Energy-momentum relation for polarons in quantum-well wires

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The static and dynamical properties of electrons confined in quantum-well-wire structures are modified because of the interaction with unconfined phonon modes. The interaction with virtual phonons leads to a mass renormalization, a binding energy, and a nonparabolic energy-momentum relation. Using the improved Wigner-Brillouin perturbation theory, we have investigated the energy-momentum relation for electrons confined in rectangular quantum-well wires of GaAs surrounded by $Ga_{1-x}Al_xAs$, as a function of the transverse sizes of the wire. There is observed a significant energy lowering when the electron momentum k approaches k_{LO}, and this bending over of the dispersion curve increases when the electron confinement is enhanced.

High-quality quasi-one-dimensional (Q1D) semiconductor structures have been constructed with the advances in material fabrication techniques. The electron confinement can be realized by etching techniques,[1–5] by selective-ion implantation,[6,7] by using the field effect to create quasi-one-dimensional conducting channels[8–10] or by pinching off a two-dimensional conducting channel using a split gate.[11,12] From a fundamental point of view there are many fascinating and interesting reasons to study quasi-one-dimensional systems. On the other hand, the technological importance in high-speed-device applications has motivated theorists as well as experimentalists to investigate various properties of such systems.

Recently the mobility modulation was observed[13] as an increase in the mobility in the lowest subband of the Q1D wires as suggested by Sasaki.[14] The static and dynamical conductivity have been also measured.[5,8,9] Most of the theoretical studies have investigated the static and dynamical conductivity,[15,16] collective excitations,[17] mobility of electrons scattered by ionized donors as well as by the optical and acoustic phonons,[18–20] binding energies of hydrogenic impurities, and excitons.[21,22]

The electron-phonon interaction in quantum-well wires of GaAs surrounded by $Ga_{1-x}Al_xAs$ was studied recently by Degani and Hipólito,[23,24] who calculated the polaronic corrections to the electron ground-state energy and the effective-mass renormalization as a function of the transverse sizes of the wire.

In this paper we will focus our attention on the energy-momentum relation for quasi-one-dimensional polarons in an ultrathin wire of GaAs in a confining barrier material of $Ga_{1-x}Al_xAs$. The theory of the dispersion relation for tridimensional electron-phonon coupling has been given by Whitfield and Puff[25] and by Larsen.[26] By the arguments of Whitfield and Puff, the dispersion curve must bend over at one phonon energy above the shifted ground state of the system. We will show that this effect is more pronounced in the quasi-one-dimensional systems and increases when the electron confinement is increased; this occurs because in this system the electron-phonon interaction is stronger than in the tridimensional systems. In two-dimensional systems, Devresse and Peeters[27] have found a similar behavior in the region before the threshold.

In order to make the calculation feasible we will use the infinite confining potential approach, the electron–LO-phonon coupling is assumed to be described by the Fröhlich Hamiltonian, and the LO phonon is considered in the bulk phonon approximation instead of the confined phonon modes, i.e., the quasi-one-dimensional confined electrons are interacting with the bulk LO phonon mode. Although crude, this model works well for a two-dimensional electron gas. In a quasi-one-dimensional system, the subband structure, which arises from the two-dimensional confinement of the electronic motion, plays an important role. Otherwise, for wires with a large transverse cross section, the subband structure cannot be neglected. In the present study all subbands will be taken into account.

We will consider an electron confined in a two-dimensional potential $V(y,z)$ and free to move along the x direction. The energy-momentum or dispersion relation for the weakly interacting electron-polar optical-phonons system is calculated using the improved Wigner-Brillouin perturbation theory.[28] The quasiparticle energy-momentum relation is obtained as the solution of the self-consistent equation

$$E(k)=k^2+\mathrm{Re}\Sigma(k,E)\ , \tag{1}$$

where

$$\Sigma_{n_yn_z}(k,E)=\frac{\alpha}{\pi}\sum_{m_y}\sum_{m_z}\int_{-\infty}^{+\infty}\frac{F_{n_yn_zm_ym_z}(q)dq}{E-1-(k-q)^2-\Delta_{n_yn_zm_ym_z}-\Sigma_{n_yn_z}(0,0)}\ , \tag{2}$$

and

$$\Delta_{n_y n_z m_y m_z} = \left[\frac{\pi}{L_y}\right]^2 (m_y^2 - n_y^2) + \left[\frac{\pi}{L_z}\right]^2 (m_z^2 - n_z^2) , \tag{3}$$

and $F_{n_y n_z m_y m_z}(q)$ is the form factor of a Q1D system which is given by

$$F_{n_y n_z m_y m_z}(q) = \int_0^\infty \frac{|G_{n_y m_y}(\eta)|^2 H_{n_z m_z}(q,\eta)}{(q^2+\eta^2)^{1/2}} d\eta , \tag{4}$$

with

$$G_{n_y m_y}(\eta) = \int \Phi^*_{n_y}(y)\Phi_{m_y}(y) e^{i\eta y} dy , \tag{5}$$

and

$$H_{n_z m_z}(q,\eta) = \int dz \int dz' \, \Phi^*_{n_z}(z)\Phi^*_{m_z}(z) \times e^{-q'|z-z'|}\Phi_{n_z}(z')\Phi_{m_z}(z') . \tag{6}$$

Here Φ_j's are the electron wave functions for the motion along y or z directions of an infinite one-dimensional well and $q' = (q^2+\eta^2)^{1/2}$, α is the standard Fröhlich coupling constant which is equal to 0.07 in GaAs. We have used energy in units of $\hbar\omega_{\mathrm{LO}}$ and length in units of k_{LO}^{-1}, which is defined as the wave vector of an electron with kinetic energy equal to the longitudinal optical-phonon energy $\hbar\omega_{\mathrm{LO}}$. L_y and L_z are the transverse sizes of the wire, and n_y, n_z, m_y, m_z are the subband index.

The numerical solution of Eq. (1) was obtained for the case where $n_y = 1$ and $n_z = 1$ for two different transverse sizes of the wire, $L_y = L_z = 50$ Å, and $L_y = L_z = 200$ Å. In Fig. 1 we have plotted the dispersion relation as a function of k/k_{LO} and for the sake of comparison we have plotted the parabolic dispersion. We observe that for low momentum the dispersion is essentially parabolic, therefore when k approaches k_{LO} there is a significant energy lowering and the dispersion becomes strongly nonparabolic. This bending over of the dispersion curve increases with the electron confinement because phonons with larger transverse momentum can contribute to the energy lowering. This bending over is similar to that predicted by Withfield and Puff and by Larsen for three-dimensional polarons with intermediate coupling, but the energy shifts are much larger in the quasi-one-dimensional case, even for small coupling materials such as GaAs.

We expect that effects of the bending over should appear in the transport characteristics of polarons. As we have seen in Fig. 1, the electron-phonon interaction induces a negative effective-mass region below the optical-phonon energy. A polaron moving in the x direction under the influence of a weak electric field accelerates normally until it reaches the negative-effective-mass region, therefore the strong contribution of the electron-phonon interaction to the effective mass slows, and eventually stops the polaron motion. In other words, the group velocity reaches a maximum and then decreases until zero. Above the threshold, for large momentum, the effective mass tends to the bare value because sufficiently fast electrons in the band do not polarize the lattice.

In conclusion, we have calculated the energy-momentum relation for polarons confined in GaAs quantum-well wires with rectangular cross sections as a function of the transverse sizes of the wires using the improved Wigner-Brillouin perturbation theory. We found that the dispersion relation bends over when $k \approx k_{\mathrm{LO}}$ and this effect is increased when the cross section is reduced, i.e., the electron confinement is increased. The dispersion relation for polarons confined in quasi-one-dimensional systems is qualitatively similar to the tridimensional case, but quantitatively is enhanced.

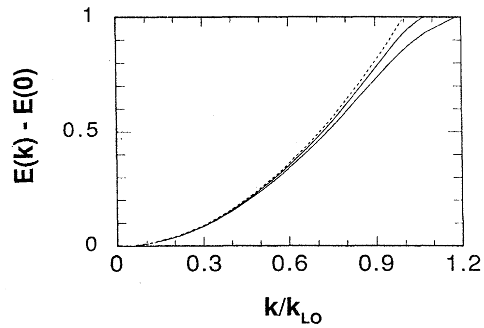

FIG. 1. Energy-momentum relation for polarons confined in quantum-well wires with rectangular cross section. The dashed line is the parabolic dispersion, and the other two curves are the dispersion relation for two different transverse sizes of the wire, $L_y = L_z = 50$ Å and $L_y = L_z = 200$ Å. The dispersion curves become strongly nonparabolic near the region where $k \approx k_{\mathrm{LO}}$ and this effect increases when the electronic confinement is increased.

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