PHYSICAL REVIEW B VOLUME 31, NUMBER 8 15 APRIL 1985

Screening of polar interaction in quasi-two-dimensional semiconductor microstructures

S. Das Sarma and B. A. Mason
Center for Theoretical Physics, Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
(Received 14 January 1985)

The effect of free-carrier screening on polarons in semiconductor heterostructures and quantum wells is considered with particular reference to GaAs-based experimental systems. It is shown that screening has an appreciable effect on quantities like the polaronic binding energy and the effective-mass renormalization as well as on the polar scattering rate. Different models for the screened polar interaction are compared quantitatively and the importance of using wave-vector-dependent screening in the theory is established.

A thorough quantitative understanding of the polar electron-LO phonon ("polaron") interaction in high-mobility two-dimensional (2D) systems like GaAs-AlGaAs heterostructures and quantum wells is very important with respect to both the device operation and the fundamental physics of these systems. The polaron interaction is an important factor in determining the high-temperature mobility[1] and the hot-electron properties[2] of these systems. On a microscopic level this interaction renormalizes the carrier effective mass, an effect which may show up in cyclotron resonance experiments[3] under suitable conditions.

Our objective in this paper is to obtain a quantitative estimate of the free-carrier screening effect on the polar optical-phonon interaction in quasi-two-dimensional semiconductor microstructures. With the exception of a publication[4] by one of us, screening effects have virtually been completely ignored in the literature on polar optical-phonon interaction in quasi-two-dimensional structures. This is surprising in view of the fact that 2D screening is stronger than the corresponding 3D effect and for three-dimensional doped polar semiconductors (e.g., InSb) free-carrier screening was shown to be important as early as 1959 by Ehrenreich.[5] In this Rapid Communication we provide a rather complete quantitative picture of screening effects on various polaronic quantities like the binding energy, the polaronic-mass renormalization, and the electron-LO phonon scattering rate in realistic confined semiconductor structures. Our actual numerical results are for the well-studied modulation-doped GaAs-AlGaAs system, even though the theory itself is quite general and applies to all 2D structures. We find that screening effects are substantial and, for GaAs systems, one would make quantitative errors by as much as a factor of 10 by neglecting screening. This calls into question most of the theoretical work[6] done on this subject to date since screening is usually neglected[7] (except for a formal discussion in Ref. 7) in these calculations. In fact, we find that for the usual range of electron densities in GaAs heterostructures screening is more effective in reducing the strength of the polar interaction than the usual form factor effect[8,9] arising from the subband wave functions associated with the carrier confinement. Screening and form-factor effects together reduce polaronic-interaction effects in these 2D structures below the corresponding 3D results even though the intrinsically pure 2D polaronic effects are much stronger[4,9] than the corresponding 3D situation.

The central quantity in our calculation is the electronic self-energy due to the polar interaction, which in the leading-order approximation is given by ($\hbar=1$ throughout),

$$\sum_{ij}(\mathbf{k},i\omega_n) = -(\beta^{-1})\sum_{\mathbf{q}}\sum_{i\nu_l}\sum_{\lambda_1\lambda_2} u_{i\lambda_1\lambda_2 j}(\mathbf{q},i\nu_l)\,G_{\lambda_1\lambda_2}(\mathbf{k}-\mathbf{q};i\omega_n-i\nu_l)\ , \tag{1}$$

where $\beta=(k_BT)^{-1}$; i,j,λ_1,λ_2 are subband indices, u is the screened electron-phonon-electron interaction, and G is the electron Green's function. The frequencies $\omega_n=(2n+1)\pi/\beta$ and $\nu_l=2l\pi/\beta$ with $n,l=0,\ \pm1,\ \pm2$, etc., are the standard Matsubara frequencies and $\mathbf{k},\mathbf{q}$ are 2D wave vectors. The leading-order self-energy approximation has been shown[9] to be quite good for systems of our interest with their weak polar coupling. We evaluate the self-energy given in Eq. (1) by following the prescription[9] of Das Sarma and Mason. In evaluating the self-energy we make only the following approximations. (i) We make a 1-subband approximation which should be valid in GaAs systems for $N_s<7\times10^{11}\ \mathrm{cm}^{-2}$. (ii) We calculate the screened polar interaction by using the static random-phase approximation (RPA) whence the interaction becomes

$$u(q,i\nu_l)=\left(\frac{\pi\alpha}{q}\right)\left(\frac{2\omega_{\mathrm{LO}}^3}{m}\right)^{1/2}\left(\frac{2\omega_{\mathrm{LO}}}{(i\nu_l)^2-\omega_{\mathrm{LO}}^2}\right)F(q)[\epsilon(q,0)]^{-2}\ , \tag{2}$$

where $F(q)$ is the form factor[8,9] associated with the 2D confinement and $\epsilon(q,0)$ is the static dielectric function[8,9] of the system. The use of the static screening has been shown[5] to be quantitatively accurate in 3D systems and we assume its applicability in our systems as well. The electron-phonon coupling strength is given by the dimensionless Fröhlich coupling constant α which for GaAs is 0.07. (iii) The subband wave functions are obtained in the Stern-Howard variational scheme which has recently been shown[10] to be a fairly accurate description for the GaAs heterostructure.

The calculation of polaron binding energy (E_p), polaron effective mass (m_p), and the electron-phonon scattering rate (Γ) from the polaron self-energy Σ [Eq. (1)] is standard and has been described in detail[9] elsewhere. In this Rapid Communication we will only give representative results for E_p, m_p, and Γ for GaAs-based quasi-2D systems using a variety of screening approximations.

In Fig. 1 we show the weak-coupling polaron binding en-

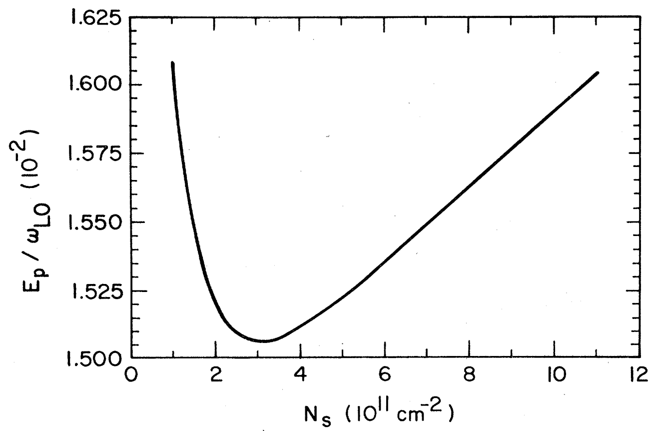

FIG. 1. Shows the polaronic-binding energy E_p (in units of $\omega_{LO} \simeq 35$ meV for GaAs) as a function of 2D carrier density N_s in a GaAs heterostructure (purely 2D and 3D unscreened values are, respectively, 0.11 and 0.07).

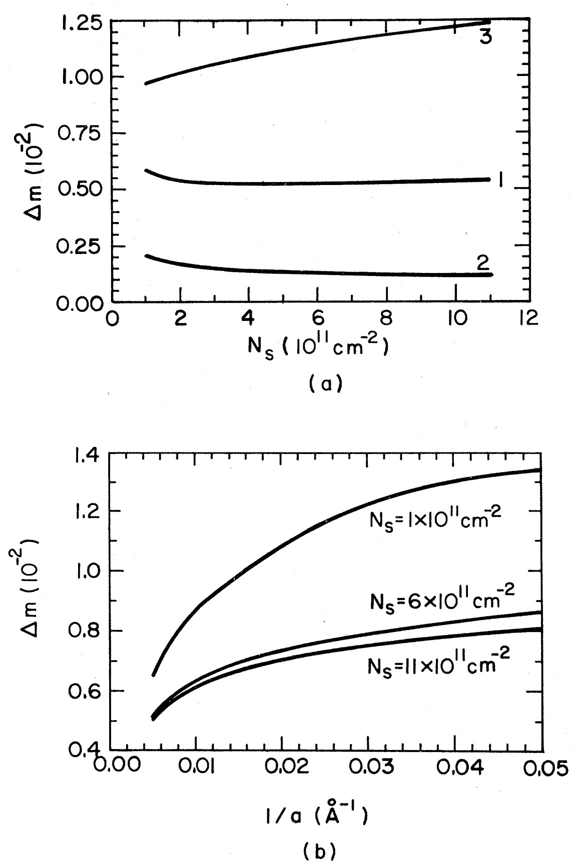

Fig. 2. (a) shows the effective-mass renormalization $\Delta m = (m_p - m)/m$, where m_p, m are polaron and band masses, respectively) as a function of N_s in a GaAs heterostructure. Curves 1, 2, and 3 correspond, respectively, to the unscreened approximation, 2D screening result without form factor, and the complete result with both screening and form factor (purely 2D and 3D unscreened values for Δm are, respectively, 0.027 and 0.012). (b) shows Δm as a function of $1/a$ (where a is the well thickness) in a GaAs quantum well structure. The three curves correspond to three different values of $N_s = 1, 6, 11 \times 10^{11}$ cm^{-2}. (N_s and a are assumed to be independent of each other.) Results include screening and form-factor effects.

ergy E_p as a function of 2D carrier density N_s for a GaAs heterostructure ($\alpha = 0.07$) in the units of ω_{LO}($\simeq 35$ meV for GaAs). The results[4,9] for the purely 2D and 3D unscreened limits are 0.11 and 0.07, respectively. There are two important aspects of Fig. 1 which we want to emphasize. The first one is that E_p is substantially (by about a factor of 7) reduced from the purely 2D result by the combined effects of subband form-factor and free-carrier screening. The second point is the interesting variation in E_p as a function of the 2D carrier density N_s. The minimum in Fig. 1 arises from a competition between screening and subband-confinement effects—screening effects increase with increasing N_s whereas the form factor is reduced since the inversion layer is becoming more two dimensional at higher N_s. Even though the variation in E_p is small (of the order of only 10%), the minimum in E_p as a function of N_s is an interesting result of the effect of the full random-phase approximation (RPA) screening (i.e., *wave-vector-dependent* screening) that we employ in our theory as against the Thomas-Fermi (i.e., the long-wavelength) approximation which is commonly used. Thomas-Fermi screening in 2D is independent of N_s (Ref. 11) and, therefore, would not produce[4] the interesting variation shown in Fig. 1. It may be worthwhile to remark that the actual magnitude for E_p($\simeq 0.016$ ω_{LO}) is only about 0.5 meV in GaAs systems and is not an experimentally relevant quantity. On the other hand, in a more polar material like CdTe, E_p could be of the order of 5 meV producing experimentally relevant shifts of band edge and affecting the impurity-binding energies.

In Fig. 2 we show the polaronic mass renormalization $\Delta m = (m_p - m)/m$ (scaled with respect to bare mass m) which has a value of $\pi\alpha/8$ ($\simeq 0.027$ for GaAs) in the purely 2D unscreened limit. We show Δm in Fig. 2(a) as a function of N_s in a GaAs heterostructure for three different approximations: (1) Screening (full RPA) and form-factor effects both included; (2) form-factor effect excluded but purely 2D screening effect included; (3) no screening but form-factor effect included. There are a number of significant features of Fig. 2(a) worth mentioning. Note that the curve 2 is monotonically decreasing (since screening increases with N_s) and curve 3 is monotonically increasing (since the form-factor effect decreases as the system is becoming more 2D at large N_s). These two variations tend to cancel each other somewhat (as for E_p) and the actual variation in Δm (as shown in curve 1) with N_s is rather small ($\Delta m \simeq 0.005$, a factor of 5–6 smaller than the purely 2D result) with a shallow minimum because of the competition between screening and form-factor effects. These results also make explicit the fact that for actual GaAs heterostructures screening and form-factor effects are both essential for obtaining quantitative polaronic corrections. We also conclude (compare curve 3 with curve 2) that purely 2D screening overestimates the screening effect (this is even more true if one uses the long-wavelength Thomas-Fermi formula which will reduce Δm by almost a factor of 2 even compared with curve 2 in Fig. 2).

In Fig. 2(b) we show the mass renormalization Δm for a GaAs quantum-well structure as a function of the (inverse) well thickness (a) in angstroms. For this calculation we assume that the well thickness (a) and the 2D electron density (N_s) in the well are independent variables. We obtain[9] the form factor by making the usual square-well approximation which should be good at low N_s. The difference in Δm in Fig. 2(b) for different values of N_s (but fixed a) is entirely due to screening. We conclude that screening effects could be substantial.

In Fig. 3 we show the electronic scattering rate (Γ) due to the polar Fröhlich interaction. Formally[9] it is just the imaginary part of the polaron self-energy given in Eq. (1). In Fig. 3(a) we show Γ as a function of the temperature (T) for a fixed electron density of $N_s = 3\times 10^{11}$ cm^{-2} in a GaAs heterostructure. Six different screening approximations have been employed which have been labeled 1–6 in order of increasing sophistication: (1) purely 2D result without any screening or form-factor effect; (2) no screening, but includes form-factor effect; (3) classical Debye screening;[9] (4) zero-temperature Thomas-Fermi screening; (5) zero-temperature finite wave-vector RPA screening;[11] and (6) finite-temperature finite wave-vector screening[12] [the results in (2)–(6) include quasi-2D form-factor effect].

In Fig. 3(b) we show the scattering rate as a function of quasiparticle energy E (measured from the Fermi energy) at a fixed low temperature ($T = 50$ K) for a GaAs heterostructure with fixed electron density $N_s = 3\times 10^{11}$ cm^{-2}. At such a low temperature ($k_B T/\omega_{LO} \simeq 0.1$) most of the scattering is due to LO-phonon emission and, therefore, Fig. 3(b) has a sharp threshold at $E = \omega_{LO}$ above which phonon emission is allowed. The behavior of the scattering rate at the threshold is much sharper in 2D systems compared with the corresponding 3D systems as has been emphasized[9] by us elsewhere. The six curves in Fig. 3(b) correspond to the same six screening approximations employed for Fig. 3(a). Screening is seen to have a substantial effect on the calculated scattering rate.

On the basis of the above results we conclude that for obtaining results which are quantitatively correct to within 10%, one has to use finite wave-vector RPA screening for calculating polar interaction, except at rather high temperatures (>300 K) where classical Debye screening seems to be a good approximation. This conclusion is similar to that[13] of Stern who concluded, for entirely different reasons, that finite wave-vector screening effects are important for impurity-scattering limited transport in 2D systems. It seems that long-wavelength Thomas-Fermi screening approximation is quantitatively a poor approximation for 2D semiconductor systems and should be avoided if possible.

We conclude by stating that we have calculated polaronic-binding energy and mass, and polar scattering rate in realistic quasi-2D microstructures like GaAs heterostructures and quantum wells by using a variety of screening approximations for the polar interaction. To our knowledge this is the first such calculation including form-factor, screening, and Fermi statistics effects in realistic systems. Our calculation clearly shows the quantitative importance of finite wave-vector screening in understanding polar interaction in realistic quasi-2D systems.

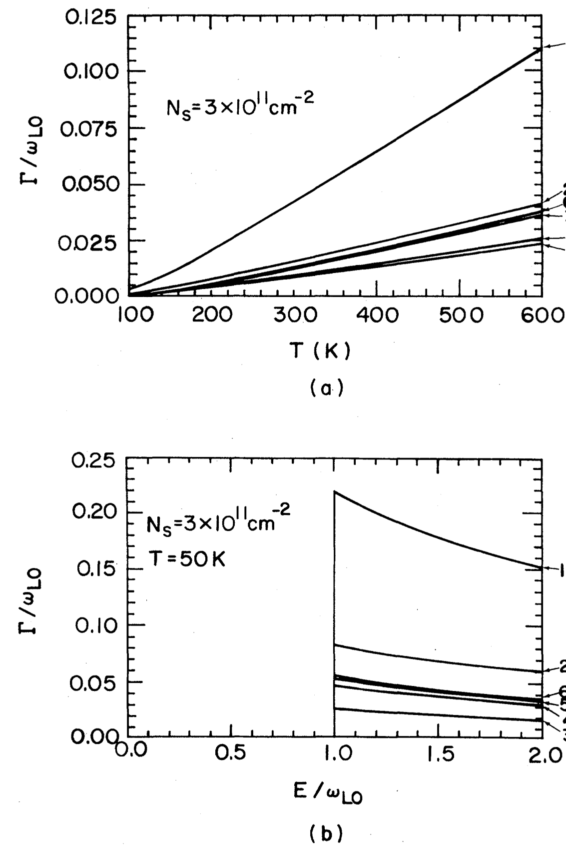

FIG. 3. (a) shows the polar scattering rate Γ as a function of temperature T in a GaAs heterostructure for six different screening approximations labeled 1–6 (as explained in the text) at a fixed $N_s = 3\times 10^{11}$ cm^{-2}. (b) shows $\Gamma(E)$ as a function of electron energy E (measured from E_F) in a GaAs heterostructure at fixed N_s ($=3\times 10^{11}$ cm^{-2}) and T ($=50$ K) for the same six screening approximations as in (a).

The work has been supported in part by the Office of Naval Research through Contract No. N00014-84-K-0586 and by the National Science Foundation under Grant No. NSF-DMR-82-13768. We are grateful to the University of Maryland Computing Center for providing the computer time.

[1]B. Vinter, Appl. Phys. Lett. **45**, 581 (1984).
[2]J. Shah, A. Pinczuk, H. L. Störmer, A. C. Gossard, and W. Wiegmann, Appl. Phys. Lett. **44**, 322 (1984); **42**, 55 (1983).
[3]M. Horst, U. Merkt, and J. P. Kotthaus, Phys. Rev. Lett. **50**, 754 (1983).
[4]S. Das Sarma, Phys. Rev. B **27**, 2590 (1983).
[5]H. Ehrenreich, J. Phys. Chem. Solids **8**, 130 (1959).
[6]See, for example, M. Walukiewicz *et al.*, Phys. Rev. B **30**, 4571 (1984), and references therein.
[7]P. J. Price, J. Vac. Sci. Technol. **19**, 599 (1981).
[8]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[9]S. Das Sarma and B. A. Mason, Ann. Phys. (N.Y.) (to be published).
[10]F. Stern and S. Das Sarma, Phys. Rev. B **30**, 840 (1984).
[11]F. Stern, Phys. Rev. Lett. **18**, 546 (1967).
[12]P. Maldague, Surf. Sci. **73**, 296 (1978).
[13]F. Stern, Phys. Rev. Lett. **44**, 1469 (1980).