Distributions of delay times and transmission times in Bohm's causal interpretation of quantum mechanics

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In Bohm's causal or trajectory interpretation of quantum mechanics, it is straightforward to determine, from a sufficiently large number of calculated particle trajectories, probability distributions for time delays caused by a potential barrier, or for transmission times through a barrier. We show that these distributions can be calculated directly and more efficiently from probability currents, without the calculation of Bohm trajectories as an intermediate step. The ideas are illustrated for Gaussian wave packets incident on a square potential barrier and used to explain why average causal delay times differ from the average delay times calculated in other approaches.

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I. INTRODUCTION

Consider an ensemble of N single-particle scattering experiments. In each experiment, a particle is launched at $t=0$ in the normalized state $\psi(z,t=0)$ from the left of and at normal incidence to a potential barrier $V(z)\theta(z)\theta(d-z)$ which varies only in the z direction. (The Heaviside unit step functions θ ensure that the barrier is confined to $0\le z\le d$.) Beyond the barrier is an ideal detector that responds if and only if the particle reaches the plane $z=b>d$, recording the arrival time $t(b)$. The initial centroid $z_0\equiv\langle\psi^*(z,0)z\psi(z,0)\rangle$ of the wave packet is chosen far enough to the left of the barrier that the integrated probability density from $z=0$ to ∞ is negligibly small compared to the transmission probability $|T|^2$. Then, for sufficiently large N, the N experiments give good estimates for both the transmission probability

$$|T|^2\equiv\lim_{t\to\infty}\int_d^\infty dz\,|\psi(z,t)|^2\approx\frac{N_T}{N}\ , \tag{1}$$

and the distribution of arrival times for transmitted particles [1,2]

$$P(t(b))\equiv\frac{j(b,t(b))}{|T|^2} \tag{2a}$$

$$\approx\frac{\delta N_T(t(b)-\frac{\delta t(b)}{2},t(b)+\frac{\delta t(b)}{2})}{N_T\delta t(b)}\ , \tag{2b}$$

where $j(z,t)\equiv(\hbar/m)\mathrm{Im}[\psi^*(z,t)\partial\psi(z,t)/\partial z]$ is the probability current density, N_T is the total number of triggered detectors, and $\delta N_T(t(b)-\delta t(b)/2,t(b)+\delta t(b)/2)/N_T$ is the fraction of these for which the recorded arrival time lies within $\pm\delta t(b)/2$ of $t(b)$. [$\delta t(b)$ must be small enough that $j(b,t(b))$ varies slowly with $t(b)$ on the scale of $\delta t(b)$. A derivation using Bohmian mechanics of (2a), clearly showing its range of validity, is given in [2].]

Several other characteristic times for the one-dimensional scattering of wave packets have been introduced into the theoretical literature [3]. It is widely agreed that the mean dwell time or sojourn time $\tau(z_1,z_2)$, defined as the average time spent subsequent to $t=0$ in the region $z_1\le z\le z_2$ by particles with initial wave function $\psi(z,0)$, is correctly given by the expression

$$\tau(z_1,z_2)=\int_0^\infty dt\int_{z_1}^{z_2}dz\,|\psi(z,t)|^2\ . \tag{3}$$

On the other hand, a great deal of controversy has stemmed from attempts to decompose $\tau(0,d)$, the mean dwell time for the barrier region, into "to be transmitted" and "to be reflected" components according to

$$\tau(0,d)=|T|^2\tau_T(0,d)+|R|^2\tau_R(0,d)\ , \tag{4}$$

involving mean transmission and reflection times $\tau_T(0,d)$ and $\tau_R(0,d)$, respectively. (Here $|R|^2=1-|T|^2$ is the reflection probability.) Many, including us, believe that this cannot be meaningfully done within conventional interpretations of quantum mechanics.

One approach that leads to further characteristic times without bending the rules of orthodox quantum mechanics, is to study the effect of the barrier on the mean time spent by the particles in a much larger spatial range $a\le z\le b$ containing the barrier. For this purpose a second ensemble is introduced, identical to the one considered above except that $V(z)$ is zero everywhere. [We label all quantities associated with this ensemble of freely evolving particles with a superscript (f).] Jaworski and Wardlaw [4] use the mean dwell times for the two ensembles to define the mean delay time for the region $a\le z\le b$ as

$$\Delta\tau(a,b)=\tau(a,b)-\tau^{(f)}(a,b)\ . \tag{5}$$

In a similar vein, they define the mean delay time for transmitted particles arriving at $z=b>d$ by

$$\Delta\tau_T^{(\mathrm{JW})}(b)=\lim_{z_2\to\infty}\left[\tau^{(f)}(b,z_2)-\frac{1}{|T|^2}\tau(b,z_2)\right]\ . \tag{6}$$

They then use

$$\Delta\tau(a,b)=|T|^2\Delta\tau_T^{(\mathrm{JW})}(b)+|R|^2\Delta\tau_R^{(\mathrm{JW})}(a,b) \tag{7}$$

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to obtain the mean delay time $\Delta\tau_R^{(JW)}(a,b)$ for reflected particles. Equation (6) involves the assumption $|T^{(f)}|^2=1$. This assumption is not true in general; for example, an initial Gaussian wave packet with zero mean velocity has $|T^{(f)}|^2=1/2$, and, strictly speaking, any Gaussian wave packet has $|T^{(f)}|^2<1$. But the difference $1-|T^{(f)}|^2$ can be made arbitrarily small by making the spread of momentum of the wave packet sufficiently small compared to the average momentum. Taking $|T^{(f)}|^2=1$ is an excellent approximation for the cases considered below. The expressions for $\Delta\tau_T^{(JW)}(b)$ and $\Delta\tau(a,b)$ in the limits $a\to-\infty$ and $b\to+\infty$ in general depend on the arguments b or a and b, respectively. However, if the potential barrier is symmetric about some point $z=z'$, then $\Delta\tau(a\to-\infty,b\to\infty)$ is independent of a and b if the natural restriction $b-z'=z'-a$ is adopted. It is clear from the analysis of Jaworski and Wardlaw that attempts to localize the entire transmission time delay to the barrier region, for example by defining the mean transmission time $\tau_T(0,d)$ to be $\tau^{(f)}(0,d)+\Delta\tau_T^{(JW)}(b)$, are not justified.

Jaworski and Wardlaw [5] also extended the method of analysis of Hauge, Falck, and Fjeldly [6] to define mean transmission and reflection time delays based on the arrival times of the centroids of wave packets at $z=b$ and $z=a$, with and without the barrier. They found that the two approaches give identical results for wave packets with vanishingly small dispersion in energy, but in general lead to different results.

Although Jaworski and Wardlaw suggested the desirability of extending their work to distributions of transmission and reflection delays, this has not been done. The approach based on the work of Hauge, Falck, and Fjeldly [6] involves the time evolution of the centroids of incident, reflected, and transmitted wave packets at small or large times. Since each of these centroids is by definition the same for each member of the ensemble, it is clear that this approach cannot be extended to the calculation of distributions. To see the difficulties involved in calculating distributions in orthodox quantum mechanics, consider how to interpret the results of two independent scattering experiments, each of N trials, one with a barrier and the other without a barrier, but otherwise identical. The data consist of N_T arrival times $\{t_i(b)|i=1,\ldots,N_T\}$ for the "with barrier" ensemble and $N_T^{(f)}$ arrival times $\{t_j^{(f)}(b)|j=1,\ldots,N_T^{(f)}\}$ for the reference or "without barrier" ensemble. How does one construct a set of transmission time delays from the N_T arrival times $t_i(b)$ and the larger number $N_T^{(f)}$ of reference arrival times $t_j^{(f)}$, faced with the impossibility of experimentally correlating a given $t_i(b)$ with a particular $t_j^{(f)}(b)$? (This question is related to the problem of constructing a joint probability distribution for $t_i(b)$ and $t_j^{(f)}(b)$, given only the individual (or marginal) distributions for $t_i(b)$ and $t_j^{(f)}(b)$. Even in classical probability theory this cannot be done in general [7].) Consistent with the inherent randomness of conventional quantum mechanics, one might try to pair every measured result for one ensemble with every one of the other, assigning equal weight to every pair. This leads to the set $\{\Delta t_{ij}(b)\equiv t_i(b)-t_j^{(f)}(b)|i=1,\ldots,N_T;j=1,\ldots,N_T^{(f)}\}$ of $N_T N_T^{(f)}$ individual transmission time delays with which to generate the desired distribution. This is consistent with the approach of Jaworski and Wardlaw for the mean transmission time delay. But now consider the case in which $V(z)$ goes to zero. Since time delays for the finite barrier case are attributed solely to the presence of the barrier, it seems logical to require that time delays should be zero for a barrier of zero height, as is the case classically. But the above quantum prescription obviously generates a distribution of time delays of nonzero width for a barrier of zero height, even though the mean transmission time delay $\Delta\tau_T^{(JW)}(b)$ is zero.

Rather than abandon the concept of delay time distribution altogether, we think it worthwhile to take a fresh look at it from the point of view of Bohm's causal or trajectory interpretation of quantum mechanics [8–11]. Since the concept of delay time is fundamentally different within this interpretation we use a new name, causal delay time, to make this clear. In the next section, we briefly introduce the relevant parts of Bohm's interpretation, then define the causal transmission delay time. Then we discuss an efficient way to calculate these distributions without calculating Bohm trajectories, and apply this technique to several examples.

To reduce the number of subscripts needed to distinguish all the different types of times we discuss, we allow the meaning of the symbol $t(\ )$ to depend on the number of arguments. Thus, for example, $t(b)$ denotes the time of arrival at $z=b$ with a barrier potential present and $t^{(f)}(b)$ the time of arrival of a free particle (no barrier); $\Delta t(b)$ denotes the delay time, the difference between the arrival times with and without a barrier; $t(a,b)$ denotes the dwell time, the time spent in the region $z=a$ to $z=b$; and $\Delta t(a,b)$ denotes the difference in dwell times with and without a barrier. The symbol $\tau(\ )$ is used similarly for average values. Subscripts T and R on τ indicate averages for transmitted or reflected particles only.

II. BOHM'S INTERPRETATION OF QUANTUM MECHANICS AND CAUSAL DELAY TIMES

Within Bohm's causal "hidden variable" interpretation of nonrelativistic quantum mechanics [8–11], a quantum entity such as an electron is a particle with, at each instant of time, a well-defined position and velocity causally determined by an objectively real (complex-valued) field $\psi(z,t)$. Although this basic postulate is completely contrary to the fundamental tenets of conventional quantum mechanics, it leads to the same results for all experimentally observable quantities when augmented by the following three secondary postulates: (1) the guiding field $\psi(z,t)$ satisfies the time-dependent Schrödinger equation (TDSE); (2) when the particle is at the position z at time t its velocity is given by

$$v(z,t)=\frac{j(z,t)}{|\psi(z,t)|^2}\ ; \tag{8}$$

(3) the quantity $|\psi(z,t)|^2dz$ is the probability of the particle being between z and $z+dz$ at time t even in the absence of a position measurement. For a particle prepared at $t=0$ in the state described by $\psi(z,0)$, uncertainty

enters only because the initial position of the particle is not known precisely. If the initial position is $z^{(0)}$ then the subsequent trajectory $z(z^{(0)},t)$ is uniquely determined by simultaneous integration of the TDSE and the guidance equation $dz(t)/dt = v(z,t)|_{z=z(t)}$.

We now consider the various characteristic times discussed in the Introduction from the point of view of Bohm's causal approach to quantum mechanics [12]. Bohm trajectories, although unobservable or hidden, are to be interpreted not as abstract mathematical constructs but as possible particle trajectories, one of which the particle actually follows in a given scattering experiment. Hence the methods of classical statistical mechanics can be applied to an ensemble of such scattering experiments using the possible particle trajectories $\{z(z^{(0)},t)| -\infty \le z^{(0)} \le \infty\}$ appropriate to the initial state $\psi(z,0)$ and barrier potential $V(z)$. For a particle that is at $z=z^{(0)}$ at $t=0$ the time spent thereafter in the region $z_1 \le z \le z_2$ is given by the classical stopwatch expression

$$t(z_1,z_2;z^{(0)}) = \int_0^\infty dt \int_{z_1}^{z_2} dz\, \delta(z - z(z^{(0)},t)) . \tag{9}$$

The mean dwell time is then given by

$$\tau(z_1,z_2) = \int_{-\infty}^{\infty} dz^{(0)} |\psi(z^{(0)},0)|^2 t(z_1,z_2;z^{(0)}) . \tag{10}$$

There is no integration over initial momenta $p^{(0)}$ in these expressions because $p^{(0)} \equiv mv^{(0)} = mj(z^{(0)},0)/|\psi(z^{(0)},0)|^2$ is uniquely determined by $z^{(0)}$ for given $\psi(z^{(0)},0)$. Inserting Eq. (9) into Eq. (10) and noting that

$$|\psi(z,t)|^2 = \int_{-\infty}^{\infty} dz^{(0)} |\psi(z^{(0)},0)|^2 \delta(z - z(z^{(0)},t)) \tag{11}$$

immediately gives the expression (3) for the dwell time.

A crucial property of Bohm trajectories $z(z^{(0)},t)$ with different $z^{(0)}$ is that they do not intersect each other [11,12]: if $z_i^{(0)} \ne z_j^{(0)}$, then $z(z_i^{(0)},t) \ne z(z_j^{(0)},t)$ for any t. This fact allows the probability density $|\psi(z,t)|^2$ for a scattering experiment to be decomposed at any time $t \ge 0$ into components $|\psi(z,t)|^2\theta(z - z_c(t))$ and $|\psi(z,t)|^2\theta(z_c(t) - z)$ associated with transmission and reflection, respectively. (See Fig. 1 of Ref. [2] for an example.) The bifurcation curve $z_c(t)$ separating transmitted trajectories from reflected ones is the Bohm trajectory $z(z_c^{(0)},t)$ given implicitly by

$$|T|^2 = \int_{z_c(t)}^{\infty} dz |\psi(z,t)|^2 \tag{12}$$

with $z_c^{(0)} \equiv z_c(0)$. The mean dwell time $\tau(z_1,z_2)$ given by Eq. (3) is readily decomposed into components associated with transmission and reflection, as in Eq. (4). The resulting mean transmission and reflection times are given by

$$\tau_T(z_1,z_2) = \frac{1}{|T|^2} \int_0^\infty dt \int_{z_1}^{z_2} dz |\psi(z,t)|^2 \theta(z - z_c(t)) , \tag{13}$$

$$\tau_R(z_1,z_2) = \frac{1}{|R|^2} \int_0^\infty dt \int_{z_1}^{z_2} dz |\psi(z,t)|^2 \theta(z_c(t) - z) . \tag{14}$$

For these average quantities it is sufficient to calculate a single Bohm trajectory, namely $z_c(t)$. The most straightforward way to calculate numerically the distribution of transmission times,

$$P_T(t(z_1,z_2)) \equiv \frac{1}{|T|^2} \int_{z_c^{(0)}}^{\infty} dz^{(0)} |\psi(z^{(0)},0)|^2 \times \delta(t(z_1,z_2) - t(z_1,z_2;z^{(0)})) , \tag{15}$$

is to construct a histogram by computing a large number of trajectories $z(z^{(0)},t)$ with $z^{(0)} \ge z_c^{(0)}$, and for each trajectory adding the weight $|\psi(z^{(0)},0)|^2$ to the histogram channel determined by $t(z_1,z_2;z^{(0)})$. A more efficient numerical method is discussed in the next section.

Equation (9) for the dwell time automatically takes into account the possibilities that a given particle never enters the region of interest or that it enters the region more than once. These possibilities are not so easily dealt with in calculations of arrival times and delay times. We consider the concept of the time of arrival $t(z^{(0)};b)$ of a particle at the point $z=b$ to be meaningless if the particle following its trajectory $z(z^{(0)},t)$ never actually reaches $z=b$ for $t>0$. We do not consider $t(b;z^{(0)})$ for such a trajectory to be $+\infty$; if this were the case then the mean arrival time at a point $b>d$ would in general be infinite. We exclude such trajectories from the outset by considering for $b \ge d$ only those for which $b > z^{(0)} > z_c^{(0)}$. This involves the implicit assumption that a reflected particle never reaches a point z in the region of zero potential $z>d$ and that a transmitted particle with $z^{(0)} < z$ arrives there once and only once. Within Bohm's interpretation, this is equivalent to the assumption that $j(z,t)$ is nonnegative for $z \ge d$. If this is indeed the case, then the arrival time distribution at $z=b \ge d$ is given by [2]

$$P(t(b)) = \frac{j(b,t(b))}{|T|^2} \quad (b \ge d) . \tag{16}$$

If for some particular case $j(b,t)$ becomes negative for $b \ge d$ and $t>0$ then Eq. (16) is no longer applicable, and reentrant trajectories must be allowed for in the analysis. The analysis along the lines of [2] necessarily becomes complicated. A negative value of $j(b,t)$ implies trajectories are crossing $z=b$ from right to left. For the cases we consider, all but a negligible number of trajectories begin to the left of $z=b$ at $t=0$, so trajectories associated with negative $j(b,t)$ must have crossed $z=b$ from left to right at least once at some earlier time. If we wish to calculate delay or dwell times for such trajectories, we must keep track of the entire history of these trajectories. One way to do this is outlined below.

In conventional interpretations, all particles belonging to the "with barrier" and "without barrier" ensembles are identical at $t=0$, because they are described by the same initial wave function $\psi(z,0)$. Within Bohm's causal interpretation, however, complete specification of the initial state of the particle also requires its initial position $z^{(0)}$. Hence, for a given value of $z^{(0)} > z_c^{(0)}$ the causal delay in the arrival time at $z=b \ge d$ due to the presence of the barrier is quite naturally defined to be

$$\Delta t(b;z^{(0)}) = t(b;z^{(0)}) - t^{(f)}(b;z^{(0)}) . \tag{17}$$

The distribution of such causal arrival time delays is given by

$$P(\Delta t(b))=\frac{1}{|T|^2}\int_{z_c^{(0)}}^{\infty}dz^{(0)}|\psi(z^{(0)},0)|^2 \times\delta(\Delta t(b)-\Delta t(b;z^{(0)})) \ . \quad (18)$$

Note that $P(\Delta t(b))$ does not contain a δ-function contribution at $\Delta t(b)=+\infty$, because we have excluded from the analysis those particles that do not reach $z=b$. Equation (18) is obviously equal to $\delta(\Delta t(b))$ for the special case $V(z)=0$ considered above. That part of the delay actually occurring in the barrier region is

$$\Delta t(0,d;z^{(0)})=t(0,d;z^{(0)})-t^{(f)}(0,d;z^{(0)}) \ , \quad (19)$$

and the corresponding distribution is

$$P_T(\Delta t(0,d))=\frac{1}{|T|^2}\int_{z_c^{(0)}}^{\infty}dz^{(0)}|\psi(z^{(0)},0)|^2 \times\delta(\Delta t(0,d)-\Delta t(0,d;z^{(0)})) \ . \quad (20)$$

For the initial wave function

$$\psi(z,0)=\frac{1}{[2\pi(\Delta z)^2]^{1/4}}\exp\left[-\left[\frac{z-z_0}{2\Delta z}\right]^2+ik_0z\right] \quad (21)$$

used in this paper the free-particle motion is readily obtained. Using (8)

$$v^{(f)}(z,t)=\frac{\left[\frac{\hbar k_0}{m}+\frac{\hbar^2(z-z_0)t}{4m^2(\Delta z)^4}\right]}{\left[1+\frac{\hbar^2t^2}{4m^2(\Delta z)^4}\right]} \ . \quad (22)$$

Integration of $dz/dt=v$ then gives

$$z^{(f)}(z^{(0)},t)=z_0+v_0t+(z^{(0)}-z_0)\left[1+\frac{\hbar^2t^2}{4m^2(\Delta z)^4}\right]^{1/2} \quad (23)$$

for the Bohm trajectory starting from $z=z^{(0)}$ at $t=0$. Transmitted trajectories are those for which

$$\lim_{t\to\infty} z(z^{(0)},t)=\infty \ , \quad (24)$$

which is equivalent to $z^{(0)}>z_c^{(0)}$, where for the free-particle case $z_c^{(0)}=z_0-2k_0(\Delta z)^2$. The arrival time $t^{(f)}(b;z^{(0)})$ for the Bohm trajectory starting at $z^{(0)}$ is defined implicitly by $z^{(f)}(z^{(0)},t^{(f)}(b;z^{(0)}))=b$ for $z_c^{(0)}\le z^{(0)}\le b$ (otherwise the particle never reaches $z=b$ for $t\ge 0$). This is readily solved to give

$$t^{(f)}(b;z^{(0)})=\frac{(b-z_0)+(z_0-z^{(0)})\left[1+\frac{(b-z^{(0)})(b+z^{(0)}-2z_0)}{4k_0^2(\Delta z)^4}\right]^{1/2}}{v_0\left[1-\left[\frac{z_0-z^{(0)}}{2k_0(\Delta z)^2}\right]^2\right]} \ . \quad (25)$$

III. EFFICIENT METHOD FOR CALCULATING DISTRIBUTIONS

So far we have considered an ideal detector that registers when a particle arrives. The quantities to be introduced in this section are closer to a different but related thought experiment. Consider as in the Introduction a series of experiments in which a particle is released at time $t=0$ in a state $\psi(z,0)$. At a time t, create an infinitesimally thin, perfectly reflecting potential barrier at a point $z=b$ to the right of where $|\psi(z,0)|^2$ is non-negligible. Such a barrier divides space into the region to the right and left of b, and once it is in place we can determine whether the particle was to the left or the right of it at time t. Repeating this sufficiently many times for particular values of b and t determines to any desired accuracy the probability $Q(b,t)$ that a particle in the ensemble is found to the right of b at time t. In terms of the wave function $\psi(z,t)$,

$$Q(b,t)=\int_b^{\infty}|\psi(z,t)|^2dz \ . \quad (26)$$

We consider only Gaussian wave packets initially localized sufficiently far to the left of the barrier so that the transmission probability $|T|^2$ is well defined and given by the limiting value of $Q(b,t)$ as t tends to infinity. From the continuity equation it follows that

$$\frac{dQ(b,t)}{dt}=\int_b^{\infty}\frac{\partial|\psi(z,t)|^2}{\partial t}dz =\int_b^{\infty}-\frac{\partial j(z,t)}{\partial z}dz =j(b,t) \ . \quad (27)$$

In the causal interpretation the distribution of arrival times, $P(t(b))$, is related to $j(b,t(b))$ by Eq. (16), provided there are no reentrant trajectories through $z=b$. Then

$$P(t(b))=\frac{1}{|T|^2}\left.\frac{\partial Q(b,t)}{\partial t}\right|_{t=t(b)} \ . \quad (28)$$

In probability theory, this relation implies that $Q(t(b))\equiv Q(b,t=t(b))$ is $|T|^2$ times the cumulative distribution function corresponding to $P(t(b))$ [7]. If $j(b,t)$ is known from a solution to the TDSE, $Q(t(b))$ can be calculated from the integral of Eq. (27),

$$Q(t(b))=\int_{-\infty}^{t(b)}j(b,t)dt \ . \quad (29)$$

[We normalize $Q(t(b))$ to the number of particles released from the source, rather than to the number of transmitted particles, to simplify the expressions derived below.]

We turn now to probability distributions of delay and transmission times. Rather than express these distributions in terms of integrals over trajectories, as in Sec. II, we shall relate them to pairs of distributions of arrival times. Since this approach avoids the calculation of trajectories, it is more efficient numerically than evaluating the integrals of Sec. II.

As an example, Fig. 1 shows $Q(t(a))$ and $Q(t(b))$ for $a=0$ Å and $b=20$ Å for a free electron that initially has a minimum-uncertainty-product Gaussian wave packet; the details will be discussed in the next section. We wish to calculate from these two functions a third function $Q(t(a,b))$ which gives the cumulant distribution function for the time $t(a,b)$ that a transmitted particle spends between a and b.

This is impossible without knowing how each particle travels from a to b. Suppose for a moment that Fig. 1 applies to a classical system, where each particle in the ensemble follows a classical trajectory from source to detector, but only the information $Q(t(a))$ and $Q(t(b))$ is available for analysis. Since the two curves are almost the same except for a translation along the time axis, it would be natural to assume that each particle in the ensemble took about the same time to cross from a to b. If so, the transmission time distribution would be sharply peaked near 1.5 fs. But without knowing the trajectories of the particles, we cannot rule out other (perhaps contrived) possibilities, such as one in which the last particles to arrive at a are rapidly accelerated between a and b, and actually are the first to arrive at b, and conversely that the first to arrive at a are the last to arrive at b. In such a case, the transmission time distribution would be broad, extending from about 0 to 5 fs. As a third possibility, we could match all points in one arrival time distribution with all points in the other, as discussed in the Introduction; this would also lead to a broad transmission time distribution. The problem, obviously, is to match points in one arrival time distribution with points in the other.

In the causal interpretation of quantum mechanics, there is a well-defined procedure to do this matching, even when there is a potential barrier in the region between $z=a$ and $z=b$, as long as there are no reentrant transmitted trajectories through either of these points. Let $z^{(0)}(t(b))$ denote the origin of the trajectory that crosses b at time $t(b)$. Since trajectories do not cross, all trajectories that begin to the right of $z^{(0)}(t(b))$ must lie to the right of b at time $t(b)$. Thus

$$Q(t(b))=\int_{z^{(0)}(t(b))}^{\infty} dz^{(0)}|\psi(z^{(0)},0)|^2 \ . \tag{30}$$

Because of this relation, we can use $Q(t(b))$ instead of $z^{(0)}$ to label the trajectories that actually reach $z=b$.

If $Q(t(b))$ is not monotonic, then $j(b,t)$ must be negative for some times, implying reentrant trajectories through b. Because trajectories do not cross each other, each time a trajectory crosses b it must do so at the same value of Q. (This is because at the instant a trajectory crosses b, all those trajectories that were to the right of it in the starting distribution must be to the right of b, and all those that were to the left of it in the starting distribution must be to the left of b.) Thus all the arrival times of a given trajectory can be read off the points where a horizontal line at a given Q intersects a plot of $Q(t(b))$ versus $t(b)$. It is readily shown from such a construction, or by the type of analysis given in [2], that the arrival time distribution is given by

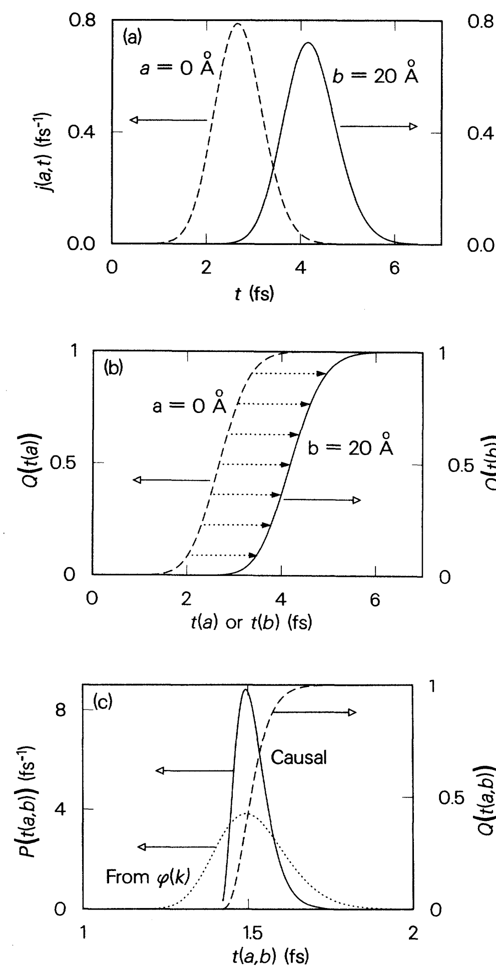

FIG. 1. Calculating the causal dwell time of a free particle, with initial wave function as given in the text. (a) Probability current density at $a=0$ Å (dashed curve) and $b=20$ Å (solid curve). (b) Cumulative distribution functions $Q(t(a))$ (dashed curve) and $Q(t(b))$ (solid curve) for arrival times $t(a)$ and $t(b)$ calculated by integrating the currents in (a) through Eq. (29). The horizontal dashed arrows indicate the matching of equal values of Q central to the calculation of the distribution of causal dwell times. (c) Cumulative distribution function $Q(t(a,b))$ (dashed curve) of causal dwell times $t(a,b)$ between a and b, calculated from (b) through Eq. (32), and corresponding probability distribution $P(t(a,b))$ (solid curve). The dotted curve in (c) is the probability density calculated from Eq. (34) based on the (unjustified) assumption that a given particle has a constant but unknown velocity $\hbar k/m$.

$$P(t(b))=\frac{|j(b,t(b))|}{\int_0^{\infty}dt'|j(b,t')|} \tag{31}$$

allowing for multiple arrival times, both from the left and right, associated with any reentrant trajectory that might occur. Moreover, if the sense of the crossing is needed, as it is in determining the dwell time, it can be read off from the slope of $Q(t(b))$; trajectories cross b from left to right when $Q(t(b))$ is increasing and from right to left when $Q(t(b))$ is decreasing. Although it is, therefore, possible to treat these more complicated cases, there is no need to do so in the examples that follow.

As discussed earlier, to calculate the distribution of transmission times for the region $a \le z \le b$, we consider the time spent in that region for each transmitted trajectory. Since each such trajectory is associated with a unique value of Q, it can be labeled by Q, giving

$$t(a,b;Q)=t(b;Q)-t(a;Q) \ . \tag{32}$$

Inverting this relation gives $Q_T(t(a,b))$ for the causal transmission time $t(a,b)$, and differentiating $Q_T(t(a,b))$ with respect to $t(a,b)$ and normalizing with $|T|^2$ gives the transmission time distribution $P_T(t(a,b))$.

To obtain a distribution of arrival time delays, we compare the distribution of arrival times $Q(t(b))$ of transmitted particles with the barrier in place and the distribution $Q^{(f)}(t(b))$ for the free particle (no barrier). The delay time $\Delta t(b)$ for a particular trajectory is given by the difference between the arrival time $t(b)$ at b with the barrier and the value $t^{(f)}(b)$ for the corresponding trajectory (the same $z^{(0)}$) without the barrier. Again, because trajectories do not cross, corresponding trajectories are uniquely specified by their common value of Q. The causal delay time $\Delta t(b)$ for a given Q is given by

$$\Delta t(b;Q)=t(b;Q)-t^{(f)}(b;Q) \ . \tag{33}$$

Inverting this gives $Q(\Delta t(b))$ for the delay time $\Delta t(b)$ at the point b. Differentiating $Q(\Delta t(b))$ with respect to $\Delta t(b)$ and normalizing with $|T|^2$ gives the arrival time delay distribution $P(\Delta t(b))$.

Equations (32) and (33) relate $Q_T(t(a,b))$ and $Q(\Delta t(b))$ to $Q(t(a))$, $Q(t(b))$, and $Q^{(f)}(t(b))$, which through Eq. (29) are related to probability currents, and hence to wave functions. Thus $Q_T(t(a,b))$ or $Q(\Delta t(b))$ can be calculated directly from solutions of the TDSE (subject to the above proviso regarding reentrant trajectories); no intermediate calculations of trajectories are needed. The next section shows calculated distributions of delay and transmission times for electron wave packets tunneling through a square potential. The quantities $Q_T(t(a,b))$ or $Q(\Delta t(b))$ also simplify derivation of relations between average causal dwell times and arrival times; as an example, we discuss why the average causal delay time differs from results derived in conventional approaches.

IV. NUMERICAL RESULTS

In this section, we demonstrate the accuracy of the approach of the previous section in calculations of transmission and delay times for electron wave packets. We compare the probability distributions of these times calculated directly from the Bohm trajectories to those calculated from the integrated current density using the results of Sec. III.

A. Free-electron transmission time distribution

As a first example, consider the time that a free electron spends in the region between a and b. The starting wave function $\psi(z,t=0)$ is assumed to be a minimum-uncertainty-product Gaussian wave packet with centroid at $z_0=-35.58$ Å, and initial spread in wave vector k of $\Delta k=0.08$ Å^{-1}. (The reason for the particular choice of initial centroid will emerge below in the analysis of the same wave packet incident on a barrier.) Figure 1(a) shows $j^{(f)}(z,t)$ at $z=a=0$ and $z=b=20$ Å as a function of time, and Fig. 1(b) the corresponding results for $Q(t(a))$ and $Q(t(b))$ calculated by Eq. (29). The arrows in Fig. 1(b) show schematically how $Q(t(a,b))$ for the dwell time is calculated through Eq. (32) by connecting equal values of Q, and Fig. 1(c) shows the results of that (numerical) calculation.

Also shown in Fig. 1(c) is the distribution of dwell times based on the *unjustified* assumption that each electron in the ensemble has a constant but unknown velocity $\hbar k/m$ distributed according to $m|\phi(k)|^2/2\pi\hbar$, where $\phi(k)=\int_{-\infty}^{\infty}\psi(z,0)e^{-ikz}dz$ is the Fourier transform of $\psi(z,0)$. The resulting probability density for the transmission time $t(a,b)=(b-a)m/\hbar k$ is

$$P(t(a,b))=\frac{m(b-a)}{2\pi\hbar[t(a,b)]^2}|\phi(k)|^2 \ . \tag{34}$$

This quantity differs from the causal result because in Bohm's interpretation the particle velocity is not necessarily equal to $\hbar k/m$. The particle is not "free" in the classical sense within the causal interpretation—it is guided by the wave function and hence subject to the quantum potential $-(\hbar^2/2m)|\psi(z,t)|^{-1}\partial^2|\psi(z,t)|/\partial z^2$ [8–11]. Holland [11] discusses this in more detail.

B. Causal distribution of arrival time delays

We now consider the distribution of arrival time delays $P(\Delta t(b))$ produced by a barrier of height 10 eV extending from $a=0$ to $b=5$ Å, for the same initial wave packet used in Fig. 1. The initial centroid z_0 of the wave packet was chosen so that only $10^{-4}|T|^2$ of the initial probability density was to the right of $z=0$. Figure 2(a) shows the probability current $j(b,t)$ and $j^{(f)}(b,t)$, and Fig. 2(b) the corresponding values of $Q(t(b))$ and $Q^{(f)}(t(b))$, obtained by integration through Eq. (29) with and without the barrier, respectively. Note that $Q(t(b))$, normalized to the number of electrons incident on the barrier, tends to $|T|^2$ at long times. Thus in calculating the arrival time delay [Eq. (33)], we need only those values of $Q^{(f)}(t(b))$ less than $|T|^2$; that is, we consider only the free-electron trajectories corresponding to those which are transmitted when the barrier is in place. Figure 2(c) shows the calculated cumulative distribution function $Q(\Delta t(b))$ and the resulting distribution

$P(\Delta t(b))$ of arrival time delays. The circles show the distribution calculated by direct numerical evaluation of Eq. (18) using about 10^4 transmitted Bohm trajectories. The two calculations agree as they should except for the scatter of the circles, which could be eliminated by following a much larger number of trajectories or using a better sampling technique.

The peak in $P(\Delta t(b))$ of Fig. 2(c) is at about 1.5 fs. According to Fig. 2(a), most electrons arrive between 2 and 3 fs with the barrier in place, and most free electrons starting from the same region in the initial distribution arrive at about 1 fs. Thus in Bohm's interpretation the barrier delays the electrons between about 1 and 2 fs. We would arrive at a very different conclusion if we compared the peaks in the probability current in Fig. 2(a); we would conclude, in fact, that the delay is negative, or that, on average, electrons travel faster in the region $z \leq b$ with the barrier than without. This conclusion, incorrect in the Bohm interpretation (and unjustified in conventional interpretations), is the result of ignoring the difference in behavior of free electrons that would be transmitted and those that would be reflected, were the barrier in place. We return to this point below.

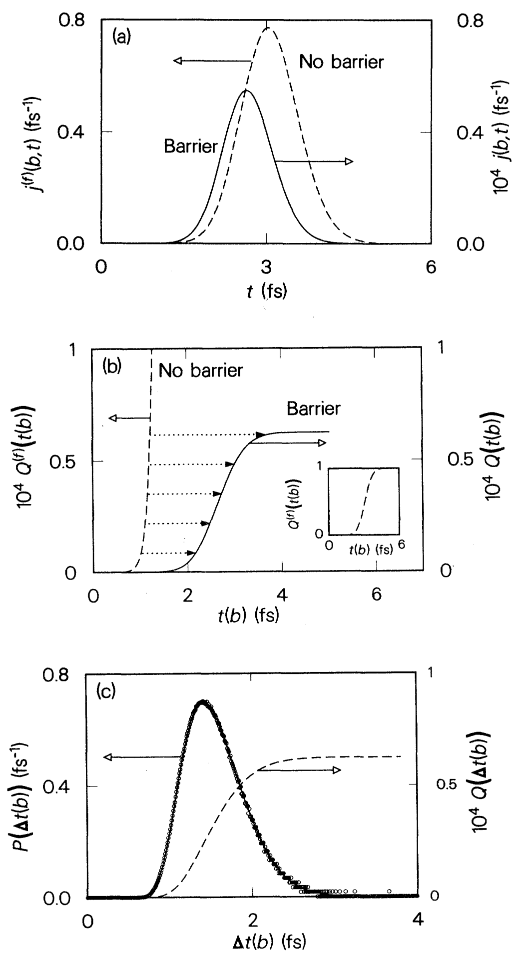

FIG. 2. Calculating the causal delay time associated with a constant potential barrier of 10 eV extending from $z=0$ Å to $z=5$ Å. The same initial wave function is used as in Fig. 1. (a) Probability current density at $b=5$ Å without a potential barrier (dashed curve) and with a barrier (solid curve). Note the different vertical scales for the two curves in (a). (b) $Q^{(f)}(t(b))$ without the barrier (dashed curve) and $Q(t(b))$ with the barrier (solid curve) calculated from the integral of the currents in (a) through Eq. (29). The insert shows that $Q^{(f)}(t(b))$ for the free particle (no barrier) reaches a value close to unity at long times. The dashed arrows connect equal values of Q, as used in the calculation of (c). (c) Causal distribution function $Q(\Delta t(b))$ of causal delay time $\Delta t(b)$ at b (dashed curve) calculated from (b) through Eq. (33), and corresponding probability distribution $P(\Delta t(b))$ (solid curve). The circles in (c) were calculated from the integral in Eq. (18) using 10^4 Bohm trajectories.

C. Causal transmission time distribution

Figure 3(a) shows the probability current density at the front ($z=a=0$) and at the rear ($z=b=d$) of the same barrier as above, for the same starting wave packet. Note the difference in scales for the two currents. The probability current density at the front of the barrier goes negative, corresponding to Bohm trajectories that are reflected after penetrating part way into the barrier. (These trajectories are illustrated in Fig. 3 of Ref. [12].) The functions $Q(t(a))$ and $Q(t(b))$ calculated by Eq. (29) are shown in Fig. 3(b). As shown by the insert, the peak in $Q(t(a))$ is much higher than its final value $|T|^2$, indicating that nearly all the trajectories crossing $z=0$ are turned back. The calculation of Eq. (32) leads to the distribution of transmission times in Fig. 3(c).

In this example, the distribution of arrival time delays $P(\Delta t(b=d))$ of Fig. 2(c) is almost the same as the distribution of transmission times $P_T(t(a=0,b=d))$ of Fig. 3(c). This similarity suggests that most of the arrival time delay occurs while the particle is inside the barrier. The trajectories in Fig. 3 of Ref. [12] confirm this.

In the insert to Fig. 3(b), $Q(t(a))$ has a peak because there are reentrant reflected trajectories at $z=a$. A reflected trajectory that penetrates the barrier enters it at $t=t_{\text{in}}(a)$ with a positive velocity [$j(a,t_{\text{in}}(a))$ is positive] and leaves it at a later time $t_{\text{out}}(a)$ with a negative velocity [$j(a,t_{\text{out}}(a))$ is negative]. With arguments similar to those used in deriving the distribution of transmission times in Eq. (32), we could calculate the distribution of reflection times for the region $z>a$ from the difference $t_{\text{out}}(a)-t_{\text{in}}(a)$ at a fixed Q, with $t_{\text{out}}(a)$ to the right of the peak in $Q(t(a))$ and $t_{\text{in}}(a)$ to the left of the peak, such that $Q(t_{\text{out}}(a))=Q(t_{\text{in}}(a))=Q$.

V. AVERAGE DELAY TIMES

The distributions for delay and dwell times within Bohm's theory are derived from differences in arrival times. Similarly, the mean delay and dwell times can also be expressed as differences in mean arrival times. As an example, we consider the average transmission delay time, and show that it involves a quantity that is undefined in conventional quantum mechanics.

In the Bohm interpretation, the mean arrival time of the particle at $z=b>d$ with the barrier in place is

$$\tau(b)=\int_0^\infty t(b)P(t(b))dt(b) \ . \tag{35}$$

We now change variables in the integral from t to Q, using Eq. (28) to relate $P(t(b))$ to $dQ(t(b))/dt(b)$,

$$\begin{aligned}\tau(b)&=\frac{1}{|T|^2}\int_0^\infty t(b)\frac{dQ(t(b))}{dt(b)}dt(b)\\ &=\frac{1}{|T|^2}\int_0^{|T|^2} t(b;Q)dQ \ .\end{aligned} \tag{36}$$

The expression for mean arrival time without the barrier is

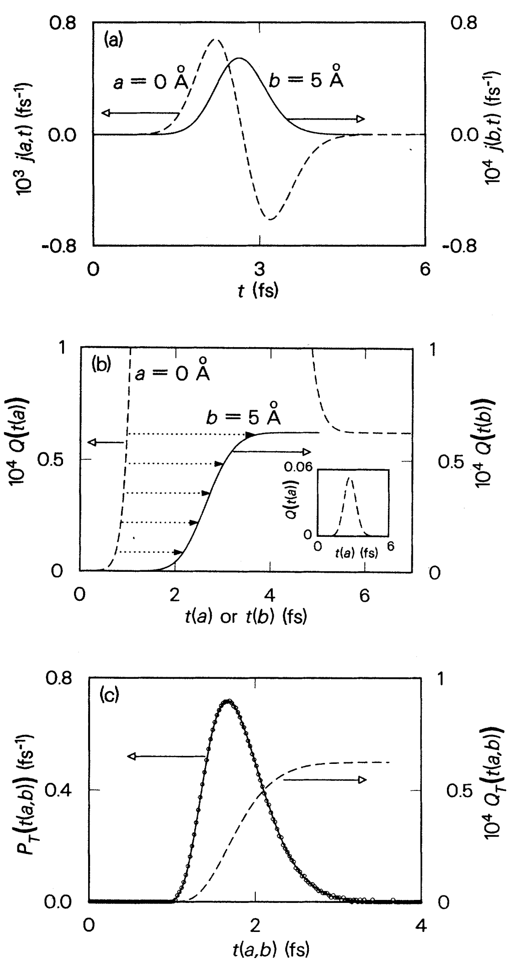

FIG. 3. Calculating the causal transmission time. The potential barrier and incident wave packet are the same as in Fig. 2. (a) Probability current density at $a=0$ Å (dashed curve) and at $b=5$ Å (solid curve). Note the different vertical scales for the two curves in (a). (b) $Q(t(a))$ at $z=a=0$ Å (dashed curve) and $Q(t(b))$ at $z=b=5$ Å (solid curve) calculated from the integral of the currents in (a) through Eq. (29). The insert shows the peak and subsequent drop in $Q(t(a))$ due to the reentrant trajectories of reflected particles. The dashed arrows connect equal values of Q, as used in the calculation of (c). (c) $Q_T(t(a,b))$ of causal transmission time $t(a,b)$ calculated from (b) through Eq. (32), and corresponding probability distribution $P_T(t(a,b))$ (solid curve). The circles in (c) were calculated from the integral in Eq. (15) using 10^4 Bohm trajectories.

$$\begin{aligned}\tau^{(f)}(b)&=\frac{1}{|T|^{(f)}|^2}\int_0^{|T^{(f)}|^2} t^{(f)}(b;Q)dQ\\ &=\int_0^1 t^{(f)}(b;Q)dQ \ ,\end{aligned} \tag{37}$$

where we have followed Jaworski and Wardlaw in assuming that the free-particle transmission probability $|T^{(f)}|^2$ is unity. A similar equation follows for the mean delay time:

$$\Delta\tau(b)=\frac{1}{|T|^2}\int_0^{|T|^2}\Delta t(b;Q)dQ \ . \tag{38}$$

The delay and arrival times at a given Q are related by Eq. (33). Substituting this relation into the integrand of Eq. (38) gives

$$\begin{aligned}\Delta\tau(b)&=\frac{1}{|T|^2}\left[\int_0^{|T|^2} t(b;Q)dQ-\int_0^{|T|^2} t^{(f)}(b;Q)dQ\right]\\ &=\tau(b)-\frac{1}{|T|^2}\int_0^{|T|^2} t^{(f)}(b;Q)dQ\\ &=\tau(b)-\tau^{(T)}(b) \ ,\end{aligned} \tag{39}$$

where $\tau^{(T)}(b)$ is defined as

$$\tau^{(T)}(b)\equiv\frac{1}{|T|^2}\int_0^{|T|^2} t^{(f)}(b;Q)dQ \ . \tag{40}$$

(Note that T, not $T^{(f)}$, enters this definition.)

This quantity $\tau^{(T)}(b)$ is not defined in conventional interpretations of quantum mechanics, because we cannot ask whether a given particle would have been transmitted if there had been a barrier, when in fact there was no barrier. It is, however, well defined in Bohm's interpretation. As an example, let us compare the causal delay time in Eq. (39) with the transmission time $\Delta\tau_T^{\rm JW}(b)$ considered by Jaworski and Wardlaw [4], given above in Eq. (6). To see the difference, we cast their expression in a form like Eq. (39). From Eq. (26), the probability for finding a particle to the right of $z=b$ at time t is $\mathcal{Q}^{(f)}(b,t)$ without the barrier and $\mathcal{Q}(b,t)$ with the barrier. Consider the latter case first. The dwell time for the region $b\le z\le\infty$ is

$$\tau(b,\infty)=\lim_{t_2\to\infty}\int_0^{t_2}\mathcal{Q}(b,t)dt \ . \tag{41}$$

Integrating by parts gives

$$\begin{aligned}\tau(b,\infty)&=\lim_{t_2\to\infty}\left[\mathcal{Q}(b,t_2)t_2-\int_0^{\mathcal{Q}(b,t_2)} t(b;Q)dQ\right]\\ &=\lim_{t_2\to\infty}[\,|T|^2t_2]-\int_0^{|T|^2} t(b;Q)dQ \ ,\end{aligned} \tag{42}$$

where we have used $\mathcal{Q}(b,\infty)=|T|^2$ and assumed that $\mathcal{Q}(b,0)$ is negligible. The last term in Eq. (42) is $|T|^2\tau(b)$. Thus

$$\tau(b,\infty)=\lim_{t_2\to\infty}[\,|T|^2t_2]-|T|^2\tau(b) \ . \tag{43}$$

A similar expression follows for $\tau^{(f)}(b,\infty)$, except with $|T|^2$ replaced by $|T^{(f)}|^2=1$:

$$\tau^{(f)}(b,\infty)=\lim_{t_2\to\infty}[t_2]-\tau^{(f)}(b)\ . \qquad (44)$$

Substituting (43) and (44) into (6) cancels the terms in t_2, giving

$$\Delta\tau_T^{(\mathrm{JW})}(b)=\tau(b)-\tau^{(f)}(b)\ . \qquad (45)$$

This expression differs from the average causal delay time $\Delta\tau(b)$ in Eq. (39) because of the following inequality:

$$\tau^{(f)}(b)\neq\tau^{(T)}(b)\ . \qquad (46)$$

In words, $\tau^{(f)}(b)$, the average arrival time without the barrier, is not the same as $\tau^{(T)}(b)$, the average arrival time of only those particles with $z^{(0)}>z_c^{(0)}$, which would have been transmitted had the barrier been in place. This statement is meaningless in conventional interpretations of quantum mechanics, but in Bohm's interpretation it makes sense, both in words and mathematically as expressed above. The difference between $\tau^{(f)}(b)$ and $\tau^{(T)}(b)$ can be large, especially when $|T|^2$ is small, because only those trajectories that reach the barrier first are transmitted in Bohm's interpretation. Those trajectories originate in the forward tail of the starting Gaussian wave packets used in Fig. 2.

VI. DISCUSSION AND CONCLUSIONS

We have given a prescription for calculating causal transmission times or causal delay times in the Bohm interpretation directly from a solution of the TDSE, with out calculating Bohm trajectories as an intermediate step. With these expressions, we derived the delay time of Jaworski and Wardlaw, and showed why their expression differs from the corresponding causal time: they assume that each particle in a scattering experiment is identical, and has the same probability of being transmitted as any other, whereas the causal time is based on the idea that a particle's fate is decided by its starting position, and so is already determined before the particle reaches the barrier. (The starting position, however, is not controllable.) Jaworski and Wardlaw say, "The point is that quantum mechanically there is no sense in speaking about transmitted and reflected particles before they are detected as such." We agree, but only in the conventional interpretation of quantum mechanics. In Bohm's approach this does make sense; the quantity $\tau^{(T)}(b)$ is well defined, and enters the expression for $\Delta\tau(b)$.

The assumption of Jaworski and Wardlaw that all particles are equally likely to be transmitted has been called into question by recent experiments on the time delay of transmitted photons [13,14]. The authors of these experiments interpret their results as evidence that the transmitted packet comes from the front of the incident packet, a particular case of what they call pulse reshaping. According to them [13], Bohm's causal interpretation provides "the closest there is to an explanation of why only the early part of an incident wave packet traverses a tunnel barrier." This is certainly true in our opinion when the particles involved are electrons, but there is no consensus on the correct form of a causal interpretation for photons [15]. Dumont and Marchioro [1], who observed pulse reshaping in quantum and semiclassical calculations for tunneling through one-dimensional Gaussian and Lorentzian potentials, describe the process as the barrier acting as a filter for the large-momentum components of the initial wave packet, as proposed by Hartman [16]. The Bohm interpretation clearly gives a different picture.

Even if a delay time distribution can be determined experimentally, the theoretical causal expressions for it will be of relevance to the experiment only if the measuring process does not strongly perturb the intrinsic quantity. It would be interesting to calculate how much a quantum clock or other measuring apparatus changes the distribution. It may be that the causal delay times for an unperturbed system have little or no relation to measured times. If so, these times would be analogous to the causal momentum of an electron in a stationary s state. In the causal interpretation, an electron in an s state is at rest. But, as Bohm discusses [8], in a time-of-flight measurement the quantum potential accelerates the electron as soon as the confining potential is removed, and the causal interpretation predicts the same experimental result as the conventional interpretation for the distribution of arrival times at a distant detector. So in the causal interpretation a time-of-flight measurement of momentum does not reveal the intrinsic value of momentum in the stationary state. Perhaps the same is true of the causal times we have considered here.

In summary, we have shown that distributions of causal arrival times, causal transmission times, and causal arrival time delays, all well-defined quantities in Bohm's interpretation of quantum mechanics, can be obtained directly from the probability current density without a calculation of Bohm trajectories as an intermediate step.

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