Solid State Communications, Vol. 76, No. 3, pp. 253-261, 1990.
Printed in Great Britain.

0038-1098/90$3.00+.00
Pergamon Press plc

TRAVERSAL TIMES FOR RECTANGULAR BARRIERS WITHIN BOHM'S CAUSAL INTERPRETATION OF QUANTUM MECHANICS

C.R. Leavens

Institute for Microstructural Sciences,
National Research Council of Canada, Ottawa K1A 0R6

(Received 5 July 1990 by R. Barrie)

In sharp contrast to the conventional interpretation of quantum mechanics, Bohm's causal or trajectory interpretation provides a unique, well-defined, and unambiguous prescription for calculating the average time spent by a transmitted particle inside a one-dimensional barrier. Numerical results for such traversal times are presented for the special case of a particle described initially by a minimum-uncertainty-product wavepacket incident on a rectangular barrier. These are very different from the corresponding Larmor clock or time-modulated barrier results unless the transition probability is close to unity.

For the one-dimensional scattering problem in which a particle with wave function $\Psi(z,t)$ is incident normally (from the left) on the potential barrier $U(\vec{r}) = V(z)\Theta(z)\Theta(d-z)$, the following three characteristic times[1] are of considerable current interest[2,3,4]: the transmission and reflection times $\tau_T(a,b)$ and $\tau_R(a,b)$ are the (ensemble) average times spent in the region $a \le z \le b$ by transmitted and reflected particles respectively; the dwell time $\tau_D(a,b)$ is the average time spent between a and b irrespective of whether the incident particle is ultimately transmitted or reflected. The quantity of primary interest here is the so-called traversal time $\tau_T \equiv \tau_T(a=0,b=d)$.

In quantum mechanics time is regarded not as an observable represented by a Hermitian operator but rather as a parameter or 'c-number'.[5] Hence, there is no automatic prescription in the basic formalism for calculating the above characteristic times. Moreover, within the conventional interpretation a microscopically well-defined particle trajectory is a meaningless concept and, consequently, it is sometimes claimed that the traversal time is also a meaningless concept. Despite this, many different approaches for calculating the traversal time have been invented. However, there is no consensus on which, if any, is (are) correct. It is sometimes argued that much of the resulting controversy and confusion stems from the fact that two approaches give different results simply because they are concerned with different characteristic transmission times, at least one of which is not the traversal time as defined above. However, for each of the approaches discussed in this paper a case can be made that the characteristic transmission time involved is, in fact, the above traversal time.

Disregarding quantum mechanics for the moment, consider a classical point-particle propagating in one dimension under the influence of the potential $V(z)\Theta(z)\Theta(d-z)$ along the precisely determined trajectory $z(t)$. The time spent by this particle in the region $a \le z \le b$ is exactly and unambiguously given by

$$t(a,b) \equiv \int_{-\infty}^{+\infty} dt\,\Theta[z(t)-a]\,\Theta[b-z(t)] \quad . \tag{1}$$

If the particle is transmitted completely through the region of non-zero potential $0 \le z \le d$ then its traversal time is clearly $t(0,d)$.

The classical result given by Equation (1) was the starting point of Sokolovski and Baskin's Feynman path-integral approach[6] to the calculation of a quantum mechanical traversal time. They generalized (1) for the classical path $z(t)$ to an arbitrary path and then averaged the resulting functional, using the complex Feynman weight factor[7], over all possible paths subject to the appropriate stationary-state scattering boundary conditions. The resulting traversal time for an incident particle with precisely known energy $E \equiv \hbar^2k^2/2m$ is

$$\tau_T^{SB}(k) \equiv \tau_T^{SB}(k;0,d) = i\hbar \int_0^d \frac{\delta \ln T[k;V(z)]}{\delta V(z)} dz \tag{2}$$

where $T[k;V(z)]$ is the plane-wave transmission probability amplitude for the barrier $V(z)$. The real and imaginary parts of this complex traversal time are identical to the spin-precession traversal time of Rybachenko[8] and (minus) the spin-rotation traversal time of Büttiker[1]. These transmission times were derived, following Baz'[9], from an analysis of the effect of an infinitesimal uniform magnetic field confined to the barrier region $0 \le z \le d$ on the components of the average spin per transmitted particle in the plane perpendicular to the field and in the field direction respectively. Büttiker[1] identified the actual traversal time with the square-root of the sum of the squares of the spin-precession and spin-rotation traversal times (i.e. with $|\tau_T^{SB}(k)|$). This quantity is referred to as the Larmor clock traversal time in the rest of the paper. It is identical to the Büttiker-Landauer traversal time[10] derived by considering the sensitivity of the transmission probability amplitude to the instantaneous height of a time-modulated barrier. In view of the above exact relations linking the spin-precession and Larmor clock or modulated barrier traversal times with that of Sokolovski and Baskin it is difficult not to believe that all these approaches attempt to calculate the same characteristic time. Moreover, since the method of Sokolovski and Baskin is based on the classical result (1), the meaning of which is perfectly clear, there is a strong case for arguing that all these approaches address the same problem, namely the calculation of the traversal time as defined at the beginning of the paper. A somewhat weaker case can be made for including all those approaches based on the sensitivity of the transition probability amplitude to the energy E of the incident particle. For example, Huang et al.[11] have repeated the Larmor clock analysis[1] but with the infinitesimal uniform magnetic field extending from $-\infty$ to $+\infty$ rather than being confined to the barrier region. They obtained spin-precession and spin-rotation transmission times that differ from those of Rybachenko[6] and Büttiker[1] respectively (the difference between the two spin-precession times diverges as the incident energy goes to zero!). Their spin-precession time is in fact identical with the Bohm-Wigner phase transmission time[12,13] obtained by tracking the peak[14] (or centroid[15]) of a sufficiently wide wavepacket through the barrier region. This involves an extrapolation through the region in front of the barrier where there is strong interference between the incident and reflected components of the wavefunction. In fact, all the approaches involving the sensitivity to E lead to a different result from Rybachenko's not because they are concerned with a different characteristic transmission time but because they ignore in one way or another this quantum mechanical interference[16,4]. Such approaches are not considered further in this paper.

As argued above, the spectrum of different results for the traversal time obtained within the conventional interpretation of quantum mechanics cannot be swept under the rug by simply claiming that approaches that lead to different results are actually concerned with different characteristic transmission times. In the author's opinion the traversal time problem has not been satisfactorily resolved within the conventional interpretation despite many serious attempts and it might prove worthwhile to approach the problem from the point of view of an alternative interpretation, in particular Bohm's causal or trajectory interpretation[17-21]. At first sight this might seem pointless because of the well known claim that Bohm's interpretation leads to exactly the same results as the conventional one for all measurable quantities.[18] However, it is possible that this applies only to observables represented by Hermitian operators and not to the characteristic times of interest here (recall that time is only treated as a parameter in quantum mechanics). In any case, within Bohm's interpretation it is almost trivial to write down formal expressions for these quantities[22] and the numerical results presented below for the traversal time of a rectangular barrier are, to the author's knowledge, qualitatively different from any in the literature. This, of course, does not necessarily mean that one cannot invent an approach within the conventional interpretation that gives identical results. However, that remains an interesting possibility especially if, as some maintain, the concept of traversal time is not a meaningful one within the conventional interpretation because it implies precisely defined particle trajectories which are expressly forbidden. This is obviously not the case in Bohm's trajectory interpretation which does not require an observer at the most fundamental level and hence regards pre-existing properties of particles such as instantaneous positions and velocities as meaningful.

In the one-electron version of Bohm's theory[18] a non-relativistic (spinless) electron is a particle the motion of which is determined by an objectively real complex-valued field

$$\Psi(z,t) \equiv R(z,t)\exp[iS(z,t)/\hbar] \qquad \text{(R and S real)}, \tag{3}$$

satisfying the time-dependent Schrödinger equation via the guidance condition

$$v(z,t) = \frac{1}{m}\frac{\partial S(z,t)}{\partial z} \tag{4}$$

on the instantaneous velocity of the particle. Given $\Psi(z,t{=}0)$, if the particle's initial position $z^{(0)}$ is also known exactly at $t = 0$ then its trajectory $z(z^{(0)},t)$ is uniquely determined by simultaneous integration of the Schrödinger equation and $dz(t)/dt = v(z,t)$. Alternatively, the trajectory can be obtained by simultaneously integrating the Schrödinger equation and Newton's equation of motion with the usual potential energy $V(z)$ augmented (in the latter only) by the "quantum potential"

$$Q(z,t) \equiv -\frac{\hbar^2}{2m}\frac{\partial^2 R(z,t)}{\partial z^2}/R(z,t) \quad . \tag{5}$$

The particle's initial position is never known exactly in practice and uncertainty enters Bohm's deterministic theory through the postulated probability distribution for the initial position of the particle: $|\Psi(z^{(0)},0)|^2\, dz^{(0)}$ is the probability of the particle being between $z^{(0)}$ and $z^{(0)} + dz^{(0)}$ at $t = 0$ even if a position measurement is not made at that instant. For a point-particle that is at $z^{(0)}$ at $t = 0$ the time spent thereafter in the region $a \le z \le b$ is exactly and unambiguously given by

$$t(z^{(0)};a,b) = \int_0^\infty dt\, \Theta[z(z^{(0)},t) - a]\,\Theta[b - z(z^{(0)},t)] \quad . \tag{6}$$

It is always assumed in the following discussion of the characteristic times $\tau_T(a,b)$, $\tau_R(a,b)$ and $\tau_D(a,b)$ that the initial wavepacket described by $\Psi(z,t{=}0)$ is sufficiently far to the left of the barrier region $0 \le z \le d$ that the probability density $|\Psi(z,t)|^2$ is completely negligible for $z \ge 0$ for all $t \le 0$. It is also assumed that each trajectory $z(z^{(0)},t)$ with non-negligible weight $|\Psi(z^{(0)},0)|^2$ can be followed (numerically) for a sufficiently long time that it can confidently be labelled as either transmitted or reflected. In this case

$$\Theta_T(z^{(0)}) + \Theta_R(z^{(0)}) = 1 \tag{7}$$

where

$$\begin{aligned} &\Theta_T(z^{(0)}) = 1 \ , \ \Theta_R(z^{(0)}) = 0 \ \text{(transmission)} \\ &\Theta_T(z^{(0)}) = 0 \ , \ \Theta_R(z^{(0)}) = 1 \ \text{(reflection)} \quad . \end{aligned} \tag{8}$$

The transmission and reflection probabilities for the wavepacket are obviously given by

$$|T|^2 = \langle \Theta_T(z^{(0)}) \rangle \ , \ |R|^2 = \langle \Theta_R(z^{(0)}) \rangle \tag{9}$$

where

$$\langle f(z^{(0)}) \rangle \equiv \int_{-\infty}^{+\infty} dz^{(0)} |\Psi(z^{(0)},0)|^2 f(z^{(0)}) \tag{10}$$

for any function f of $z^{(0)}$. The transmission, reflection, and dwell times as defined at the beginning of the paper are uniquely given by

$$\tau_T(a,b) \equiv \langle \Theta_T(z^{(0)})\, t(z^{(0)};a,b) \rangle / \langle \Theta_T(z^{(0)}) \rangle \ , \tag{11a}$$

$$\tau_R(a,b) \equiv \langle \Theta_R(z^{(0)})\, t(z^{(0)};a,b) \rangle / \langle \Theta_R(z^{(0)}) \rangle \ , \tag{11b}$$

$$\tau_D(a,b) \equiv \langle t(z^{(0)};a,b) \rangle = |T|^2 \tau_T(a,b) + |R|^2 \tau_R(a,b) \ , \tag{11c}$$

which clearly are real, non-negative quantities.
Equation (11c) can be written in the equivalent form

$$\tau_D(a,b)=\int_0^\infty dt\int_a^b dz|\Psi(z,t)|^2 \tag{12}$$

by introducing unity in the form of an integral over all z of the delta function $\delta[z-z(z^{(0)},t)]$ and noting that $|\Psi(z,t)|^2=\langle\delta[z-z(z^{(0)},t)]\rangle$. Equation (12) was derived by Sokolovski and Baskin[6] using their Feynman path-integral approach. From (12) one can derive Büttiker's expression[1]

$$\tau_D(k;a,b)=\frac{1}{j_k^{inc}}\int_a^b dz\,|\psi_k(z)|^2 \tag{13}$$

relating the dwell time $\tau_D(k;a,b)$ for an incident particle of well-defined energy $E\equiv\hbar^2k^2/2m$ to the incident flux $j_k^{inc}\equiv\hbar k/m$ and the stationary-state wavefunction $\psi_k(z)$.[6,4] Sokolovski and Baskin have proven that

$$\tau_D(k;a,b)=|T|^2\tau_T^{SB}(k;a,b)+|R|^2\tau_R^{SB}(k;a,b) \tag{14}$$

(the imaginary parts of the two terms on the right-hand-side exactly cancel). Hence, it follows from (11c) that the Sokolovski-Baskin and Bohm trajectory approaches should give precisely the same result for the stationary-state transmission (reflection) time whenever $|T(k)|^2=1$ ($|R(k)|^2=1$). This exact agreement only holds in the perfect transmission or perfect reflection limits because $\tau_T^{SB}(k;a,b)$ and $\tau_R^{SB}(k;a,b)$ are in general complex for $0<|T(k)|^2<1$.

As a concrete application of the Bohm trajectory approach consider a particle with initial wavefunction

$$\Psi(z,t=0)=\frac{1}{[2\pi(\Delta z)^2]^{1/4}}\exp\left[-\left(\frac{z-z_0}{2\Delta z}\right)^2+ik_0z\right] \tag{15}$$

incident on the rectangular barrier $V_0\,\Theta(z)\,\Theta(d-z)$ of height $V_0=10$ eV and width d. The width Δz of this minimum-uncertainty-product wavefunction is related to the width Δk of its Fourier transform $\phi(k)$ by $\Delta z\Delta k=1/2$; z_0 is the centroid of $|\Psi(z,t{=}0)|^2$ and k_0 the centroid of $|\phi(k)|^2$. The centroid z_0 must be chosen far enough to the left of the barrier that $|\Psi(z,t{=}0)|^2$ is negligible in the region $z>0$. The criterion used in this paper to determine z_0 is

$$\int_0^\infty dz^{(0)}\,|\Psi(z^{(0)},0)|^2=10^{-4}\,|T|^2 \tag{16}$$

with $|T|^2$ calculated from the stationary-state scattering transmission probability $|T(k)|^2$ using

$$|T|^2=\int_{-\infty}^{+\infty}\frac{dk}{2\pi}|\phi(k)|^2\,|T(k)|^2 \quad . \tag{17}$$

The numerical method used to solve the time-dependent Schrödinger equation was the fourth order (in time step δt) symmetrized product formula method developed by De Raedt[23]. The resulting transmission probability

$$|T|^2=\lim_{t\to\infty}\int_d^\infty dz\,|\Psi(z,t)|^2 \tag{18}$$

converges very satisfactorily with decreasing δt to the value given by (17). After every time step δt each Bohm trajectory was advanced by $\delta z=v(z,t)\,\delta t$ with $v(z,t)$ given by (4). Since Bohm trajectories do not intersect there is a particular starting point $z_c^{(0)}$ such that for all $z^{(0)}$ to the left (right) of $z_c^{(0)}$ the trajectory $z(z^{(0)},t)$ is a reflected (transmitted) one. Provided the initial wavepacket is far enough to the left of the barrier, $z_c^{(0)}$ is given by

$$|T|^2=\int_{z_c^{(0)}}^\infty dz^{(0)}\,|\Psi(z^{(0)},0)|^2 \quad , \tag{19}$$

i.e. $z_c^{(0)}=z_0+\mathrm{erf}^{-1}(1-|T|^2)\,\Delta z$. For the calculations of the traversal time τ_T about 4,000 trajectories with starting points $z^{(0)}$ between $z_c^{(0)}$ and 0 were used. Since the error in the calculated Bohm trajectories is of order $(\delta t)^2$ the convergence of the transmission probability given by Equation (9) is much slower than that given by (18), but is still satisfactory. Fortunately, the errors in the numerator and the denominator of expression (11a) for the traversal time cancel to a large extent and the convergence is much better for this quantity.

Figure 1 shows for $\Delta k=0.04$ and 0.08 Å^{-1} a selection of de Broglie-Bohm trajectories with starting points $z^{(0)}$ in the vicinity of the transmission-reflection divergence at $z^{(0)}=z_c^{(0)}$. The barrier width d is 10 Å and the energy $E_0\equiv\hbar^2k_0^2/2m$ of the incident wavepacket is half of the barrier height V_0. For the wavepacket with the larger width Δk the trajectories are qualitatively very similar to those shown in Figure 3 of the paper by Dewdney and Hiley[24]. However, for the wavepacket with the narrower spread in wavenumber those trajectories with $z^{(0)}$ very close to $z_c^{(0)}$ no longer oscillate within the barrier before escaping.

Figure 2 shows for $\Delta k=0.04$ Å^{-1} a selection of de Broglie-Bohm trajectories for the special case in which the energy E_0 of the incident wavepacket coincides with $E_r^{(1)}$, the energy of the first transmission resonance ($|T(k_r^{(1)})|^2=1$) of the rectangular barrier of height $V_0=10$ eV and width $d=5$ Å. It should be noted that there are no trajectories that describe a particle oscillating back and forth within the barrier region.

In the following comparisons of Bohm trajectory and Larmor clock traversal times, the latter quantity is defined for a finite wavepacket as

$$\int_0^\infty\frac{dk}{2\pi}|\phi(k)|^2\,|T(k)|^2\,|\tau_T^{SB}(k;0,d)|\,/\,|T|^2 \quad , \tag{20}$$

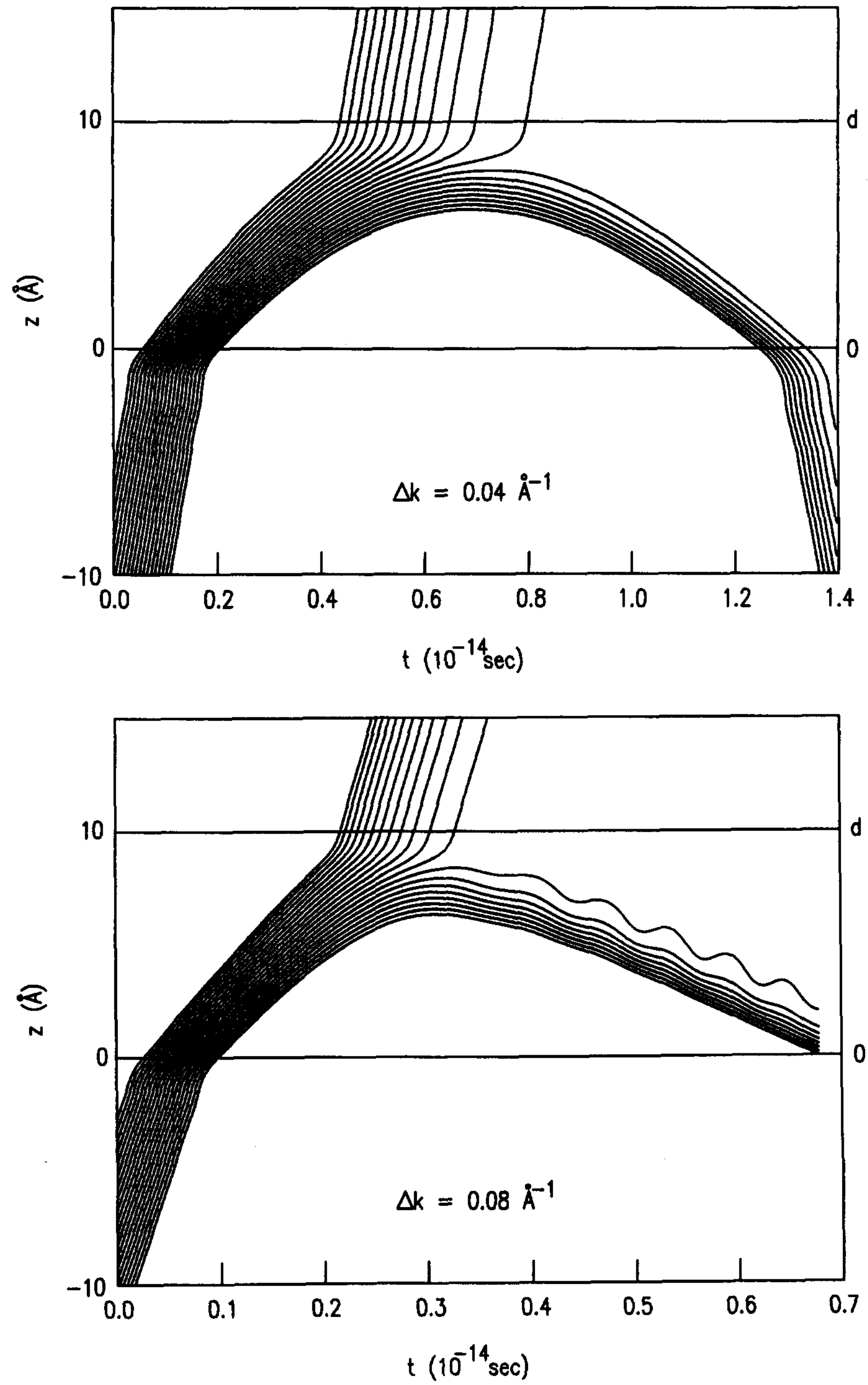

Fig. 1 De Broglie-Bohm trajectories in the vicinity of the transmission-reflection divergence for an initial ($t = 0$) minimum-uncertainty-product wavepacket incident on a rectangular barrier of height $V_0 = 10$ eV and width $d = 10$ Å. The energy $E_0 \equiv \hbar^2 k_0^2/2m$ is 5 eV ($k_0 \sim 1$ Å^{-1}). The other initial wavepacket parameters are: width $\Delta z = 12.5$ Å, i.e. $\Delta k = 0.04$ Å^{-1}, and centroid $z_0 = -92.60$ Å (top); $\Delta z = 6.25$ Å, i.e. $\Delta k = 0.08$ Å^{-1}, and $z_0 = -44.97$ Å (bottom).

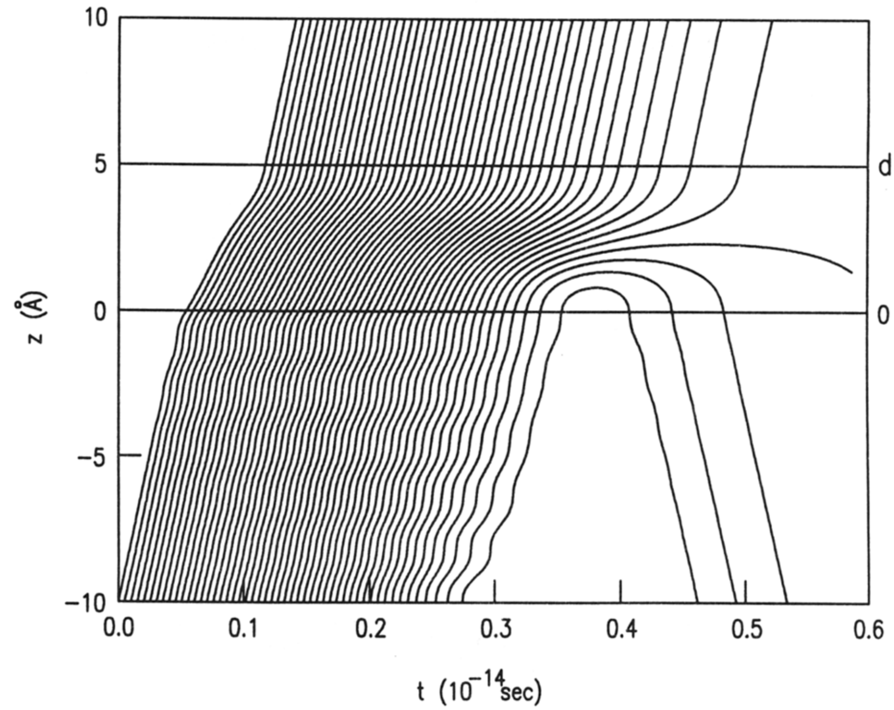

Fig. 2 De Broglie-Bohm trajectories for an initial (t = 0) minimum-uncertainty-product wavepacket incident on a rectangular barrier of height $V_0 = 10$ eV and width d = 5 Å. The energy E_0 coincides with the energy $E_r^{(1)} = 11.503$ eV of the first transmission resonance above the barrier. The other initial wavepacket parameters are width $\Delta z = 12.5$ Å ($\Delta k = 0.04$ Å^{-1}) and centroid $z_0 = -47.275$ Å.

assuming that $|\phi(k)|^2$ is negligible for $k < 0$.

The dependence of the traversal time $\tau_T(0,d)$ on the energy E_0 of a wavepacket with $\Delta k = 0.04$ Å^{-1} incident on a rectangular barrier of height $V_0 = 10$ eV and width d = 3 Å is shown in Figure 3. For E_0 below the top of the barrier the Bohm trajectory traversal time rises with decreasing E_0 while the Larmor clock traversal time falls so that they differ by an order of magnitude when E_0 has decreased to half the barrier height. Above the barrier the agreement between the two traversal times becomes quite good when the transmission probability $|T|^2$ is close to unity and, for the range of E_0 shown, is particularly good in the immediate vicinity of $E_0 = E_r^{(1)} = 14.2$ eV.

Figure 4 shows the dependence of the traversal time $\tau_T(0,d)$ calculated using the Bohm trajectory and Larmor clock approaches on the width d of the barrier for a wavepacket with $E_0 = V_0/2$ and $\Delta k = 0.04$ or 0.08 Å^{-1}. As d approaches zero both approaches lead to a traversal time that merges with the free-particle ($V(z) = 0$) result

$$\tau_T^{(0)}(0,d) = \int_0^\infty \frac{dk}{2\pi}\left(\frac{md}{\hbar k}\right)|\phi(k)|^2\,|T(k)|^2 \,/\, |T|^2 \quad . \qquad (21)$$

From the expression for the traversal time in Büttiker's paper[1] it follows that $\tau_T(k;0,d) = (md/\hbar k)\,[1 + (\kappa d)^{-2}]^{1/2}\tanh \kappa d$ for the special case $k = \kappa \equiv [2m(V_0-E)/\hbar^2]^{1/2}$, i.e. $E = V_0/2$. This is equal to the free-particle result $\tau_T^{(0)}(k) \equiv md/\hbar k$ both in the transparent ($\kappa d \to 0$) and opaque ($\kappa d \to \infty$) barrier limits and remains within 10% of that result for all values of κd. Hence, for $E_0 = V_0/2$ and for Δk sufficiently small the Larmor clock traversal time should not depart significantly from the free-particle result $\tau_T^{(0)}(k_0)$ indicated by the dashed line in the figure. For the range of d shown this is true for $\Delta k = 0.04$ Å^{-1}. However, for $\Delta k = 0.08$ Å^{-1} the decrease of $|\phi(k)|^2 \propto \exp[-(k-k_0)^2/2(\Delta k)^2]$ as k increases from k_0 is not strong enough at large d compared to the rapid increase of $|T(k)|^2 \propto \exp(-2\kappa d)$ to constrain the dominant contributions of the integrands in (20) to the immediate vicinity of $k = k_0$ and the traversal time rises significantly above the free-particle result. For neither $\Delta k = 0.04$ or 0.08 Å^{-1} is there any qualitative change in behaviour of the Larmor clock traversal time as d increases through the region $d \sim \kappa_0^{-1} = 0.873$ Å. On the other hand, the Bohm trajectory traversal time increases dramatically as d increases through a relatively narrow region centred on $d \cong 2\kappa_0^{-1}$ and rapidly becomes much larger than the Larmor clock traversal time. That this

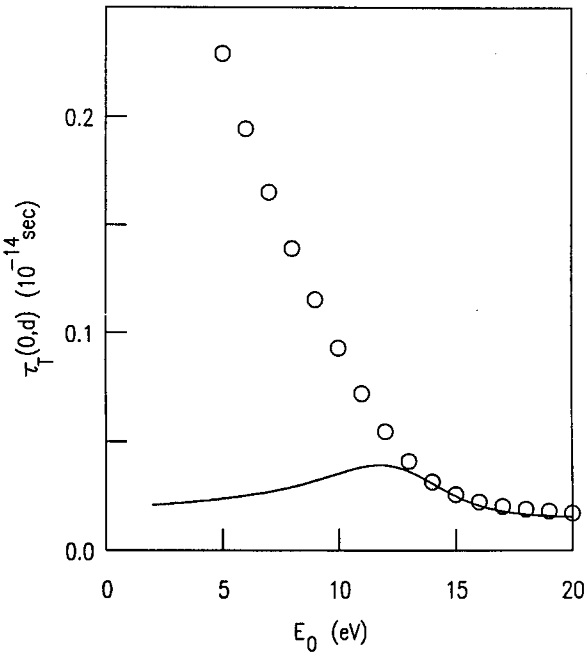

Fig.3 Dependence of the traversal time $\tau_T(0,d)$ on the incident energy E_0 for a rectangular barrier of width d = 3 Å and height V_0 = 10 eV. The width $\Delta z = (2\Delta k)^{-1}$ of the initial (t = 0) incident minimum-uncertainty-product wavepacket is 12.5 Å corresponding to $\Delta k = 0.04$ Å^{-1}. The Larmor clock results are shown by the solid line and the de Broglie-Bohm trajectory results by the circles. The first above-barrier transmission resonance $E_r^{(1)}$ occurs at 14.175 eV.

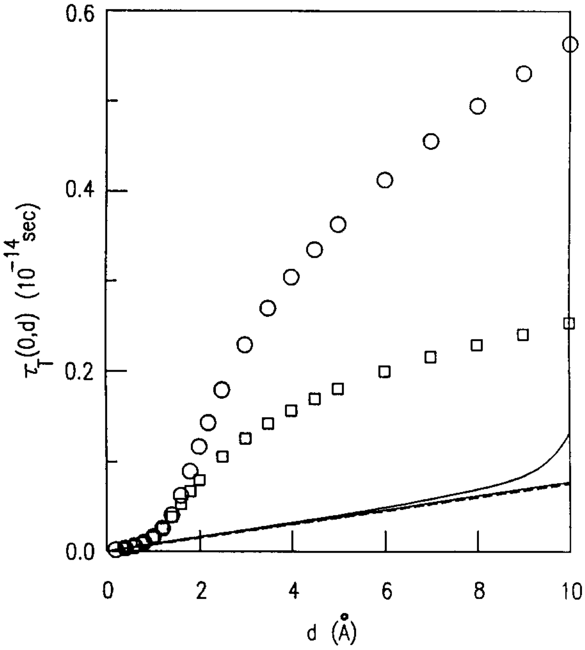

Fig. 4 Dependence of the traversal time $\tau_T(0,d)$ on the thickness d of a rectangular barrier of height V_0 = 10 eV for an incident energy

$E_0 \equiv \hbar^2 k_0^2/2m$ of 5 eV ($k_0 \sim 1$ Å^{-1}). The lower and upper solid curves show the Larmor clock results for initial (t = 0) incident minimum-uncertainty-product wavepackets of width $\Delta z = 12.5$ Å ($\Delta k = 0.04$ Å^{-1}) and $\Delta z = 6.25$ Å ($\Delta k = 0.08$ Å^{-1}) respectively. The corresponding de Brogie-Bohm trajectory results are shown by circles for $\Delta z = 12.5$ Å and squares for $\Delta z = 6.25$ Å. The free-particle (plane-wave) traversal time $d/(\hbar k_0/m)$ is indicated by the dashed straight line.

switchover from transparent to opaque barrier behaviour occurs when the barrier width is approximately twice the characteristic tunneling length κ_0^{-1} is intuitively plausible because one can associate a tunneling length with each side of the barrier. Another striking feature of the Bohm trajectory traversal time is the strong dependence on Δk which sets in for much smaller d than is the case for the Larmor clock traversal time. These results for $\Delta k = 0.08$ and 0.04 Å^{-1} and additional ones for $\Delta k = 0.16$ and 0.02 Å^{-1} indicate that convergence to the plane-wave ($\Delta k \to 0$) limit is very slow and, unfortunately, for numerical reasons (i.e. $\Delta z \to \infty$) the author has not been able to come close to that limit for the opaque rectangular barrier.

The switchover with increasing barrier width d from the transparent to opaque barrier regimes seen in Figure 4 for the Bohm trajectory traversal time $\tau_T \equiv \langle t(0,d)\rangle_T$ is even more sharply defined for the corresponding quantity

$$[\langle t(0,d)^2\rangle_T^{1/2} - \langle t(0,d)\rangle_T]/\langle t(0,d)\rangle_T \quad , \quad (22)$$

with

$$\langle f(z^{(0)})\rangle_T \equiv \langle \Theta_T(z^{(0)}) f(z^{(0)})\rangle / \langle \Theta_T(z^{(0)})\rangle \quad , \quad (23)$$

shown in Figure 5. This quantity which is a measure of the width of the transmission time distribution function $P_T(t(a,b))$ is sharply peaked near $d = 2\kappa_0^{-1}$ for both $\Delta k = 0.04$ and 0.08 Å^{-1}.

The probability that a transmitted particle has a transmission time between t and t + dt is $P_T(t)dt$. The traversal time and mean-square traversal time are, of course, given by

$$\tau_T(0,d) = \int_0^\infty dt\, P(t) t \quad , \quad \langle t(0,d)^2\rangle = \int_0^\infty dt\, P(t) t^2 \qquad (24)$$

respectively. Transmission time probability distributions are shown in histogram form in Figure 6 for barrier width d well below (0.4 Å), near (2.0 Å), and well above (5.0 Å) the 'switchover' width $d \sim 2\kappa_0^{-1}$ (1.75 Å). (10^4 trajectories were used in the construction of each distribution.) In each case, it is clear that there is a well defined minimum transmission time. However, particularly

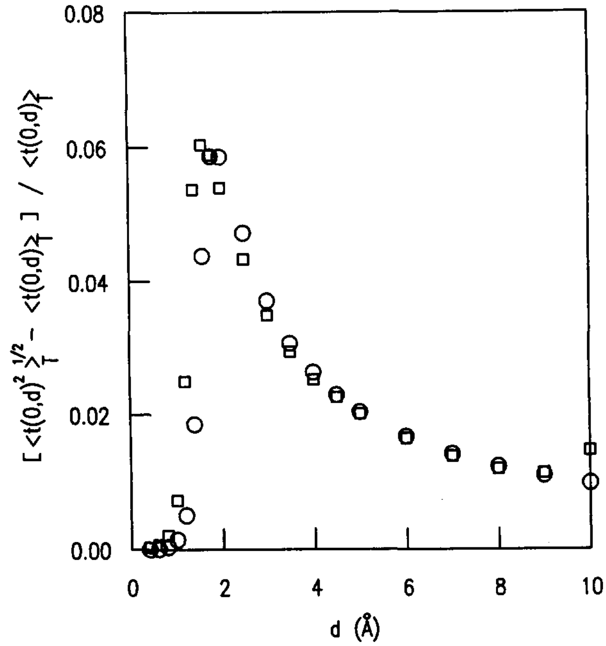

Fig. 5 Dependence of $[< t(0,d)^2 >_T^{1/2} - < t(0,d) >_T]/ <t(0,d)>_T$ calculated using the de Broglie-Bohm approach on barrier width d for the two cases considered in Figure 4: $\Delta z = 12.5$ Å (O) and 6.25 Å (□).

for $d \geq \kappa_0^{-1}$, the distributions have long tails on the high transmission time side of the peaks reflecting the fact that transmission times very much in excess of the average, although rare, are possible. This could have implications for submicron devices where the response time is limited by the time taken for an electron to tunnel through a barrier.

An interesting question[25,2] is "How much time, on average, does an incident particle that is finally reflected spend in some region $z_1 \leq z \leq z_2 = z_1 + \Delta$ on the far side ($z_1 \geq d$) of the potential barrier $V_0\, \Theta(z)\, \Theta(d-z)$?". Intuitively, one might think that the result must be zero. The Larmor clock approach has been applied to the problem[25,2] and leads to the result

$$|\tau_R^{SB}(k;z_1,z_1+\Delta)| = \frac{4m\kappa^2\, |\sin k\Delta|}{\hbar(k^2+\kappa^2)[4k^2\kappa^2+(k^2+\kappa^2)^2\sinh^2\kappa d]^{1/2}\sinh\kappa d}\ . \quad (25)$$

This result is independent of z_1 and is non-zero unless $k\Delta = n\pi$ ($n = 0,1,2,\ldots$). The dependence on Δ is most peculiar because it is oscillatory rather than monotonically non-decreasing. Although (25) is proportional to $\exp[-2\kappa d]$ for $\kappa d >> 1$ one should not regard this as essentially zero because in the same limit $|R(k)|^2 / |T(k)|^2$ contains a compensating factor of $\exp[2\kappa d]$. Hence, for $\kappa d >> 1$ the quantity $|R(k)|^2\, |\tau_R^{SB}(k;z_1,z_1+\Delta)| / [|T(k)|^2\, \tau_T^{(0)}(k;z_1,z_1+\Delta)]$, a reasonable measure of the importance of a non-zero value of $|\tau_R^{SB}(k;z_1,z_1+\Delta)|$, is $|\sin k\Delta| / k\Delta$. This is a disturbing result. It implies that there is the possibility that a particle detected to the right of the barrier and labelled as transmitted should in fact have been labelled as reflected because in the absence of the right-hand detector it would have returned through the barrier and ultimately been detected on the left side of the barrier. Hence (25) seems inconsistent with the usual operational definitions of transmission and reflection probabilities. Since (25) is independent of z_1 one cannot get around the problem simply by moving the right-hand detector further from the barrier. This problem does not appear to arise with the Bohm trajectory approach because a careful search has failed to find a single trajectory that re-enters the barrier after leaving it.

In a recent paper[26], Spiller et al. also suggested calculating traversal times within Bohm's interpretation of quantum mechanics. However, they did not consider the time evolution of an incident wavepacket as in Reference 22. Instead they looked at the stationary-state (Δk=0) scattering problem and identified the barrier traversal time with the quantity

$$\tau_T^{SCPP}(k;0,d) = \int_0^d \frac{dz}{v_k(z)} \quad (26)$$

where the time-independent particle velocity is given by $v_k(z) \equiv m^{-1}\, dS_k(z)/dz$ with $S_k(z)/\hbar$ the phase of the stationary-state wavefunction. For the special case of a rectangular barrier they obtained

$$\tau_T^{SCPP}(k;0,d) = \frac{m}{4\hbar k\kappa^3}[(k^2+\kappa^2)\sinh 2\kappa d - 2(k^2-\kappa^2)\kappa d] \quad (27)$$

which is proportional to $\exp(2\kappa d)$ for $\kappa d >> 1$ (in the same limit the spin-precession time of Rybachenko is independent of d and the Larmor clock time is linear in d).

Equations (26) and (27) were written down by Hirschfelder, Christoph and Palke[27] in '74. However, they regarded this time as having "little physical significance". The present author also fails to appreciate the significance of (26) as a traversal time except for the special case of perfect transmission. For each of the other approaches considered in this paper it is obvious how to convert an expression for the average transmission time into the corresponding expression for the average reflection time. For the Bohm trajectory approach, as shown explicitly in equations (11a) and (11b), one simply replaces $\Theta_T(z^{(0)})$ by $\Theta_R(z^{(0)})$; for the other approaches one replaces the transmission probability amplitude T by the reflection probability amplitude R. However, for the average transmission time of Spiller et al. there is nothing in the right-hand-side of (26) to indicate that it is a property of transmitted rather than reflected particles. Hence, it is not at all obvious what the corresponding expression for the average reflection time might be.

Equation (4) for the particle velocity can also be written as the probability current density divided by the probability density, i.e.

$$v(z,t) = j(z,t) \,/\, |\Psi(z,t)|^2 \quad (28)$$

For a stationary-state this becomes $v_k(z) = j_k / |\psi_k(z)|^2$ where $j_k = |T(k)|^2\, j_k^{inc}$ is independent of z. Since $v_k(z)$ is positive for all z there can be no reflected trajectories. Moreover, comparison of (26) with (13) immediately gives

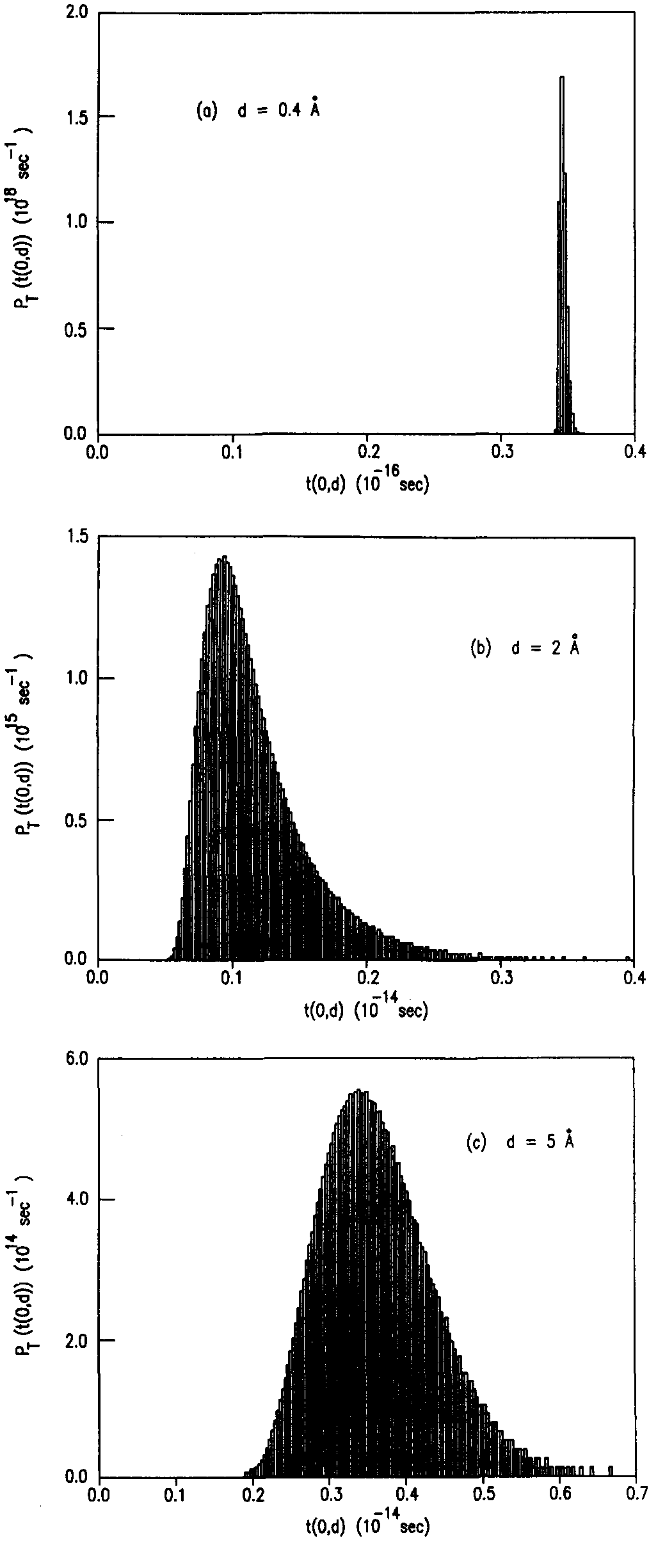

Fig. 6 Traversal time distributions $P_T[t(0,d)]$ calculated using the de Broglie-Bohm trajectory approach for a barrier of height $V_0 = 10$ eV and width d of 0.4 Å (a), 2.0 Å (b) and 5.0 Å (c). For each case the wavepacket parameters are $E_0 = 5$ eV ($k_0 \sim 1$ Å^{-1}) and $\Delta z = 12.5$ Å ($\Delta k = 0.04$ Å^{-1}).

$\tau_T^{SCPP}(k;0,d) = |T(k)|^{-2}\ \tau_D(k;0,d)$ which is compatible with (11c) in the $\Delta k = 0$ limit only if $|R(k)|^2\ \tau_R(k;0,d) = 0$. Except for the special case of perfect transmission, these are both very strange results.

Unfortunately, the author has not been able to compute $\tau_T(0,d)$ given by (11a) for small enough Δk to make a direct comparison with (27). However, averaging $\tau_T^{SCPP}(k;0,d)$ over k with weight factor $|\phi(k)|^2\ |T(k)|^2 / 2\pi|T|^2$ as in (20) and (21) gives traversal times for the wavepacket and barrier parameters of Figure 4 that are orders of magnitude larger for $\kappa_0 d >> 1$ than the corresponding Bohm trajectory results shown in that figure.

In this paper the traversal time for the important case of a gaussian wavepacket incident on a rectangular barrier has been investigated within Bohm's causal interpretation of quantum mechanics and results obtained that are in qualitative disagreement with the corresponding Larmor clock results unless the transmission probability is close to unity. Clearly, experiments are in order. Unfortunately, the Bohm trajectory calculations presented here are for the traversal time in the absence of any measuring device (a meaningless concept within the conventional interpretation). Hence, before comparison with experiment can be seriously contemplated a method of carrying out the measurement must be specified and the effect of the interaction between the propagating particle and the apparatus included in the calculation.[28] Unfortunately, as Bohm has emphasized in connection with measurement of the momentum of a particle[18], the quantity actually measured may have no relation to the quantity of actual interest, in this case the unperturbed traversal time. Furthermore, the predicted strong dependence of the traversal time for an opaque barrier on the width of the incident packet, if true, will necessitate very stringent control of the initial state preparation.

An important feature of the causal interpretation is that, since it gives a well-defined and unique prescription for calculating the traversal time, it is refutable provided that the Bohm trajectory calculation of the (perturbed) traversal time and corresponding experiment can both be carried out to sufficient accuracy. On the other hand, since there is no prescription in the basic tenets of the conventional interpretation for calculating the traversal time, that interpretation is not refutable via comparison of calculated and experimental traversal times. Lack of agreement can always be blamed on an incorrect choice of theoretical approach and it is highly unlikely that one could ever prove that all possible approaches have been invented. Furthermore, there is the ultimate fallback position in the conventional interpretation that the concept of traversal time is meaningless because particles do not have microscopically well-defined trajectories.

It should be emphasized that nowhere in this paper has the author claimed that the Larmor clock (or modulated barrier) approach is incorrect because it leads to traversal times in disagreement with those of the Bohm trajectory approach (or vice versa). However, at the moment, the author prefers the latter approach in part because, unlike the former, it supports the common sense view that a reflected particle spends no time on the far side ($z \geq d$) of the barrier $V_0\ \Theta(z)\ \Theta(d-z)$ and leads to mean transmission and reflection times that satisfy the 'weighted average rule', Equation (11c), and are additive (i.e. $\tau_T(a,c) = \tau_T(a,b) + \tau_T(b,c)$ and similarly for τ_R, with $a \leq b \leq c$).[22]

Acknowledgements: The author has benefited from discussion with G.C. Aers, M. Büttiker and R. Landauer.

REFERENCES

1. M. Büttiker, Phys. Rev. B27, 6178 (1983).
2. E.H. Hauge and J.A. Stovneng, Rev. Mod. Phys. 61, 917 (1989) and references therein.
3. M. Büttiker, to appear in "Electronic Properties of Multilayers and Low Dimensional Semiconductor Structures", edited by J.M. Chamberlain, L. Eaves and J.C. Portal (Plenum, New York) and references therein.
4. C.R. Leavens and G.C. Aers, to appear in "Basic Concepts and Applications of Scanning Tunneling Microscopy and Related Techniques", edited by R.G. Behm (Kluwer, Dordrecht) and references therein.
5. D. Park, "Fundamental Questions in Quantum Mechanics", edited by L.M. Roth and A. Inomata (Gordon and Breach, New York, 1985).
6. D. Sokolovski and L.M. Baskin, Phys. Rev. A36, 4604 (1987).
7. R.P. Feynman and A.R. Hibbs, Quantum Mechanics and Path Integrals (New York, McGraw Hill, 1965).
8. V.F. Rybachenko, Sov. J. Nucl. Phys. 5, 635 (1967).
9. A.I. Baz', Sov. J. Nucl. Phys. 4, 182 (1967).
10. M. Büttiker and R. Landauer, Phys. Rev. Lett. 49, 1739 (1982); Phys. Scr. 32, 429 (1985), Equation (4.5).
11. Z. Huang, P.H. Cutler, T.E. Feuchtwang, R.H. Good Jr., E. Kazes, H.Q. Nguyen and S.K. Park, Journal de Physique C6, 17 (1988).
12. D. Bohm, Quantum Theory (Prentice-Hall, New York, 1951).
13. E.P. Wigner, Phys. Rev. 98, 145 (1955).
14. T.E. Hartman, J. Appl. Phys. 33, 3427 (1962).
15. E.H. Hauge, J.P. Falck and T.A. Fjeldly, Phys. Rev. B36, 4203 (1987); J.P. Falck and E.H. Hauge, Phys. Rev. B38, 3287 (1988).
16. C.R. Leavens and G.C. Aers, Phys. Rev. B39, 1202 (1989).
17. L. De Broglie, "An introduction to the Study of Wave Mechanics", (E.P. Dutton, New York, 1930).
18. D. Bohm, Phys. Rev. 85, 166 (1952); 85, 180 (1952).
19. D. Bohm and B.J. Hiley, Foundations of Physics 14, 255 (1984).
20. D. Bohm, B.J. Hiley and P.N. Kaloyerou, Physics Reports 144, 323 (1987).
21. J.S. Bell, "Speakable and Unspeakable in Quantum Mechanics" (Cambridge University Press, Cambridge, 1987).
22. C.R. Leavens, Solid State Commun. 74, 923 (1990).
23. H. De Raedt, Computer Physics Reports 7, 1 (1987).
24. C. Dewdney and B.J. Hiley, Foundations of Physics 12, 27 (1982).
25. C.R. Leavens and G.C. Aers, Phys. Rev. B40, 5387 (1989).
26. T.P. Spiller, T.D. Clark, R.J. Prance and H. Prance, Europhys. Lett. 12, 1 (1990).
27. J.O. Hirschfelder, A.C. Christoph and W.E. Palke, J. Chem. Phys. 61, 5435 (1975).
28. A. Peres, Am. J. Phys. 48, 553 (1980).