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Theory of Electron Resonant Tunnelling through Localized States in the Presence of Hot Acoustic Phonons

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We use nonequilibrium Green functions to consistently describe electron resonant tunnelling through localized states in the presence of hot phonons. Thereby we are able to study in details effects related to nonequilibrium steady-states of such systems in the presence of dc bias and hot phonon fields. The method is applied to a model of a delta-doped GaAs/AlGaAs double barrier heterostructure, where simulation of the hot phonons is performed by the change of their distribution function. The results are in qualitative agreement with the recent experiments performed on similar systems.

This study originates from recent experiments on resonant tunnelling through impurity levels confined in a quantum well assisted by a beam of hot acoustic phonons [1]. Our model system [2] is formed by a delta-doped GaAs/AlGaAs double barrier heterostructure, where the donor level is confined in the well and coupled via the tunnelling barriers to two 2D reservoirs and by a deformation potential to bulk LA phonons [3]. We apply the following spinless Hamiltonian

$$\begin{aligned} H = & \sum_{k;\ \alpha=\mathrm{L,R}} E_{k,\alpha} c^+_{k,\alpha} c_{k,\alpha} + E_0 d^+ d + \sum_{k;\ \alpha=\mathrm{L,R}} \gamma_{k;\ \alpha} (c^+_{k,\alpha} d + \mathrm{h.c.}) \\ & + \sum_q \hbar\omega_q b^+_q b_q + \sum_q F(q)\ M(q)\ d^+ d (b_q + b^+_{-q})\ , \end{aligned} \tag{1}$$

where $c^+_{k,\alpha=\mathrm{L,R}}$ ($c_{k,\alpha=\mathrm{L,R}}$) and $E_{k,\alpha=\mathrm{L,R}}$ are the creation (annihilation) operators and energies for conduction electrons in the left (L) and right (R) reservoirs. $d^+(d)$ and E_0 are the creation (annihilation) operators and energy for the donor level, respectively, $\gamma_{k,\alpha=\mathrm{L,R}}$ are the coupling parameters between the level and the reservoirs, b^+_q (b_q) are the phonon creation (annihilation) operators for wave vector q, $\hbar\omega_q$ is the phonon energy and $M(q)$ is the matrix element for electron interaction with LA phonons. We take the deformation potential constant $D = 11$ eV [3]. $F(q)$ is the square of the donor wave function in momentum representation. In real space this is taken to be a Gaussian function of half-width $\sigma = 10$ nm, multiplied by the wave function for the lowest subband of a quantum well of width $w = 5$ nm [4]. The reservoirs are assumed to have constant densities of states (2D) and the Fermi energy in the emitter reservoir is taken to be

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1 meV. The dc bias is approximated by taking different chemical potentials in the reservoirs $\mu_{\mathrm{L,R}}$, assuming these shift under bias by the same amount but in opposite directions with respect to their equilibrium value μ_0 and the fixed position of the donor level E_0 measured from μ_0.

The system is described by nonequilibrium correlation functions (NGF), which fulfil a set of integral Kadanoff–Baym equations in a frequency representation [5]

$$G^<(\omega) = G^{\mathrm{r}}(\omega)\ \Sigma^<(\omega)\ G^{\mathrm{a}}(\omega)\ , \qquad G^>(\omega) = G^{\mathrm{r}}(\omega)\ \Sigma^>(\omega)\ G^{\mathrm{a}}(\omega)\ . \tag{2}$$

We solve the quantum well diagonal part of these equations in the presence of the tunnelling and the electron–phonon interaction, described by the Migdal approximation for the self-energy [3].

From the resulting correlation functions we calculate the nonequilibrium spectral function $A(\omega) = G^<(\omega) + G^>(\omega)$, which is used to obtain the total resonant tunnelling current [6]. The current from the left leading to the level J_{L} is equal to the current from the right leading to the level J_{R}, but has the opposite sign. These currents can be found from the formula [7]

$$J_{\mathrm{L,R}} = \frac{e}{\hbar} \int \frac{\mathrm{d}\hbar\bar{\omega}}{2\pi}\ |\gamma_{\mathrm{L,R}}|^2 \left[G^<_{\mathrm{L,R}}(\bar{\omega})\ A(\bar{\omega}) - A_{\mathrm{L,R}}(\bar{\omega})\ G^<(\bar{\omega})\right], \tag{3}$$

where $\gamma_{\mathrm{L,R}}$ are the effective coupling constants, $G^<_{\mathrm{L,R}}(\omega)$ and $A_{\mathrm{L,R}}(\omega)$ are the local correlation and spectral functions for the leads, calculated in equilibrium but with different chemical potentials $\mu_{\mathrm{L,R}}$.

In Fig. 1 we show the nonequilibrium (equilibrium) spectral functions $A(\omega)$ by solid (dotted) lines and the nonequilibrium correlation function $G^<(\omega)$ by dashed lines. These are calculated for the coupling parameters $\gamma_{\mathrm{L}} = 7$ meV, $\gamma_{\mathrm{R}} = 5$ meV, the energy of the level $E_0 = 20$ meV and the temperature $T = 1$ K. The three diagrams a) to c) correspond to the biases $\mu_{\mathrm{L}} = -\mu_{\mathrm{R}} = 18,\ 20,\ 22$ meV, respectively. The thin vertical lines define an excitation window (populated emitter band) determined by the bottom of the emitter band (left line) and the Fermi level inside this band (right line). The spectral function for the level is shifted to lower energies as μ_{L} increases due to repulsion by the moving emitter band and below the bottom of this band it becomes narrower. The correlation function $G^<(\omega)$, related to the level population $f(\omega) = G^<(\omega)/A(\omega)$, has the same order of magnitude as $A(\omega)$ in the ex-

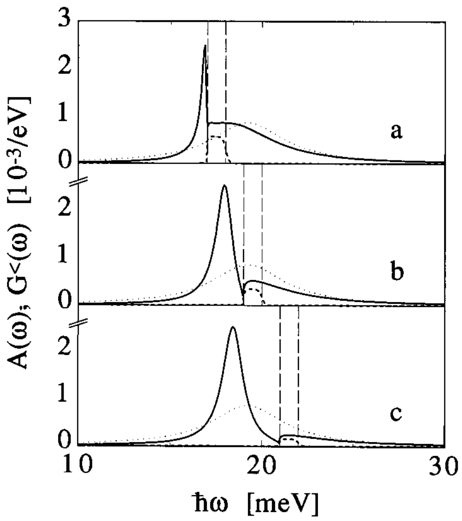

Fig. 1. The nonequilibrium (equilibrium) spectral functions $A(\omega)$ solid (dotted) line and correlation function $G^<(\omega)$ (dashed line) at different biases a) $\mu_{\mathrm{L}} = -\mu_{\mathrm{R}} = 18$, b) 20, c) 22 meV. The dashed vertical lines show the bottom of the emitter band (left line) and the Fermi level in this band (right line)

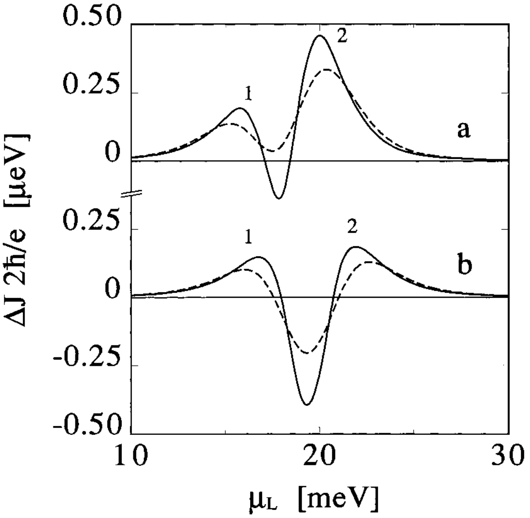

Fig. 2. The induced current by hot phonons with the temperature $T_{\rm h} = 10$ K (solid lines), calculated for low (upper picture) and high (lower picture) level populations. The dashed lines show the same in the presence of inhomogeneous level broadening $\sigma_{\rm i} = 1$ meV

ciation window. Outside, its amplitude is about 250 times smaller and follows the dependence of $A(\omega)$. This small contribution to $G^<(\omega)$ describes the relaxation of the level in the presence of phonons. This is very sensitive to hot phonons and is reflected in the asymmetry of the induced current [2].

In Fig. 2 we present the calculated change of the dc current (3) induced by non-equilibrium phonons, resulting by subtracting the current for the Bose-Einstein distribution $n_{\rm BE}(\hbar\omega, 1\ {\rm K})$ from that in the presence of hot phonons, which is modeled by the weighted phonon distribution $f_{\rm P}(\omega) = [n_{\rm BE}(\hbar\omega, 1\ {\rm K}) + n_{\rm BE}(\hbar\omega, 10\ {\rm K})]/2$. It is assumed that the phonon pulse does not heat the electrons, which remain at $T = 1$ K (see also [2]). The solid curves are the calculated signals for two sets of effective coupling parameters [2] $\gamma_{\rm L} = 7$ meV, $\gamma_{\rm R} = 5$ meV (a) and $\gamma_{\rm L} = 5$ meV, $\gamma_{\rm R} = 7$ meV (b). Two peaks can be seen, 1 and 2, separated by a negative minimum, which coincides with the resonant donor peak, in qualitative agreement with recent experiments [1]. Peaks 1 and 2 result from assisted tunneling involving absorption (emission) of acoustic phonons, respectively. The minimum at resonance results from the shift of the oscillator strength to the phonon induced peaks. The increased population of the level due to the smaller coupling ratio $\gamma_{\rm R}/\gamma_{\rm L}$ in Fig. 2a is reflected in a slight asymmetry of the response current and smaller negative values [2]. The dashed lines show the effect of inhomogeneous broadening of the level with a Gaussian distribution function of a half-width $\sigma_{\rm i} = 1$ meV. This reduces the size of the minimum, since the correlation function term $G^<(\omega)$ dominates in the current (3) even for small inhomogeneous broadening, since the contributions from the shifted spectral functions $A(\omega)$ for different levels largely cancel each other [2].

We have also linearized the transport equations (2) with respect to the phonon population and calculated from the resulting system of equations the response to monochromatic phonon waves with small amplitudes. These studies reveal a shift in the position of the phonon induced peaks, 1 and 2, with phonon energy and a cut-off in the response for energies higher than $\hbar\omega_q \approx 5$ meV, due to confinement of the level. The shift of the peaks is small and the cut-off is less effective if the system is excited by a heated phonon distribution, which is also observed in experiments [1]. If the phonon energy is smaller than the homogeneous or the inhomogeneous width of the spectral function, then both the magnitude of the response current and the shift of the peaks also decrease [2].

In summary, we have calculated the resonant tunnelling current assisted by hot phonons by the NGF method. The phonon induced current shows two peaks which result from the phonon absorption and emission processes and it agrees qualitatively with recent experiments [8]. However, the present calculations do not include the effect of heating the electron gas in the contacts, which would give a larger response than the phonon assisted signal but with a different dependence on the bias [2,8]. Our model does not also include the Coulomb interaction between the charged impurities in the well and the electrons in the emitter, which could lead to an increase in the electron–phonon coupling and hence the phonon-assisted signal [8]. Heating might also play a different role in this more complex model.

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