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POLARON PROBLEM IN QUANTUM WELLS*

W. BARDYSZEWSKI AND M. PRYWATA

Institute of Theoretical Physics, Warsaw University
Hoża 69, 00-681 Warszawa, Poland

The effect of polar interaction between an electron in a quantum well and bulk longitudinal optical phonons is analysed. Electron spectral density function is calculated in the lowest order cumulant approximation. The position and linewidth of the quasiparticle peak are obtained as a function of quantum well width and temperature.

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1. Introduction

The problem of the polaron ground state energy and of effective mass renormalization in quantum wells has been widely discussed in literature [1, 2]. Considerably less attention has been paid to the quantum well polaron lifetime [3], or more generally, to the spectral density function which is closely related to the excitonic absorption lineshape function. We employ the cumulant expansion method which has been proved to be very accurate in the case of three-dimensional polarons [4]. The main idea of this method is to expand the correction to the phase of the time dependent Green's function in powers of the coupling constant. Such an expansion is much faster convergent than a standard perturbation series for the Green's function. In practice, already the lowest order term provides a very reasonable approximation.

2. Electron Green's function

The presence of a quantum well generally affects bulk phonons by introducing interface and confined modes. These modifications are weak in many materials, so we adopt a model of a quantum well confined electron interacting with unperturbed bulk phonons. With this simplification we can write the electron–phonon Hamiltonian in the following form:

$$H = \sum_{p,n} E_n(p) c^\dagger_{n'p} c_{np} + \sum_q \hbar\omega_0 b^\dagger_q b_q + \sum_{n'n\,pq} V_q c^\dagger_{n'p+q_\parallel} c_{np} M_{n'n}(q_z)(b_q + b^\dagger_{-q}). \tag{1}$$

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The electron and phonon annihilation operators are denoted by c_{np} and b_q, respectively while ω_0 is LO phonon frequency and V_q represents the three-dimensional Fröhlich coupling potential. The electron confinement introduces the factor $M_{nn'}(q_z) = \int \mathrm{d}z \mathrm{e}^{-\mathrm{i}q_z z} F_n(z) F_m(z)$ with $F_n(z)$ denoting electron envelope function for the n-th subband with the dispersion given by $E_n(p)$.

The time dependent propagator for an electron with the momentum p parallel to the well plane can be expressed in terms of the cumulant series [5]

$$G_n(p,t) = G_n^o(p,t) \exp\left\{-\mathrm{i}\sum_{m=1}^{\infty} \frac{(-\mathrm{i})^m}{m!}\left[\mathbf{T}\left(\int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \Sigma_n(p,\tau-\tau')\right.\right.\right.$$
$$\left.\left.\left. \times \exp(\mathrm{i}E_n(p)(\tau-\tau'))\right)^m\right]_c\right\}, \tag{2}$$

where Σ_n denotes the retarded self-energy function in the subband n. In the lowest order with respect to the electron–phonon coupling one obtains

$$G_n(p,t) = G_n^o(p,t) \exp\left(\Phi_n(p,t)\right), \tag{3}$$

where the phase correction for the electron propagator is given by

$$\Phi_n(p,t) \approx -\mathrm{i}\int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \Sigma_n^{(0)}(p,\tau-\tau') \exp\left(\mathrm{i}E_n(p)(\tau-\tau')\right). \tag{4}$$

Thus the lowest order cumulant expansion is reduced to the evaluation of the lowest order self-energy with respect to the electron–phonon coupling $\Sigma_n^{(0)}(p,\tau-\tau')$. This is a very good approximation for the systems with a weak coupling such as in the GaAs/AlGaAs lattice matched quantum wells.

The self-energy function can be easily evaluated for various quantum well models.

3. Quasi two-dimensional limit

The limit of infinite confinement is particularly interesting. Since for a well width $L \to 0$ we have $M_{nm} \approx \delta_{nm}$, so for large t

$$\Phi_n(p,t) = -\mathrm{i}t\Sigma_n^{2\mathrm{D}}(p) - L_n^{2\mathrm{D}}(p) \tag{5}$$

with the two-dimensional on-shell self-energy

$$\Sigma_n^{2\mathrm{D}}(p) = -\alpha\omega_0 \left[(N_0+1)K\left(\sqrt{\frac{E_n(p)}{\omega_0}}\right)\right.$$
$$\left. +\mathrm{i}N_0\sqrt{\frac{\omega_0}{\omega_0+E_n(p)}}K\left(\sqrt{\frac{E_n(p)}{\omega_0+E_n(p)}}\right)\right] \tag{6}$$

and the renormalization factor

$$L_n^{2\mathrm{D}}(p) = \frac{1}{2}\left[(N_0+1)\Pi\left(-\frac{E_n(p)}{\omega_0}, \sqrt{\frac{E_n(p)}{\omega_0}}, \frac{\pi}{2}\right)\right.$$
$$\left. -\mathrm{i}N_0\left(\frac{\omega_0}{\omega_0+E_n(p)}\right)^{3/2}\Pi\left(-\frac{E_n(p)}{\omega_0+E_n(p)}, \sqrt{\frac{E_n(p)}{\omega_0+E_n(p)}}, \frac{\pi}{2}\right)\right], \tag{7}$$

where N_0 denotes Bose–Einstein occupation factor for phonons, and K and Π are elliptic functions of the first and of the third kind. The Fröhlich coupling constant

is given by $\alpha = e^2\sqrt{m^*/2\omega_0}(1/\epsilon_\infty - 1/\epsilon_0)$, where m^* denotes the corresponding effective mass. For the polaron with $p = 0$ one obtains an expression which is identical to the three-dimensional one up to the multiplicative constant of $\pi/2$ [6].

The resulting spectral density function is given by a simple asymmetric Lorentzian function

$$A_n(p,E) = -\frac{1}{\pi}\mathrm{Im}G_n(p,E) = -2\mathrm{Im}\frac{e^{-L}}{E - E_n(p) - \Sigma_n^{2D}(p)}. \tag{8}$$

This asymptotic result should be reasonably accurate in the vicinity of the resonance. The quality of this approximation can be judged from Fig. 1, in which three model spectral density functions are presented. The Lorentzian curve (solid

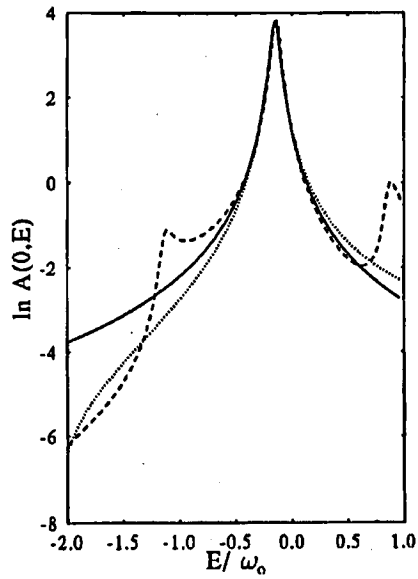

Fig. 1. Log of the polaron spectral density function at $p = 0$ for an infinitely narrow GaAs/GaAlAs quantum well at 300 K; cumulant expansion — dashed line, asymmetric Lorentzian — dotted line and Lorentzian model — solid line.

line) decays much slower than the other two. The dotted line representing the asymmetric Lorentzian follows rather closely the exact, dashed curve. However, it obviously does not reproduce the satellite structures present at the energy offset of $\pm\omega_0$ from the central peak. The calculations are performed for the GaAs/GaAlAs quantum well at 300 K.

4. Finite well width limit

The electron–phonon-coupling in realistic quantum wells is much more complicated due to their finite thickness. In this case, the envelope function form-factor M_{nm} will couple many subbands. In fact, it has been pointed out that it is impossible to recover the bulk, $L \to \infty$, limit without inclusion of the intersubband electron–phonon scattering processes. In order to analyze the relative contribution

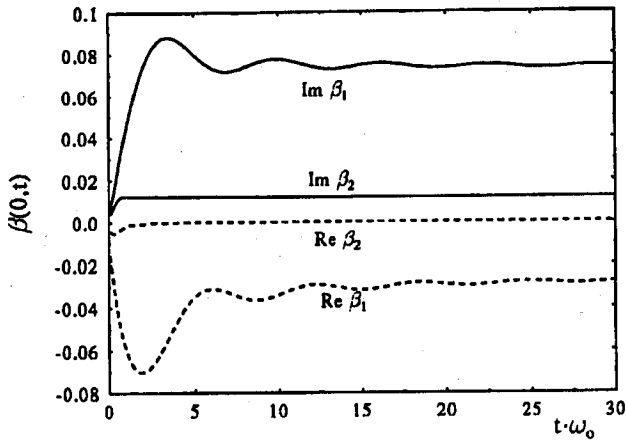

Fig. 2. Real and imaginary part of the contributions from the intrasubband (β_1) and the lowest order intersubband transitions (β_2) to the coefficient β in the phase function Φ_1 for the lowest subband. The GaAs/GaAlAs quantum well width is assumed to be equal to 100 Å.

of the intrasubband and intersubband transition for a finite confinement quantum well we first represent Φ_n as $\Phi_n = \sum_{n'} t\beta_{n'}(t)$ with $\beta_{n'}(t)$ corresponding to the n' level contribution to Φ_n and evaluate separately the coefficients $\beta_{n'}$. In Fig. 2 the contributions from the lowest order intrasubband and first order intersubband transitions are presented with solid line corresponding to the imaginary, and the dashed line to the real part of β. The calculation are performed for a 100 Å GaAs/GaAlAs QW at 300 K for an electron state with $p = 0$. As one can easily see, the intrasubband processes give the dominant contribution while the intersubband transitions can be neglected in this case. The asymptotic behaviour of the coefficients β corresponds to the limit of the asymmetric Lorentzian model (Eq. (8)). In the first approximation the asymptotic values of β determine the energy renormalization and damping constant for a polaron.

5. Conclusions

We have presented a simple model for the polaron lineshape function in a quantum well. Our calculation, based on the cumulant resumation principle, takes into account multiphonon processes up to infinite order. The resulting spectral density function has a proper asymptotic behaviour both in the limit of small and large frequencies. Using our model, we have found that for most standard quantum well structures, the intrasubband electron–phonon processes are dominant. However, even in the single subband approximation the finite well thickness modifies the effective electron–phonon coupling. In the extremely narrow confinement situation one can obtain a simple working formula for the spectral density function of a polaron at the subband bottom.

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