \equiv (t - t_i)/(t_f - t_i)$ , for  $\Delta p = 0.1$  a.u. and  $d = 2, 4,$  and  $8$  a.u. (b) Expectation values (indistinguishable on the present scale) of  $\hat{J}^{(+)}(X)$  and  $\hat{J}(X)$  (in  $10^{-6}$  a.u.) as a function of  $t_n$ , for  $\Delta p = 0.1$  a.u. and  $d = 8$  a.u.

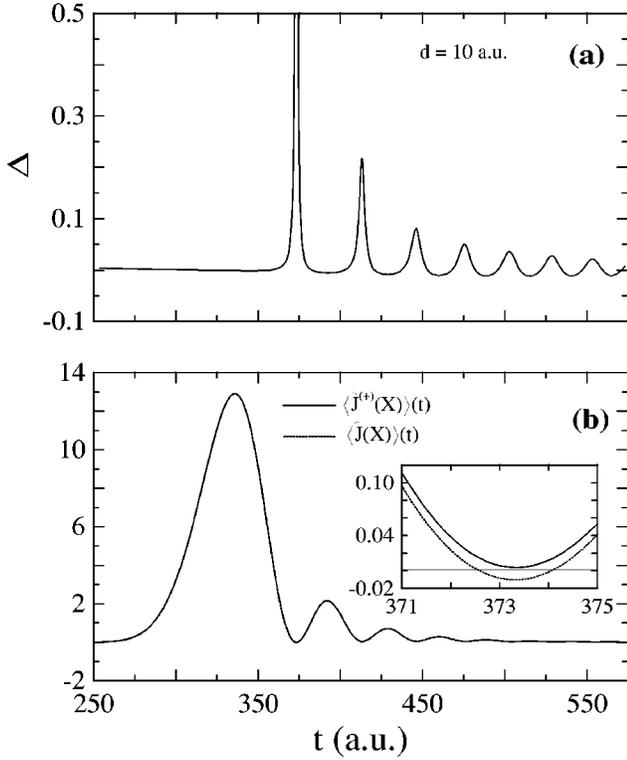


FIG. 7. (a) Relative difference  $\Delta$  as a function of the time of arrival  $t$ , for  $\Delta p = 0.1$  a.u. and  $d = 10$  a.u. (b) Expectation values (indistinguishable on the present scale) of  $\hat{J}^{(+)}(X)$  and  $\hat{J}(X)$  (in  $10^{-6}$  a.u.) as a function of  $t$ , for  $\Delta p = 0.1$  a.u. and  $d = 10$  a.u.

density. Were we to plot the relative difference between  $\langle \hat{J}^{(+)}(X) \rangle(t)$  and  $|\langle \hat{J}(X) \rangle(t)|$ , the only relevant change in Fig. 7(a) would be the transformation of the first maximum  $\Delta(t = 373.3 \text{ a.u.}) = 3.92$  into a minimum ( $3.92 \rightarrow -1.92$ ). Consequently, a considerable discrepancy would still survive.

## VI. CONCLUSION

In the present work we have compared the proposal made in previous papers [12,13] for a quantum probability distribution of the time of arrival at a certain point with that based on the probability current density (or alternatively on its modulus), with the aim of establishing conditions under which the proposals might be tested by experiment. To this end, we began by obtaining (under certain particular conditions) an analytical approximation for the expectation value of  $\hat{J}^{(+)}(X)$  valid up to order  $(\Delta p/p_0)^2$ , and we have performed a quantitative analysis of the corresponding relative differences as a function of the initial state of the particle

TABLE II. Parameters corresponding to  $\Delta p = 0.1$  a.u. All values in atomic units.

$d$	$x_0$	$t_i$	$t_f$	$X$
2	-20.15	145.7	530.0	112.9
4	-22.48	137.0	470.0	108.5
8	-25.84	141.1	390.0	117.3
10	-28.30	254.0	573.0	229.4

(both in the case of free evolution and in the presence of an intermediate potential barrier).

We have found that quantum regime conditions produce the biggest differences between the formulations which are otherwise near indistinguishable. In fact, in the semiclassical regime, for electrons in quantum states with a well-defined momentum  $p_0 \gg \Delta p$  (thus having a clear classical analog), the relative discrepancy can be typically of order 0.2%, and this figure would be even smaller if one restricted attention to arrival times having an appreciable probability. Therefore, in this regime the probability distribution proposed in Refs. [12,13] becomes indistinguishable in practice from the corresponding probability current density. Important discrepancies only occur in the purely quantum regime, for states of genuinely quantum character, having no classical analog. Indeed, the appearance of important relative differences can be straightforwardly related to the existence or emergence of a marked interference pattern in the probability current density (or alternatively in the position probability density), irrespective of the fact that such quantum interference was already present in the initial state or was generated dynamically through the temporal evolution of the system (as can be the case in the presence of a scattering potential). Furthermore, a closer analysis reveals that such quantum effects are mainly localized about arrival times having a negligible probability and/or occur over short time scales in comparison with the relevant time interval. These results indicate that in order to discriminate conclusively among the different alternatives, the corresponding experimental test should be performed in the quantum regime and with sufficiently high resolution as to resolve small quantum effects. Hopefully, the recent advances in the development of experimental techniques as well as in the preparation and manipulation of atomic systems will make such experiments feasible.

## ACKNOWLEDGMENTS

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## APPENDIX A

Let us introduce the state  $|p-\rangle \equiv \hat{\Omega}_- |p\rangle$ , which is the solution of the Lippmann-Schwinger equation corresponding to an outgoing plane wave  $|p\rangle$ , i.e.,

$$|p-\rangle = |p\rangle + (p^2/2m - i0 - \hat{H})^{-1} V(\hat{X}) |p\rangle. \quad (\text{A1})$$

In terms of these states one can define the projector

$$\hat{\mathcal{P}} \equiv \hat{\Omega}_- \Theta(\hat{P}) \hat{\Omega}_-^\dagger = \int_0^\infty dp |p-\rangle \langle p-|, \quad (\text{A2})$$

which selects that part of a given state vector that will be finally transmitted. Taking into account that  $\hat{\Omega}_\pm^\dagger \hat{\Omega}_\pm = \hat{1}$  and  $\hat{S} = \hat{\Omega}_-^\dagger \hat{\Omega}_+$ , it follows from Eq. (A2) that

$$\hat{\Omega}_-^\dagger \hat{\mathcal{P}} \hat{\Omega}_+ = \Theta(\hat{P}) \hat{S}. \quad (\text{A3})$$

By using the intertwining relations for the Møller operators [29],

$$\hat{\Omega}_{\pm}^{\dagger} \hat{H} \hat{\Omega}_{\pm} = \hat{H}_0, \quad (\text{A4})$$

as well as Eq. (A3), it can be readily shown that

$$e^{-i\hat{H}_0 t/\hbar} \Theta(\hat{P}) \hat{S} = \hat{\Omega}_{-}^{\dagger} \hat{P} e^{-i\hat{H} t/\hbar} \hat{\Omega}_{+}. \quad (\text{A5})$$

Taking advantage of this relationship and recalling that  $|\psi_{\text{tr}}\rangle = \Theta(\hat{P}) \hat{S} |\psi_{\text{in}}\rangle$ , we can write

$$|\psi_{\text{tr}}(t)\rangle = e^{-i\hat{H}_0 t/\hbar} \Theta(\hat{P}) \hat{S} |\psi_{\text{in}}\rangle = \hat{\Omega}_{-}^{\dagger} \hat{P} |\psi(t)\rangle, \quad (\text{A6})$$

where we have used that  $e^{-i\hat{H} t/\hbar} \hat{\Omega}_{+} |\psi_{\text{in}}\rangle = e^{-i\hat{H}_0 t/\hbar} |\psi(0)\rangle = |\psi(t)\rangle$ . In particular, for  $t=0$ , Eq. (A6) reduces to

$$|\psi_{\text{tr}}\rangle = \hat{\Omega}_{-}^{\dagger} \hat{P} |\psi(0)\rangle. \quad (\text{A7})$$

Substitution of Eq. (A6) [or alternatively Eq. (A7)] into Eq. (15) leads to Eq. (20).

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