Ground-state energy of the polaron gas in two-dimensional semiconductor microstructures

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The properties of the ground-state energy of a gas of quasi-two-dimensional interacting polarons are investigated by using the self-consistent theory of Singwi, Tosi, Land, and Sjölander to the response function of the electron system. The electron-phonon contribution to the ground-state energy is calculated for the electron gas confined in GaAs-$Al_xGa_{1-x}As$ heterojunctions and quantum wells with appropriate form factors to take the finite width of the electron layer into account. For the sake of comparison, different approximations (Hubbard, random-phase approximation, and Hartree-Fock) for the screening are also considered.

I. INTRODUCTION

A very exciting application of the polaron theory involves many-body systems, where we have to include the electron-electron interaction along with the electron-phonon interaction. A suitable three-dimensional (3D) system in which we must consider both interactions is a highly doped polar semiconductor.[1] In two dimensions (2D), electrons trapped in GaAs-$Al_xGa_{1-x}As$ heterojunctions and quantum wells have served as an ideal system for studying the electron-phonon interaction screened by the interacting electron gas. In these systems, the density of electrons can be experimentally varied over a wide range and, in some modulation-doped samples, the electrons are far apart from the impurities in such a way that the high-temperature mobility is limited only by the electron coupling to phonons. In addition, correlation effects are much stronger in 2D than in 3D.[2-4]

Das Sarma[5] was the first to incorporate screening effects in the polar-optical-phonon interaction in order to understand surprising experimental results which indicated that polaronic effects in quasi-2D semiconductor structures are much smaller than those in the 3D counterpart. The screening was treated within the Thomas-Fermi approximation (TFA), which has the undesirable property of giving density-independent results for the polaronic quantities. Even though the effects of the finite width of the electron layer, by itself, could not explain the experimental data, it should also be included to interpret correctly the cyclotron-resonance measurement.[5-7]

More recently, Das Sarma and Mason[8] have used the static dielectric function $\epsilon(q,0)$ in the random-phase approximation (RPA) to screen the electron-phonon interaction in single-particle expressions of polaron quantities such as the binding energy and the renormalized mass.

Screening effects in quasi-2D systems have also been studied by Wu, Peeters, and Devreese[9] by using a different approach, which was previously developed to investigate the ground-state properties of an interacting polaron gas in degenerate semiconductors.[10] In this theory, the ground-state energy of the polaron gas is expressed in terms of the structure factor of the electron system in the absence of the electron-phonon interaction. Then, the structure factor was evaluated within the RPA. However, it is well known that the RPA only gives good results at high densities and it has shown a number of quantitative deficiencies. The failure of the RPA manifests itself in the large negative values of the pair correlation function, the Fourier transform of the structure factor, at small distances. As a consequence, the RPA grossly overestimates the correlation energy of the electron gas. Another deficiency of the RPA is that, as in the TFA, it leads to a free value of the screening length. This fact is essential from the point of view of describing screening effects on the electron-phonon interaction. Then, it is necessary to go beyond RPA in order to get a quantitative understanding of the screening of polaron effects.

In this paper we calculate the electron-phonon contribution to the ground-state energy of a quasi-two-dimensional polaron gas by treating the electron-electron interaction effects in mean-field approximations beyond RPA. The electron-phonon coupling is considered within a lowest-order perturbation scheme. We use the dynamical screening approach, as discussed in Ref. 9. The structure factor of the interacting electron system is calculated by a new method recently developed by de Freitas *et al.*[3] This approach provides an accurate way to incorporate local-field corrections in several approximations to the density-density response function. The local-field factors are calculated in the approximation of Singwi, Tosi, Land, and Sjölander (STLS) and in the Hubbard approximation (HA).[11] Even though there is some

experimental evidence[12,13] of the electron interaction with interface modes in semiconductor heterojunctions, we here consider only the coupling of the confined electrons to the relevant bulk LO phonons. Previous studies are concerned with polaron effects in the quasi-two-dimensional electron gas (2D EG) in a single heterojunction only. We shall also extend these studies to include the influence of the thickness of the electron layer in semiconductor quantum wells.

The paper is organized as follows: in Sec. II, for the sake of completeness, we present a brief outline of the canonical transformation theory as generalized for a many-polaron system in order to obtain the electron-phonon correction to the ground-state energy. We review the essentials of the calculation of the structure factor in the self-consistent STLS theory and in the HA. Section III contains the numerical results, discussions, and conclusions in the case of GaAs-$Al_xGa_{1-x}As$ heterojunctions and quantum wells. For comparison, we also show the results within the Hartree-Fock approximation (HFA) and the RPA.

II. THEORETICAL FORMULATION

We consider a 2D interacting polaron gas, at zero temperature, which is described by the Hamiltonian

$$H=H_0+H_{e\text{-}e}+H_{e\text{-ph}} , \tag{1a}$$

where

$$H_0=\sum_k \frac{\hbar k^2}{2m} c_k^\dagger c_k+\sum_q \hbar\omega_{\rm LO} a_q^\dagger a_q , \tag{1b}$$

$$H_{e\text{-}e}=\tfrac{1}{2}\sum_{k,p_1,p_2} V(p_2) c_{k+p_2}^\dagger c_{p_1-p_2}^\dagger c_{p_1} c_k , \tag{1c}$$

$$H_{e\text{-ph}}=\sum_{k,q} M_q (a_q^\dagger + a_{-q}) c_{k+q}^\dagger c_k . \tag{1d}$$

Here $a_q^\dagger$ and a_q are the creation and annihilation operators for bulk LO phonons with energy $\hbar\omega_{\rm LO}$ and wave number q, whereas $c_k^\dagger$ and c_k, respectively, create and annihilate an electron with a 2D wave vector k, which is described by the wave function

$$\psi(\mathbf{r},z)=\psi_0(z)\exp(i\mathbf{k}\cdot\mathbf{r}) . \tag{2}$$

We do not consider here the electron intersubband scattering because the transition rate is quite small, and we restrict ourselves to the extreme quantum limit, where only the lowest subband is occupied. H_0 includes both the kinetic energy of the electrons and the contribution of free phonons. $H_{e\text{-}e}$ describes the interaction between electrons and the interaction with the positive background (the term $k=0$ is omitted in the summation). The potential $V(k)$, which takes the finite thickness of the electron layer into account, is given by

$$V(k)=\frac{2\pi e^2}{\epsilon k}F(k) , \tag{3}$$

where

$$F(k)=\int dz \int dz' \, |\psi_0(z)|^2 \, |\psi_0(z')|^2 \times \exp[-k(z-z')] \tag{4}$$

is the form factor to the Coulomb interaction due to the layer width. For electrons moving in the GaAs side in a single heterojunction (SH), the lowest subband wave function is well approximated by the Fang-Howard variational function,[14]

$$\psi_0(z)=\left[\frac{b^3}{2}\right]^{1/2} z\exp\left[-\frac{bz}{z}\right] . \tag{5}$$

Then, for a SH, we have

$$F(k)=\frac{b}{8}\left[\frac{8b^2+9bk+3k^2}{(b+k)^3}\right] , \tag{6}$$

where b is a variational parameter determined by minimizing the total energy. The result is

$$b=(48\pi m^* e^2 N^*/\epsilon h^2)^{1/3} ,$$

where m^* and ϵ are, respectively, the effective mass and dielectric constant of GaAs, and $N^*=N_d+\frac{11}{32}n$. Here N_d is the depletion charge density in GaAs and n is the electron density. The second system to be considered here is a double heterojunction which forms a quantum well (QW) of width d. For a QW, the lowest subband wave function is approximated by that of a square-well potential with infinitely deep barriers,

$$\psi_0(z)=\left[\frac{2}{d}\right]^{1/2}\sin\left[\frac{\pi z}{d}\right] . \tag{7}$$

In this case, we obtain ($u=kd$)

$$F(k)=\frac{2(u^2+8\pi^2)}{(u^2+4\pi^2)^2}(1-e^{-u})+\frac{u}{u^2+4\pi^2}+\frac{2}{u}\left[1-\frac{1}{u}(1-e^{-u})\right] . \tag{8}$$

In a purely 2D EG with δ-function probability density, we must have $F(k)=1$ in Eq. (3). The electron-phonon coupling is represented by $H_{e\text{-ph}}$ in Eq. (1d). The interaction strength is given by

$$M_q=i\hbar\omega_{\rm LO}\left[\frac{4\pi\alpha}{\Omega q^2}\right]^{1/2}\left[\frac{\hbar}{2m\omega_{\rm LO}}\right]^{1/4}\langle\psi_0|e^{iqz}|\psi_0\rangle , \tag{9}$$

where Ω is the volume and α is the standard Fröhlich coupling constant of the electron-phonon interaction.

A. Ground-state energy of the polaron gas

We review briefly the canonical transformation theory, discussed in earlier works,[9,10] as applied to the many-polaron system. The method consists in subjecting the bare Hamiltonian [Eq. (1)] to a similarity transformation given by

$$U=\exp Q \ , \tag{10}$$

with

$$Q=\sum_{k,q} f_q \langle \psi_0 | e^{iq_z z} | \psi_0 \rangle (a_q - a^{\dagger}_{-q}) c^{\dagger}_k c_{k+q} \ , \tag{11}$$

where f_k are unknown functions. The canonical transformation U is referred to as the Lee-Low-Pines transformation. The expectation value of the transformed Hamiltonian over the vacuum phonon state leads to a reduced Hamiltonian, which has the same form as the original one, but with an effective potential between electrons given by

$$V_{\rm eff}(k)=V(k)-2(M_k f^*_k + M^*_k f_k - \hbar\omega_{\rm LO} f_k f^*_k) \ . \tag{12}$$

The second term of Eq. (12) corresponds to the contribution of the electron-phonon coupling to the electron-electron interaction. Next, the ground-state energy is obtained by calculating the expectation value of the reduced Hamiltonian over the ground-state wave function of the electron gas. Finally, f_k are determined by minimizing the ground-state energy. The calculation is straightforward and gives the following result to the ground-state energy per particle:

$$E=K+\sum_k V(k)[S(k)-1]+E_p \ , \tag{13}$$

where the first two terms correspond to the usual ground-state energy of the electron gas, including the exchange and correlation contribution, and

$$E_p=-\sum_k \frac{|M_k|^2 S(k)}{\hbar\omega_{\rm LO}+\hbar^2k^2/2mS(k)} \tag{14a}$$

or

$$E_p=-\alpha\hbar\omega_{\rm LO}k_{\rm LO}^{-1}\int_0^{\infty} dk \frac{S^2(k)}{S(k)+k^2k_{\rm LO}^{-2}} \tag{14b}$$

is the correction of the electron-phonon interaction to the ground-state energy. In Eq. (14b), $k_{\rm LO}=(2m\omega_{\rm LO}/\hbar)^{1/2}$. The static structure factor is a key quantity in determining the screening properties of the interacting system. In Eq. (14), $S(k)$ is the structure factor of the electron gas in the absence of the electron-phonon interaction.

B. Structure factor of the quasi-2D EG

A new method has been proposed recently to determine the structure factor of the quasi-2D EG in the mean-field approximation. Here we give only the essentials of the method and we refer the reader to Ref. 3 for details. The structure factor is related to the density response function through the fluctuation-dissipation theorem as

$$S(k)=-\frac{\hbar}{2\pi n}\int_{-\infty}^{\infty}\chi(k,i\omega)d\omega \ . \tag{15}$$

The density response function is written as

$$\chi(k,\omega)=-i\int_0^{\infty} dt\, e^{i\omega t}\langle [\rho^{(t)}_k,\rho^{(0)}_{-k}]\rangle \ , \tag{16}$$

where the electron-density operator is

$$\rho_k(t)=\sum_p c^{\dagger}_{k+p}(t)c_p(t) \ . \tag{17}$$

As pointed out in Ref. 9, it is worthwhile to remark that $S(k)$ is different from $S(k,0)$, the static limit of the dynamic structure factor $S(k,\omega)$, since $S(k)$, which appears in Eq. (15), is obtained from the evaluation of $\chi(q,\omega)$ for all frequencies. In this sense, this approach could be called a "dynamical screening" to make the distinction with the usual procedure[8] which consists of replacing the strength coefficients $|M_k|^2$ by $|M_k|^2/\epsilon^2(k,0)$ with $1/\epsilon(k,0)-1=V(k)\chi(k,0)$. In general, $\chi(k,\omega)$ could be calculated in terms of a diagrammatic formalism. However, in the mean-field theory, the density response function can be written as

$$\chi(k,\omega)=\frac{\chi_0(k,\omega)}{1-V(k)[1-G(k)]\chi_0(k,\omega)} \ , \tag{18}$$

where $\chi_0(k,\omega)$ is the response function in the absence of the Coulomb interaction. $G(k)$ is the local-field correction which takes the short-range exchange-correlation effects into account in the density response function. The effect of $G(k)$ is to reduce the electron-electron interaction at small distances. Note that if we set $G(k)=0$, we recover the RPA response function. Thus, the RPA neglects all short-range correlations in the system. This is the underlying reason why we must go beyond the RPA.

Using a very simple expression for $\chi_0(k,i\omega)$, obtained by a suitable transformation to new coordinates, de Freitas and Studart[4] showed that the structure factor can be written as

$$S(k)=\frac{k}{\pi k_F^2}\int_0^{\alpha(k)}\left[(4k_F^2-k^2\sin^2\theta)^{1/2}+\frac{4k_F^2\cot^2\theta}{(4k_F^2-k^2\sin^2\theta)^{1/2}}\right]\frac{(1-\cos\theta)}{1+V(k)[1-G(k)](1-\cos\theta)m/\pi\hbar^2}d\theta \ , \tag{19}$$

where

$$\alpha(k)=\begin{cases}\pi/2, & k\le 2k_F\\ \sin^{-1}(2k_F/k), & k>2k_F \ .\end{cases}$$

The Fermi wave number $k_F=(2\pi n)^{1/2}$ in 2D. It is important to note that Eq. (19) contains a single integral over a finite interval; thus, it can be numerically calculated with great accuracy. By making $G(k)=1$ in Eq. (19),

we get the structure factor in the HFA. The analytical result is

$$S_{\mathrm{HFA}}(k)=\frac{2}{\pi}\left[\sin^{-1}\left[\frac{k}{2k_F}\right]+\frac{k}{2k_F}\left[1-\frac{4k_F^2}{k^2}\right]^{1/2}\right]\times\Theta\left[\frac{2k_F}{k}-1\right]+\Theta\left[1-\frac{2k_F}{k}\right], \quad (20)$$

where $\Theta(x)$ is the step function. In the self-consistent STLS approximation, the choice of $G(k)$ arises from an ansatz in decoupling the two-body Wigner distribution function.[11] The local-field function in STLS is given by

$$G(k)=-\frac{1}{n}\int d\mathbf{q}\frac{1}{(2\pi)^2}\frac{V(q)}{V(k)}\frac{\mathbf{q}\cdot\mathbf{k}}{k^2}[S(\mathbf{k}-\mathbf{q})-1]\,. \quad (21)$$

The local field $G(k)$ and the structure factor $S(k)$ are calculated by solving self-consistently Eqs. (19) and (21). In the HA, $G(k)$ is determined by substituting $S_{\mathrm{HFA}}(k)$ from Eq. (20) into Eq. (21).

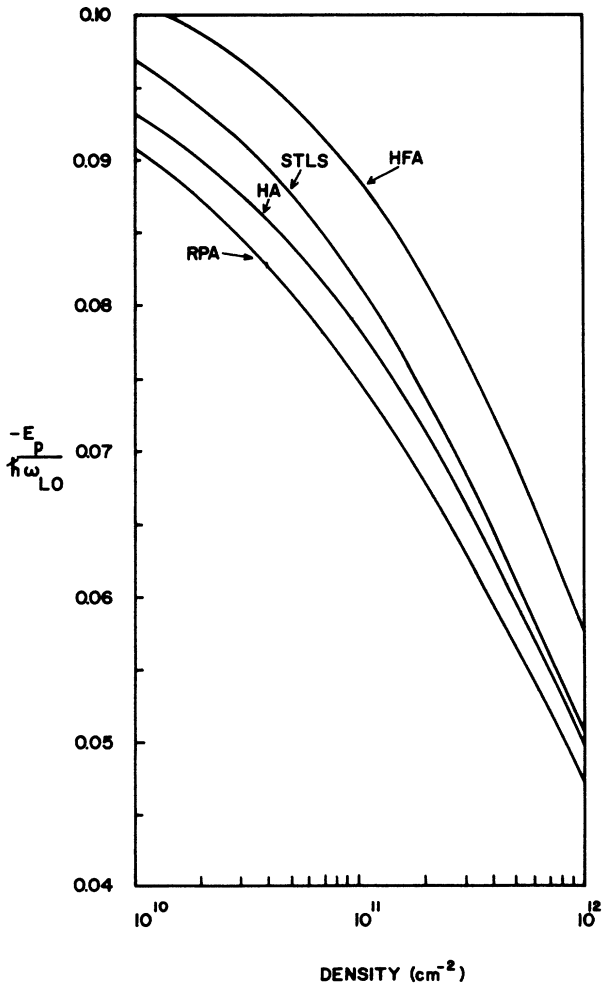

FIG. 1. Polaronic-binding energy as a function of the electron density within different approximations in a purely 2D system.

III. RESULTS

The structure factor obtained by the solution of Eqs. (19) and (21) is substituted into Eq. (14b) to get the polaronic-binding energy. The physical parameters that we use in our calculations are those of the GaAs, i.e., $\hbar\omega_{\mathrm{LO}}=36.77$ meV, $\epsilon=10.9$, $m^*=0.0657m_0$, and $\alpha=0.068$. In Fig. 1 we show the electron-phonon contribution to the ground-state energy of a purely 2D polaron gas in the self-consistent STLS approximation, the HA, the RPA, and the HFA. It is noted that in all of these approximations, the polaronic-binding energy $|E_p|$ decreases as the density increases. As we expected, the screening effects on the electron-phonon interaction increase with increasing density. However, it is clear from Fig. 1, that the RPA (HFA) overestimates (underestimates) the screening effects. As we include the short-range correlations, first through the HA, which only takes the Pauli-hole exchange effect into account, and then through the STLS scheme, we observe a gradual reduction of the screening on the electron-phonon interaction. This result arises from a more correct treatment of the short-range correlation effects provided by the STLS approach. In the limit of very low density, we recover the 2D single-polaron limit $E_p=\pi\alpha\hbar\omega_{\mathrm{LO}}/2$, as may be easily seen by neglecting interaction effects [set $S(k)=1$] and taking the zero-thickness approximation [set $F(k)=1$] in Eq. (14).

In the next figures, we show the influence of the subband confinement by considering the electron gas in a single heterojunction (Fig. 2) and in quantum wells of 50-

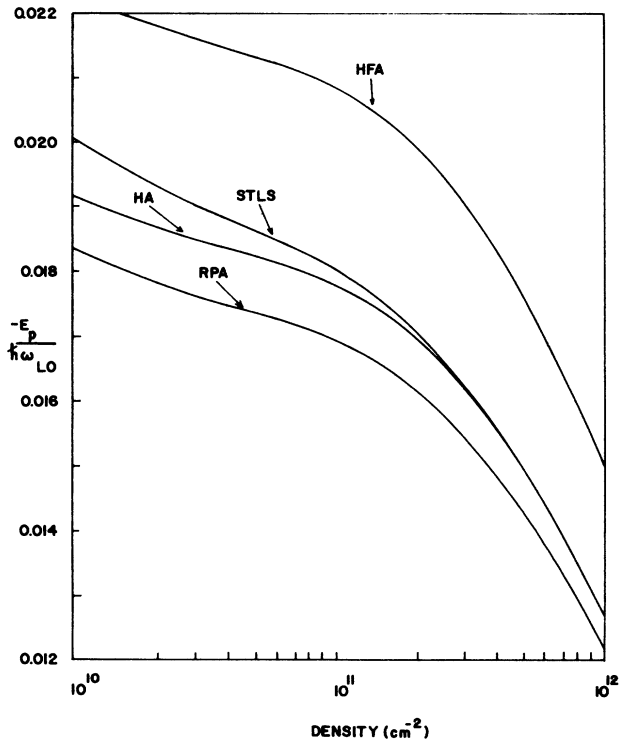

FIG. 2. Polaronic-binding energy vs the electron density in the GaAs-$Al_xGa_{1-x}As$ heterojunction.

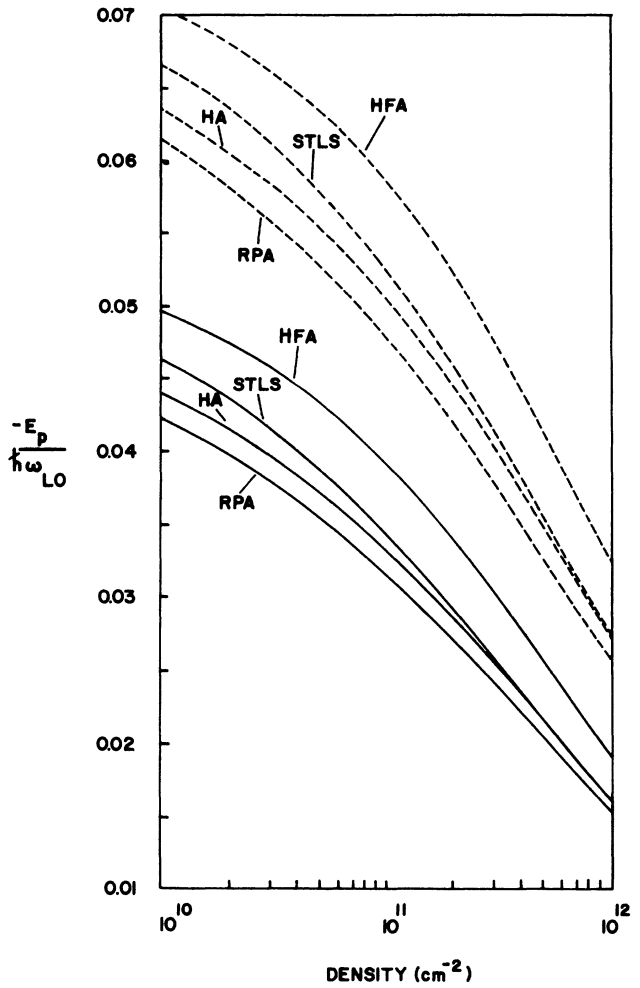

FIG. 3. Same as Fig. 1, but now showing the effects of screening in the polaronic energy in quantum wells of 50 Å (dashed lines) and 150 Å (solid lines).

and 150-Å widths (Fig. 3). We see in Fig. 2 that $|E_p|$ is substantially reduced (by a factor of 5) from the strictly 2D results because of the combinations of the effects of the electron-electron interaction and the subband confinement. Again it is clearly observed that $|E_p|$ monotonically decreases with increasing density, and both effects contribute to reducing the electron-phonon interaction. This is in contrast to the result of the static RPA approach (screening of the electron-phonon interaction by the wave-vector-dependent dielectric function at zero frequency), which exhibits a minimum in $|E_p|$ at $n \cong 3\times 10^{11}$ cm^{-2}. At high densities, the STLS approximation and the HA give the same results and approach the RPA values of the binding energy. When n goes to infinity, the electron-phonon interaction is fully screened out and $|E_p|$ goes to zero. As we can see from Fig. 3, the results of $|E_p|$ for a quantum well show a smaller reduction as compared with those of the 2D EG in a heterojunction. Furthermore, the binding energy is quite sensitive to the thickness of the electron layer. As we increase the well width for a fixed density, the wave function spreads out, and the binding energy decreases. However, we cannot get, in this model, the bulk value of the binding energy, which could be obtained, in principle, by taking the limiting value of $F(k)$ as b goes to zero or d goes to infinity. When b is small or d is large, the energy difference between the levels of the lowest subbands becomes comparable and we have to include the population of higher subbands. We must recall that in this limit the electron-electron interaction behaves like $\ln r$, the potential of an infinite string of charges, instead of the actual 3D $1/r$ potential. Then, we have to sum up over all electron subbands in Eq. (4) in order to get the correct result. Furthermore, in this case, we also have to consider explicitly the z dependence of the screening in our approach.

Even though the correction to the subband energy due to the electron-phonon interaction is quite small for experimental electron densities in GaAs systems, it could be important in heterostructures of more polar materials, as discussed by Das Sarma and Mason.[8]

In conclusion, we have shown that screening and subband-confinement effects are important to reduce the electron-phonon interaction, and an improved treatment of the short-range correlations in the polaron gas is necessary to obtain a quantitative picture of the electron-phonon interaction in semiconductor microstructures.

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