On the approach to the stationary-state-scattering limit within Bohmian mechanics

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On the approach to the stationary-state-scattering limit within Bohmian mechanics

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Abstract

For an initial minimum-uncertainty-product Gaussian wave packet incident on an opaque barrier we investigate how small its spread Δk in wave number must be in order that the Bohm trajectory mean transmission time be well approximated by the stationary-state ($\Delta k = 0$) expression of Spiller, Clark, Prance and Prance.

1. Introduction

Many different theoretical approaches (see Refs. [1–4], and references therein) have been applied to the calculation of various characteristic times associated with a particle interacting with a potential barrier. This Letter ties up a loose end associated with the approach based on Bohmian mechanics.

Consider an ensemble of a very large number of identically prepared single-particle one-dimensional scattering experiments. In each, a Schrödinger electron with the same initial wavefunction $\psi(z, 0)$, normalized to unity, is incident from the left on a static potential barrier which, for simplicity, is assumed to be zero outside the range $0 \leqslant z \leqslant d$. The mean transmission time $\tau_T(z_1, z_2)$ is defined as the average time spent in the region $z_1 \leqslant z \leqslant z_2$ subsequent to $t = 0$ by those electrons that are ultimately transmitted; the mean reflection time $\tau_R(z_1, z_2)$ is the corresponding quantity for those that are reflected. Finally, the mean dwell time $\tau_D(z_1, z_2)$ is the average time spent between z_1 and z_2 irrespective of whether the scattered particle is transmitted or reflected. It is assumed that the probability of the particle being either absorbed or trapped for an infinitely long time by the scattering potential is zero so that the transmission and reflection probabilities, $|T|^2$ and $|R|^2$ respectively, sum to one. It is also assumed that the initial centroid $z_0 \equiv \langle \psi^*(z, 0) z \psi(z, 0) \rangle$ of the wave packet is chosen so that the integrated probability density $|\psi(z, 0)|^2$ from $z = \mathrm{Min}[z_1, 0]$ to ∞ is negligibly small compared to $|T|^2$ (by a factor of 10^{-4} in the calculations presented here).

According to Bohmian mechanics [5–12] an electron is an actual particle the motion of which is causally

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determined by the wavefunction $\psi(z, t)$ so that it has, at each instant t of time, a well-defined position $z(t)$ and velocity

$$v[z(t), t] = \left. \frac{J(z, t)}{|\psi(z, t)|^2} \right|_{z=z(t)}, \tag{1}$$

where $J(z, t) \equiv (\hbar/m)\,\mathrm{Im}[\psi^*(z, t)\partial\psi(z, t)/\partial z]$ is the probability current density. The electron's trajectory $z(z^{(0)}, t)$ is uniquely specified by $\psi(z, 0)$ and its initial position $z^{(0)} \equiv z(z^{(0)}, 0)$. The latter is unknown but statistically distributed according to $P(z^{(0)}) = |\psi(z^{(0)}, 0)|^2$. It readily follows [13] that

$$\tau_D(z_1, z_2) = |T|^2 \tau_T(z_1, z_2) + |R|^2 \tau_R(z_1, z_2), \tag{2}$$

with

$$\tau_D(z_1, z_2) = \int_0^\infty \mathrm{d}t \int_{z_1}^{z_2} \mathrm{d}z\, |\psi(z, t)|^2 = \int_0^\infty \mathrm{d}t\, t[J(z_2, t) - J(z_1, t)], \tag{3}$$

$$\tau_T(z_1, z_2) = \frac{1}{|T|^2} \int_0^\infty \mathrm{d}t\, t[J_T(z_2, t) - J_T(z_1, t)], \tag{4a}$$

$$\tau_R(z_1, z_2) = \frac{1}{|R|^2} \int_0^\infty \mathrm{d}t\, t[J_R(z_2, t) - J_R(z_1, t)]. \tag{4b}$$

The first expression in (3) is well known, the second follows upon multiplying the continuity equation $\partial|\psi(z, t)|^2/\partial t + \partial J(z, t)/\partial z = 0$ by t and then integrating over z from z_1 to z_2 and over t from 0 to ∞ [14]. The components of $J(z, t)$ associated with transmission and reflection are given by

$$J_T(z, t) \equiv J(z, t)\Theta[z - z_c(t)], \tag{5a}$$

$$J_R(z, t) \equiv J(z, t)\Theta[z_c(t) - z], \tag{5b}$$

where $z_c(t) \equiv z(z_c^{(0)}, t)$, the bifurcation line separating transmitted from reflected trajectories, is defined implicitly by

$$|T|^2 = \int_{z_c(t)}^\infty \mathrm{d}z\, |\psi(z, t)|^2 \tag{6}$$

($\Theta(z)$ is the unit step function equal to 0 for $z < 0$ and 1 for $z > 0$).

Rather than consider the time-evolution of an incident wave packet of finite spatial extent, Spiller, Clark, Prance and Prance (SCPP) [15] applied Bohmian mechanics to the stationary-state scattering problem. For "incident" electrons of wave number k and energy $E \equiv \hbar^2k^2/2m$ they identified the mean transmission time, assuming that the transmission probability $|T(k)|^2$ is non-zero, with the quantity

$$\tau_T(z_1, z_2; k) = \int_{z_1}^{z_2} \frac{\mathrm{d}z}{v_k(z)}, \tag{7}$$

where $v_k(z)$ is the stationary-state particle velocity

$$v_k(z) \equiv \frac{J_k}{|\psi_k(z)|^2} = \frac{|T(k)|^2(\hbar k/m)}{|\psi_k(z)|^2}. \tag{8}$$

Here, $\psi_k(z)\exp(-\mathrm{i}Et/\hbar)$ and $J_k(z) = J_k$ (independent of z) are the stationary-state wavefunction and probability current density respectively (the wavefunction is now normalized so that the incident flux $J_{k,\mathrm{I}}$ is $\hbar k/m$). SCPP applied (7), (8) to the special case of a rectangular barrier $V(z) = V_0\Theta(z)\Theta(d - z)$. Twenty years ago Hirschfelder et al. [16] also considered the quantity on the right-hand-side of (7) from the point of view of Bohmian mechanics but regarded it as having "little physical significance". On the other hand, many authors [17–22] have used (7), (8) to study the dynamics of electronic transport in devices, a few apparently not aware of the connection with Bohm's theory.

If the stationary-state limit of Eq. (3) is derived [23] taking into account the different prescriptions for normalization, the well-known result [24]

$$\tau_D(z_1, z_2; k) = \frac{m}{\hbar k}\int_{z_1}^{z_2} dz\,|\psi_k(z)|^2 \tag{9}$$

for the mean dwell time is obtained. Comparing (9) with (7) and (8) it follows immediately that

$$\tau_T(z_1, z_2; k) = |T(k)|^{-2}\tau_D(z_1, z_2; k). \tag{10}$$

Application of (2) then leads to the surprising conclusion

$$\tau_R(z_1, z_2; k) = 0 \qquad \left(0 < |T(k)|^2 < 1\right). \tag{11}$$

That reflected electrons never enter the region $z > z_1$ with z_1 arbitrary, not even when the transmission probability is exceedingly small (but finite), also follows from (8) because $v_k(z)$ is never negative ($k > 0$ for electrons incident from the left).

Leavens and Aers [13] expressed reservations about determining the temporal characteristics of a scattering process by studying only the stationary-state ($\Delta k = 0$) case. They attempted to test the validity of (7), (8) via (11) by carrying out accurate numerical calculations of $\tau_R(0, d)$ for the special case of Gaussian wave packets of average wave number $k_0 \sim 1$ Å^{-1} and spread $\Delta k = 0.08$, 0.04, 0.02 and 0.01 Å^{-1} incident on a rectangular barrier of height $V_0 = 2E_0 \equiv 2\hbar^2 k_0^2/2m = 10$ eV and width $d = 5$ Å. The results were inconclusive: even though the calculated values for $|R|^2\tau_R(0, d)$ can convincingly be extrapolated linearly to a value at $\Delta k = 0$ that is very close to $\tau_D(0, d; k_0)$, apparently disproving (11), they actually do not rule out the possibility that $|R|^2\tau_R(0, d)$ eventually plummets to zero for sufficiently small Δk. In this paper it is shown that the latter behaviour is in fact the correct one. In Section 2 a method is discussed for deriving approximate, closed form expressions for $\psi(0, t)$ and $J(0, t)$ that are accurate in the regime $\Delta k/k_0$ very much less than unity. Also, a simple expression is suggested for estimating how small $\Delta k/k_0$ must be before the stationary-state regime, defined here by the condition $|R|^2\,\tau_R(0, d) \ll \tau_D(0, d)$, is effectively reached. In Section 3 calculated results for the dependence of $|R|^2\tau_R(0, d)$ on Δk as Δk approaches zero are presented. They confirm the correctness (within Bohmian mechanics) of the expression for the mean transmission time in the stationary-state limit given by Spiller et al. [15]. Concluding remarks are made in Section 4.

2. A method for approaching the stationary-state limit

The approach to the stationary-state limit $\Delta k = 0$ is made here assuming that the Fourier transform $\phi(k)$ of the incident component $\psi_I(z, t = 0)$ of the initial wavefunction is Gaussian, i.e.

$$\phi(k) = \frac{(2\pi)^{1/4}}{(\Delta k)^{1/2}}\exp\left[-\left(\frac{k - k_0}{2\Delta k}\right)^2 - i(k - k_0)z_0\right], \tag{12}$$

where k_0 is the centroid of $|\phi(k)|^2$ and z_0 that of $|\psi_I(z, 0)|^2$. In the calculations presented below, z_0 is chosen so that the integral of $|\psi_I(z, 0)|^2$ over the region $0 \leqslant z \leqslant \infty$ is equal to $10^{-4}|T|^2$, i.e. $\lambda \equiv -z_0\Delta k = \frac{1}{2}N^{-1}(1 - 10^{-4}|T|^2)$ where $N^{-1}(x)$ is the inverse of the normal distribution function. The dependence of λ on Δk as Δk approaches zero is negligible (λ is between 2 and 3 for the two examples considered in the next section). With the above choice for $\phi(k)$ the time-evolved incident component

$$\psi_I(z, t) = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\phi(k)\,\exp(ikz)\,\exp(-i\hbar k^2 t/2m) \qquad (z \leqslant 0) \tag{13}$$

can be evaluated analytically in closed form but the reflected component

$$\psi_R(z,t)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\phi(k)R(k)\exp(-ikz)\exp(-i\hbar k^2t/2m)\qquad(z\leqslant 0)\tag{14}$$

in general cannot. In (14), $R(k)\equiv|R(k)|\exp[i\varphi_R(k)]\equiv\exp[\ln|R(k)|+i\varphi_R(k)]$ is the reflection probability amplitude. Now, in the approach $\Delta k\to 0$ to the stationary-state limit ($\Delta k=0$), it should ultimately be an excellent approximation to expand $\ln|R(k)|$ and $\varphi_R(k)$ in the integrand of (14) about the peak wave number $k=k_0$ of $|\phi(k)|^2$ to order $(k-k_0)^2$ (hereafter referred to as the quadratic approximation). Then (14) becomes a Gaussian integral which can be evaluated analytically. Using the resulting expressions for $\psi_I(z,t)$ and $\psi_R(z,t)$ in $\psi(z\leqslant 0,t)=\psi_I(z,t)+\psi_R(z,t)$, the corresponding analytic approximation to the probability current density $J(z,t)\equiv(\hbar/m)\,\mathrm{Im}[\psi^*(z,t)\partial\psi(z,t)/\partial z]$ for $z\leqslant 0$ follows. Now consider the usual case in which there are no reentrant *transmitted* Bohm trajectories through the leading edge of the barrier at $z=0$ (this is certainly the case for the two systems studied in Section 3). Since Bohm trajectories do not intersect each other [9,13], there is then a time t_{TR} defined implicitly by $z_c(t_{TR})=0$ such that only "to be transmitted" electrons enter the barrier for $t<t_{TR}$ and only "to be reflected" ones for $t>t_{TR}$. Then $J(0,t)_R=J(0,t)\Theta(t-t_{TR})$ and it follows from (4b) that

$$|R|^2\tau_R(0,d)\leqslant|R|^2\tau_R(0,\infty)=-\int_{t_{TR}}^{\infty}dt\,tJ(0,t).\tag{15}$$

In the next section, where the behaviour of $|R|^2\tau_R(0,\infty)$ as $\Delta k\to 0$ is studied, there are no reentrant trajectories through $z=d$ for the two barriers considered. Hence $\tau_R(0,d)$ is equal to $\tau_R(0,\infty)$ and the distinction is dropped.

Unfortunately, the above-mentioned analytic approximations for $\psi(z,t)$ and $J(0,t)$ are too lengthy to be transparent and are not written down here. Hence, for purposes of discussion it is convenient to use the much simpler expressions obtained by replacing $R(k)$ by

$$|R(k_0)|\exp\left\{i\left[\varphi_R(k_0)+\left(\frac{\partial\varphi_R(k)}{\partial k}\right)_{k_0}(k-k_0)\right]\right\}.\tag{16}$$

and then retaining only terms that contribute to $v(0,t)$ to order $\Delta k/k_0$. (For the opaque barriers considered in Section 3, neglect of the partial derivatives of $|R(k)|$ should be well justified.) With these approximations, one obtains

$$J(0,t)\simeq\left(\frac{2}{\pi}\right)^{1/2}\Delta k\left(\frac{\hbar k_0}{m}\right)\exp\left(-\frac{2\lambda^2(t-t_0)^2}{t_0^2}\right)\left\{|T(k_0)|^2-4\lambda|R(k_0)|\right.$$
$$\left.\times\left[\sin\varphi_R(k_0)+k_0|R(k_0)|\left(\frac{\partial\varphi_R(k)}{\partial k}\right)_{k_0}\right]\frac{t-t_0}{t_0}\frac{\Delta k}{k_0}\right\}\qquad(\Delta k/k_0\to 0),\tag{17}$$

where $t_0\equiv|z_0|/(\hbar k_0/m)$. The corresponding expression for the probability density at the leading edge of the barrier is

$$|\psi(0,t)|^2\simeq\left(\frac{2}{\pi}\right)^{1/2}\Delta k\exp\left(-\frac{2\lambda^2(t-t_0)^2}{t_0^2}\right)\left[1+|R(k_0)|^2+2|R(k_0)|\cos\varphi_R(k_0)\right.$$
$$\left.+4\lambda|R(k_0)|[|R(k_0)|+\cos\varphi_R(k_0)]\left(\frac{\partial\varphi_R(k)}{\partial k}\right)_{k_0}\frac{t-t_0}{t_0}\Delta k\right]\qquad(\Delta k/k_0\to 0).\tag{18}$$

The prefactor of Δk common to $J(0, t)$ and $|\psi(0, t)|^2$ cancels in the expression $v(0, t) \equiv J(0, t)/|\psi(0, t)|^2$ for the Bohm particle velocity at the leading edge of the barrier. Clearly, to order $\Delta k/k_0$, $v(0, t)$ is equal to the positive stationary-state ($\Delta k = 0$) result $v_{k_0}(0)$ of SCPP given by (8) plus a term proportional to $\Delta k/k_0$ that changes sign at $t = t_0$. Let us consider the usual situation in which $J(0, t)$ changes sign only once, from plus to minus at $t = t_{\pm}$. It then follows from (15) that

$$|R|^2\tau_R(0, d) \leqslant -\int_{t_{\mathrm{TR}}}^{t_\pm} \mathrm{d}t\, tJ(0, t) + \int_{t_\pm}^{\infty} \mathrm{d}t\, t|J(0, t)| \leqslant \int_{t_\pm}^{\infty} \mathrm{d}t\, t|J(0, t)|. \tag{19}$$

Because the first term in expression (17) for $J(0, t)$ is positive (assuming $|T(k_0)|^2 \neq 0$) and the second changes sign at $t = t_0$, it is clear that $t_{\pm} > t_0$. However, because of the Gaussian factor $\exp[-2\lambda^2(t - t_0)^2/t_0^2]$ in (17), if $t_{\pm}$ exceeds the peak time t_0 by significantly more than the characteristic width [1] $\Delta t = t_0/2^{1/2}\lambda$ then it follows from (19) that $|R|^2\tau_R(0, d)$ is negligibly small. Hence, an order of magnitude estimate for how small $\Delta k/k_0$ must be before reaching the effective stationary-state regime, $|R|^2\tau_R(0, d) \ll \tau_D(0, d)$, is obtained by demanding that $J(0, t = t_0 + \Delta t) = 0$ and solving (18) for $\Delta k/k_0$. This gives

$$\frac{\Delta k}{k_0} \lesssim \frac{2^{1/2}|T(k_0)|^2}{4|R(k_0)|\{\sin \varphi_R(k_0) + k_0|R(k_0)|(\partial\varphi_R(k)/\partial k)_{k_0}\}} \tag{20}$$

for the regime in which reflected electrons spend a negligible amount of time within the barrier and the SCPP result (7), (8) provides a good approximation to $\tau_T(0, d)$.

3. Results

In this section, scattering by rectangular barriers $V(z) = V_0\Theta(z)\Theta(d - z)$ of finite height $V_0 = 2E_0 \equiv 2\hbar^2k_0^2/2m$ and width d is considered. For this special case, $|R(k_0)| = \tanh(k_0 d)$, $\varphi_R(k_0) = -\pi/2$ and $(\partial\varphi_R(k)/\partial k)_{k_0} = 2k_0^{-1}\tanh(k_0 d)$. The fact that $\sin[\varphi_R(k_0)] = -1$ clearly shows the importance of the $(\partial\varphi_R(k)/\partial k)_{k_0}$ term in (17). If this term is replaced by zero then the leading order correction to the (positive) $\Delta k = 0$ result for $v(0, t)$ is negative for $t < t_0$ and positive for $t > t_0$. This implies that $v(0, t) > 0$ for $t > t_0$ and hence rules out the possibility of any "to be reflected" electrons entering the barrier. Such electrons would have $v(0, t) < 0$ at the instant t when they ultimately returned to the region $z < 0$ and, because of the non-intersecting property of the trajectories, could not then be followed by transmitted electrons in the ensemble with $v(0, t) > 0$. At least for the special case under consideration, reinstating the $(\partial\varphi_R(k)/\partial k)_{k_0}$ term in (17) changes the sign of the correction term so that $v(0, t)$ can become negative for sufficiently large t, corresponding to reflected electrons eventually leaving the barrier after spending a finite amount of time there.

For the opaque, rectangular barriers with $V_0 = 2E_0$ considered in this section, (20) can be replaced to a good approximation by $\Delta k/k_0 \lesssim 2^{1/2}\exp(-2k_0 d)$. It is now clear why the accurate numerical calculations of $|R|^2\tau_R(0, d)$ carried out by Leavens and Aers [13] were unable to confirm SCPP's expression for $\tau_T(0, d; k_0)$. For the parameters $V_0 = 2E_0 = 10$ eV ($k_0 = 1.146$ Å^{-1}) and $d = 5$ Å considered it was not feasible for them to perform accurate numerical solutions of the time-dependent Schrödinger equation, using the real-space fourth order (in time step) method of Ref. [25], for Δk significantly less than 0.01 Å^{-1}. This value of Δk although very small compared to k_0 still lies far outside the estimated range $\Delta k \lesssim 1.7 \times 10^{-5}$ Å^{-1} for the stationary-state regime given by either (20) or the above simplified expression. Fig. 1 shows $|R|^2\tau_R(0, d)$ for the region below $\Delta k = 0.01$ Å^{-1} calculated using the approximation (17) for $J(0, t)$ based on (16). (The corresponding results obtained with the more accurate quadratic approximation differ by considerably less than 1 part in 10^3 over the

[1] The Gaussian factor is reduced from its peak value by a factor of e^{-1} for $|t - t_0| = \Delta t$.

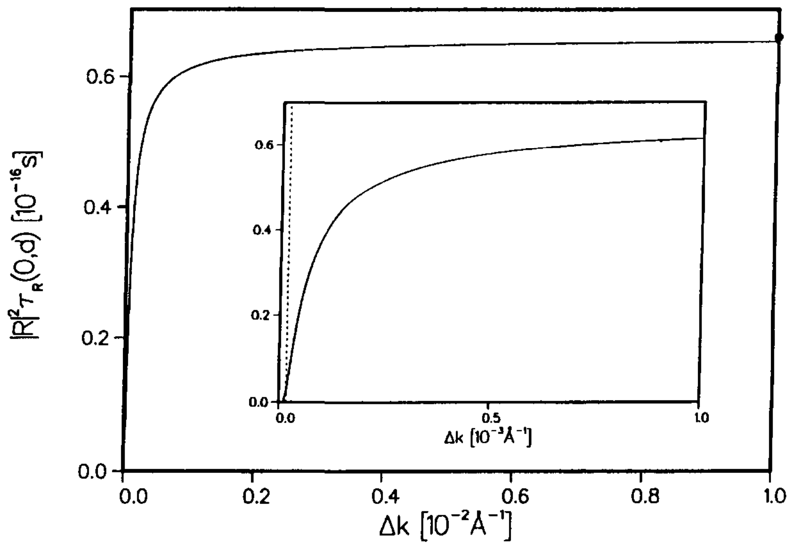

Fig. 1. Dependence of $|R|^2\tau_R(0, d)$ on Δk for an initial minimum-uncertainty-product wavefunction with centroid $z_0 = -\lambda/\Delta k$ ($\lambda = 2.88$) and mean wave number $k_0 = (2mE_0)^{1/2}/\hbar$ incident on a rectangular barrier of height $V_0 = 2E_0 = 10$ eV and width $d = 5$ Å. The solid curve was calculated using the quadratic approximation; (●) result for $\Delta k = 0.01$ Å^{-1} based on accurate numerical solution of the time-dependent Schrödinger equation. The value of Δk given by (20), below which the stationary-state limit is expected to be applicable, is indicated by the vertical dashed line in the inset. The transmission probability $|T|^2$ varies by less than 0.6% over the range $0 \leqslant \Delta k \leqslant 0.01$ Å^{-1}.

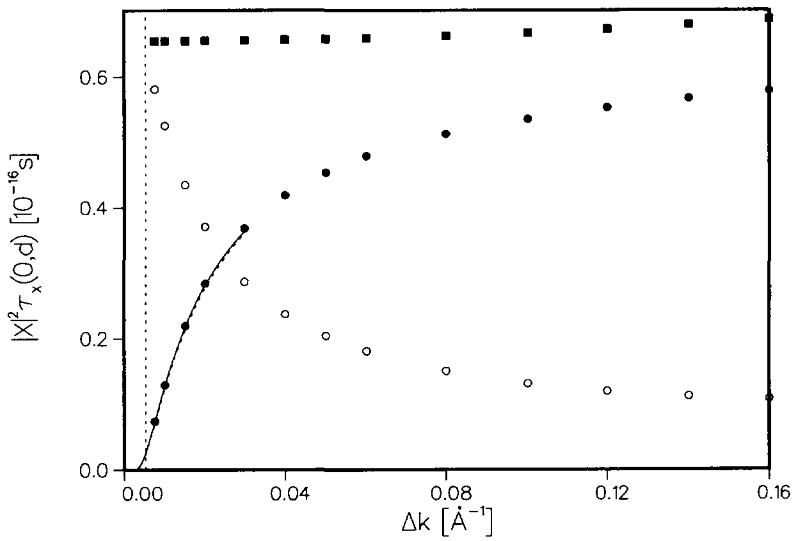

Fig. 2. Dependence of Δk of the transmission (○) and reflection (●) contributions, $|T|^2\tau_T(0, d)$ and $|R|^2\tau_R(0, d)$ respectively, to the mean dwell time $\tau_D(0, d)$ (■). The initial spatial wavefunction is a minimum-uncertainty-product Gaussian with centroid $z_0 = -\lambda/\Delta k$ ($\lambda = 2.35$) and mean wave number $k_0 = (2mE_0)^{1/2}/\hbar$ with $E_0 = 5$ eV. The scattering potential is a rectangular barrier of height $V_0 = 2E_0$ and width $d = 2.5$ Å. (○), (●) and (■) denote results based on accurate numerical solution of the time dependent Schrödinger equation while the solid and broken curves (for $|R|^2\tau_R$ only) denote results based on the quadratic approximation and on (16) respectively. The value of Δk below which the stationary-state limit is expected to be applicable is indicated by the vertical dashed line. The transmission probability $|T|^2$ varies by less than 9% over the range $0 \leqslant \Delta k \leqslant 0.08$ Å^{-1}.

range of Δk shown.) The results for $|R|^2\tau_R(0, d)$ do eventually plummet to negligibly small value and, as indicated in the inset, the effective stationary-state regime is reasonably well delineated by (20).

Results for $|R|^2\tau_R(0, d)$ based on the quadratic approximation and on (16) are now compared with accurate numerical results over an extended range of Δk by considering a $d = 2.5$ Å barrier for which the effective stationary-state regime is estimated to be $\Delta k/k_0 \lesssim 2^{1/2}\exp(-2k_0 d) = 4.6 \times 10^{-3}$ Å^{-1}. The Δk dependence of each of $\tau_D(0, d)$, $|T|^2\tau_T(0, d)$ and $|R|^2\tau_R(0, d)$, calculated from (2)–(6) using accurate numerical solutions of the time-dependent Schrödinger equation [25], is shown in Fig. 2. The results for $|R|^2\tau_R(0, d)$ based on the quadratic approximation and on (16) are also shown [2] for $\Delta k \leqslant 0.03$ Å^{-1}. They are both in good agreement, in the region of overlap, with the accurate numerical results. Moreover, the estimate (20) for the region of applicability of the stationary-state limit result of Spiller et al. [15] is again reasonable.

It is interesting to note that for a typical planar metal–insulator–metal barrier width d of 10 Å (with $V_0 = 2E_0 = 10$ eV as above), the right-hand-side of (20) is 1.6×10^{-10} Å^{-1} corresponding to a spatial width $\Delta z \equiv 1/2\Delta k$ for the initial Gaussian wave packet of almost 30 cm! According to the prescription adopted here, the initial centroid z_0 is located about 2.3 m from the barrier. The question that leaps to mind is whether such a single-particle wavefunction could maintain its coherence for the duration of the scattering process in the presence of a realistic finite temperature solid-state environment.

For a more optimistic case, consider ultracold neutrons in vacuum scattering from a planar rectangular Cu barrier of width $d = 400$ Å and height $V_0 = 2E_0 = 1.65 \times 10^{-7}$ eV [26]. For these parameters, the region of applicability of the SCPP result for τ_T is $\Delta k/k_0 \lesssim 0.91 \times 10^{-2}$. This degree of monochromaticity has been achieved in practice for neutrons exhibiting wave function coherence over macroscopic distances.

4. Concluding remarks

Many of the prescriptions that have been proposed for calculating the mean transmission time $\tau_T(z_1, z_2)$ share the convenient property that it can be obtained directly from the corresponding stationary-state quantity $\tau_T(z_1, z_2, k)$ by integrating $|\phi(\mathrm{k})|^2 |T(k)|^2 \tau_T(z_1, z_2; k)/2\pi |T|^2$ over k from 0 to ∞. This is, for example, the case for all of the prescriptions contained within the systematic projector approach of Brouard, Sala and Muga [3] but, as shown by Leavens [13], is in general *not* the case for the approach based on Bohmian mechanics. Hence, attempting to calculate $\tau_T(z_1, z_2)$ from the stationary-state result (7), (8) in the above direct way can lead to extremely large errors if Δk is significantly outside the effective stationary-state regime.

Strictly speaking, the stationary-state scattering limit $\Delta k = 0$ is an idealization that can never be realized exactly, not even in principle, because it implies complete coherence of a single-particle state over all of space and of time from $t = -\infty$. Of course, what is relevant in practice is how small Δk must be before the quantity of interest, say $F(\Delta k)$, is adequately approximated by $F(0)$ and whether or not, for such a Δk, the required coherent single-particle state can be prepared and then survive as such for the duration of the scattering experiment. It is clear from the examples presented in this paper, which are far from extreme, that convergence of $|T|^2\tau_T(0, d)$ and $|R|^2\tau_R(0, d)$ to their stationary-state values can require Δk very much smaller than is the case for either $|T|^2$ or $\tau_D(0, d)$. Hence, the dependence of $|R|^2\tau_R(0, d)$ on Δk calculated by Leavens and Aers [13] for the range $0.01 \leqslant \Delta k/k_0 \leqslant 0.08$ could easily lead to a completely incorrect estimate for the stationary-state limit of this quantity.

In the Bohm picture, transmitted particles originate in the leading $|T|^2$ part of the wave packet and are delayed relative to the corresponding free particles with the same initial positions $z^{(0)}$ so that this part of the packet can evolve into the entire transmitted packet. In the stationary-state limit, the average time that these

[2] Over this range of Δk, the quadratic approximation for $J(0, t)$ leads to a transmission probability $|T|^2$ that agrees to better than 1% with the numerically exact one obtained by integrating $|\phi(k)|^2 |T(k)|^2/2\pi$ over positive k.

particles are delayed in the region $z < 0$ in front of the barrier diverges and, moreover, for an opaque barrier is very large relative to the (infinite) mean arrival time at $z = 0$ of the corresponding free particles. It seems somewhat arbitrary to ignore this important perturbation of the particle motion by the barrier and to focus only on the mean transmission time for the barrier region. Neither of these quantities is directly measurable in general because of the position–momentum uncertainty relation. On the other hand, the mean arrival time of transmitted particles at a point $z > d$ on the far side of the barrier is experimentally observable in principle but is of interest only for finite initial wave packets because it necessarily diverges in the stationary-state limit.

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