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LETTER TO THE EDITOR

Tunnelling through a time-modulated barrier—relation to tunnelling times

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Abstract. We analyse tunnelling through time-modulated barriers. Our numerical results for the transmitted sideband intensities, obtained with wave-packet simulations, are in quantitative agreement with the analytical results of Büttiker and Landauer. For opaque barriers the asymmetry of the sideband intensities can be characterised with a single frequency whose inverse Büttiker and Landauer interpret as the traversal time. This simple behaviour does not hold in general, and we discuss some of the difficulties one meets in an attempt to generalise the one-parameter description to arbitrary barriers. Furthermore, we examine analytically the transmitted wavefunction in the adiabatic limit, and show that the related density and current involve both the dwell time, and the Büttiker time, defined in the context of a Larmor clock. This suggests the possibility that experiments probing different aspects of the transmitted wavefunction may yield different, but complementary, information about the tunnelling process.

In recent years experimental and/or theoretical studies of tunnelling in semiconductor heterostructures have attracted widespread interest. Most of the theoretical models have been time-independent, even though many experiments would, in principle, require an explicitly time-dependent treatment. As an example we mention the theoretical estimation of the ultimate speed limit of a double-barrier, resonant-tunnelling device. Phenomenological discussions often require as input an estimate of the tunnelling time: the time a charge carrier spends in the classically forbidden barrier region. Several different tunnelling times have been suggested [1–6]; however, due to the lack of conclusive experiments no single theoretical tunnelling time has been universally accepted. Indeed, it is not even clear if a unique tunnelling time exists [7, 8].

In the present Letter we address several aspects of time-dependent tunnelling. First, we briefly describe a numerical method that is suitable for studying explicitly time-dependent situations. Next, as an application, we compare our numerical results to a case where analytical results are known [1, 2]: a square barrier with an imposed weak harmonic perturbation. We hasten to point out that the numerical method employed in this work can with equal ease be applied to arbitrary tunnelling structures and/or time modulations (which do not have to be small). The harmonically perturbed square barrier has been used by Büttiker and Landauer to construct a theory for the traversal time for tunnelling, and we proceed with a discussion of this model, and its generalisations and their relation to tunnelling times. We conclude by presenting and analysing the results of an analytical calculation of the transmitted electron density, and current in the adiabatic limit, and the relation of these observables to tunnelling times.

Our numerical method is based on wave-packet simulations (i.e. direct numerical forward integration of the time-dependent Schrödinger equation with a given initial state). The numerical integration procedure is standard and it has been discussed elsewhere [9]. Here we only want to make a few points which are of special importance for the present study.

(i) Choice of the initial state. Predictions for tunnelling times for 25–50 Å thick $Al_xGa_{1-x}As$ range typically between 1 and 10 femtoseconds. These times correspond to energies of the order of 0.6 to 0.06 eV, and in order to yield quantitative results the energy resolution of the simulation must be better than the above values. This implies that the spatial width of the initial wave packet, which is inversely proportional to the momentum width, and hence also determines the energy width, must be chosen accordingly. In practice we find that wave packets with half width $\sigma \geqslant 1000$ Å $[\psi(t=0) \sim \exp(-x^2/2\sigma^2)]$ yielded sufficient accuracy. This, in turn, required long 'contact' regions (in order to prevent the initial state overlapping with the tunnelling barrier); typically we chose 1 μm-long flat regions outside the barriers.

(ii) Discretisation of the potential. The thinnest barriers in our simulations contain only ~10 mesh points which requires some care when choosing the discretisation procedure. We found out that the procedure suggested by Collins and co-workers [5] was sufficient to lead to stable results.

(iii) Momentum representation. We found it extremely useful to work simultaneously in momentum space and real space. The point is that even the slightest numerical instability immediately reflects itself in the momentum representation of the wavefunction: thus the 'cleanness' of the momentum spectrum was an indispensable tool in judging the convergence and quality of the numerics.

(iv) Consistency with static transmission coefficient. Another measure of the sharpness of the energy distribution of the initial state can be obtained by comparing the simulated transmission coefficient with the exactly known static value. For the parameters used in our calculations the agreement was always within a couple of percent; the error was larger for the thinner barrier presumably because the finite mesh size plays a more important role there. In addition, to make connection to the weak time-dependent perturbation considered by Büttiker and Landauer, the amplitude of the time-dependent modulations was chosen to be so small ($V_1 = V_0/20$ in our simulations) that the total transmission coefficient is independent of the modulation frequency, and that higher-order processes (emission/absorption of several modulation quanta) are negligible.

The physics of tunnelling through a time-modulated barrier has been elucidated by Büttiker and Landauer (BL) [1, 2]. The tunnelling particles may absorb, or emit, modulation quanta, and thus in momentum (or energy) space the reflected and transmitted parts of the wavefunction consist of a main feature with the initial energy E, and sidebands at $E \pm n\hbar\omega$. Below we discuss the relation of these sidebands to tunnelling times.

We now turn to our numerical results. Figure 1 shows a temporal evolution of a typical simulation, and as seen there the sidebands at energies $E \pm \hbar\omega$ are clearly resolved. Thus a quantitative evaluation of the sideband intensities is possible (this was

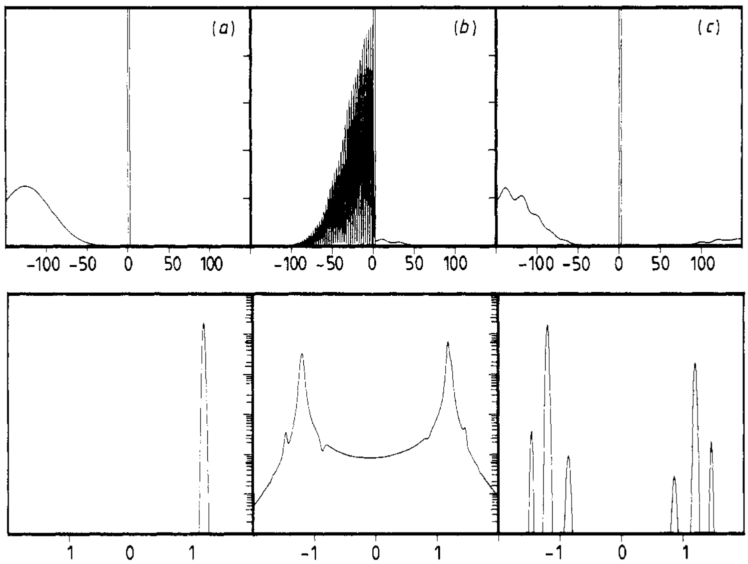

Figure 1. A Gaussian wave packet of mean energy, E, is shown colliding with a sinusoidally modulated square barrier, $V(x, t) = (V_0 + V_1 \sin(\omega t))\ \theta(x)\theta(d - x)$, where $V_0 = 0.23$ eV, $V_1 = 0.05\ V_0$, $\hbar\omega = 0.35\ V_0$, and $d = 50$ Å. The square modulus of the wave packet for $E = 0.72\ V_0$ is plotted both in real space (top: linear y axis, length unit = 22.22 Å) and in momentum space (bottom: logarithmic y axis, momentum $\hbar k = \sqrt{2}$ corresponds to energy $E = V_0$), for three characteristic time instants during the simulation: (a) before collision, (b) 'mid-collision' and (c) after collision. After a completed collision (c) the momentum representation of the transmitted pulse (positive momentum) and the reflected pulse (negative momentum) contains well resolved sidebands corresponding to emission or absorption of one modulation quantum.

not the case for our preliminary data reported earlier [10] for which we gave an erroneous interpretation).

In figure 2 we show the sideband intensities obtained both from our simulations, and from the analytical results of BL. As seen in the figure, the two totally independent approaches are in quantitative agreement. This serves as a stringent test for the accuracy of the numerical method, and suggests its applicability to a wide range of other time-dependent phenomena.

Büttiker and Landauer [1, 2] have suggested using the side-band intensities for defining a tunnelling time. For simplicity, let us first consider opaque barriers ($k_0 d \gg 1$, $k_0 = (2mV_0/\hbar^2)^{1/2}$, V_0 is the height of the barrier, and d is its thickness). In this case BL find that the intensities of the sidebands $T_\pm$ ($\equiv T(E \pm \hbar\omega)$, E being the energy of the incoming particle, and ω the modulation frequency) are given by

$$T_\pm = (v_1/2\hbar\omega)^2(\exp(\pm\omega md/\hbar\kappa) - 1)^2 T(E) \tag{1}$$

where $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$, V_1 is the modulation amplitude (it is assumed that $v_1 \ll \hbar\omega$), and $T(E) = |D(E)|^2$ are the transmission coefficient and the transmission amplitude of the static barrier, respectively.

Next BL define an asymmetry function

$$f(\omega) = (T_+ - T_-)/(T_+ + T_-) \tag{2}$$

which for the opaque barrier acquires the simple form

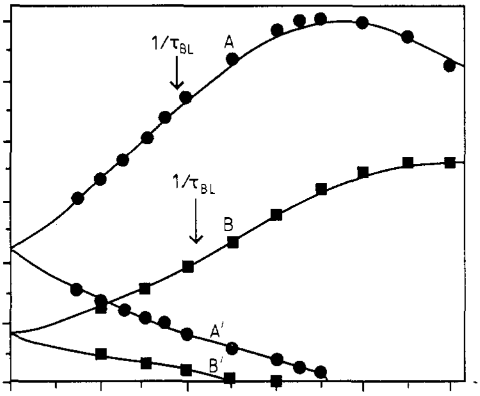

Figure 2. Sideband intensities, $T_{\pm}$, as a function of modulation frequency obtained from a series of simulations of the kind shown in figure 1. Curves A, B and points, T_+; curves A', B' and points, T_-. ●, $E = 0.72\ V_0$; ■, $E = 0.50\ V_0$. It can be shown for Gaussian wave packets narrow in momentum space, that $T_{\pm} = (k_{\pm}/k)|D_{\pm}|^2$, and can thus be compared directly with the analytical results of [2], which are shown as full curves. A quantitative agreement is found with the analytical and simulated results. Note that T_- vanishes for $\hbar\omega > E$, where $E = \hbar^2k^2/2m$ and $\hbar k$ is the mean momentum of the incoming pulse. The barrier parameters are as in figure 1.

$$f_{\text{opaque}}(\omega) = \tanh(\omega md/\hbar\kappa). \tag{3}$$

Thus, in this case the asymmetry function is characterised by a single quantity with the dimension of time, $\tau_{BL} = md/\hbar\kappa$, that separates characteristic low- and high-frequency behaviours. Therefore BL identify τ_{BL} as the traversal time for tunnelling. It is interesting that for an *opaque* barrier the same traversal time appears from an analysis of field emission [11]. There a time-dependent field due to charge oscillations (surface plasmons) plays a similar role as the time-dependent barrier height (phonons) do in the problem discussed here.

Let us now consider general barriers. Büttiker and Landauer [1, 2] discuss the crossover behaviour of the asymmetry function *explicitly* only in the opaque limit, but their arguments suggest the approach might have a more general validity. However, if one constructs the asymmetry function according to equation (2), and uses the results of BL for square barriers, it is seen that the resulting (complicated) expression cannot be characterised by a single quantity of dimension time. Even worse, for general barriers the asymmetry function is known only numerically, and some kind of operational procedure is called for. One may again examine the crossover from low to high frequencies as a suitable criterion. It appears obvious that (i) for low frequencies $f(\omega)$ is linear in ω, and that (ii) for high frequencies $f(\omega)$ saturates to unity. The characteristic (or crossover, in the terminology of BL) frequency could therefore be *defined* by the relation

$$\omega_c f'(0) = \lim_{\omega\to\infty} f(\omega). \tag{4}$$

We observe that in the opaque limit the above prescription gives the BL traversal time as the inverse of the characteristic frequency. However, this method cannot always be applied. For example, thin barriers ($d \simeq 25$ Å) the asymmetry function has a *negative* slope at the origin, and (4) has no solutions (see also [7], where similar conclusions have been obtained). It is possible, of course, to construct other *ad hoc* procedures which do yield a critical frequency; the two points we want to make here are that (i) a simple generalisation of the crossover analysis in the opaque limit is not viable, and (ii) that the connection of the tunnelling time and the inverse of a characteristic frequency does not appear immediate for a general barrier.

Let us now consider the adiabatic limit. Physically, it does not appear surprising that a finite frequency object (such as $T(E \pm \hbar\omega)$) does not directly yield intrinsic information of a static quantity (tunnelling time through a static barrier), and thus this limit may provide a more direct connection. Actually the generalised traversal time introduced by BL in [2], $\tau_{\mathrm{BL}} = \hbar|\mathrm{d} \ln D/\mathrm{d} V|^{1/2}$, emerges from an analysis of an adiabatic limit. After first identifying a traversal time τ_{BL} for an opaque barrier from a crossover behaviour at *finite* frequency of the asymmetry function of (2), BL notice that $T_\pm \propto \tau_{\mathrm{BL}}^2$ in the limit $\omega \to 0$. Their generalised traversal time appears when the limiting value of $T_\pm$ for an arbitrary barrier is forced to have the same quadratic form.

The adiabatic limit of the modulated barrier bears a close analogue to the Larmor clock [12] where one extracts a tunnelling time in the limit of a vanishing magnetic field. In this context it is interesting to observe that by adding the static part of the transmitted wavefunction, $D \exp(\mathrm{i}kx - \mathrm{i}Et/\hbar)$, and the one-phonon sideband terms, $D_\pm \exp(\mathrm{i}k_\pm x - \mathrm{i}E_\pm t/\hbar)$, the total transmitted wavefunction, in the limit of low frequency and amplitude of the modulation, can be written as a single term

$$\psi(x,t) = D(E,\bar{V})\exp\{\mathrm{i}[k(\tau_D^{\bar{V}})x - E(\tau_D^{\bar{V}})t/\hbar] + \eta\}. \tag{5}$$

This result, which is valid for a general form of the potential barrier if $t \ll 1/\omega$ and $x \ll v(k)/\omega$, is obtained by relating the sideband amplitudes, $D_\pm$, to the *static* transmission (D) and reflection (A) amplitudes. A generalisation of the discussion in [2] gives

$$\begin{aligned} D_\pm = -\frac{\mathrm{i}}{2}\frac{V_1}{2\hbar\omega} D(E \pm \hbar\omega, \bar{V}) \bigg[&(1 + k/k_\pm)\left(1 - \frac{D(E,\bar{V})}{D(E,\bar{V} \mp \hbar\omega)}\right) \\ &+ (1 - k/k_\pm) A(E,\bar{V})\left(1 - \frac{D(E,\bar{V})}{D(E,\bar{V} \mp \hbar\omega)}\frac{A(E,\bar{V} \mp \hbar\omega)}{A(E,\bar{V})}\right)\bigg] \end{aligned} \tag{6}$$

where $\bar{V}$ is the average height of the barrier, $\bar{V}_\mp = \bar{V} \mp \hbar\omega$, $E_\pm = E \pm \hbar\omega$, and $k_\pm = \sqrt{2mE_\pm/\hbar^2}$. The sideband intensities are given as $T_\pm = |D_\pm|^2$. In the wavefunction matching procedure that leads to (6) we have used the fact that the eigenfunctions $\varphi_{1,2}(E, \bar{V})$ in the barrier region are approximately the same if the parameters $(E_\pm, \bar{V})$ are changed to $(E, \bar{V}_\mp)$. Within the WKB approximation, where $V(x)$ and E always appear in the combination $V(x) - E$, this is an exact relation. Upon expanding (6) to lowest order in ω and summing the static and sideband terms as described above, one finds (5), where

$$E(\tau_D^{\bar{V}}) = E + V_1 \omega \tau_D^{\bar{V}} \tag{7}$$

and

$$k(\tau_D^{\bar{V}}) = k + (V_1/2E)(\omega\tau_D^{\bar{V}})k. \tag{8}$$

The complex quantity

$$\tau_D^{\bar{V}} = \mathrm{i}\hbar \,\mathrm{d} \ln D(E, \bar{V})/\mathrm{d}\bar{V} \tag{9}$$

has the dimension of time and is closely related to the complex times introduced by Sokolovski and Baskin [3] and Leavens and Aers [13]. Note that for the presently considered symmetric barrier the real [14] and imaginary parts of equation (9) are the well known dwell time, $\tau_{\rm dwell}$, and the so-called Büttiker time [12], τ_z, as here $\tau_d^V = \tau_{\rm dwell} - i\tau_z$. The generalisation of $\tau_{\rm BL}$ to arbitrary potential barriers [2, 6, 12] is related to (6) as $\tau_{\rm BL} = |\tau_D^V|$. The factor η in (5) is quite complicated and will not be given explicitly here.

In deriving equations (5)–(9) we took the modulating potential to be $V_1 \sin(\omega t)$, i.e. $V_1 \omega t$ for $t \ll 1/\omega$. From (7) it is therefore tempting to interpret the modified energy and momentum of the transmitted wavefunction to be the result of an adiabatic interaction between the tunnelling electron and the rising barrier during a traversal time τ_D^V. Such an interpretation is not meaningful, however, as τ_D^V is complex and any measurable traversal time must certainly be real. Some insight into the role of τ_D^V can be gained by calculating the transmitted electron density and current density. If x_0 and x are points beyond the barrier and $t_0, t \ll 1/\omega$, one finds to lowest order in ω

$$\rho(x, t) = |\psi(x, t)|^2 = \rho(x_0, t_0) \exp\{-2V_1(\omega\tau_z)[(t - t_0) - (x - x_0)/v(k)]/\hbar\} \tag{10}$$

and

$$J(x, t) = v(k)\rho(x, t) + (V_1/2E)(\omega\tau_{\rm dwell})v(k)\rho(x_0, t_0). \tag{11}$$

One notes that the decrease in the transmitted density with time is related to the Büttiker time, τ_z, i.e. to the imaginary part of τ_D^V. The result for the transmitted current density is a sum of two terms. The first simply reflects the change of the transmitted density with time while the second comes about because the change in density inside the barrier is associated with a change in current (to conserve charge). The latter term can also, from (8), be interpreted as arising from an adiabatic change of the momentum of the tunnelling electron while it interacts with the barrier during the well time, $\tau_{\rm dwell}$, given by the real part of τ_D^V.

The result for the transmitted current is in a sense reminiscent of the results of Büttiker's analysis [12] of the Larmor clock. There a beam of electrons, spin-polarised in the x direction, is travelling in the y direction impinging on a barrier. A magnetic field in the z direction inside the barrier gives the spin of the transmitted electrons a y-component proportional to $\omega_{\rm L}\tau_{\rm dwell}$, where $\omega_{\rm L}$ is the Larmor frequency. In addition, Büttiker showed that the transmitted electrons also acquire a spin component in the z direction. This is because the incoming electrons, which have no spin component in the z direction, can be thought of as a superposition of a spin-up and a spin-down state. Because of the Zeeman interaction these states have different energies and therefore the energy dependence of the barrier transmission probability results in a non-zero z-component of the spin proportional to $\omega_{\rm L}\tau_z$.

Hence both for the Larmor clock and the time-modulated barrier systems part of the effect on the transmitted current of electrons is due to a dependence of transmission probability on the barrier height and is characterised by the Büttiker time, τ_z, part is due to an interaction process within the barrier during a time $\tau_{\rm dwell}$.

For the case of the Larmor clock Büttiker [12] has argued that the magnitude of the spin in the yz plane can be used to define a traversal time, and thus identifies $\tau = \sqrt{\tau_z^2 + \tau_{\rm dwell}^2}$. Though plausible, this reasoning does not appear forceful and we speculate, in the light of (10) and (11), that experiments probing different aspects of the transmitted wavefunction (5) may yield different, but complementary information about the tunnelling process. A related discussion of the non-uniqueness of the tunnelling time appears in [8].

After this manuscript was completed we received a preprint by Støvneng and Hauge [7], which asserts that no direct general relation exists between the characteristic frequency of a time modulated barrier, and the duration of the tunnelling process. Their conclusion appears consistent with our work.

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