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Numerical simulations of resonant tunneling in the presence of inelastic processes

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We describe simulations of resonant tunneling through a time-modulated double-barrier potential. The harmonic modulation of frequency ω leads to emission and/or absorption of modulation quanta of energy $\hbar\omega$ in close analogy with emission and/or absorption of dispersionless bosons (optical phonons, photons, plasmons, etc.). The transmission coefficient shows satellite peaks in addition to the main resonance. Momentum space snapshots can be used to extract detailed information of the dynamics of the inelastic tunneling processes, such as opening and closing boson-mediated resonant channels, their relative importance, and related time scales.

Resonant tunneling in semiconductor heterostructures[1,2] is currently a very active area of research featuring both device applications and questions of basic physics. Traditionally most current versus voltage curves are analyzed with the Tsu-Esaki[3] tunneling formula (or its modifications[4])

$$\mathbf{J}=\frac{2e}{(2\pi)^3}\int d\mathbf{k}\,v(\mathbf{k})[f_{\rm FD}(E)-f_{\rm FD}(E+eV)]\,|T|^2, \quad (1)$$

where $f_{\rm FD}$ is the Fermi-Dirac distribution, $T(E,V)$ the transmission coefficient obtained from the solution of the static Schrödinger equation, E the total energy of the tunneling particle, and V the applied voltage. The use of (1) implies several assumptions, the following of which are of relevance to the present work: (i) use of equilibrium distribution functions (even though a biased resonant tunneling diode is manifestly in a nonequilibrium state), and (ii) scattering is not accounted for. A complete theoretical description would require a numerically tractable quantum kinetic theory for nonstationary and spatially inhomogeneous systems. No such theory exists as of today; for a status report of some candidate theories see Ref. 5. As a natural first step several research groups have recently addressed partial aspects of the problem. Phenomenological theories where the main effect of inelastic collisions is to broaden the resonant transmission coefficient have been reported.[6] Wigner function simulations, with simplified collision operators, have been performed to obtain the nonequilibrium distribution function, from which the current can be extracted.[7] Several analytic calculations of the transmission coefficient in the presence of optical-phonon scattering have recently been reported.[8] These calculations have been motivated by the observation of optical-phonon related features in the I-V curves.[9]

The purpose of this paper is to introduce a different approach for studying energy exchange, i.e., inelastic scattering, in resonant tunneling physics. The proposed method does not overrule any of the above-mentioned theoretical approaches but rather complements them by providing a means of obtaining additional insight on details of various tunneling processes. Our method consists of solving the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=\left[\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x,t)\right]\Psi(x,t), \quad (2)$$

where the potential $V(x,t)$ contains the heterojunction band-edge potential *and* a harmonic modulation of frequency ω. By starting from a given initial state, the transmission coefficient can be obtained by integrating (2) forwards in time until the asymptotic state has been reached. A time-modulated single-barrier has been considered in a different context by Büttiker and Landauer[10] (analytical work), and by Jauho and Jonson[11] (numerical work; the Schrödinger equation solver and numerical details are described in this reference). The phenomenology is as follows:[10] The incoming particles of energy E may either emit or absorb modulation quanta of energy $\hbar\omega$, and consequently the reflected and transmitted beams contain sidebands at $E\pm n\hbar\omega$. Thus there is a close analogy to interaction with a dispersionless boson field. The analogy is not complete: Effects related to statistics and/or temperature are not included. In a sense the present approach is an infinite temperature calculation: Absorption and emission of modulation quanta have the same probability. We do not exclude the possibility of extending the present approach to include temperature effects.

Despite this restriction the present approach has several advantages. No heavy numerical work is required as is the case for the Wigner-function simulations. The coupling to the external time modulation can be of arbitrary strength, and no truncation to low-order processes is necessary as is customarily done in the analytic calculations. Further, the shape of the heterostructure potential can be arbitrary, and the bias and energy dependence of the transmission coefficient is accounted for exactly. The part of the structure which is affected by the time-modulation can be chosen at will. This allows one to analyze the relative importance of inelastic processes occurring in the barriers, or in the quantum well (see below).

As an illustration of the method we have calculated the transmission coefficient for a symmetric double-barrier structure with 50-Å barriers and a quantum well. The other parameters in the simulation were as follows: V_0 (barrier height relative to contacts and quantum well) $=0.23$ eV, V_1 (amplitude of harmonic modulation) $=0.05\times V_0$, and $\hbar\omega=0.3\times V_0$. The initial Gaussian wave packet had a half width of 1000 Å which was required for sufficient energy resolution. The simulated transmission coefficient is depicted in Fig. 1, where we show results for

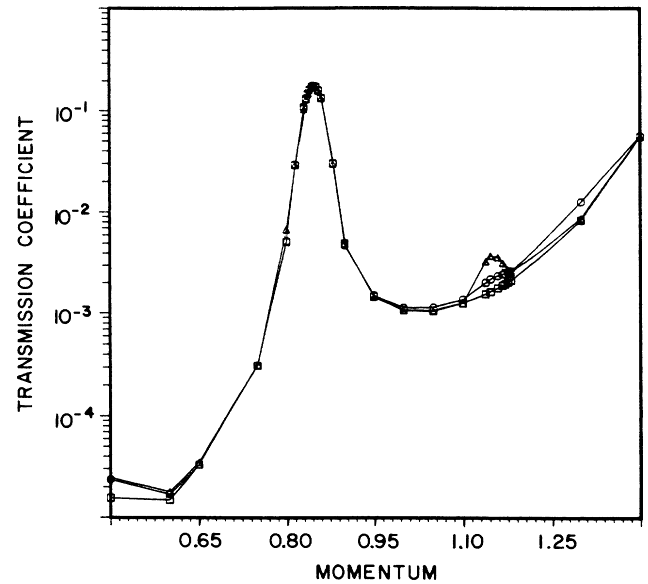

FIG. 1. Transmission coefficient as a function of momentum for a $50\times50\times50$ Å^3 double-barrier structures. Units are chosen so that $p=\sqrt{2}$ corresponds to an energy equaling the static barrier height. Squares, static structure; circles, modulated barriers; triangles, modulated quantum well. In addition to the main resonance at $p_r=0.864$ the satellite at $p=(p_r^2+2\hbar\omega)^{1/2}$ is seen. The feature corresponding $p=(p_r^2-2\hbar\omega)^{1/2}$ is weak (not shown in the figure) and best analyzed in momentum space snapshots (see Fig. 2).

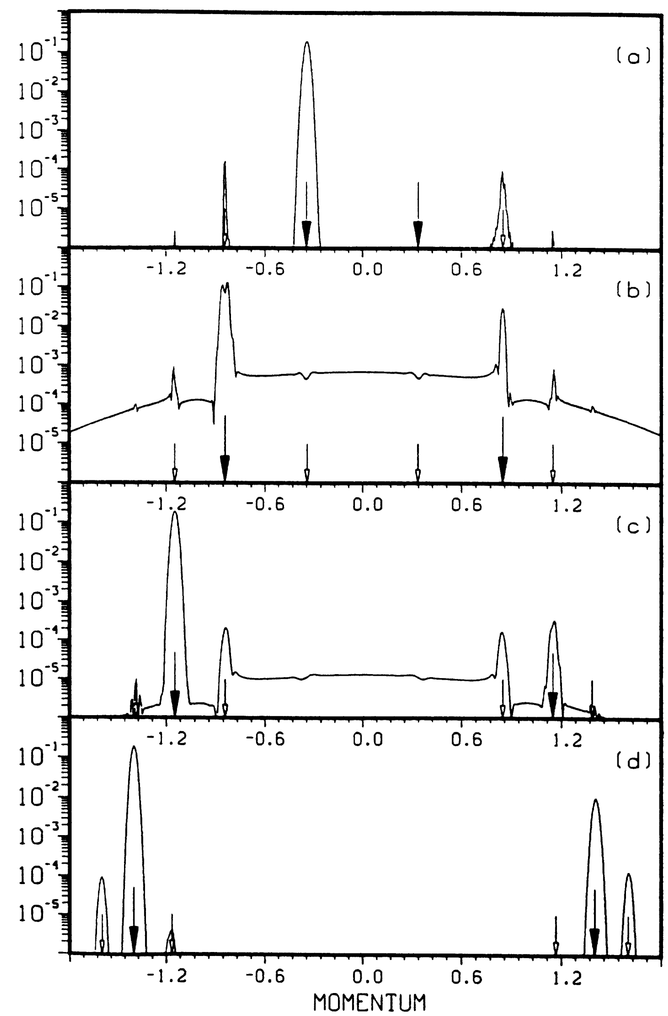

FIG. 2. Square modulus of the momentum space wave function during the simulation for four different incident energies: (a) $E=E_r-\hbar\omega$, (b) $E=E_r$, (c) $E=E_r+\hbar\omega$, and (d) $E=0.9\times V_0$. The large solid arrows show the incident momentum, while the small open arrows indicate the locations of the $n=\pm1$ sidebands (the $n=-1$ sideband does not exist for the lowest energy).

the static double barrier (squares), modulated barriers (circles), and modulated well (triangles). The satellite at $E_r+\hbar\omega$ (E_r is the resonant energy) is clearly visible for the case of the modulated quantum well while it is barely discernable for the modulated barriers case. To our knowledge this effect has not been discussed previously, and it can be understood as follows. The tunneling particles pass through the classically forbidden region so fast (typical estimate for a tunneling time for a 0.23 eV high and 50-Å broad barrier at energy 0.1 eV would be a few femtoseconds) that they do not have time to absorb or emit a modulation quantum.[10] However, once in the quantum well the particles stay there so long (semiclassically, they reflect back and forth several times before tunneling out) that a sideband has time to form, and therefore the modulated well shows a stronger effect than modulated barriers. This seems to suggest that in experimental situations barrier phonons are of minor importance. Interfaces, however, which are probed many times (within the semiclassical picture) may have an important effect.

Further insight on the dynamics of the tunneling processes can be extracted by analyzing the wave-packet in momentum space.[11] In Fig. 2 we show the momentum space wave function for four different energies at the time instant when the simulation was terminated. Two different criteria were used to determine this time: (i) The transmission coefficient had converged to its asymptotic value [Figs. 2(a) and 2(d)], or, equivalently, there was no wave function left in the quantum well. In the case of a strong resonant coupling to the quasibound state in the well a second criterion was used: (ii) The part of wave function trapped in the quantum well had reached its asymptotic exponentially decaying time dependence [Figs. 2(b) and 2(c)]. Let us now examine in detail the transmitted part of the wave function, i.e., positive momenta (similar considerations can be made for the reflected pulse). Starting from low energies [Fig. 2(a)], $E=E_r-\hbar\omega$, we observe that the transmitted pulse does not have *any* amplitude at the incoming energy E: all its weight is located at channels $E+\hbar\omega$ and $E+2\hbar\omega$. Thus we have a very clear case of velocity filtering: the transmitted pulse has a different velocity, or energy, than the incoming one. The mechanism leading to this behavior is easily understood by recalling that the transmission coefficient is very small for small energies (see Fig. 1), and that by absorbing a modulation quantum the tunneling particles are excited to the resonant channel with an enhanced probability for transmission. For $E=E_r$ [Fig. 2(b)] the momentum space wave function is characterized by a very broad uniform background, with a sharp peak at the incoming energy and small features corresponding to emission and absorption of modulation quanta. The background corresponds to the trapped part of the wave function which slowly leaks out from the quantum well. For $E=E_r+\hbar\omega$ [Fig. 2(c)] we also observe a large background; the interesting feature is the large feature at $E-\hbar\omega$, which corresponds to the particles that have emitted a modulation quantum, and therefore are at resonance, and thus contribute strongly to the transmitted pulse. Particles that have absorbed modulation quanta, however, do not contribute significantly to the tunneling current. At even higher energies [Fig. 2(d)] the situation differs in two aspects: first, there is hardly any uniform background, which shows that tunneling is fast and dominated by nonresonant effects, and second, the dominant sideband now occurs at $E+\hbar\omega$, which corresponds to particles that by absorbing a quantum are excited above the barriers, and therefore can contribute to the transmitted pulse.

In summary, we have described a numerical procedure which is simple and straightforward to apply, allows the simulation of inelastic processes, and gives insight to the dynamics of tunneling in the presence of inelastic effects. The method can be applied to many other tunneling problems where scattering or relaxation effects are important. Examples of potential applications include studies of stochastic time modulation, and sequential tunneling and relaxation in biased multiple quantum well systems.[12]

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