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Plasmon-phonon coupling in one-dimensional semiconductor quantum-wire structures

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Collective excitation modes of coupled one-dimensional electron–longitudinal-optical-phonon systems (as occurring, for example, in GaAs quantum wires) are calculated in the mean-field approximation. In sharp contrast to higher-dimensional systems, the plasmon-phonon coupling is found to be strong at all densities. We also calculate the inelastic scattering rate of energetic quantum-wire electrons in the random-phase approximation, finding sharp thresholds in the scattering rate corresponding to the emission of coupled plasmon-phonon modes.

In a doped polar semiconductor (e.g., n-type GaAs) the free carriers couple to the longitudinal-optical (LO) phonons of the underlying lattice via the long-range polar Fröhlich coupling. On a microscopic level[1] this electron–LO-phonon interaction leads to polaronic many-body renormalization of the single-particle free-carrier properties, e.g., polaronic effective mass renormalization, lowering of the effective band edge, broadening of the quasiparticle spectral function, etc. For weakly polar material (e.g., GaAs or other III-V systems) such polaronic many-body quasiparticle renormalization (i.e., self-energy) corrections are small because the Fröhlich coupling constant $\alpha \ll 1$. For example, the typical polaronic effective-mass renormalization in GaAs is of the order of a few percent. There is, however, a much stronger quantitative manifestation of electron–LO-phonon coupling in doped polar semiconductors, which is the macroscopic coupling of the electronic collective modes (plasmons) to the LO phonons of the system via the long-range Fröhlich coupling. This mode-coupling phenomenon, which hybridizes the collective plasmon modes of the electron gas with the LO-phonon modes of the lattice, gives rise to the coupled plasmon-phonon modes (sometimes also referred to as the hybrid modes), which have been extensively studied[2] both experimentally and theoretically in bulk and two-dimensional GaAs electron systems. A good understanding of plasmon-phonon coupling phenomena is important in developing quantitative theories for many different experimental studies in doped polar semiconductors including light scattering spectroscopy,[2] hot-electron energy-loss processes,[3] transport properties,[4] and ballistic electron transistors.[5] In this paper we calculate the coupled plasmon-phonon modes in one-dimensional (1D) GaAs-based quantum-wire structures, and use our theory to obtain the inelastic scattering rate of energetic quantum-wire electrons as a function of their energy. Our most significant finding is that the one-dimensional plasmon-phonon mode-coupling effect is substantially "stronger" than that in higher- (two- and three-) dimensional systems, and, in contrast to higher dimensions, mode coupling is significant in one-dimensional quantum wires at all electronic densities.

In this calculation we assume the extreme quantum limit with the occupancy of the lowest 1D subband only, and obtain the Coulomb interaction matrix element $v_c(q)$ by taking the quantizing confinement potential to be of infinite square well type.[6] Quantum wires with only single subband occupancy are now available,[7] and our interest in this paper is the investigation of plasmon-phonon coupling in this extreme 1D limit. Note that the details of the confinement potential (e.g., rectangular, parabolic, etc.) do not affect our qualitative results. Our model consists of a one-dimensional electron gas (1DEG) coupled to bulk dispersionless LO phonons at zero temperature. Electrons interact among themselves through the Coulomb interaction and through virtual–LO-phonon exchange via the Fröhlich interaction. In calculating the effective 1D electron-phonon interaction we sum over the phonon wave vector in the other two dimensions in the standard manner.[1] The Coulomb interaction is logarithmically divergent in the 1D wave-vector space, and therefore we use the more realistic finite width quantum-wire model.[6] The LO-phonon mediated electron-electron interaction is dependent on both wave vector and frequency,

$$v_{\mathrm{ph}}(q,\omega)=M_q^2 D^0(\omega). \tag{1}$$

M_q is the 1D Fröhlich interaction matrix element given by ($\hbar=1$ throughout this paper)

$$M_q^2=v_c(q)\frac{\omega_{\mathrm{LO}}}{2}\left[1-\frac{\epsilon_\infty}{\epsilon_0}\right], \tag{2}$$

where ω_{LO} is the LO-phonon frequency, ϵ_0 (ϵ_∞) is the static (high-frequency) dielectric constant. The unperturbed LO-phonon propagator is given by

$$D^0(\omega)=\frac{2\omega_{\mathrm{LO}}}{\omega^2-\omega_{\mathrm{LO}}^2}\,. \tag{3}$$

The total effective electron-electron interaction is obtained in the random-phase approximation (RPA) (Ref. 1) by summing all the bare bubble diagrams,

$$v_{\mathrm{eff}}(q,\omega)=\frac{v_c(q)+v_{\mathrm{ph}}(q,\omega)}{1-[v_c(q)+v_{\mathrm{ph}}(q,\omega)]\Pi_0(q,\omega)}=\frac{v_c(q)}{\epsilon_t(q,\omega)}\,, \tag{4}$$

where $\Pi_0(q,\omega)$ is the complex irreducible 1D polarizability[6,8] given by the bare bubble diagram. The total dielectric function within the RPA contains contributions both from electrons and LO phonons:

$$\epsilon_t(q,\omega)=1-v_c(q)\Pi_0(q,\omega)+\frac{1-\epsilon_\infty/\epsilon_0}{\epsilon_\infty/\epsilon_0-\omega^2/\omega_{\rm LO}^2}. \quad (5)$$

The collective modes are given by the zeros of the complex total dielectric function:

$$\epsilon_t(q,\omega)=0. \quad (6)$$

In the long-wavelength limit ($q\rightarrow 0$) we get the following coupled $\omega_\pm$ collective modes from Eq. (6):

$$\omega_+(q)=\omega_{\rm LO}\left[1+\frac{\omega_{\rm LO}^2-\omega_{\rm TO}^2}{\omega_{\rm LO}^4}2r_s|\ln(qa)|q^2+O(q^4)\right], \quad (7)$$

and

$$\omega_-(q)=\frac{\omega_{\rm TO}}{\omega_{\rm LO}}2q\sqrt{r_s|\ln(qa)|}+O(q^3), \quad (8)$$

where a is the width of the 1DEG (i.e., the confinement width) and $r_s=4me^2/(\pi k_F\epsilon_0)=8/(\pi^2 n_0 a_B^*)$ with k_F as the 1D Fermi wave vector (n_0 is the 1D electron density of the sample and a_B^* the effective Bohr radius). In the long-wavelength limit ω_+ is slightly greater than $\omega_{\rm LO}$ and ω_- is slightly less than the corresponding uncoupled 1D plasmon mode ω_0:[6–8]

$$\omega_0(q)|_{q\rightarrow 0}=2q\sqrt{r_s|\ln(qa)|}. \quad (9)$$

In Fig. 1 we show our numerically calculated coupled plasmon-phonon collective modes for two different densities. We show the coupled modes ($\omega_\pm$) as well as the pure plasmon mode (ω_0) without the electron-phonon coupling. We use the parameters $\omega_{\rm TO}=33.8$ meV, $\omega_{\rm LO}=36.7$ meV, $a_B^*=0.85\times 10^{-6}$ cm for GaAs, and $a=100$ Å. It is clear from Fig. 1 that mode coupling is strong at both densities and shows up at wave vectors far from the resonance where $\omega_0(q)\approx\omega_{\rm LO}$. This 1D situation is substantially different from the corresponding 2D (Refs. 1 and 9) case where plasmon-phonon mode coupling is significant only at high densities or, equivalently, at wave vectors around the resonance ($\omega_0\approx\omega_{\rm LO}$) condition. This strong 1D plasmon-phonon coupling is a direct consequence of the logarithmic singularity in the 1D polarizability, which makes it possible for ω_0 to exist for all wave vectors leading to strong plasmon-phonon coupling. In two dimensions the low-density plasmon disappears below the LO-phonon frequency due to Landau damping, leading to weak plasmon-phonon coupling except at higher densities. Note that the plasmon-like mode ω_- in Fig. 1 vanishes at a critical wave vector, $q_c\simeq -1+\sqrt{1+\omega_{\rm TO}^2}$, and for $q>q_c$ we find only the phonon-like mode (ω_+), which approaches ω_0 for large q. This behavior is similar to the corresponding high-density 2D situation. Note that in three dimensions, with the plasmon energy (ω_0) being finite at zero wave vector, the nature of plasmon-phonon coupling is substantially different and strong mode coupling occurs[2] only for densities satisfying the resonant condition $\omega_0\approx\omega_{\rm LO}$.

The dynamical structure factor $S(q,\omega)$, which gives the spectral weight of the collective modes, is proportional to the imaginary part of the inverse dielectric function

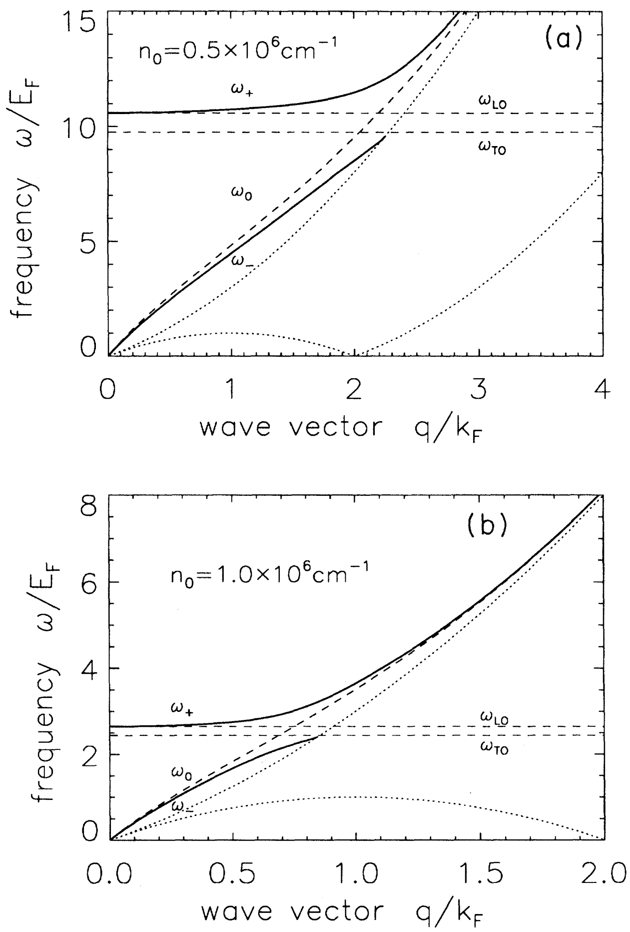

FIG. 1. Calculated collective mode dispersions ω are shown as a function of the wave vector q for two different 1D densities: (a) $n_0=0.5\times 10^6$ cm^{-1} and (b) 1.0×10^6 cm^{-1}. The plasmon dispersion without the electron-phonon coupling is shown by the dashed line (ω_0). The dotted lines are the boundaries of the 1D electron-hole single-particle excitation continuum.

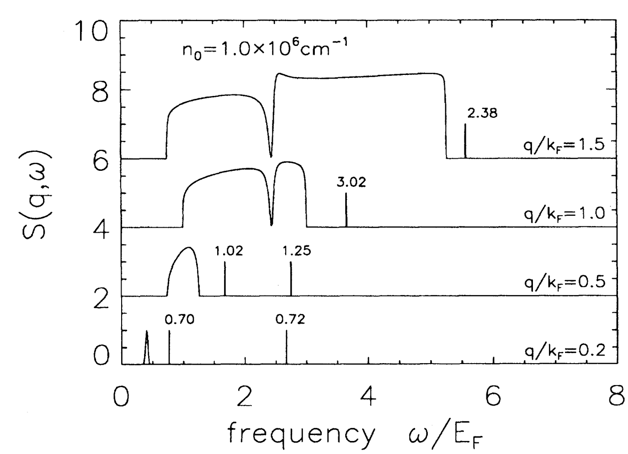

FIG. 2. Calculated structure factor $S(q,\omega)$ as a function of the frequency ω for different wave vectors q. The delta function peaks are the collective excitations with the weights written above the peaks. The strength of the electron-hole continuum has been enhanced ten times larger than the actual value for visual clarity.

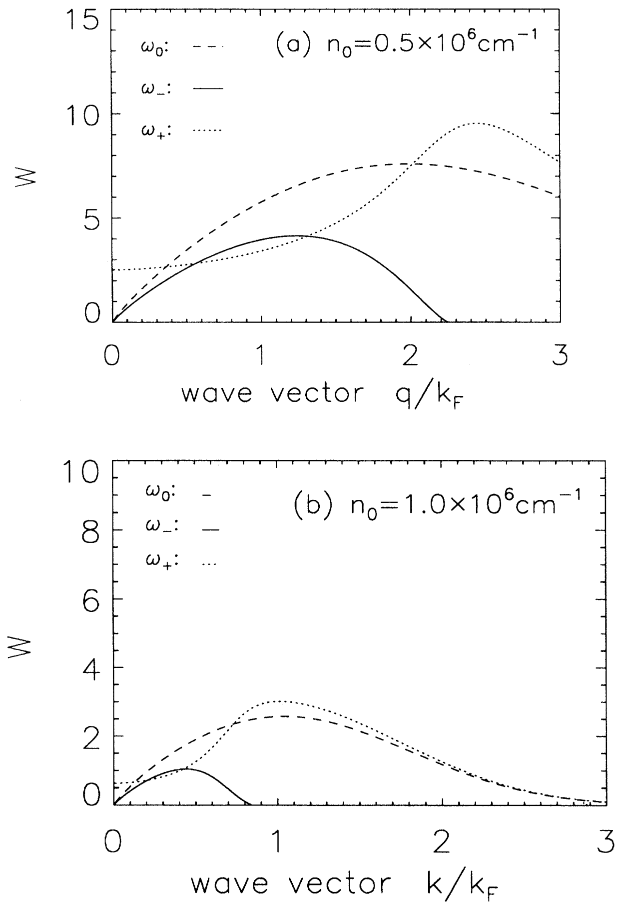

FIG. 3. Spectral weights $W(q)$ for the coupled $\omega_\pm$ and the uncoupled ω_0 modes are shown as a function of q for different densities: (a) $n_0=0.5\times10^6$ cm^{-1} and (b) 1.0×10^6 cm^{-1}.

$$S(q,\omega)=-\frac{1}{n_0 v_c(q)}\mathrm{Im}\left[\frac{1}{\epsilon_t(q,\omega)}\right]. \tag{10}$$

For a true collective mode with zero Landau damping both Im[$\epsilon_t(q,\omega)$] and Re[$\epsilon_t(q,\omega)$] vanish, and the inverse dielectric function becomes a delta function with weight

$$W(q)=\frac{\pi}{\frac{\partial}{\partial\omega}\mathrm{Re}[\epsilon_t(q,\omega)]|_{\omega=\omega_i(q)}}, \tag{11}$$

where $\omega_i(q)$, defined by Eq. (6), is the collective mode frequency at wave vector q. In the long-wavelength ($q\rightarrow0$) limit the weight of the plasmonlike mode vanishes as

$$W(q)|_{\omega_-}=\pi\left(\frac{\omega_{\mathrm{TO}}}{\omega_{\mathrm{LO}}}\right)^3 q\sqrt{r_s|(qa)|}\left[1-\left(\frac{\omega_{\mathrm{LO}}}{\omega_{\mathrm{TO}}}\right)^2\frac{2}{r_s|\ln(qa)|}\right], \tag{12}$$

and the weight of the LO-phononlike mode is finite,

$$W(q)|_{\omega_+}=\frac{\pi}{2}\frac{\omega_{\mathrm{LO}}^2-\omega_{\mathrm{TO}}^2}{\omega_{\mathrm{LO}}}. \tag{13}$$

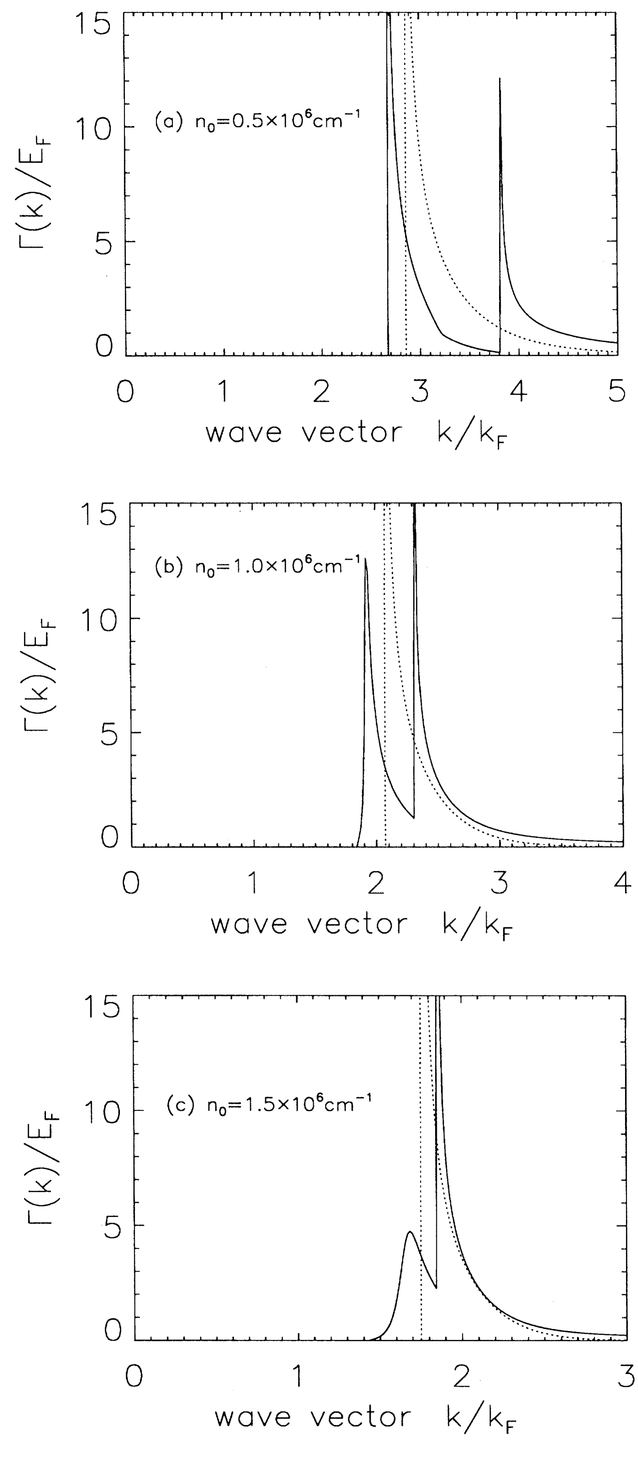

FIG. 4. Damping rates $\Gamma(k)$ of energetic 1D electrons for the uncoupled (dotted line) and the coupled (solid line) 1DEG for three different densities: (a) $n_0=0.5\times10^6$ cm^{-1}, (b) 1.0×10^6 cm^{-1}, and (c) 1.0×10^6 cm^{-1}.

In Fig. 2 the calculated RPA structure factor is shown for different wave vectors and for density $n_0=1.0\times10^6$ cm^{-1}. The weight of the electron-hole continuum is enhanced in Fig. 2 by a factor of 10 for visual clarity, and the numbers on peaks indicate the actual strengths of the collective modes. In

Fig. 3 the calculated weight W [Eq. (11)] is shown for two different densities: (a) $n_0 = 0.5 \times 10^6$ cm^{-1} and (b) $n_0 = 1.0 \times 10^6$ cm^{-1}. (Dotted and solid curves indicate the weights of the ω_- and ω_+, respectively.) For the sake of comparison we also show the weight (dashed curve) of the corresponding uncoupled plasmon ω_0, neglecting any electron-phonon coupling. The weights $W(q)$ are not normalized and only the relative weights are meaningful. In the long-wavelength limit the phononlike mode has most of the weight. In the intermediate wave-vector range, however, the plasmonlike mode becomes stronger. For large wave vectors, the weight of the ω_- mode vanishes again because the plasmonlike mode merges with the electron-hole continuum at a critical wave vector and becomes overdamped by Landau damping.

As an example of the role of plasmon-phonon coupling in a physical process we calculate the scattering rate of energetic electrons injected into the 1D quantum wire. The damping rate $\Gamma(k)$ is given by the imaginary part of the self-energy

$$\Gamma(k) = |\mathrm{Im}\Sigma[k, \xi(k)]|, \tag{14}$$

where $\xi(k) = k^2/2m - \mu$ is the energy of the "hot" electron (or, equivalently the quasiparticle energy measured with respect to the chemical potential $\mu = E_F$). The quasiparticle scattering rate $2\Gamma(k)$, the inelastic lifetime $[2\Gamma(k)]^{-1}$, and the inelastic mean free path $l(k) = k/[2m\Gamma(k)]$ can be calculated from the damping rate Γ. In Fig. 4 we show the damping rate for the uncoupled (dotted line) and the coupled (solid line) 1D system, for three different densities: (a) 0.5×10^6 cm^{-1}, (b) 1.0×10^6 cm^{-1}, and (c) 1.5×10^6 cm^{-1}. For the uncoupled 1DEG the quasiparticle scatters by plasmon emission,[6] which corresponds to the sharp threshold peak in the dotted line in Fig. 4. There is no 1D single-particle electron-electron scattering below a threshold critical wave vector because the conservation of energy and momentum restricts electron-electron scattering to an exchange of particles.[6] For the coupled 1DEG the quasiparticle decays via the emission of coupled plasmon-phonon modes (ω_- and ω_+), which correspond to the two peaks in the solid lines of Fig. 4. At low density the damping rate due to the plasmonlike ω_- mode is stronger than that due to the ω_+ mode. At high density, however, the ω_+ mode is stronger, and the situation is reversed. For very high electron density [Fig. 4(c)] we observe the excitation of an electron-hole pair just below the plasmonlike mode threshold.

In summary, we have calculated the dispersion and the spectral weight of the plasmon-phonon mode coupling in 1D semiconductor quantum wires at zero temperature and within RPA. We also calculate the 1D electronic inelastic scattering rate due to coupled plasmon-phonon mode emission. Our most important qualitative result is that the mode-coupling effect is strong in a 1DEG at all densities and wave vectors in contrast to the corresponding higher-dimensional situations.

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