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Phonon confinement and screening effects on the polaron energy in quantum wires

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Abstract. We study the contribution of confined phonons to the polaron energy in quantum-well wires. We use a dispersionless, macroscopic continuum model to describe the phonon confinement in quantum wires of square cross section. The polaron energy is calculated variationally incorporating the dynamic screening effects. We find that the confined phonon contribution to the polaron energy is comparable to that of bulk phonons in the density range $N = 10^4$–10^7 cm^{-1}. Screening effects within the random-phase approximation significantly reduce the electron-confined phonon interaction, whereas the correlation effects tend to oppose this trend.

A great deal of effort has been expended on the study of quasi-one-dimensional (Q1D) semiconductor structures in recent years. In these systems, based on the confinement of electrons, the carrier motion is quantized in two transverse directions, and thus the charge carriers essentially move only in the longitudinal direction. Interest stems from fundamental and applied points of view, because of new physical phenomena involved and their potential applications in high-speed optoelectronic devices. Progress in fabrication techniques such as molecular beam epitaxy and lithographic deposition has made possible the realization of such Q1D systems [1].

The interaction strength of electrons with LO phonons in low-dimensional structures is strongly affected by phonon confinement, as well as by the changes in the electronic wavefunction brought about by the confining potential. Phonon confinement causes changes in the electron–phonon interaction, modifying properties like scattering and relaxation rates from those in the bulk phonon case. Stroscio [2] has applied the dielectric continuum model to describe the confined LO phonons in rectangular quantum wires. Similar calculations using different models of a quantum wire have also been performed [3]. A calculation of confined and interface phonon scattering rates in finite barrier, multisubband quantum wires was presented by Jiang and Leburton [4]. A microscopic calculation for rectangular wires has been reported by Rossi *et al* [5].

The energy and the effective mass of an electron in a quantum wire including the subband effects were calculated in the presence of electron–LO-phonon interaction by Degani and Hipólito [6]. The ground-state energy of the Q1D polaron gas in a rectangular quantum-well wire has been calculated by Campos *et al* [7] and very recently by Hai *et al* [8]. The latter group has investigated the polaron energy in different quantum-well wire models and the effects of screening. Coupling to phonons of a Q1D electron–hole plasma was considered by Güven and Tanatar [9]. In most previous works, LO phonons have been treated in the bulk, neglecting the phonon confinement effects. The effects of phonon confinement in a quantum-well wire were considered by Zhu and Gu [10], Degani and Farias [11] and Li *et al* [12] using various models and approximations. In the present calculation the electrons are coupled to the confined phonon modes, and we are interested in the combined effect of phonon confinement and carrier screening. We note that the polaron energy is not an observable quantity in itself, but the results of our calculation will provide insight into the relative contribution of the various LO phonon modes in quantum wires. Inelastic light scattering measurements by Klein [13] suggest the importance of confined phonon and interface modes. Hot-electron energy-loss studies [14] offer the possibility of distinguishing the phonon modes involved in polar semiconductors of reduced dimensionality. Experimentally, the more relevant problem of magnetopolarons, especially in connection with cyclotron resonance measurements, has been explored by different groups [15].

The purpose of this paper is to study the contribution of confined phonon modes to the ground-state energy of an electron–phonon system in Q1D structures, and in particular to investigate the effects of screening. Phonon confinement is treated within a macroscopic approach, one in which electrostatic boundary conditions are used [2, 16]. Although the actual spectrum for phonon modes in confined structures is more complicated than those described by the macroscopic models, they lend themselves to simplified

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expressions and provide qualitative understanding. In the electrostatic model, the standard boundary conditions are applied to the electrostatic potential. This gives rise, for the LO phonons, to travelling waves in the direction of the wire and standing waves in the confined, transverse directions. We employ a variational approach to estimate the confined phonon contribution, and investigate the effects of screening in various approximations.

For the Q1D system of electrons we consider a square well of width a with infinite barriers. This may be built, for instance, by embedding a thin wire of GaAs in a barrier material of AlAs. We restrict our attention to the extreme quantum limit, where only the first subband is occupied. This approximation will hold as long as the subband separation remains much larger than the phonon energy in quantum wires. Furthermore, we assume for simplicity a complete confined phonon picture. In an interesting work, Zhu and Chao [17] have shown that only a fraction of the LO phonon modes are confined in the quantum well.

We study the Q1D polaron gas using the Lee–Low–Pines unitary transformation approach as introduced by Lemmens *et al* [18] and Wu *et al* [19] in applications to 3D and Q2D systems. It is harder to incorporate the screening effects (especially the dynamic screening) within the perturbation theory approach [20], and thus a variational method seems more suitable. Following the usual procedure [6, 7, 18, 19] of assuming that the ground state may be written as a product of the phonon vacuum state and ground-state wavefunctions of electrons, and minimizing the energy with respect to the variational parameter, we arrive at the ground-state energy of the polaron gas:

$$E_{\mathrm{p}} = -\sum_q \sum_{mn} \frac{|M_{mn}(q)|^2 S^2(q)}{\omega_{\mathrm{LO}} S(q) + q^2/2m} \qquad (1)$$

where the sum over the discrete labels is due to confined phonons in two transverse directions, and the wavevector q is along the wire direction. In the above expression, $S(q)$ is the static structure factor determining the screening properties of the electron–phonon system. Setting $S(q) = 1$, in the unscreened limit, we recover the result from perturbation theory for the polaron energy.

In the extreme quantum limit, when the electrons are in the lowest subband, the Q1D electron–phonon interaction matrix element for confined phonons in quantum-well wires of infinite potential and square cross section is

$$|M_q|^2 = \frac{2\alpha\omega_{\mathrm{LO}}^2}{\sqrt{2m\omega_{\mathrm{LO}}}} \sum_{mn} F_{mn}$$

where [2, 16]

$$F_{mn}(q) = \frac{32\pi}{a^2} \frac{|P_{mn}|^2}{q^2 + (m\pi/a)^2 + (n\pi/a)^2} \qquad (2)$$

with

$$P_{mn} = \frac{(8/\pi)^2}{mn(4-m^2)(4-n^2)} \sin(m\pi/2)\sin(n\pi/2). \qquad (3)$$

Owing to symmetry considerations [2, 16], in the electrostatic confinement model we sum only over the odd values of m and n. We have taken dispersionless LO phonons in the description of confined phonon modes, for simplicity.

The static structure factor $S(q)$ is obtained from the full frequency-dependent dielectric function $\varepsilon(q, \omega)$ by integrating over all frequencies, and thus it inherently carries dynamic information. For Q1D electron systems the collective excitations (plasmons) have a strong wavevector dependence without damping. Thus, along with the single-particle excitations, plasmons have to be taken into account explicitly in the calculation of $S(q)$. We consider the expression $S(q) = S_{\mathrm{sp}}(q) + S_{\mathrm{pl}}(q)$, and use the random-phase approximation (RPA) forms of the individual contributions as given by Hai *et al* [8].

We illustrate our calculations of the confined phonon contribution to the ground-state energy of a quantum wire by choosing a GaAs system for which the relevant parameters are $m = 0.067\, m_{\mathrm{e}}$, $\omega_{\mathrm{LO}} = 36.5$ meV and the coupling constant $\alpha = 0.07$.

In figure 1 we show the polaron energy of a quantum wire with lateral widths $L_y = L_z = a = 100$ Å. The contributions of the electron–phonon interaction to the ground-state energy of a polaron gas are plotted as a function of the 1D carrier density N. The dotted and broken curves are for the Hartree–Fock (HF) approximation and RPA respectively. It is seen that the confined phonon contribution is quite significant, especially at low densities. Figure 2 shows the polaron energy as a function of the quantum wire width a, for an electron density of $N = 10^6$ cm^{-1}. The dotted and broken curves give the width dependence using HF and RPA structure factors respectively. A comparison of our results with the calculations of Hai *et al* [8], who employed bulk phonons, indicates that the polaron gas energy due to the confined phonons is comparable to that of bulk phonons.

The static structure factor $S(q)$, as set out in the previous section, determines the screening properties of the

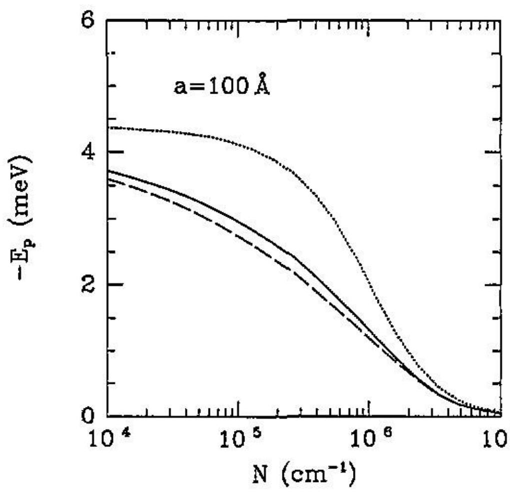

Figure 1. Polaron energy due to confined phonons, as a function of electron density N, for a 100 × 100 Å^2 GaAs quantum wire. The dotted and broken curves indicate HF and RPA respectively. The full curve represents the Hubbard approximation.

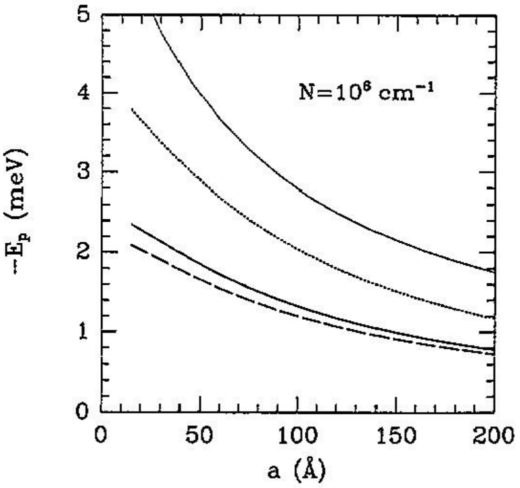

Figure 2. Polaron energy due to confined phonons, as a function of quantum wire width a, for an electron density $N = 10^6$ cm^{-1}. The dotted and broken curves indicate HF and RPA respectively. The thick full curve represents the Hubbard approximation, whereas the thin full curve corresponds to the unscreened limit.

electron–phonon system. It has been known that the RPA, although exact in the high density limit, fails to take the short-range electron correlations into account properly in the lower density regime. To improve the RPA, we introduce the vertex corrections (to the dynamic susceptibility) in the mean-field sense using the local-field corrections $G(q)$. A variety of many-body schemes exist to calculate $G(q)$, including the self-consistent field approach of Singwi *et al* [21], which is known to yield good results in 3D and 2D calculations. We use the equivalent of the Hubbard approximation for $G(q)$ in one dimension [21]:

$$G(q) \approx \frac{1}{2}\frac{V\left(\sqrt{q^2+k_F^2}\right)}{V(q)}. \tag{4}$$

The physical nature of the Hubbard approximation is such that it takes exchange into account and corresponds to using the Pauli hole in the calculation of the local-field correction between the particles. The local-field effects are implemented in the calculation with the replacement of the effective Coulomb interaction $V(q)$ by $V(q)(1 - G(q))$ in the expressions for $S(q)$.

The dependence of the confined phonon energy on screening within the Hubbard approximation is illustrated in figures 1 and 2 by the full curves. When the correlation effects are included within the Hubbard approximation (full curves), we obtain a slight increase in the magnitude of the polaron energy with respect to the RPA. We observe that, on going from the HF approximation to the RPA, the screening reduces the electron–phonon interaction appreciably as the carrier density increases. The correlation effects, on the other hand, when treated within the mean-field model (i.e. Hubbard approximation) tend to increase the electron–phonon interactions, giving rise to anti-screening. Qualitatively similar results were found by Campos *et al* [7] for bulk phonons in quantum-well wires, where they used the self-consistent field approximation in $S(q)$. As the electron density becomes large, screening effects dominate and we observe that the HF, RPA and Hubbard approximation curves in figure 1 become similar. In order to reliably assess the importance of correlations beyond the RPA, better approximations to the local-field factor $G(q)$ could be employed.

In the unscreened limit, i.e. $S(q) = 1$, the polaron energy becomes

$$E_p = -\frac{32\pi}{a^2}\alpha\omega_{LO}\sum_{mn}|P_{mn}|^2 \times\frac{[(m\pi/a)^2+(n\pi/a)^2]^{-1/2}}{(2m\omega_{LO})^{1/2}+[(m\pi/a)^2+(n\pi/a)^2]^{1/2}}. \tag{5}$$

The thin full curve in figure 2 indicates the unscreened polaron energy due to confined phonons.

It has been noted [22] that the static screening has a stronger effect in the renormalization (of polaron energy and mass) than the dynamic screening, because in the static approximation only the long-time response of the system is taken into account. Similar conclusions have been drawn by Hai *et al* [8] in their calculation that takes the dynamic screening effects into account for Q1D systems. We have not attempted a perturbative calculation including dynamical screening, but we expect the polaron energy E_p to increase in magnitude if such an approach is considered.

For the Q1D electron system we have used the infinite barrier, square cross-sectional wire model. There are various other models of the quantum-well wire structures making use of parabolic confining potentials and geometrical reduction of dimensionality [8]. The general trends obtained here for the carrier density and screening dependence should be valid irrespective of the details of the model chosen. We have neglected the interface phonon modes, which are expected to be appreciable only for very narrow wires since they have exponentially decaying amplitudes. The interaction of electrons in a Q2D structure with interface and bulk LO phonons was considered by Degani and Hipólito [23]. They found that interface phonons give a significant contribution to the polaron energy and effective mass. Polaron effects due to interface phonons in lateral quantum wires were considered by Degani and Farias [11]. It would be interesting to include the interface phonon modes in quantum wires, particularly in the studies of electron relaxation processes.

In summary, we have calculated the polaron energy in a Q1D GaAs quantum-well wire, using the confined phonons. We have included the screening effects within the RPA and Hubbard approximation. We find that the approximate local-field corrections tend not to change the magnitude of the polaronic corrections significantly.

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