The quantum mechanical tunnelling time problem-revisited

J. Phys. C: Solid State Phys. **20** (1987) 6213–6232. Printed in the UK

The quantum mechanical tunnelling time problem—revisited

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Received 14 January 1987, in final form 2 June 1987

Abstract. A long-standing argument in elementary quantum mechanics concerns the prescription which specifies how long it takes for a particle to tunnel through a classically forbidden region. In this paper, the controversy is reviewed by analysing a selection of principal contenders and comparing with our own analytic expressions and numerical simulations. Our overall conclusion is that the phase-time result originally obtained by Wigner and Hartman is the best expression to use for a wide parameter range of barriers, energies and wavepackets.

1. Introduction

Occasionally in physics a problem arises which, although on an almost trivial level of complexity, leads to an extensive and often controversial debate. One such question which has yet to be satisfactorily resolved concerns the time that one may identify for a particle to tunnel through a classically forbidden region.

Addressed naïvely this is a problem that ought to be decided by a solution of the time-dependent Schrödinger equation (which is linear since the complications of charge redistribution through a Poisson correction are ignored). In the general case this may only be accomplished in an approximate fashion, even formally, leading to the possibility of argument concerning the validity of the approximations used. However one could have expected an argument *a priori* over the question of 'How long does it take for an electron to tunnel through a barrier?'. This is because *time* in quantum mechanics does not have the status of a dynamical variable, and cannot have that status since its 'conjugate' variable, the energy operator or the Hamiltonian is a bounded function from below. This is what restricts the introduction of time as an observable in quantum theory (see for instance, [1, 2] and references therein) and why time–energy uncertainty relations have to be handled with care. Therefore the inherent lack of a unique definition of time as an observable leads to interpretational problems, even for formally precise results.

The controversy surrounding this question is evident in the history of the solution of the problem. The dynamics of the tunnelling electron was emphasised as long ago as

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1931 by Condon [3] and MacColl in 1932 [4]. The conclusion then was that there is no appreciable delay in the transmission of a wavepacket through a potential barrier.

However there are current technological motivations for attempting to quantify the dynamics of the tunnelling event more precisely. For instance if tunnelling is a slow process relative to the inelastic scattering time of a semiconductor, then one might expect that there was not sufficient time available for the coherent tunnelling of electrons to take place. This would influence the design of ultra small logic transistors composed out of layered heterostructures exploiting a large tunnelling current density at resonance. Similarly, if the motion of a tunnelling electron is faster than the inverse plasma frequency of an electron gas, then one would not expect the dynamic image force induced by a tunnelling electron to have any feedback on that electron as it tunnelled through an insulator, or escaped from a surface for instance [5, 6]. In addition, whether one employed the static or optical dielectric constants in calculations in small scale opto-electronic devices exploiting the tunnel effect, would be determined by the relative celerity of the tunnelling event. These are problems relating the many particle nature of tunnelling electrons, and although there have been notable attempts to treat the time-dependent many body tunnelling problem consistently (for instance [7]) this note is concerned solely with the one-electron problem.

Many authors since 1930 have obtained tunnelling time expressions. These expressions tend to fall into one of four general groups which we may label the scattering time, the dwell time, the semi-classical time, and the phase time.

The scattering-time group (see for instance [8]) base their results on the decay of metastable states as described by a transition probability matrix calculated under time independent perturbation theory. The incident electrons are viewed as metastable to the tunnelling process transforming them into another state on the far side of a potential barrier. The tunnelling time is thus characterised by the inverse of this transition matrix.

The dwell-time group [9–12] obtain a result for the mean interaction time based on the ratio of the probability density in the barrier region to the incident current flux density. For an electron of mass m and energy E tunnelling through a rectangular barrier of width d and height V_0 the dwell time takes the form

$$\tau_d = \left(\frac{mk}{\hbar\kappa}\right)\left(\frac{2\kappa d(\kappa^2 - k^2) + k_0^2 \sinh(2\kappa d)}{4k^2\kappa^2 + k_0^4 \sinh^2(\kappa d)}\right) \tag{1}$$

where

$$E = \frac{\hbar^2 k^2}{2m} \qquad V_0 = \frac{\hbar^2 k_0^2}{2m} \qquad V_0 - E = \frac{\hbar^2 \kappa^2}{2m}.$$

The semi-classical group of results include the recent works of Büttiker [12], Büttiker and Landauer [13, 14] and Stevens [15] (see also [16]). In this scheme one may visualise the tunnelling particle as moving freely in the inverted potential with an imaginary velocity of $i\hbar\kappa/m$. Therefore the relevant tunnelling time expression for the simple square barrier problem becomes

$$\tau_s = -i(md/(\hbar\kappa)). \tag{2}$$

We have retained the $-i$ factor to emphasise the fact that this tunnelling time is imaginary as discussed by Pollak and Miller [17] and implicitly assumed by Jonson [5]. Büttiker and Landauer [14] argue that it is this imaginary time which is of importance for dynamic tunnelling events, and Stevens has ascribed this time with the physical

notion of the signal velocity of a truncated wavepacket. A relationship between the real and imaginary times in scattering theory has been discussed by Pollak and Miller [17]. Note that the real time discussed by Pollak and Miller is not the dwell time of Smith, but actually is the phase time of Wigner (introduced below). The fact that Smith [9] erroneously equated the dwell time with the phase time was due to an ensemble averaging of the phase time in a particular problem with an infinite potential barrier dividing the half plane so that there were no transmitted electrons.

Although we have included Büttiker [12] in this semi-classical time category, more precisely he derived an entirely separate time which may be expressed as

$$\tau_B = (\tau_d^2 + \tau_z^2)^{1/2} \tag{3}$$

where

$$\tau_z = \left(\frac{mk_0^2}{\hbar\kappa^2}\right)\left(\frac{(\kappa^2 - k^2)\sinh^2(\kappa d) + (\kappa d k_0^2/2)\sinh(2\kappa d)}{4k^2\kappa^2 + k_0^4\sinh^2(\kappa d)}\right). \tag{4}$$

However, for a wide range of energies $E < V_0$ and for an opaque barrier, the Büttiker expression reduces to the magnitude of the semi-classical time τ_s which is why Büttiker identifies the semi-classical time as the appropriate one to use as a transit tunnelling time.

The final category is the phase time group [18–20]. In this methodology, the time delay due to an electron wavepacket tunnelling is associated with the energy derivative of the phase shift η of the complex transmission coefficient, i.e. $\tau_\varphi = \hbar\, \mathrm{d}\eta/\mathrm{d}E$. For the simple case under study here, this produces an expression of the form

$$\tau_\varphi = \left(\frac{m}{\hbar k\kappa}\right)\left(\frac{2\kappa d k^2(\kappa^2 - k^2) + k_0^4\sinh(2\kappa d)}{4k^2\kappa^2 + k_0^4\sinh^2(\kappa \mathrm{d})}\right). \tag{5}$$

Although quite similar, these results lead to distinct limiting behaviour either for low energies or wide or thin barriers which can be orders of magnitude apart. Therefore it is desirable to decide which, if any, of these expressions is the most suitable. The following section presents some of our reservations for rejecting the first three categories. A comparison with numerical simulations of wavepackets is reserved until § 4.

2. Critique

In this section we present arguments as to why we believe the scattering time, the dwell time, and the semi-classical time are not the physically relevant or accurate expressions to employ for the dynamical transit tunnelling times of electrons through potential barriers.

The scattering time, defined through the inverse of the transition probability matrix, is not related to the dynamical transport behaviour of electron tunnelling. It is associated with the finite lifetime and decay of metastable states—the metastable states in this case being the tunnelling electrons treated as quasi-particles which are decaying from a state on one side of the potential barrier into another state on the opposite side of the barrier. Since this quantifies the decay of metastable states and not the transit time of an electron across a barrier, this time can be quite large and is a steady-state picture which does not reflect the dynamic nature of the tunnelling particles. It can be seen on the basis of the time-independent picture and by analogy with α-particle decay, that the scattering time

represents a mean time in which a certain likelihood of a tunnelling event may take place. Specifically, after a certain time τ_Γ then it is probable that approximately half of the original density of electrons has managed to tunnel away. This does not reflect the actual time of a tunnelling process.

The dwell time (1) is also not the relevant transport time for tunnelling electrons to transit a classically forbidden region. The physical motivation for the dwell time is that if a barrier is present, then a measure of the characteristic time associated with the potential profile may be obtained from the total electron density in the barrier region divided by the incoming flux density in steady-state conditions. As pointed out by Büttiker [12], this definition makes no distinction between transmitted and reflected components—both are given equal weight in the ensemble average to obtain a measure of the total delay induced by the presence of the potential. Therefore the dwell time, although it may be interpreted as a mean interaction time of a collision event, is not the appropriate physically relevant quantity to describe the time for a *transmitted* electron to pass through the barrier.

We now address the semi-classical tunnelling time (2). Pollak and Miller [17] have identified this time as the imaginary component of an approximate scattering S-matrix. Jonson [5] identifies an imaginary velocity of a tunnelling electron which is related to the damping wavevector $\kappa \propto (E - V)^{1/2}$ of the WKB wavefunction, by analogy with the travelling-wave solution. This imaginary velocity thus converts into the semiclassical imaginary time. The same expression is obtained from the phase-time equation if the WKB wavefunction is employed and an identification of the imginary phase with the damping wavevector is made. This is not a satisfactory method to obtain a tunnelling time.

Stevens [15] also obtains this tunnelling time by analysing an initial value problem of a semi-infinite truncated cisoidal function moving towards a step potential (the third problem considered in [15]). The wavefunction within the step region at time t is considered by employing a complex-variable analysis integrating over the frequency rather than the wavevector. This problem, which is equivalent to a WKB analysis of a rectangular potential profile (since contributions from $\exp(+\kappa x)$ are neglected), produces the result that the *signal velocity* of the considered wavepacket within the barrier region is proportional to the damping factor κ. It is not apparent that the signal velocity should be the appropriate physical concept to describe the transit of an electron from one side of a barrier to the other. Since information in a dispersive medium is carried by the *group* velocity, and we are considering the real appearance of an electron after a tunnelling event has occurred, there would appear to be stronger arguments in support of the group velocity as the appropriate concept, in preference to the signal velocity. In addition, if the analysis is repeated using a more traditional wavevector integration to reconstruct the wavepacket (in which case one is allowed to let the integration run from $-\infty$ to ∞, rather than from 0 to ∞ as is the case for the energy integration considered in [15]) and employing the same contour one does not obtain the same result. Specifically, the initial condition considered in [15] may be expressed as the contour integral

$$\psi(x, t = 0) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty + \mathrm{i}\varepsilon}^{\infty + \mathrm{i}\varepsilon} \frac{\exp[\mathrm{i}k_0 x + ik(x - x_0)]}{k - k_0} \, \mathrm{d}k \tag{6}$$

where the integration line runs just above the real axis. This is a cisoidal function with velocity $\hbar k_0/m$ and extending over all space for $x < x_0$ and zero for $x \geqslant x_0$ (hence the origin of the pole at $k = k_0$).

Therefore, the wavefunction at time t within the potential step (height V_0 for $x \geqslant 0$) is represented by an integration of the Fourier components of this initial condition modulated by the connection coefficient of the potential profile and a time evolution exponential factor

$$\psi_{II}(x, t) = \frac{1}{2\pi i} \int \frac{2k \exp[-i(kx_0 + \hbar k^2 t/2m) - \kappa x]}{(k - k_0)(k + \kappa)} \, dk \tag{7}$$

where $\kappa = (2mV_0/\hbar^2 - k^2)^{1/2}$. The integral runs from $-\infty$ to ∞ just above the real axis although the contour is closed in a manner depending on the time t. This closure is performed on the arcs of the great circle linked by a straight line of angle $3\pi/4$ crossing through the real axis at $K = (x - x_0)m/\hbar t$, since this gives a line contribution to the integral which for large distances r along the line is proportional to $\exp(-r^2\hbar t/2m)$ and hence is negligible sufficiently far away from the real axis. The contributions stemming from the angled line have been described [15] as fore and after-runners of the wavepacket which, because of its sharp nature, is composed out of an infinite number of wavevector components spanning the range $[-\infty, \infty]$. Since there are significant components of arbitrarily high velocity, this initial wavepacket very quickly decomposes, and loses its initial form which therefore explains the existence of the fore and after-runners. Now the only poles which can contribute to the integral stem from the pulse edge ($k = k_0$) and the barrier ($k = -\kappa = -mV_0/\hbar^2$) which do not produce a substantial increase in the wavefunction as the line contribution crosses through $K = (2mV_0/\hbar^2 - k_0^2)^{1/2}$. However, if instead we had introduced a new variable into the integration procedure, $Z^2 \equiv 2mV_0/\hbar^2 - k^2$, then this would appear to produce poles at $Z \propto \pm(V_0 - \hbar^2 k_0^2/2m)^{1/2}$ which *would* have this effect. However it is not permissible for us to make this change of variables in our analysis due to the uncertainty introduced into the integration limits by the squaring operation. Consequently, there appears to be a mathematical difficulty arising from whether the complex integration reconstructing the wavefunction is performed over energy or wavevector values, and what contour should be employed.

Büttiker and Landauer [13] obtained the semi-classical time from considerations of a square-barrier system subjected to a uniform time-varying oscillatory potential. By working within the WKB approximation for energies well away from the barrier peak, a *real* time of tunnelling propagation

$$\tau = \int_{x_1}^{x_2} [m/2(V_0 - E)]^{1/2} \, dx$$

was estimated. Quite aside from the approximations assumed and the operational methodology used (which only permit an order of magnitude estimate of tunnelling times), this approach is suspect since it attempts a treatment of an *open* quantum system by techniques designed for conservative quantum mechanics. Specifically, if the externally acting, explicitly time-dependent force is confined to the barrier region alone (which is the situation one would wish to consider for this problem) then the Schrödinger equation of the whole system is not separable in time (an attempt to separate variables would lead to the time dependent coefficients satisfying a differential equation which also depends on position). This implies that an eigenvalue decomposition cannot be made and the Schrödinger equation has to be solved by other methods.

Alternatively, if the externally acting force is *uniform* across the system, then although a separation of time variables may be performed, physically this corresponds

to adiabatically redefining the energy labels of the entire system at each instant in time. In this situation it should not be permissible to fix one value of energy on one side of the barrier region and match to the oscillating levels within the barrier, since relative to one level, *all* levels remain constant. In either situation, the formal analysis of Büttiker and Landauer is suspect since it seems to combine the problems of both a spatially uniform, and a confined external time-dependent force.

Another very good candidate for a tunnelling time theory, that of Büttiker [12] can also obtain the semi-classical time under certain approximations (essentially those under which the WKB approximation should become more accurate). However, in our view the analysis which Büttiker employed to obtain his tunnelling time (3) is erroneous on several points which we now discuss.

The theory considers the interaction of a spin polarised beam of electrons with a potential barrier containing a magnetic field. In the limit of small magnetic field, it is claimed that the motion of the tunnelling electrons are governed by three characteristic times, the dwell time (1), a traversal time (3) and a reflection time.

The first problem is that the Pauli spin matrices are not correctly normalised. This manifests itself in two ways. Firstly, if the equations (2.12) and (2.14) from [12] are used to calculate the total spin in the reflected and transmitted beams, the result is twice the total spin of the incident beam. Specifically, the expressions for the three transmitted spin components according to [12] are

$$\begin{aligned}
\langle S_z \rangle &= \frac{\hbar}{2}\frac{T_+ - T_-}{T_+ + T_-} \\
\langle S_y \rangle &= -\hbar \sin(\Delta\varphi_+ - \Delta\varphi_-)\frac{(T_+T_-)^{1/2}}{T_+ + T_-} \\
\langle S_x \rangle &= \hbar \cos(\Delta\varphi_+ - \Delta\varphi_-)\frac{(T_+T_-)^{1/2}}{T_+ + T_-}
\end{aligned} \tag{8}$$

and the corresponding expressions for the reflected spin components are

$$\begin{aligned}
\langle S_z \rangle_R &= \frac{\hbar}{2}\frac{R_+ - R_-}{R_+ + R_-} \\
\langle S_y \rangle_R &= -\hbar \sin(\Delta\varphi_+ - \Delta\varphi_-)\frac{(R_+R_-)^{1/2}}{R_+ + R_-} \\
\langle S_x \rangle_R &= \hbar \cos(\Delta\varphi_+ - \Delta\varphi_-)\frac{(R_+R_-)^{1/2}}{R_+ + R_-}
\end{aligned} \tag{9}$$

where $R_\pm$, $T_\pm$ are the reflection and transmission probabilities including the effects of the Larmor frequency of a magnetic field. It is a straightforward matter to see that

$$\langle S \rangle_T^2 = \hbar^2/4$$
$$\langle S \rangle_R^2 = \hbar^2/4$$

in spite of the fact that the incident beam had a total spin of $\hbar/2$ in the x direction.

Secondly, the total reflected (or transmitted) spin components are independent of the barrier reflection and transmission coefficients which lead to an anomaly if no barrier is present.

One should realise that the measurement of a spin component in the transmitted

beam is *conditional* upon transmission through the potential barrier. Therefore the Pauli spin matrices should be normalised to account for this joint probability. This criticism does not have a significant impact on the results of the paper since it only modifies the amplitudes of the various components and so we consider this problem to be minor.

A more serious oversight arises in the subsequent treatment of the transmitted spin components $\langle S_x\rangle$, $\langle S_y\rangle$, $\langle S_z\rangle$. All three components are treated equally until a Taylor expansion is employed on two of them ($\langle S_z\rangle$, $\langle S_y\rangle$) in order to define appropriate times τ_z (an unidentified time) and τ_y (the dwell time) whilst employing the normalisation condition

$$\langle S_x\rangle = (\langle S_z\rangle^2 + \langle S_y\rangle^2)^{1/2}$$

restricting the third spin component.

This yields a tunnelling time τ_x

$$\tau_x = (\tau_z^2 + \tau_y^2)^{1/2}.$$

However, if τ_x had been treated equivalently with τ_y to the same order in ω_L (the Larmor frequency) the more satisfactory result

$$\tau_x = \tau_y$$

would have been obtained, in which case the derived tunnelling time would be the dwell time (1). This argument is supported by the author himself. If the results of his Appendix (A5), i.e.

$$\langle S_x\rangle = \frac{\hbar}{2}[1 - (1/2)(md/\hbar k)^2\omega_L^2]$$

are compared with his equation (2.17), i.e.

$$\langle S_x\rangle = \frac{\hbar}{2}[1 - \omega_L^2\tau_x^2/2]$$

the identification

$$\tau_x = \tau_y = \frac{md}{\hbar k}$$

can be made.

In addition there is a physical basis for the equivalence of τ_x and τ_y. The experimental situation which Büttiker considers involves an electron beam moving along the y-axis, spin polarised along the x axis, incident upon a barrier containing a magnetic field parallel to the z axis and therefore three times may be identified in the limit of vanishing magnetic field according to the three distinct components along x, y, z. We can interpret these components as follows. S_z may be understood as arising from the differential rejection of the particles aligned against the magnetic field due to the difference in the effective potentials for spin-up and spin-down electrons. This does not have a valid physical basis to be interpreted as giving rise to a relevant transit tunnelling time. However, relative changes in S_x and S_y both arise from the Larmor precession around the z axis, and one can visualise that the amount of Larmor precession depends on the mean time the electron is subjected to the field in the barrier region. It would be expected that since the physical mechanism giving rise to the two spins is the same (the loss in S_x is a gain for S_y and vice versa), then τ_x and τ_y ought to be equivalent, which is what Büttiker actually obtains in his Appendix. Therefore Büttiker should only be able to derive a dwell time.

To summarise this section, we have presented arguments why the scattering, dwell and semi-classical results are not appropriate concepts to describe the transit time of tunnelling electrons through classically forbidden regions. The one remaining step is to illustrate why we believe the phase time result to be the best all round solution.

3. Analysis of the tunnelling problem

It is our intention to obtain the phase-time result using a combination of conventional state space analysis, and a phase space description of the quantum dynamics. The state space analysis is developed in detail in spite of its textbook nature. This is because many assumptions that are important in this problem are often glossed over in treatments of the tunnelling problem which tend to submerge the approximations involved.

3.1. Conventional state space analysis

A convenient method of solution of the dynamical tunnelling problem is to decompose the initial condition into eigen-states of the potential profile and evolve each component separately. Then one can exploit the linearity of the problem by resumming to obtain the wavefunction at a time t. Consider the basis set for a single barrier of width a and height V shown in figure 1 which have yet to be orthonormalised. The orthogonality of the basis set is easily proven: the non-degenerate pairs must be orthogonal [21] whilst the degenerate pairs are orthogonal because they are of opposite parity. However the *normalisation* of each state give rise to a problem. For example, the normalisation integral for an even parity state with energy less than the barrier height is

$$\langle\psi|\psi\rangle = 2\int_0^{a/2} (B^{+2}\cosh^2(\kappa x) - A^{+2}\cos^2(kx - \delta^-))\,\mathrm{d}x + 2\int_0^{\infty} A^{+2}\cos^2(kx - \delta^-))\,\mathrm{d}x \tag{10}$$

where A^+, B^+, $\delta^\pm$ are functions that have yet to be determined by boundary conditions.

The normalisation integral has two components, one of which requires delta function normalisation, whilst the other requires a normalisation to unity. These conditions are

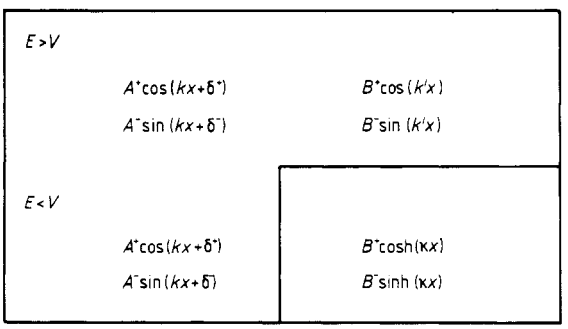

Figure 1. The basis set used for a single square barrier. The figure only illustrates one half of the potential. The wavefunction on the side not shown, only differs by the sign of the phase factors ($\delta^\pm$).

mutually incompatible and so we choose to normalise to a delta function by ignoring the contribution which stems from the integral corresponding to the barrier region. This choice is made on the basis that the contribution from the small region of space occupied by the barrier when compared to the free space contribution will be negligible. This approach yields a normalisation constant of $A^{\pm} = 1/\sqrt{\pi}$. The remaining functions $B^{\pm}$, $\delta^{\pm}$ may be calculated in terms of $k = (2mE/\hbar^2,\ k')^{1/2} = [2m(E - V)/\hbar^2]^{1/2}$ and $\kappa = [2m(V - E)/\hbar^2]^{1/2}$ by imposing continuity of the wavefunction and its derivative. Specifically we find

$$\begin{aligned}
\delta^+ &= ka + \tan^{-1}(\kappa \tanh(\kappa a)/k) && E < V \\
\delta^+ &= ka - \tan^{-1}(k' \tan(k'a)/k) && E > V \\
\delta^- &= ka - \tan^{-1}(k \tanh(\kappa a)/\kappa) && E < V \\
\delta^- &= ka - \tan^{-1}(k \tan(k'a)/k') && E > V.
\end{aligned} \tag{11}$$

Any initial condition may now be expanded in terms of the basis set, and its time development calculated. It is important to realise that in tunnelling problems there are two mutually exclusive initial conditions which one may consider: the energy of the incident wavepacket can be restricted to below the barrier height, or the spatial location of the wavepacket can be restricted to one side of the barrier. In the first case there will be no superbarrier components, but there will be some leakage of the initial wavepacket throughout the barrier region and into the transmitted region. In the second situation, there will be superbarrier momentum components but at least one can be sure that any transmitted components have traversed the barrier region. We denote the half-space region to which the initial wavepacket is confined, region 1 and the other half, region 2. Then the wavefunction in region 1 is

$$\psi_1(x, t) = \frac{1}{2\pi}\left(\int_{-\infty}^{\infty} f(k)\, \mathrm{e}^{-\mathrm{i}kx - \mathrm{i}\omega t}\, \mathrm{d}k + \int_{-\infty}^{\infty} f(k) \times \sin(\delta^+ - \delta^-) \exp[\mathrm{i}(kx - \omega t + \delta^+ + \delta^-)]\, \mathrm{d}k\right) \tag{12}$$

and the wavefunction in the region 2 is

$$\psi_2(x, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(k) \cos(\delta^+ - \delta^-) \exp[\mathrm{i}(kx - \omega t + \delta^+ + \delta^-)]\, \mathrm{d}k. \tag{13}$$

A simple interpretation arises if one considers that the wavefunction in free space is

$$\psi(x, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(k) \exp[\mathrm{i}(kx - \omega t)]\, \mathrm{d}k.$$

The two components in region 1 are the incident and reflected wavepackets, while the single contribution in region 2 is the transmitted wavepacket. This interpretation allows the identification of the reflection (r) and transmission (t) coefficients from which follows:

(i) the condition $t^2 + r^2 = 1$ is automatically satisfied;

(ii) the phase shifts of the reflected and transmitted components differ by $\pi/2$;

(iii) since both phase angles $\delta^{\pm}$ tend to zero as the barrier width tends to zero, then the solution to the freely evolving wavepacket is easily recovered;

(iv) the transmission probability and the phaseshifts are those which are calculated

by solving the time independent Schrödinger equation assuming unit incident flux in region 1.

Note that this interpretation means that expressions (12) and (13) correspond to the results that are commonly assumed to be correct without comment. However, as the analysis demonstrates, the integrals must be performed over *all k* (so that all negative as well as positive momentum components contribute—this contrast with Hartman's [19] analysis), the initial conditions have to be localised to one side of the barrier region, and in addition an approximate eigen-state normalisation has had to be employed. The validity of these assumptions and approximations will be checked in § 4. This analysis depends only on the finite extent of the potential, and so the method may be applied to any suitable spatially localised barrier. Thus the procedure to calculate the time development is a three-stage process;

(i) Fourier transform the initial condition

(ii) solve the time-independent equation assuming unit incident flux to obtain $t(k)$ and $r(k)$

(iii) integrate the expressions (12), (13).

Knowing the wavefunction at a time t would allow us to introduce a tunnelling time by considering the transmitted probability density at a time t as considered by Hartman [19]. Dealing with the probability density directly necessitates the introduction of the stationary phase approximation (see [19]). To avoid this approximation, and in addition, to highlight the approximations involved in obtaining the phase time expression, we choose to consider the problem in a phase space description. As it is more closely allied with classical techniques, this approach also provides additional physical insight which is denied by the state space interpretation.

3.2. Phase-space analysis

We employ a phase-space description using the Wigner distribution function $F(x, p, t)$, a simultaneous function of position and momentum, which may be defined in terms of the momentum components $\varphi(p, t)$ of a wavefunction as [22]

$$F(x,p,t) = \int_{-\infty}^{\infty} \varphi^*(p + p'/2, t)\varphi(p - p'/2, t)\, e^{ip'x/\hbar} \frac{dp'}{2\pi\hbar}.$$

The Wigner distribution in free space evolves as a classical distribution (note that not all quantum distributions have this property) so that if the distribution at time $t = 0$ is $F_0(x, p)$ then the distribution at time t would be given by $F_0(x - \hbar\langle p\rangle t/m, p, t)$ where $\langle p\rangle$ is the mean momentum of the initial condition.

Now using the expression for the transmitted wavefunction (13), we find that the transmitted Wigner distribution is

$$F(x,p,t) = \int_{-\infty}^{\infty} t^*(p + p'/2)t(p - p'/2)f^*(p + p'/2)f(p - p'/2)\, e^{i(xp'/\hbar - pp't/m)} \frac{dp'}{2\pi\hbar}. \tag{14}$$

Note that this may be alternatively expressed in the form

$$F(x,p,t) = \int T(x - x', p)G(x', p, t)\, dx'$$

where

$$T(x,p) \equiv \int_{-\infty}^{\infty} \exp(ikx\hbar)t^*(p-k/2)t(p+k/2)\frac{dk}{2\pi\hbar}$$

is the Wigner equivalent of the transmission coefficient (i.e. is a measure of the transmissivity at a given energy conditional on x and hence the transmission probability is given by the integral of $T(x,p)$ over all space), and

$$G(x,p,t) \equiv \int_{-\infty}^{\infty} \exp(ikx/\hbar)\exp\{-i[\omega(p-k/2) - \omega(p+k/2)]t\}f^*(p-k/2)f(p+k/2)\frac{dk}{2\pi\hbar}$$

is the freely propagating Wigner distribution ($\hbar\omega(p) \equiv p^2/2m$).

To see how the phase time result may be derived, we first assume that the initial condition is highly peaked about a momentum p_0. We would expect that the dominant contribution to the above integral (14) comes from the region around p_0. If, in addition, we assume that the transmission coefficient is slowly varying about p_0, we can take a locally homogeneous approximation to the transmissivity function above by a Taylor expansion about p_0. This gives an approximate transmissivity function around $p = p_0$ of

$$T(x,p) \approx \delta(x)|t(p)|^2 + \mathrm{Im}[t^*(p)\partial_p t(p)]\frac{d\delta(x)}{dx}.$$

Note that the validity of this expansion gives the condition that

$$t(p)|_{p=p_0} \gg \frac{k}{2}\partial_p t(p)|_{p=p_0}. \tag{15}$$

If the transmission coefficient is now expressed in the form $t(p) = R(p)\exp(i\varphi(p))$ then the transmitted Wigner distribution is approximately

$$F(x,p,t) \approx |t(p_0)|^2\left[G(x,p,t) + \frac{d\varphi}{dp}\frac{\partial G}{\partial x}\right] \tag{16}$$

$$\approx |t(p_0)|^2 G[x + (d\varphi/dp)|_{p=p_0}, p, t]$$

under the approximation

$$\left.\frac{d\varphi}{dp}\right|_{p=p_0} \ll x.$$

This approximation stems from the rigid condition that we have employed for the sake of generality, that the *form* of the transmitted wavepacket should be close to the form that the packet would have had in the absence of a potential barrier. For example, the minimum uncertainty wavepacket (considered shortly) is expected to have a transmitted wavepacket which resembles a Gaussian distribution, in which case there is no difficulty in defining a tunnelling time.

To summarise, our result (16) may be interpreted in the following way. An initial condition localised in momentum, here represented by the Wigner distribution, propagates forwards. If there is no potential barrier in the way the Wigner distribution at time t will be simply $G(x,p,t)$. If a barrier is present, characterised by a transmission

coefficient $t(p) = R(p)\exp(i\varphi(p))$, then the transmitted Wigner distribution is reduced in magnitude by an amount $|t(p_0)|^2$ and delayed with respect to the corresponding freely moving wavepacket by an amount

$$\tau = \frac{m}{p_0}\left(\frac{d\varphi}{dp}\right)_{p=p_0}. \tag{17}$$

This is the characteristic tunnelling delay time of the problem which is seen to be the phase time result of Wigner and Hartman (5). Therefore the total traversal time is the delay time, plus the time it would have taken to cross the barrier region in the absence of a potential.

The analysis we have employed allows us to place bounds on its validity, and to see how to generalise the expression when the approximations break down. The principal approximation is that the initial wavepacket should have a dominant momentum component, and the transmission coefficient should be slowly varying in this region (condition (15)). Specifically, if the initial momentum distribution is characterised by a peak at $p = p_0$ with a spread of $2\sigma_p$ (where typically σ_p would be the standard deviation), then the inequality that we require to hold is

$$t(p_0) \gg \left(\sigma_p \frac{dt}{dp}\right)_{p=p_0}. \tag{18}$$

When this inequality does not hold, for instance when the initial wavepacket is broadly spread out in momentum, then momentum skewing effects have to be taken into account and the expansion made in $t(p)$ ought to take into account higher-order terms. This wavepacket-dependent effect is something the various other tunnelling time theories have not discussed.

It is possible to generalise this argument by considering the specific example of an initial Gaussian wavepacket centred at x_0 with momentum $p_0 = \hbar k_0$ and standard deviation of σ. To be consistent with our conditions, the Gaussian must be initially sufficiently distant from the barrier so that the high momentum components involved in truncating the exponential tail at the barrier are negligible. Since the Fourier transform of a truncated Gaussian is

$$f(k) = \frac{\sigma\sqrt{\pi}}{2}\{1 - \Phi[(x_0 + a/\sigma) - i(k-k_0)\sigma/2]\}\exp[-i(k-k_0)x_0 - (k-k_0)^2\sigma^2/4]$$

where $\Phi(a + ib)$ is the error function [23], then the truncation of the initial condition will not appreciably distort the momentum spectrum if the peak is sufficiently far away from the barrier region, in which case we will assume that the momentum distribution may be treated as a Gaussian distribution.

Using this initial condition the transmitted Wigner distribution takes the form

$$F(x,p,t) = |t(p_0)|^2 G(x,p,t)\left(1 - \frac{(x - x_0 - p_0 t/m)}{\sigma^2}\frac{d\varphi(p)}{dp}\right) \tag{19}$$

where $G(x, p, t)$ the freely propagating Wigner distribution is

$$G(x,p,t) \propto \exp\left(-\frac{(x - x_0 - p_0 t/m)^2}{2\sigma^2} - \frac{2\sigma^2}{\hbar^2}(p - p_0)^2\right).$$

In terms of the transmitted probability density we find

$$|\psi(x)|^2 \equiv \int\int_{-\infty}^{\infty} T(p, x-x')G(x', p, t)\,\mathrm{d}p\,\mathrm{d}x'/2\pi\hbar$$

$$\approx \int |t(p)|^2 G(x, p, t)\left(1 - \frac{(x - x_0 - pt/m)}{\sigma^2}\frac{\mathrm{d}\varphi(p)}{\mathrm{d}p}\right)\mathrm{d}p/2\pi\hbar \tag{20}$$

where we have employed the approximation inherent in the first part of equation (16) and the Gaussian nature of $G(x, p, t)$. If we consider the evolution of the *peak* of this transmitted packet, and hence consider $d_x|\psi(x)|^2 = 0$, we have the relationship

$$0 = \int |t(p)|^2 G(x, p, t)\left(\frac{(x - x_0 - pt/m)^2}{\sigma^4}\frac{\mathrm{d}\varphi(p)}{\mathrm{d}p} - \frac{(x - x_0 - pt/m)}{\sigma^2} - \frac{1}{\sigma^2}\frac{\mathrm{d}\varphi(p)}{\mathrm{d}p}\right)\frac{\mathrm{d}p}{2\pi\hbar}. \tag{21}$$

Provided that there is no momentum skewing around the peak momentum value of p_0, the expression (21) produces a quadratic equation in $(x - x_0 - p_0t/m)$. If there *is* momentum skewing, it is clear from the above equation that the weighted values of the mean and the variance of the momentum distribution are involved (the weighting function being the transmission probability $|t(p)|^2$). Neglecting the skewing factor and in the absence of a potential ($\mathrm{d}\varphi/\mathrm{d}p = 0$) we find that the peak position at time t, x_t, is just the classically expected time of $x_t = x_0 + p_0t/m$ as it should be. However if $\mathrm{d}\varphi/\mathrm{d}p \neq 0$ then the peak position at time t is

$$x_t = x_0 + p_0t/m + \Lambda(p_0)$$

where

$$\Lambda(p) \equiv \frac{\sigma^2}{2\mathrm{d}\varphi(p)/\mathrm{d}p}\left\{1 - \left[1 + \left(\frac{2\mathrm{d}\varphi/\mathrm{d}p}{\sigma}\right)^2\right]^{1/2}\right\}.$$

In the limit of small $\sigma^{-1}\,\mathrm{d}\varphi/\mathrm{d}p$ (corresponding to a narrow momentum spread) the above equation reproduces the phase time result, specifically

$$\Lambda(p) = -\frac{\mathrm{d}\varphi(p)}{\mathrm{d}p}.$$

This is a *delay* if $\mathrm{d}\varphi/\mathrm{d}p > 0$. Since we are concerned with a comparison of various tunnelling times which have been derived on implicit assumptions of wide wavepackets, we retain this approximation to the tunnelling time for the subsequent sections.

In summary, the phase-space argument illustrates that the phase-time result is the natural tunnelling time under a reasonable class of assumptions (mainly concerned with an initially narrow wavepacket in momentum and a smoothly varying transmission probability).

To further justify this claim, to validate the approximations we had to employ and to show the impact of violating the derived inequalities, the following section compares the main contenders of a tunnelling time with numerical simulations.

4. Numerical comparison of various models

We have so far employed analytical and physical arguments why the phase-time result

as a transit tunnelling time may be considered to be the most appropriate for a wide variety of relevant situations. In this section it is our intention to employ numerical simulations of wavepackets incident upon square barriers to compare with the results proposed by several of the competing theories discussed in this paper.

Such a comparison (with the phase-time result alone) has previously been performed by Schnupp [6]. However our numerical simulations do not agree with those of Schnupp and a suggestion for the source of this discrepancy will be made later. In the light of this discrepancy, it is clear that there was a need for a careful set of numerical simulations.

The numerical technique we employed for solving the discretised time-dependent Schrödinger equation was based on the algorithm of Goldberg *et al* [24]. This raises two apparent problems: the discretisation mesh must be sufficiently fine that the discrete problem adequately mimics its continuous counterpart, and secondly the discontinuous square-barrier potential profile has to be discretised in such a way that the essential physics is preserved (in particular the correct asymptotic transmission probability has to be obtained). We found that the particular choice of discretising a discontinuous potential had a significant effect on the results. A discretisation prescription which we found to accurately reproduce the analytically expected time-independent transmission probability for a square barrier is that employed by Vigneron and Lambin [25]. A more crucial test of the discretisation is if it reproduces the wavefunction itself at an arbitrary time (and not just asymptotically).

Figure 2 shows a comparison of numerical and analytic results obtained for the probability density at an instant in time when an incident Gaussian wavepacket is in the process of impinging on a square-barrier potential. The numerical results were obtained by solving the time-dependent Schrödinger equation using the Goldberg algorithm and a uniform discretisation mesh where the discontinuous potential was represented in the same manner as employed by Vigneron and Lambin. The analytic results were obtained

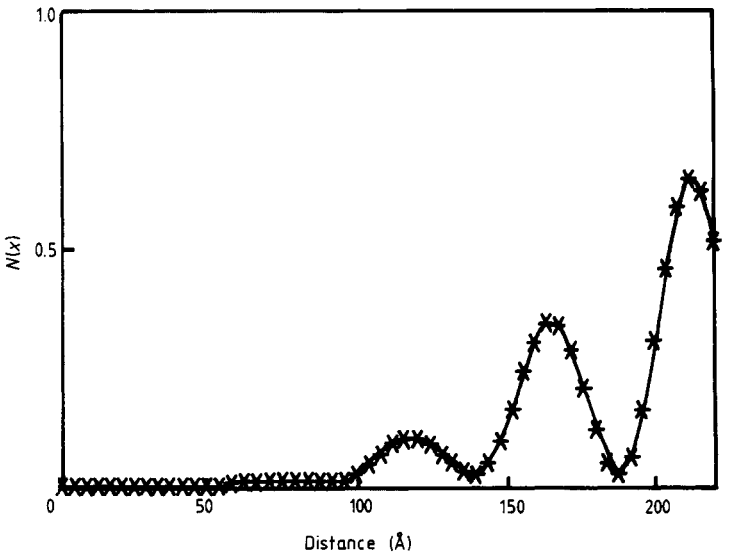

Figure 2. A comparison of the numerical (*) and analytic (——) wavefunctions a short time after a Gaussian wavepacket has impinged upon a square barrier. The abscissa is the probability density $N(x)$ and the front of the barrier forms the right had edge of the figure.

from the expression given in equation (12). As seen, good agreement is obtained between the analytic and numerical techniques in the time domain. This provides us with confidence that the data obtained from the numerical simulations is sufficiently accurate to pinpoint the tunnelling times.

The definition of the tunnelling time in the previous sections required that the overall shape of the transmitted packet be approximately the same as that obtained if no barrier were present. Therefore a convenient point of reference to employ in order to evaluate the tunnelling time is the difference in times between the impact of the incident *peak* and the emergence of the transmitted peak (note that under the assumptions we had to make, if the initial condition is tightly located in momentum and the transmission coefficient is slowly varying, then we only expect one single dominant peak in the transmitted wavepacket and so our problem is well defined). The time for the incident pulse to reach the barrier is just the classically expected time which is known. Therefore the remaining problem is the calculation of the instant when the peak emerges on the far side of the barrier. The numerical experiments consisted of a sequence of runs, where the same initial Gaussian wavepacket was evolved towards a square barrier but with gradually increasing energies on each successive run. Knowing the incident energy gave the arrival time and a peak picking technique was used to obtain the emergence time at the back of the barrier. This was performed in an iterative manner. First a large region of space on the far side of the barrier was examined at an instant when the peak of the transmitted packet had emerged. This gave an estimate of the peak position which was used to extrapolate back in time to give a more refined estimate of when the peak emerged. It was then possible to focus into the region at the back of the barrier to examine more accurately when the peak emerged. This refined result was then plotted as a function of energy and compared with the values predicted by several tunnelling time theories.

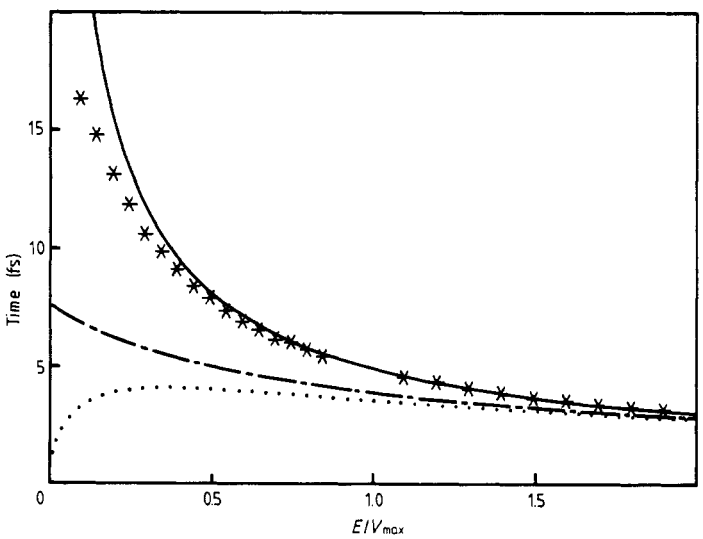

Figure 3. A comparison of numerical traversal times for a 'narrow' barrier (width 25 Å, height 0.1 eV, effective mass $m^* = 0.063$). (– – –) Büttiker's expression; (—) phase-time results; (. . .) dwell time results; (*) numerical results for Gaussian wavepackets with a standard deviation of 0.3 μm.

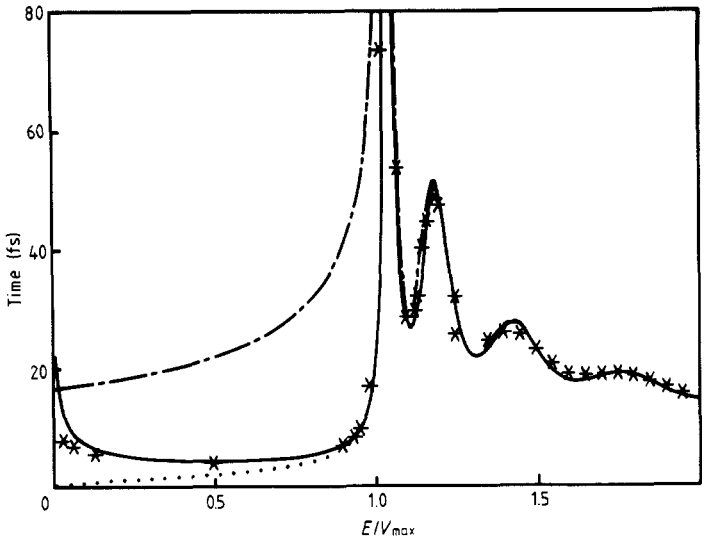

Figure 4. A comparison of numerical traversal times for a 'thick' barrier (width 200 Å, height 0.3 eV, effective mass $m^* = 0.063$). (----), Büttiker's expression; (——) phase-time results; (. . .) dwell time results; (*) numerical results for Gaussian wavepackets with a standard deviation of 0.3 μm.

The typical results of such a sequence of experiments are illustrated in figures 3 and 4. The difference between figures 3 and 4 are that they are each indicative of the behaviour one expects for a characteristically 'thin' or 'thick' barrier. Since the Schrödinger equation scales with energies and the square of linear dimensions the definition of thin and thick depend on the magnitude of L^2V for a barrier of width L and height V. In the particular simulations we made, we chose physically reasonable values appropriate to tunnelling barriers in small GaAs structures (i.e. effective mass of $0.063 \times m_e$ was used—m_e being the bare electron mass). In these units our definition of a thin barrier was one in which the width was 25 Å and the barrier height was 0.1 eV. This situation is illustrated in figure 3. On the same scales, a thick barrier limit (and the parameters employed in figure 4) correspond to a barrier width of 200 Å and a height of 0.3 eV. Incidentally, the behaviour for the thick barrier approximately corresponds to the regime considered in [12].

It is clear from these two figures that the phase-time result offers the best overall description of the times obtained from the numerical simulations, and therefore the assumptions inherent in the phase-time result and the numerical experiments regarding the definition of a tunnelling time appear to be most consistent.

It is seen that some discrepancy occurs between the numerical and phase-time result at low incident energies. This is expected, and indeed was predicted in the derivation of the phase-time result. Since the numerical data was obtained using an initial wavepacket with a fixed momentum dispersion, then as the energy decreases and the transmission coefficient becomes more rapidly varying (since the transmission coefficient is exponentially varying at low energies), then the assumption (18) begins to break down. Therefore it is expected that as $p_0 \rightarrow 0$ the numerical and phase-times disagree. To test this supposition, an initial wavepacket with a narrower momentum dispersion was employed with low incident energy, and the point of divergence between the phase and

numerical curves was seen to decrease in energy confirming the arguments. In spite of this local disagreement, which we are able to predict, the phase time is still the best contender to describe the numerical situation.

This conclusion does not confirm Schnupp's earlier analysis [6]. With the experience obtained from our own simulations we would postulate that Schnupp's work differs for one of two possible reasons: a difference in the discretisation of the discontinuous potential, or the situation considered by Schnupp was one in which the phase-time expression was not valid because of the momentum spread of the wavepacket. Unfortunately, insufficient information was given to enable us to check either of these postulates.

Thus the numerical simulations we have performed appear to agree with the phase-time results over a wide range of wavepacket energies and widths, and for a range of physically relevant barriers. It is not clear from previous derivations of the various tunnelling times what is the general range of validity of the derived expressions. It is at least evident from figures 3 and 4 that the alternative tunnelling times are not appropriate for either thin or moderately thick barriers for sub-barriers energies.

5. A particulate, semi-classical model

A consistent definition of the tunnelling time has been shown to be offered by the phase-time result. However, as we intimated in the introduction, a time for an electron to tunnel through a barrier is inherently a particulate concept which clouds the issue of its interpretation. In this section we present a semi-classical model for tunnelling electrons which allows the interpretation of the tunnelling time as an ensemble average quantity.

The simplest possible model we can consider for the simple square barrier and which still retains interesting behaviour, is to replace the barrier by two partial reflectors. Within this model, we assume that each point particle moves classically outside the barrier region and that motion between the reflectors is determined by a time characteristic of the barrier being modelled. When a particle reaches a partial reflector, it can be either transmitted or reflected with a given probability. The finite chance of reflection r at each point gives rise to an infinite number of paths that end with a particle being totally transmitted or reflected. If the partial probabilities associated with each total path is summed, expressions are obtained for the total transmission T and reflection R probabilities

$$\begin{aligned} T &= (1 - r)/(1 + r) \\ R &= 2r/(1 + r). \end{aligned} \tag{22}$$

The value of r may now be chosen to match the asymptotic value of T obtained assuming an incident unit flux of equivalent momentum. If ξ is the time it takes for the particle to move from one partial reflector to the other, then the expectation value $\langle\tau\rangle$ of the time it should take for transmission may be calculated. This produces

$$\langle\tau\rangle = \xi\left(\frac{1 + r^2}{1 - r^2}\right). \tag{23}$$

Since the model is not designed to produce the interference between the reflected and incident waves, nor the decay of the wavefunction in the barrier, the model's validity

of describing the dynamics of a tunnelling electron can only be measured by comparing with the actual transmitted or reflected probability density at a given isntant. This was performed numerically by a Monte Carlo simulation. A Gaussian initial condition was represented by 900 particles distributed uniformly in phase space within two standard deviations of the mean position and momentum of the Gaussian. Each particle was then added to the final distribution with the statistical weight of its initial condition. There are two relevant characteristic times in the particle model, the one-pass time ξ and the mean time $\langle\tau\rangle$. Initially ξ was interpreted as the phase-time result (5). When the Monte

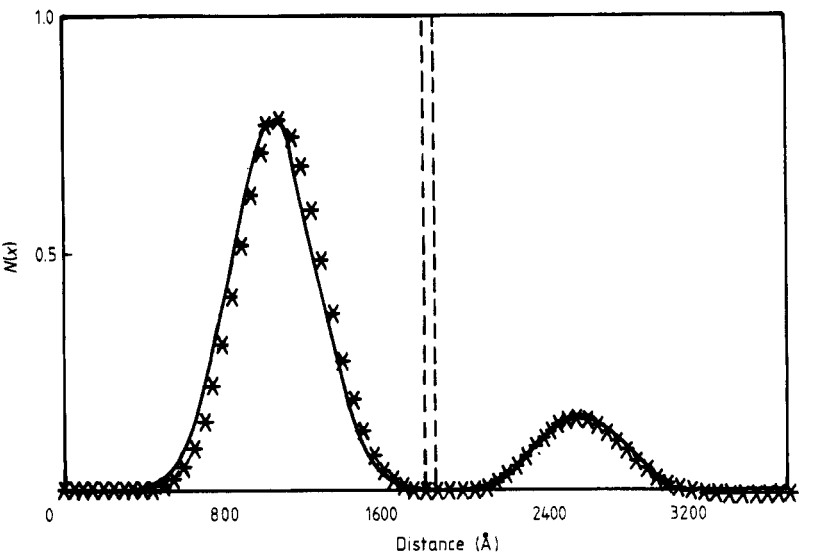

Figure 5. A comparison of the probability density calculated according to the Monte Carlo model (——) discussed in § 5, and the solution of the time-dependent Schrödinger equation (*). The locations of the edges of the barrier replaced by partially reflecting barriers, are indicated by the vertical lines.

Carlo simulation was compared with the actual numerical simulation of the exact Schrödinger equation, the results were unsatisfactory, with no general agreement. In contrast, if $\langle\tau\rangle$ is set equal to the phase-time expression (which by inverting (23) furnishes the definition of the one-pass time) the results are extremely favourable. The specific situation of an initial Gaussian wavepacket with standard deviation of 300 Å and a mean energy of 0.15 eV incident upon a barrier of width 50 Å and a height 0.2 eV are depicted in figure 5. At the instant that this snapshot was taken, the Monte Carlo simulation gave a 16.39% transmission compared to 16.40% obtained from the numerical solution of the Schrödinger equation (indicated by asterisks in the figure). Apart from the transmission probability being reproduced, it is seen that the results of the Monte Carlo simulation also reproduces the form of the actual transmitted and reflected densities quite accurately. Consequently on the basis of this figure, it is clear that the phase-time result in a semi-classical context needs to be interpreted as the ensemble average time which a particle takes to cross a potential barrier.

6. Conclusion

In this paper an expression for the tunnelling time of an electron traversing a classically forbidden region was obtained which under certain approximations was shown to be equivalent to the phase time expression derived previously by Wigner and Hartman using alternative approaches. The analysis highlighed the approximations involved and thus allowed us to obtain a criterion of when the phase-time result should break down. Since the analysis employed a basis set which could only be approximately normalised, the analytic results were compared with a direct numerical simulation of the Schrödinger equation, along with various other tunnelling time expressions. The results of our analysis indicate that the phase-time result is overall the best one to use when momentum skewing of the initial wavepacket is not significant. If momentum skewing is a problem, then the phase-time analysis indicates how the techniques may be extended to take the skewing into account.

Although we have not performed extensive simulations on a variety of different shaped wavepackets, as long as the initial conditions do not violate the restrictions expressed in our derivation we do not believe there is any reason to suppose that the conclusions obtained from Gaussian wavepacket simulations will be significantly modified. Rather, we would expect that a *minimum* criterion of a good tunnelling time theory should be that it is capable of describing the evolution of the minimum uncertainty wavepacket through a classically forbidden region, as the phase-time expression does.

Finally, by recourse to a semi-classical particle picture, it was illustrated why the phase-time expression needs to be interpreted as an ensemble average quantity. This final result should prove to be of use to Monte Carlo models of electron transport in ultra small semiconductor devices where the tunnelling problem begins to dominate the more conventional collision events without having to perform a full solution of the quantum transport problem.

Acknowledgments

The authors are grateful to the Science and Engineering Research Council who provided financial assistance during the course of this work.

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