Total dielectric function approach to the electron Boltzmann equation for scattering from a two-dimensional coupled mode system

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Abstract

The nonequilibrium total dielectric function lends itself to a simple and general method for calculating the inelastic collision term in the electron Boltzmann equation for scattering from a coupled mode system. Useful applications include scattering from plasmon-polar phonon hybrid modes in modulation doped semiconductor structures. This paper presents numerical methods for including inelastic scattering at momentum-dependent hybrid phonon frequencies in the low-field Boltzmann equation for two-dimensional electrons coupled to bulk phonons. Results for mobility in GaAs show that the influence of mode coupling and dynamical screening on electron scattering from polar optical phonons is stronger for two dimensional electrons than was previously found for the three dimensional case.

I. INTRODUCTION

The importance of hybridization of collective modes has been pointed out in the context of several semiconductor systems. Examples include hybrid optical modes in thin semiconductor layers [1], coupled intraband-interband excitations of quasi-one-dimensional electron systems [2], and, more commonly, plasmon–phonon coupled modes in doped polar semiconductors.
ductors \cite{3,5}. To the extent that electron scattering depends on the energies and interaction strengths of the system modes, a reliable theory of electron transport depends on treating mode-coupling effects accurately.

In the Born approximation, the interaction between a conduction electron and a coupled electron-phonon system can be represented as an effective electron-electron interaction screened by the nonequilibrium total dynamic dielectric function $\epsilon_T(q, \omega)$, which includes contributions from both electrons and phonons. Recent work \cite{4,5} shows that $\epsilon_T(q, \omega)$ provides a systematic way to determine the collision term in the electron Boltzmann equation for scattering against dynamically screened coupled electron-phonon modes. The result is the sum of an electron-electron collision term and an electron-LO phonon collision term that includes plasmon-phonon mode coupling. Both interactions are dynamically screened by only the electronic part of the total dielectric function for the electron-phonon system. In the random-phase approximation (RPA), the electron-phonon part contains a phonon self-energy that arises from the polarization of the electron gas. \cite{6} The self-energy correction modifies the longitudinal-optical (LO)-phonon dispersion in doped polar semiconductors, producing hybrid normal modes with phonon strength in each. Numerical results \cite{5} for bulk n-type GaAs show that mode-coupling and dynamical screening should significantly influence electron mobilities in modulation doped structures.

The present paper describes numerical methods for exactly solving the low-field Boltzmann equation for two-dimensional electrons coupled to bulk LO phonons, including dynamical screening and mode coupling for arbitrary electron degeneracy and spherical energy surfaces. In particular, the method for including phonon dispersion in the collision integrals is discussed. The phonon distribution is approximated by its equilibrium form, and the plasmon-pole approximation \cite{7} is used in the LO phonon self-energy to determine the hybrid mode frequencies. Results for GaAs show that mode coupling and dynamical screening are more important for two dimensional electrons than for the three dimensional case.
II. INELASTIC SCATTERING FROM HYBRID PHONONS WITH DISPERION

The collision integrals in the electron Boltzmann equation for doped polar semiconductors contain the momentum-dependent frequencies of the hybrid LO phonon modes [4]. Using the plasmon-pole approximation in the phonon self-energy, the differential scattering rate due to transfer of momentum $q = k - p$ to the hybrid phonons is [4,5]

$$W_{\text{LO}}(k, p) = -\frac{2 M^2_q}{\Omega h|\epsilon(q, \omega_{k,p})|^2} [N(\omega_{k,p}) + 1] \text{Im}[D^+(q, \omega_{k,p}) + D^-(q, \omega_{k,p})]$$

where $M^2_q = v_q (\epsilon^{-1}_\infty - \epsilon^0_0) h \omega^2_{\text{LO}} / 2 \omega_{\text{TO}}$ and $h \omega_{kp} = E_k - E_p$. Here, $\omega_{\text{LO}}$ and $\omega_{\text{TO}}$ are the LO and transverse optical phonon frequencies, while $\epsilon_\infty$ and $\epsilon_0$ are the high-frequency and static dielectric constants, respectively. In two dimensions, $v_q = 2 \pi e^2 / q \epsilon_\infty$. The frequencies $\tilde{\omega}_p, \omega_+,$ and $\omega_-$ are given by

$$\tilde{\omega}_p^2 = \omega^2_p [1 - \epsilon^{-1}(q, 0)]^{-1}$$

$$\omega^2_\pm = \frac{1}{2} \left\{ \omega^2_{\text{LO}} + \tilde{\omega}_p^2 \pm \left[ (\omega^2_{\text{LO}} - \tilde{\omega}_p^2)^2 + 4 \omega^4_p (\omega^2_{\text{LO}} - \omega^2_{\text{TO}}) \right]^{1/2} \right\},$$

where $\omega_p = (2 \pi n e^2 q / m^* \epsilon_\infty)^{1/2}$ is the plasmon frequency of the two-dimensional electron gas with concentration $n$ and effective mass $m^*$. The weight factors $(\omega^2_\pm - \tilde{\omega}_p^2) (\omega^2_\pm - \omega^2_{\text{TO}})^{-1}$ in $\text{Im}[D^\pm]$ give the phonon strength in each of the hybrid $\omega_\pm$ modes, so that the differential scattering rate $W_{\text{LO}}$ is the rate for scattering from only the phonon component of the hybrid modes. The screening function in [4] is the temperature-dependent RPA dielectric function, $\epsilon(q, \omega) = 1 - \nu^\infty_q P(q, \omega)$, for the two-dimensional electron gas.

The iterative procedure used here for solving the low-field Boltzmann equation was described in reference [5]. One assumes a linear form for the nonequilibrium electron distribution, $f(k) = f^0_k + x_k g_k$, where $f^0_k$ is the equilibrium (Fermi-Dirac) distribution, $x_k$ is the cosine of the angle between the electric field $F$ and $k$, and $g_k$ is an unknown function that is linear in $F$. Neglecting all scattering mechanisms except electron-LO-phonon gives
\[ g_k = \left[ \nu_{LO}[g] - \frac{eF \partial f^0_k}{\hbar} \right] \left[ \tau_{LO}^{-1}(k) \right]^{-1}, \]  
\[ \tau_{LO}^{-1}(k) = \frac{1}{\Omega} \sum_{p} \{ W^{LO}(k, p)[1 - f^0_p] + W^{LO}(p, k)f^0_p \}, \]  
\[ \nu_{LO}[g] = \frac{1}{\Omega} \sum_{p} g_{kp} \{ W^{LO}(k, p)[1 - f^0_k] + W^{LO}(p, k)f^0_k \}, \]  
and \( x_{kp} \) is the cosine of the angle between \( k \) and \( p \).

The form of the phonon Green’s function in equation (2) implies that the energy conservation relation between initial and final electron states, \( E_k - E_{k-q} = \pm \hbar \omega(q) \), is dependent on the momentum transfer \( q \) through the phonon dispersion. In three dimensions, it is convenient to choose \( q \) as an integration variable when calculating \( \nu_{LO} \) and \( \tau_{LO}^{-1} \). In this case, one must determine the integration limits by finding the points where the phonon dispersion curve \( \omega(q) \) intersects the absorption region \( q^2 + 2kq \leq 2m^*\omega(q)/\hbar \leq q^2 - 2kq \) and the emission region \( 2m^*\omega(q) \leq -q^2 + 2kq \). For the case of two-dimensional electrons, it appears that \( q \) is not a preferred choice for integration variable, since the integrand then diverges at the integration limits. Instead one can choose \( \theta_{kp} \), the angle between \( k \) and \( p \). In this case, one must determine the implicit relation between \( q \) and \( \theta_{kp} \) at each integration step by finding the (nonzero) root of the function \( f(q) = q^2 - k^2 - p_\pm^2 + 2kp_\pm \cos \theta_{kp} \) with \( p_\pm = (k^2 \pm 2m^*\omega_\pm/\hbar)^{1/2} \).

Scattering from the LO phonon part of the hybrid modes gives the inverse lifetime \( \tau_{LO}^{-1}(k) \) and functional \( \nu_{LO}[g] \),

\[ \tau_{LO}^{-1}(k) = \sum_{\lambda = \pm} \lambda \left\{ \int_0^{2\pi} d\theta_{kp} I(q, \omega_\lambda)[N(\omega_\lambda) + 1 - f^0_{k_\lambda^-}] \Theta(E_k - \hbar \omega_\lambda) + \int_0^{2\pi} d\theta_{kp} I(q, \omega_\lambda)[N(\omega_\lambda) + f^0_{k_\lambda^+}] \right\}, \]  
\[ \nu_{LO}[g] = \sum_{\lambda = \pm} \lambda \left\{ \int_0^{2\pi} d\theta_{kp} I(q, \omega_\lambda)g(k_\lambda^-) \cos(\theta_{kp}) \left[ N(\omega_\lambda) + f^0_k \right] \Theta(E_k - \hbar \omega_\lambda) + \int_0^{2\pi} d\theta_{kp} I(q, \omega_\lambda)g(k_\lambda^+) \cos(\theta_{kp}) \left[ N(\omega_\lambda) + 1 - f^0_k \right] \right\}, \]  
where \( k_\lambda^\pm = (k^2 \pm 2m^*\omega_\lambda/\hbar)^{1/2} \) and

\[ I(q, \omega_\lambda) = \frac{e^2 \omega_{LO}^2 m^*}{2q_\lambda \hbar^2} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \left| \epsilon(q, \omega_\lambda) \right|^{-2} \frac{(\omega_\lambda^2 - \omega_p^2)}{(\omega_\lambda^2 - \omega_\lambda^-)} \].
III. RESULTS AND CONCLUSIONS

Figures 1 and 2 present electron mobility as a function of concentration in GaAs at 300 K and 77 K, showing the effects of dynamic screening and mode coupling on the electron-LO phonon interaction. The mobilities were calculated by averaging the electron velocity over the nonequilibrium distribution \( f(k) \), found by solving the iterative equation (5). Without plasmon-phonon coupling, dynamic RPA screening gives mobilities that are lower than static RPA or Thomas-Fermi results, but higher than the unscreened case. The difference between static and dynamic screening has a strong momentum dependence. The inverse dynamic RPA dielectric function evaluated at \( \omega = \omega_{LO} \) has a strong peak \( (\epsilon^{-1} > 1) \) at small \( q \) where the plasmon dispersion crosses \( \omega_{LO} \), but is smaller than the inverse static dielectric function at larger \( q \) values. The small \( q \) values, where antiscreening and enhanced forward scattering occur, are accessible only for high energy electrons, since the minimum \( q \) value allowed by energy conservation is \( q_{\text{min}} = \left| k - (k^2 + 2m^*\omega_{LO}/\hbar)^{1/2} \right| \). Previous authors [8] have noted similar effects in calculations of dynamical screening of the electron-LO phonon interaction.

When plasmon-phonon coupling is included in the plasmon-pole model, the phonon spectral function \(-\pi^{-1}\text{Im}[D(q,\omega)]\) has two peaks with frequencies \( \omega_+ \) and \( \omega_- \) given by (4). Mobilities are expected to be lower when mode coupling is included, because of increased low-energy electron-phonon scattering due to the \( \omega_- \) mode. Figures 1 and 2 show that this is in fact the case. As in three dimensions [5], mode coupling works to reduce electron mobility especially for low densities at 77K where the thermal occupation of the low-energy hybrid mode is exponentially larger than the high-energy hybrid mode or uncoupled phonon mode. The effect is more pronounced in two dimensions, consistent with previous conclusions concerning the effect of dimensionality on polaronic damping. [3]
REFERENCES

[1] B.K. Ridley, “Hybrid optical modes and their interactions with electrons,” in *Phonons in Semiconductor Nanostructures*, edited by J.-P. Leburton, J. Pascual, and C. S. Torres, (Kluwer, 1993, Dordrecht), p. 25.

[2] Q.P. Li and S. Das Sarma, “Collective excitation spectra of one-dimensional electron systems,” Phys. Rev. B 40, 5860 (1989).

[3] J.F. Young and P.J. Kelly, “Many-body treatment of hot-electron scattering from quasiequilibrium electron-hole plasmas and coupled plasmon-longitudinal-optic-phonon modes in GaAs,” Phys. Rev. B 47, 6316 (1993); E.H. Hwang and S. Das Sarma, “Plasmon-phonon coupling in one dimensional semiconductor quantum wire structures,” Phys. Rev. B 52, R8668 (1995).

[4] B.A. Sanborn, “Nonequilibrium total-dielectric-function approach to the electron Boltzmann equation for inelastic scattering in doped polar semiconductors,” Phys. Rev. B 51, 14247 (1995).

[5] B.A. Sanborn, “Electron-electron interactions, coupled plasmon-phonon modes, and mobility in $n$-type GaAs,” Phys. Rev. B 51, 14256 (1995).

[6] G.D. Mahan, *Many Particle Physics* (Plenum, New York, 1990), Section 6.3.

[7] A.W. Overhauser, “Simplified Theory of Electron Correlations in Metals,” Phys. Rev. B 3, 1888 (1971);

[8] C.H. Yang and S.A. Lyon, “Dynamical Screening of the Electron-Optical Phonon Interaction in Two Dimensions,” Physica 134B, 309 (1985); P.J. Price, “Two-dimensional electron transport in semiconductor layers II: Screening,” J. Vac. Sci. Technol. 19, 599 (1981).

[9] S. Das Sarma and B.A. Mason, “Optical Phonon Interaction Effects in Layered Semiconductor Structures,” Ann. Phys. (N.Y.) 163, 78 (1985).
FIGURES

FIG. 1. Effects of screening and mode coupling on LO phonon limited mobility of two-dimensional electrons in GaAs at 300K. The dynamically screened coupled mode mobility calculation (solid curve) is compared to mobilities determined by scattering from uncoupled LO phonons screened in the Thomas-Fermi approximation (long-dashed curve), static RPA (short-dashed curve), dynamic RPA (dotted curve), and unscreened (dot-dashed curve). All other scattering mechanisms are neglected.

FIG. 2. Effects of screening and mode coupling on LO phonon limited mobility of two-dimensional electrons in GaAs at 77K. Mobility curves are represented as in Figure 1.
Mobility ($10^5 \text{ cm}^2/\text{V sec}$) vs. Electron concentration ($10^{11} \text{ cm}^{-2}$) at 77 K.