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Inelastic effects on resonant tunnelling in a double-δ-function potential

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Abstract. Inelastic effects on resonant tunnelling are considered for a model consisting of a double-δ-function potential with the region in between oscillating with amplitude V_1 and frequency ω. In the limit of small V_1/ω, we obtain analytic expressions for the transmission coefficient for the elastic and the two nearest inelastic channels. Numerically, we obtain a set of resonant sidebands around the static resonances with magnitudes proportional to $(V_1/\omega)^2$ for both symmetric and asymmetric δ functions. We discuss the conditions under which the sidebands of contiguous static resonances can superpose, producing an increase in the probabilities of both elastic and inelastic events. We also describe the feedback mechanism between the scattering of elastic and inelastic events, which modifies the probabilities of elastic events.

1. Introduction

Over the last few years there has been increasing interest in the understanding of transport properties of resonant tunnelling devices for their great technological importance. Even though dissipative effects, i.e. the effects of electron–phonon scattering on the tunnelling current, have been studied by several different methods [1–5], only a few authors have considered resonant systems and these have concentrated on isolated resonances [6–8]. In a recent paper, Cai *et al* [9] propose a general approach to the study of one-dimensional optical-phonon-associated electron tunnelling based on the polaron model, in the independent-boson approximation, which is applicable to potentials of arbitrary shape, and present results of calculations for an actual double barrier.

In this paper we consider a periodic time-dependent double-δ-function potential to model the effects of dissipation. This is the classical version of the operator of interaction introduced by Cai *et al*. As has been pointed out by Lopez-Castillo *et al* [5], this amounts to replacing phonon creation and annihilation operators by their expectation values in a phonon coherent state. In our model, an incident particle with energy E that interacts with the inelastic scattering barrier will suffer multiple inelastic collisions with the non-stationary field and will be transmitted or reflected with an energy distribution $E' = E \pm n\omega$, with n an integer.

Our objective is to calculate analytically the probabilities of transmission for the quantum problem of a system of length L, with δ functions at the boundaries ($x = 0$, $x = L$) and an oscillating region with constant amplitude V_1 and frequency ω in between ($0 \leqslant x \leqslant L$). In this classical potential model, the parameter V_1 represents a combination of both electron–phonon coupling strength and the temperature [10].

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The election of this model is based on the fact that it is a simple quantum system that can be solved analytically, giving rise to several resonant solutions. The study of inelastic effects in this system may be useful in describing the scattering properties of more realistic systems such as the quantum-well resonant-tunnelling diode whose conduction-band profile includes a double-barrier structure.

Our results show analytically, for the case of small V_1/ω, the existence of a feedback effect [4], by which the elastic processes are affected by the inelastic ones, and this is clearly appreciated in our numerical results. We also find a set of resonant inelastic sidebands around each elastic resonance with magnitude proportional to $(V_1/\omega)^2$. Our calculation predicts conditions under which the inelastic resonances can superpose to increase the probabilities of both elastic and inelastic events. In the asymmetric case we find two contributions to the elastic resonance probability maximum, due to the asymmetry of the δ functions and to the feedback mechanism.

The outline of the paper is as follows: in section 2 the model and the formal solution in the two-channel approximation are described. In section 3 the analytical results are presented and in the last section these are discussed and plots of total transmission coefficient as a function of energy are presented, with the inelastic contributions explicitly shown.

2. Model and solution

The potential function corresponding to our model can be written as

$$V(x,t) = \lambda_1\delta(x) + \lambda_2\delta(x-L) + 2V_1\cos(\omega t)\theta(x)\theta(L-x) \tag{1}$$

where λ_1 and λ_2 are the magnitudes of the δ functions, V_1 is the amplitude of the electron–phonon coupling, taken as a constant, ω is the frequency of oscillation and $\theta(x)$ is the Heaviside step function (figure 1).

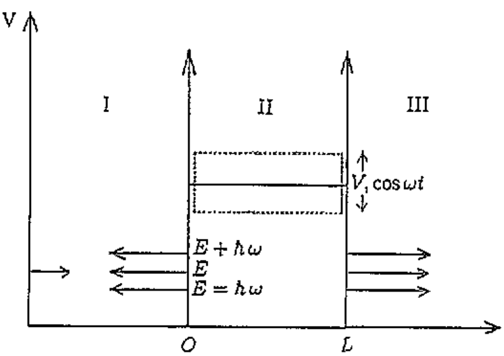

Figure 1. The double-δ-function potential of width L with the region in between oscillating with amplitude V_1 and frequency ω. Transmission and reflection occurs at energies $E \pm n\omega$.

We want to study the effects on the transmission process of an incident particle with energy E on the left (region I, $x \leqslant 0$), that interacts with the oscillating barrier and is scattered in region II ($0 \leqslant x \leqslant L$), until it finally leaves the system travelling to the right (region III, $x \geqslant L$). In region II, we need to solve the non-stationary Schrödinger equation

$$\mathrm{i}\partial\Psi^{\mathrm{II}}/\partial t = -\partial^2\Psi^{\mathrm{II}}/\partial x^2 + [\lambda_1\delta(x) + \lambda_2\delta(x-L) + 2V_1\cos\omega t]\Psi^{\mathrm{II}} \tag{2}$$

where we have used units of $\hbar = 2m = 1$. The general solution of equation (2), given that the time-dependent potential is separable, can be written as

$$\Psi^{\mathrm{II}}(x,t) = \exp\left(-2\mathrm{i}V_1 \frac{\sin\omega t}{\omega}\right) \int \mathrm{d}E' \,[B_{E'} \exp(\mathrm{i}k_{E'}x) + C_{E'} \exp(-\mathrm{i}k_{E'}x)] \exp(-\mathrm{i}E't) \tag{3}$$

where $\exp(\mathrm{i}k_{E'}x)$ and $\exp(-\mathrm{i}k_{E'}x)$ are linearly independent solutions of the stationary problem.

Assuming that an incident particle with energy E and unit amplitude enters region II, and considering V_1/ω small, then only components of $\Psi^{\mathrm{II}}(x,t)$ with energies E (elastic channel) and $E \pm \omega$ (inelastic channels) are important, and we calculate the probability current to order $(V_1/\omega)^2$. From equation (3), expanding the exponential $\exp[-2\mathrm{i}V_1(\sin\omega t)/\omega] = 1 - (V_1/\omega)\exp(\mathrm{i}\omega t) + (V_1/\omega)\exp(-\mathrm{i}\omega t)$, we can write

$$\Psi^{\mathrm{II}}(x,t) = \Psi^{\mathrm{II}}_{E+\omega}(x)\exp[-\mathrm{i}(E+\omega)t] \\ + \Psi^{\mathrm{II}}_{E}(x)\exp(-\mathrm{i}Et) + \Psi^{\mathrm{II}}_{E-\omega}(x)\exp[-\mathrm{i}(E-\omega)t] \tag{4}$$

where

$$\Psi^{\mathrm{II}}_{E+\omega}(x) = (V_1/\omega)[B_0\exp(\mathrm{i}k_0x) \\ + C_0\exp(-\mathrm{i}k_0x)] + [B_+\exp(\mathrm{i}k_+x) + C_+\exp(-\mathrm{i}k_+x)] \tag{5}$$

$$\Psi^{\mathrm{II}}_{E}(x) = [B_0\exp(\mathrm{i}k_0x) + C_0\exp(-\mathrm{i}k_0x)] \\ + (V_1/\omega)[B_-\exp(\mathrm{i}k_-x) + C_-\exp(-\mathrm{i}k_-x)] \\ - (V_1/\omega)[B_+\exp(\mathrm{i}k_+x) + C_+\exp(-\mathrm{i}k_+x)] \tag{6}$$

$$\Psi^{\mathrm{II}}_{E-\omega}(x) = -(V_1/\omega)[B_0\exp(\mathrm{i}k_0x) + C_0\exp(-\mathrm{i}k_0x)] \\ + [B_-\exp(\mathrm{i}k_-x) + C_-\exp(-\mathrm{i}k_-x)] \tag{7}$$

the subscripts 0 and $\pm$ corresponding to energies E and $E \pm \omega$, respectively. Thus, $k_0 = \sqrt{E}$ and $k_\pm = \sqrt{E \pm \omega}$. In this approximation the solution in region I is the sum of plane waves for each channel involved:

$$\Psi^{\mathrm{I}}(x,t) = \exp(\mathrm{i}k_0x - \mathrm{i}Et) + A_0\exp(-\mathrm{i}k_0x - \mathrm{i}Et) \\ + A_+\exp[-\mathrm{i}k_+x - \mathrm{i}(E+\omega)t] + A_-\exp[-\mathrm{i}k_-x - \mathrm{i}(E-\omega)t] \tag{8}$$

where A_0 and $A_\pm$ are the reflection probability amplitudes at the corresponding energies.

Similarly in region III, the solutions are outgoing plane waves for all channels:

$$\Psi^{\mathrm{III}}(x,t) = D_0\exp(\mathrm{i}k_0x - \mathrm{i}Et) + D_+\exp(\mathrm{i}k_+x - \mathrm{i}(E+\omega)t] \\ + D_-\exp[\mathrm{i}k_-x - \mathrm{i}(E-\omega)t] \tag{9}$$

with D_0 and $D_\pm$ the transmission probability amplitudes.

Using the boundary conditions for the wavefunction and its derivatives at $x = 0$ and $x = L$, which must be satisfied for all times, and solving the corresponding system of equations, it is possible to find the transmission and reflection amplitudes for channels 0 and ±. With these amplitudes we may calculate the transmitted and reflected currents, which are

$$J_0^{\mathrm{ref}} = k_0|A_0|^2 \qquad J_0^{\mathrm{trans}} = k_0|D_0|^2 \tag{10}$$

$$J_\pm^{\mathrm{ref}} = k_\pm|A_\pm|^2 \qquad J_\pm^{\mathrm{trans}} = k_\pm|D_\pm|^2. \tag{11}$$

The total transmission coefficient is the sum of the transmitted currents divided by the incident current, which in these units is simply k_0, for all the channels involved:

$$T = (1/k_0)(J_0^{\mathrm{trans}} + J_+^{\mathrm{trans}} + J_-^{\mathrm{trans}}). \tag{12}$$

3. Analytic solutions

The method used in this work to calculate all the amplitudes is the following. First, the solution for the elastic channel to order zero in V_1/ω is obtained by ignoring first-order terms in equation (6). We calculate the coefficients B_0 and C_0 and put them into the first term on the right-hand side of equations (5) and (7), and apply the corresponding boundary conditions to obtain the reflection and transmission amplitudes for the inelastic channels to first order. In this process the coefficients $B_\pm$ and $C_\pm$ are determined, which we now introduce into the terms of order V_1/ω of the elastic-channel solution (6) to find the amplitudes to first order. This correction determines how the elastic channel is affected due to the presence of inelastic channels, i.e. the feedback effect, and is a consequence of unitarity or current conservation [4].

Explicitly, by applying the boundary conditions to the elastic channel we find, for the reflection (A_0) and transmission (D_0) amplitudes to zero order,

$$A_0 = [(\lambda_2/2ik_0)(\lambda_1/2ik_0 + 1)\exp(2ik_0L) + (\lambda_1/2ik_0)(1 - \lambda_2/2ik_0)] \times [-(\lambda_1/2ik_0)(\lambda_2/2ik_0)\exp(2ik_0L) + (1 - \lambda_1/2ik_0)(1 - \lambda_2/2ik_0)]^{-1} \tag{13}$$

$$D_0 = 1/[-(\lambda_1/2ik_0)(\lambda_2/2ik_0)\exp(2ik_0L) + (1 - \lambda_1/2ik_0)(1 - \lambda_2/2ik_0)] \tag{14}$$

while the amplitudes B_0 and C_0 in region II are

$$B_0 = (1/2ik_0)D_0(2ik_0 - \lambda_2) \tag{15}$$

$$C_0 = (\lambda_2/2ik_0)D_0\exp(2ik_0L). \tag{16}$$

To determine the amplitudes for the inelastic channels let us introduce the function defined by

$$z_0(x) = (V_1/\omega)[B_0\exp(ik_0x) + C_0\exp(-ik_0x)] \tag{17}$$

so that applying the boundary conditions for these channels we find

$$A_\pm = [(-\lambda_2/2ik_\pm)\exp(2ik_\pm L)M_1/2ik_\pm + (1 - \lambda_2/2ik_\pm)M_2/2ik_\pm] \times [-(\lambda_1/2ik_\pm)(\lambda_2/2ik_\pm)\exp(2ik_\pm L) + (1 - \lambda_1/2ik_\pm)(1 - \lambda_2/2ik_\pm)]^{-1} \tag{18}$$

$$D_\pm = [-(1 - \lambda_1/2ik_\pm)M_1/2ik_\pm + (\lambda_1/2ik_\pm)M_2/2ik_\pm] \times [-(\lambda_1/2ik_\pm)(\lambda_2/2ik_\pm)\exp(2ik_\pm L) + (1 - \lambda_1/2ik_\pm)(1 - \lambda_2/2ik_\pm)]^{-1} \tag{19}$$

where the auxiliary expressions $M_{1,2}$ are defined by

$$M_1 = [\mathrm{i}k_\pm z_0(0) + z_0'(0)] - [\mathrm{i}k_\pm z_0(L) + z_0'(L)]\exp(-\mathrm{i}k_\pm L) \tag{20}$$

$$M_2 = [\mathrm{i}k_\pm z_0(0) - z_0'(0)] - [\mathrm{i}k_\pm z_0(L) - z_0'(L)]\exp(\mathrm{i}k_\pm L). \tag{21}$$

To determine $M_{1,2}$, one needs the function z_0 and its derivatives z_0' evaluated at the boundary points. These can be written in terms of $z_0(L)$, so that substituting B_0 and C_0 from (15) and (16) into (17) and evaluating at $x = 0$, $x = L$, one finds

$$z_0(L) = (V_1/\omega)D_0\exp(\mathrm{i}k_0 L) \tag{22}$$

$$z_0(0) = [z_0(L)/\mathrm{i}k_0][(\mathrm{i}k_0 - \lambda_2)\exp(-\mathrm{i}k_0 L) + \lambda_2\cos(k_0 L)] \tag{23}$$

$$z_0'(0) = z_0(L)[\mathrm{i}k_0\exp(-\mathrm{i}k_0 L) - \lambda_2\cos(k_0 L)] \tag{24}$$

$$z_0'(L) = z_0(L)[\mathrm{i}k_0 - \lambda_2]. \tag{25}$$

The next step is to calculate the expressions for the amplitudes corresponding to the elastic channel including feedback effects. This means taking into account terms of order V_1/ω in (6) and solving the corresponding boundary value problem. We obtain

$$A_0^{\mathrm{f}} = A_0 + [(-\lambda_2/2\mathrm{i}k_0)\exp(2\mathrm{i}k_0 L)L_1/2\mathrm{i}k_0 + (1-\lambda_2/2\mathrm{i}k_0)L_2/2\mathrm{i}k_0] \times [-(\lambda_1/2\mathrm{i}k_0)(\lambda_2/2\mathrm{i}k_0)\exp(2\mathrm{i}k_0 L) + (1-\lambda_1/2\mathrm{i}k_0)(1-\lambda_2/2\mathrm{i}k_0)]^{-1} \tag{26}$$

$$D_0^{\mathrm{f}} = D_0 + [-(1-\lambda_1/2\mathrm{i}k_0)L_1/2\mathrm{i}k_0 + (\lambda_1/2\mathrm{i}k_0)L_2/2\mathrm{i}k_0] \times [-(\lambda_1/2\mathrm{i}k_0)(\lambda_2/2\mathrm{i}k_0)\exp(2\mathrm{i}k_0 L) + (1-\lambda_1/2\mathrm{i}k_0)(1-\lambda_2/2\mathrm{i}k_0)]^{-1} \tag{27}$$

where the auxiliary functions $L_{1,2}$ are given by

$$L_1 = [\mathrm{i}k_0 h(0) + h'(0)] - [\mathrm{i}k_0 h(L) + h'(L)]\exp(-\mathrm{i}k_0 L) \tag{28}$$

$$L_2 = [\mathrm{i}k_0 h(0) - h'(0)] - [\mathrm{i}k_0 h(L) - h'(L)]\exp(\mathrm{i}k_0 L) \tag{29}$$

with $h(x) = z_-(x) - z_+(x)$, and the functions $z_\pm$ are defined by

$$z_\pm(x) = (V_1/\omega)[B_\pm\exp(\mathrm{i}k_\pm x) + C_\pm\exp(-\mathrm{i}k_\pm x)]. \tag{30}$$

The coefficients $B_\pm$, $C_\pm$ in region II are determined by

$$B_\pm = (1/2\mathrm{i}k_\pm)\{D_\pm[2\mathrm{i}k_\pm - \lambda_2] - [\mathrm{i}k_\pm z_0(L) + z'(L)]\exp(-\mathrm{i}k_\pm L)\} \tag{31}$$

$$C_\pm = (1/2\mathrm{i}k_\pm)\{\lambda_2 D_\pm\exp(2\mathrm{i}k_\pm x) - [\mathrm{i}k_\pm z_0(L) - z_0'(L)]\exp(\mathrm{i}k_\pm L)\} \tag{32}$$

which can be calculated since we already know the transmission amplitudes $D_\pm$ from (19), and $z_0(L)$, $z_0'(L)$ are given by (22) and (25).

Finally, we can obtain the total transmission coefficient from

$$T = |D_0^{\mathrm{f}}|^2 + (k_-/k_0)|D_-|^2 + (k_+/k_0)|D_+|^2. \tag{33}$$

4. Results and discussion

First, we know that the expression for the transmission coefficient for the double-δ-function potential in the static case is the square modulus of equation (14). It is known, furthermore, that in the symmetric case the transmission spectrum has resonant peaks with a maximum value of one. In the asymmetric case, there will still be resonances but with maximum value less than one.

Next, let us analyse the expression for the transmission amplitude for the inelastic channels, equation (19). When we compare with the static case, equation (14), we see that the denominators are equal, with the exception that they are calculated at the value $k_\pm$ corresponding to each channel. Thus, $D_\pm$ is proportional to $D_0(k_\pm)$. Furthermore, we see from equations (20) and (21) that upon substitution of z_0 and its derivatives the term $z_0(L)$ can be factorized. Therefore, the amplitudes $D_\pm$ will also be proportional to $z_0(L)$. Explicitly, we have that $D_\pm \simeq (V_1/\omega)D_0(k_0)D_0(k_\pm)$. This implies the following two observations: the inelastic channels will exhibit resonances at energies E_r and $E_r \pm \omega$, where E_r is the resonance energy for the static case, i.e. for each resonance of the static problem there will be two inelastic resonant sidebands. Also, the magnitudes of these resonant sidebands are proportional to $g = (V_1/\omega)^2$. Each channel contributes a value of g to the transmission resonance at E_r so that the total magnitude of these peaks will be $2g$. Since this could lead to a loss of unitarity in the symmetric case, it is necessary to include the following order correction terms, i.e. feedback effects (equations (26) and (27)).

When plotting the transmission coefficient as a function of energy for our model, we thus expect to see resonances at energies E_r belonging to the static case, with magnitudes decreased by feedback effects. There should also appear inelastic peaks at energies $E_r \pm \omega$ with magnitudes proportional to g.

We present plots of the total transmission coefficient, equation (33), as a function of energy for several configurations of the system, showing the inelastic contribution explicitly on a separate plot. We have fixed the values $\omega = 2.5$ and $V_1 = 0.8$ ($g = 0.1$) while varying the other parameters in the system. We study both the symmetric and asymmetric cases, for different values of L, thus varying the number of resonances in a given energy interval.

First, we show our results for the symmetric case ($\lambda_1 = \lambda_2 = 20$) for several values of L [11]. In figure 2(a) we show the case $L = 3$ where neighbouring resonances satisfy the condition

$$E_{r2} - E_{r1} > 2\omega. \tag{34}$$

In the neighbourhood of each static resonance we can observe well defined satellite peaks with magnitude, as we have pointed out, proportional to g. Similarly, the contribution of the inelastic channels to the elastic resonance magnitude is proportional to $2g$ (figure 2(b)).

When we increase L (figure 3), the number of resonances in the same energy interval increases so that condition (34) for the separation between resonances is no longer satisfied. Thus, satellite peaks belonging to neighbouring resonances may superpose, giving rise to inelastic peaks with larger magnitude. The condition for this to occur is, for resonances at E_{r1} and E_{r2},

$$E_{r2} - E_{r1} = 2\omega. \tag{35}$$

This condition is clearly observed in figure 3(b) for the inelastic peak at energy 16.3 whose magnitude is the sum of magnitudes of the satellite peaks corresponding to the two adjacent elastic resonances.

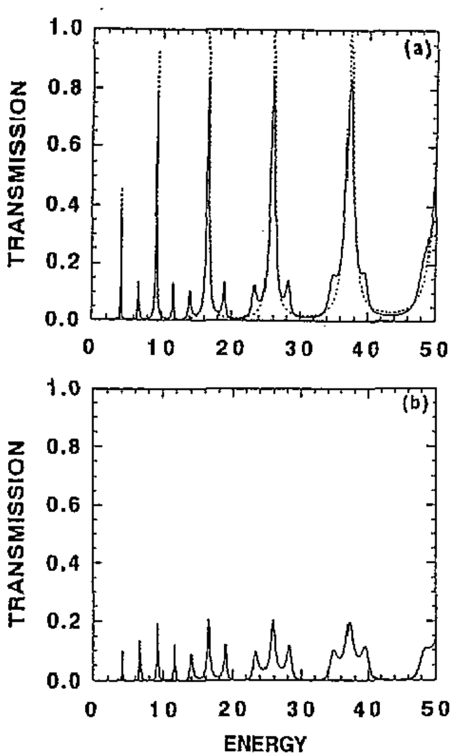

Figure 2. (*a*) Total transmission coefficient as a function of energy E for the symmetric case. The dotted curve corresponds to the static case; the full curve includes inelastic effects. The parameter values are $\lambda_1 = \lambda_2 = 20$, $L = 3$, $\omega = 2.5$, $V_1 = 0.8$. These values of ω and V_1 are kept fixed throughout. (*b*) Contribution from the inelastic channels.

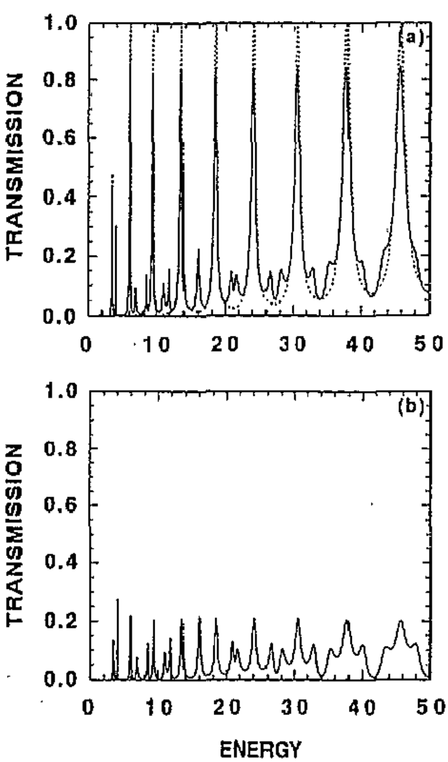

Figure 3. (*a*) Total transmission coefficient as a function of energy E for the symmetric case. The dotted curve corresponds to the static case; the full curve includes inelastic effects. The arrow indicates the superposition of neighbouring inelastic resonance peaks. The parameter values are $\lambda_1 = \lambda_2 = 20$, $L = 5$. (*b*) Contribution from inelastic channels.

Finally, in figure 4 we consider the case $L = 7$ where again we have two resonances satisfying condition (35) with the two neighbouring resonances on each side almost satisfying it. On this figure we also have a case where

$$E_{r2} - E_{r1} = \omega \tag{36}$$

i.e. the inelastic satellite peak corresponding to the resonance at E_{r1} contributes to the magnitude of the resonance at E_{r2} and vice versa. As far as we know, this superposition of satellite peaks of contiguous resonances has not been reported in the literature, since most of the work has been done for systems with isolated resonances.

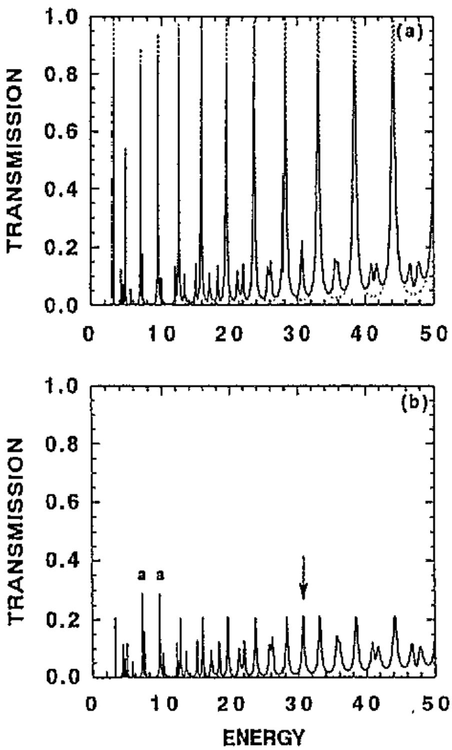

Figure 4. (*a*) Total transmission coefficient as a function of energy E for the symmetric case. The dotted curve corresponds to the static case; the full curve includes inelastic effects. The parameter values are $\lambda_1 = \lambda_2 = 20$, $L = 7$. (*b*) Contribution from inelastic channels. The arrow indicates superposition of inelastic resonance peaks, and the letter a indicates reinforcement of elastic resonances.

In these figures, the effects of feedback between elastic and inelastic channels is observed through the lowering of the magnitudes of the transmission coefficient as compared to the static case, by a factor of about 0.2. It is also interesting to note that, depending on the values of the parameters, one has competition between this effect and a reinforcement of the magnitude due to superposition of satellite peaks.

In figure 5 we show the asymmetric case. The important difference in this case is the general lowering of the transmission magnitudes due to both the asymmetry and the feedback from inelastic processes.

In all cases considered before, the intensities of the δ functions are sufficiently large that several resonances exist in the energy interval considered. Next we study the case where there are only a few resonant states (δ functions with smaller intensity). Figure 6 shows the results for the symmetric case. Again we obtain a reinforcement of resonances by inelastic contributions at the energies shown, satisfying condition (36). We also note

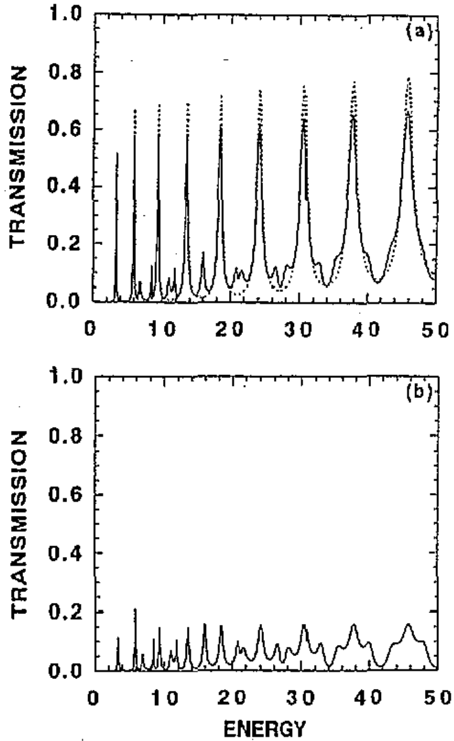

Figure 5. (*a*) Total transmission coefficient as a function of energy for the asymmetric case. The parameter values are $\lambda_1 = 20$, $\lambda_2 = 10$, $L = 5$. (*b*) Contribution from inelastic channels.

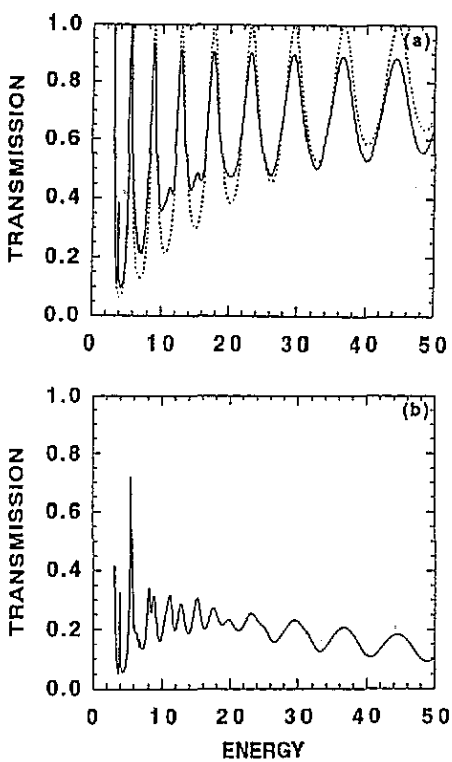

Figure 6. The symmetric case for δ functions of low intensity. Parameter values are $\lambda_1 = \lambda_2 = 5$, $L = 5$.

that for higher energies the inelastic effects are small (figure 6(*b*)). This can be understood since the contribution from inelastic channels depends on the magnitude of the transmission coefficient in the static case, which for these values of energy presents small oscillations with decreasing magnitude as the energy increases. The corresponding asymmetric case was also analysed but does not give new information.

In conclusion, we have presented an analytic solution for the inelastic effects on resonant tunnelling via a periodic time-dependent-potential model consisting of two δ functions with the region in between oscillating with frequency ω and amplitude V_1, in the limit of small V_1/ω. We observe that the effect of this potential is to give rise to satellite resonance peaks, about every static resonance, with magnitude proportional to g. We have analysed the conditions under which these satellite peaks of contiguous resonances may superpose, increasing the amplitude of both elastic and inelastic resonances and producing, on the elastic resonances, a competing effect with the feedback mechanism.

Acknowledgments

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[10] In a related study (Liu H C 1991 *Phys. Rev.* B **43** 12 538), the analysis of resonant tunnelling through a double-barrier structure under both a DC bias voltage and a small-amplitude AC modulation is undertaken to evaluate the device high-frequency response within the first-order approximation. This is different from our problem where there are no external fields and we are interested in modelling the effects of electron–phonon interactions in the region between the barriers.
[11] The unit of energy can be written as $E_I a_0^2/0.067l^2$ where $E_I = 13.6$ eV is the ionization energy of the hydrogen atom, $a_0 = 0.52$ Å is the Bohr radius, the numerical factor corresponds to the electron's effective mass and l is the length scale of the problem. In our case, choosing $l = 50$ Å gives an energy unit of 22 meV, making our results suitable for an AlAs/GaAs/AlAs double-barrier structure (see for example Tsuchiya M and Sakaki H 1986 *Appl. Phys. Lett.* **49** 88).