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Tunnelling in oscillating double-barrier heterostructures

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Abstract. One-particle wave-packet tunnelling in sinusoidally oscillating double-barrier heterostructures (DBH) is discussed here on the basis of simulation results obtained using the split operator scheme of Feit *et al* [1]. The characteristics of the side peaks in the momentum space representation of the wave packet caused by the oscillations of the potential and the effects of these on resonance tunnelling are analysed. Furthermore, the numerical results are compared with an analytical expression obtained for a spatially homogeneous Hamiltonian, giving the probabilities of inelastic interactions between the oscillating potential and the wave packet.

1. Introduction

Quantum mechanical tunnelling of electrons through ultrasmall structures has become the subject of active research during the last decade. This is largely due to the advance in the manufacturing techniques of semiconductor devices which has enabled the construction of structures whose dimensions are comparable to the de Broglie wavelength of electrons.

One of the structures that has been of particular interest is the double-barrier heterostructure (DBH) that consists of a quantum well surrounded by two barriers. This system can often be regarded as one-dimensional since it is usually made by stacking ultrathin layers of materials having different Fermi levels, e.g. GaAs and AlAs, and studying the behaviour of electrons moving perpendicular to the planes of the layers (see e.g. [2]).

DBHs and their extensions to a greater number of wells and barriers, i.e. a greater number of ultrathin layers, are of particular interest because of the existence of resonance tunnelling in which transmission currents are dramatically increased. Resonance tunnelling in DBHs occurs when the energy of the incident electron equals that of a quasi eigenstate of the quantum well between the barriers.

Here we consider the effect of sinusoidal oscillations of the DBH on the quantum mechanical tunnelling of particles. Tunnelling through various oscillating potentials has been discussed previously by, for example, Jiang [3], Büttiker and Landauer [4] and Stone *et al* [5] from a theoretical point of view, and by Jauho and Jonson [6] and Jauho [7] using a numerical approach. In these previous works the oscillations were restricted to a single sinusoidal oscillation frequency only.

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We will, in particular, consider the effect of multiple temporal frequencies of a double-barrier heterostructure on the transmission of a wave packet through the structure numerically using the algorithm of Feit *et al* [1] for the simulation of the wave packet. The simulation results will be compared with a simple analytical result describing the effect of sinusoidally oscillating potentials on tunnelling.

The physical motivation for our work comes from the fact that the realisations of DBHs are based on multicomponent layered materials with rather complicated phonon characteristics. The wave-packet approach, on the other hand, places maximum emphasis on the coherence effects in the transport properties of such devices.

2. Analytic discussion of a sinusoidally oscillating potential

Let us consider multiple sinusoidal oscillations of the DBH, that is

$$V(x,t) = V_0 + \sum_n V_n \cos(\omega_n t) \qquad \text{when } x \in [a,b] \tag{1}$$

where $[a, b]$ is the domain of the oscillating part of the structure, which is here taken as one of the spatially constant parts of the DBH. We consider only small perturbations, in which V_n is small compared to the height of the barriers. The amplitudes V_n roughly correspond to the phonon spectrum of the substance and thus equation (1) can be understood as a spatially constant potential oscillating with a discrete phonon spectrum.

It is straightforward to solve the time-dependent one-particle Schrödinger equation:

$$i\hbar\,\partial\psi(r,t)/\partial t = H(x,t)\psi(x,t) \qquad H(x,t) = (-\hbar^2/2m)\nabla^2 + V(x,t) \tag{2}$$

analytically, *if* we consider a spatially homogeneous Hamiltonian. That is, we first solve the Schrödinger equation only in the oscillating area $[a, b]$. In this case it is possible to separate the spatial and temporal parts

$$\psi(x,t;E) = u(x;E)T(t;E) \tag{3}$$

obeying

$$H_0 u(x;E) = Eu(x;E) \qquad H_0 = -(\hbar^2/2m)\nabla^2 + V_0 \tag{4}$$

and

$$i\hbar\dot{T}(t;E) - T(t;E)\sum_n V_n \cos(\omega_n t) = ET(t;E) \tag{5}$$

respectively. Equation (4) is just the time-independent Schrödinger equation of the unperturbed problem with energy equalling the separation parameter E and whose solution is of simple plane-wave form:

$$u(x;E) = \begin{cases} C_1 \exp(ikx) + C_2 \exp(-ikx) & k = \sqrt{(2m/\hbar^2)(E - V_0)} \qquad E > V_0 \\ C_3 \exp(\kappa x) + C_4 \exp(-\kappa x) & k = \sqrt{(2m/\hbar^2)(V_0 - E)} \qquad E < V_0. \end{cases} \tag{6}$$

The solution to the temporal equation is

$$T(t;E) = C_5\, e^{-i(E/\hbar)t} \prod_n \exp\left[-\frac{iV_n}{\hbar\omega_n}\sin(\omega_n t)\right] \tag{7}$$

where $\exp(-iEt/\hbar)$ is just the time behaviour of the unperturbed problem. Following

the approach of Büttiker and Landauer [4, 8] we expand the product term using the Jacobi–Anger expansion (cf [9] equation 8.511.4):

$$T(t; E) = C_5 \, e^{-i(E/\hbar)t} \prod_n \left[\sum_{m=-\infty}^{\infty} J_m \left(\frac{V_n}{\hbar\omega_n} \right) e^{im\omega_n t} \right] \tag{8}$$

where J_m is the mth cylindrical Bessel function. This form is quite informative, since it suggests the occurrence of side peaks around the non-perturbed energy E at energies that are linear combinations of the oscillation frequencies $\hbar\omega_m$. These 'side energies' can be interpreted as the emission/absorption of modulation quanta. The corresponding probabilities are given by the absolute square of a product of the Bessel functions [10]. From equation (8) it is seen that the probabilities of multiple interactions are small, if the perturbation amplitude is small ($V_n \ll \hbar\omega_n$), because of the asymptotic behaviour of the cylindrical Bessel functions for small arguments.

The separation parameter E above would equal the energy of a plane wave in the area of interest *if* the potential was static. Thus equations (6) and (8) would in the static case describe the behaviour of a *single* frequency corresponding to the energy, E, in an incoming wave packet with many frequencies. In the present case of a time-dependent potential, the separation parameter E does not, however, equal the energy due to the inelastic processes that introduce the side peaks around E. Since the side peaks occur around each of the energies in the spectrum of the incoming wave packet the side peaks can be seen as discrete peaks only if the energy width of the wave packet is small compared with the modulation energies.

At the boundaries of the area of interest (here a DBH) the wave-packet behaviour is complex and thus the wave packet coming into the oscillating area is unknown. Therefore the discussion above, which describes the behaviour of single frequencies only, is not sufficient to solve the problem of wave packets incident on an oscillating DBH. For wave packets sharp in momentum space, equation (8) gives, however, some qualitative information.

3. Numerical simulation results: emission and absorption of modulation quanta

We have used the split-operator algorithm of Feit *et al* [1] to integrate the time-dependent Schrödinger equation in order to numerically simulate the behaviour of wave packets. In the split-operator method the wave function is propagated using the following equation, where the kinetic and potential operators have been separated:

$$\psi(x, \Delta t) = \exp[-i(K/2)\Delta t] \exp(-iV(x, t)\Delta t) \exp[-i(K/2)\Delta t]\psi(x, 0) + O[(\Delta t)^3]. \tag{9}$$

Here $K(= -(\hbar^2/2m)\nabla^2)$ is the kinetic energy operator and $V(x, t)$ is the potential. The truncation term is due to the non-commutation of these. The basic idea of the method is to calculate the effect of the kinetic energy operator in momentum space and the effect of the potential operator in real space. The advantage of this is that the operators are diagonal in the respective spaces and their effect is thus reduced to plain multiplication. Moreover the split-operator equation (9) is accurate to the second order of time step Δt. The transformation between real and momentum space is performed using fast Fourier transformations and is therefore efficient and accurate.

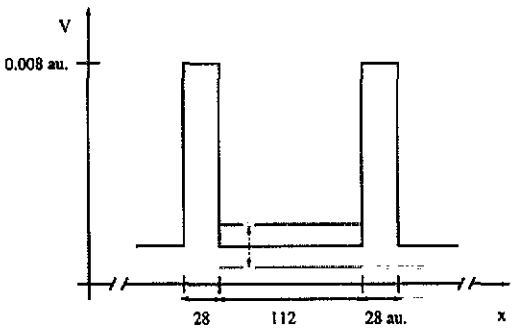

Figure 1. The symmetric static DBH potential with an oscillating quantum well.

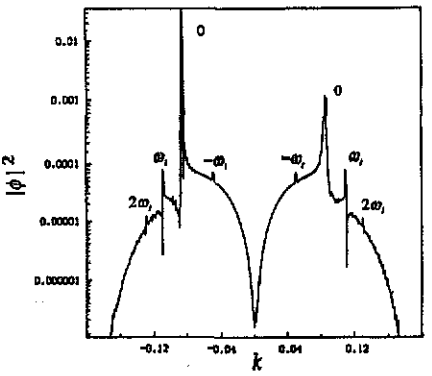

Figure 2. The probability density in momentum space for a wave packet incident on the DBH of figure 1 in which the quantum well is oscillating with a single frequency $\hbar\omega_1 = 0.0653$ eV and amplitude $V_1 = 0.0109$ eV. The mean energy of the wave packet initially equalled the second resonance energy (0.0100 eV) of the static DBH of figure 1. The side peaks around the main incident and reflected peaks corresponding to absorption/emission of modulation quanta have been indicated. The frame has been taken at a time step when the wave packet has split into transmitted, reflected and trapped parts.

We have used the split-operator algorithm to study the behaviour of an initially Gaussian wave packet incident on a symmetrical DBH in which the quantum well is oscillating and the barriers are kept constant. The dimensions of the potential structure used here are close to those of Jauho [7] and the oscillation frequencies and amplitudes are of the same order of magnitude. The height of the symmetric barriers is 0.218 eV and their width is 14.8 Å. The width of the quantum well is 59.3 Å and it is oscillating around the zero level of the potential (see figure 1).

In order for the incoming particle to 'see' the oscillations, the traversal time of the wave packet must not be too small compared with the oscillation period [4]. That is, the usual Born–Oppenheimer (BO) assumption must *not* be valid if the oscillations are to be relevant.

In the case of resonance transmission, when the transmission coefficients of the individual barriers are small, a part of the wave packet becomes trapped in the quasi-eigenstate of the quantum well. The lifetime of this localized state is proportional to the inverse of the transmission coefficients of the barriers and can thus be very long [11] and therefore the traversal time also becomes long and the BO assumption often fails. In the simulation experiments to be described here the BO assumption fails both in and off resonance.

In order to study the effects of different oscillation frequencies of the potential (equation (1)) we have studied the cases of: (i) one oscillation frequency $\hbar\omega_1 = 0.0653$ eV; (ii) two oscillation frequencies, the frequency $\hbar\omega_1$ and its double, $\hbar\omega_2 = 2\hbar\omega_1 = 0.131$ eV; and (iii) two incommensurate oscillation frequencies $\hbar\omega_1$ and $\hbar\omega_2 = (\sqrt{5} - 1)\hbar\omega_1 = 0.0807$ eV. In all these cases the oscillation amplitude was equal for all

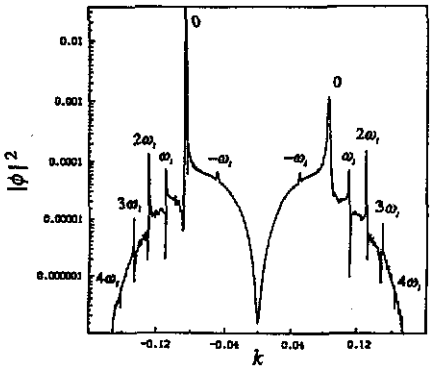

Figure 3. As figure 2, but for a quantum well oscillating with two frequencies $\hbar\omega_1 = 0.0653$ eV and $\hbar\omega_2 = 2\hbar\omega_1 = 0.131$ eV with equal amplitudes $V_1 = V_2 = 0.0109$ eV. Comparison with figure 1 clearly shows that all the side peaks are enhanced in this case.

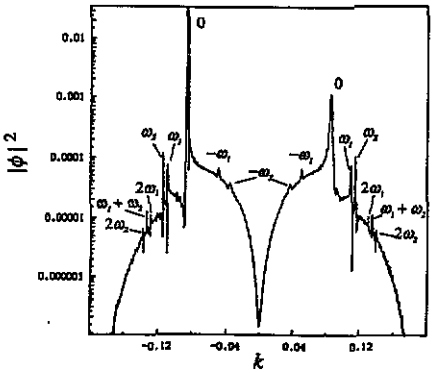

Figure 4. As figures 2 and 3, but when the quantum well is oscillating with the frequencies $\hbar\omega_1 = 0.0653$ eV and $\hbar\omega_2 = (\sqrt{5}-1)\hbar\omega_1 = 0.0807$ eV with equal amplitudes $V_1 = V_2 = 0.0109$ eV. The heights of the side peaks corresponding to integer multiples of ω_1 are almost the same as in figure 2.

the frequencies, $V_1 = V_2 = 0.0109$ eV and the other dimensions of the DBH were kept constant. The mean energy of the incident wave packet was chosen to equal the second bound state of the quantum well, i.e. the second resonance transmission energy of the system (=0.100 eV). The width of the initial wave packet in energy space was chosen so that it was somewhat smaller than the modulation energies, $\Delta E = 0.0381$ eV, which gives relatively sharp absorption/emission side-peaks.

The momentum space representations of the scattered wave packets in the three cases are shown respectively in figures 2, 3 and 4. In momentum space the side peaks corresponding to the absorption and emission of modulation quanta are clearly seen around the main peaks corresponding to the transmitted and reflected wave packets. When results of the cases of a single-frequency oscillation (i) and the case of an oscillation frequency and its double (ii) are compared, it is clearly seen that in the two-oscillation case (figure 3) the side peaks are bigger than in the single-oscillation case (figure 2). It is somewhat in contradiction with intuition that not only the side peaks corresponding to an even multiple of the single-frequency oscillation frequency ω_1 are enlarged but also those corresponding to an uneven multiple. On the other hand, when the case of the incommensurate oscillation frequencies (figure 4) is compared with the single-frequency case (figure 2) the peaks corresponding to a multiple of the single frequency ω_1 remain almost intact.

The areas under the side peaks can be interpreted as the probabilities of interaction and can thus be compared to the coefficients of the analytical expression of equation (8), where E corresponds to the initial mean energy of the wave packet and the analytical side peaks correspond to the side peaks in the momentum spectrum of the simulated wave packet. The analytical probabilities calculated from equation (8) are consistent with the trends of the numerical experiments described above.

The analytical expression is, however, only qualitative and, for example, the relative sizes of the different side peaks obtained from numerical simulation do not quantitatively agree with those obtained from equation (8). This is due to the fact that the analytical expression is valid only for a spatially homogeneous Hamiltonian and describes the

behaviour of just one of the frequencies in the incoming wave packet as discussed in the previous section.

4. Oscillating DBH and resonance transmission

When the transmission coefficients of the two individual barriers are small, resonance transmission occurs in static DBHs whenever the energy of the incoming particle is within a certain energy interval of a quasi-eigenstate energy of the quantum well [5, 12]. In resonance transmission the overall transmission coefficient is of the order of the ratio of the smaller to the larger of the individual transmission coefficients of the two barriers and not their product as in the case of off resonance. Thus in resonance, especially if the transmission coefficients of the barriers are equal, there is a dramatic increase in overall transmission of the DBH.

In the case of incoming wave packets, with a finite energy width, only the part of the wave packets that is within the resonance width of a bound state energy will be resonantly transmitted. (This is a somewhat vague notion, since the transmission decreases continuously as the energy differs from a resonance energy and the 'resonance width' is a rather arbitrary quantity [11].)

When the DBH is oscillating the situation is slightly changed. Firstly, the bound-state energies of the quantum well are not static. If the oscillations of the bound-state energies are small compared with the resonance width of the resonance energy, the movement of the bound-state energies is not very important. This is the case when the oscillation amplitudes are sufficiently small.

Secondly, when the mean energy of the incoming particle equals a resonance energy of the static system the effect of the (small) oscillations is the introduction of the side peaks to the energy spectrum of the wave packet, which generally are off-resonance and thus the overall resonance transmission is reduced [11]. If, however, one of the modulated energies $E_0 + m\hbar\omega_i$ falls within another resonance, the transmission of the part of the wave packet corresponding to the modulated energy will be enhanced. On the other hand, the other side peaks are usually off-resonance and will thus reduce the overall transmission and the effect on the overall transmission will depend on the relative importance of the in-resonance and off-resonance side peaks.

If the initial mean energy of the wave packet is off-resonance and a modulated energy is in-resonance the overall transmission will clearly increase. This was demonstrated by Jauho [7] in a numerical simulation.

These qualitative expectations were studied by simulating the behaviour of wave packets in the various oscillating DBHs and by then calculating the corresponding total transmission coefficients by numeric integration. The results are shown in table 1 and are consistent with the expectations, although the absolute differences in the transmission coeficients obtained are rather small.

5. Discussion

The split-operator algorithm of Feit *et al* [1] is a very effective method for integrating the time-dependent one-particle Schrödinger equation for an arbitrary time-dependent external potential. Here the numerical simulations have been carried out for simple one-dimensional double-barrier heterostructures, but the numerical method enables the

Table 1. The global transmission constant in various cases. ω_1 is the (single) modulation frequency and E is the average initial energy of the wave packet; $E_2 = 0.100$ eV and $E_3 = 0.202$ eV are the second and third bound-state energies of the DBH, respectively. The amplitude of oscillation $V_1 = 0.0109$ eV is kept constant. (a) The stationary resonance case. (b) The modulated energy does not equal any resonance energy. The transmission is slightly reduced compared with the stationary case. (c) One modulated energy equals resonance energy. The transmission is slightly bigger than in the previous case but still less than in the stationary case. (d) Non-resonance stationary case. Small transmission of the order of the product of the plane-wave transmissions for the individual barriers. (e) Initial energy off resonance, but modulated energy equals the third resonance energy of the well. Transmission is slightly greater than in the stationary case (d). (f) Initial and modulated energies off resonance. Transmission is comparable to the stationary case (d).

Average initial energy E (eV)	Modulation quantum $\hbar\omega_1$ (eV)	Transmission coefficient T
(a) $E_2 = 0.100$	stationary	0.1374
(b) $E_2 = 0.100$	0.0653	0.1326
(c) $E_2 = 0.100$	$E_3 - E_2 = 0.102$	0.1354
(d) 0.137	stationary	$7.202 \cdot 10^{-4}$
(e) 0.137	$E_3 - 0.137 = 0.0653$	$1.052 \cdot 10^{-3}$
(f) 0.137	$E_3 - E_2 = 0.102$	$7.527 \cdot 10^{-4}$

simulation of far more complex systems in a higher number of dimensions. We believe that numerical simulation of the behaviour of wave packets is a very effective method for studying the time-dependent quantum mechanical behaviour of particles in ultrasmall structures of interest.

The derived analytical expression for a spatially homogeneous Hamiltonian (8) describing the effect of sinusoidal oscillations proved to be of some qualitative value to the understanding of the effect of small oscillations of multiple frequencies on the behaviour of a wave packet in the DBH potentials.

The results of the numerical simulations are consistent with the expectations of the effect of the oscillations on the overall transmission coefficients of the DBH when the incident and/or modulated energies equal a resonance energy of the system as discussed in [5] and [6].

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$$\langle\psi|H|\psi\rangle = \left\langle\psi\left|\mathrm{i}\hbar\frac{\partial}{\partial t}\right|\psi\right\rangle = \left[E + \sum_{m=-\infty}^{\infty} J_{-m}\left(\frac{V_1}{\hbar\omega_1}\right) m\hbar\omega_1\right]\langle\psi|\psi\rangle.$$

Here the side peaks are at energies $m\hbar\omega_1$ and correspond to the absorption ($m > 0$) and emission ($m < 0$) of $|m|$ modulation quanta. The corresponding interaction probabilities are given by the absolute squares of the Bessel functions.
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