

## Interacting many-polaron system in degenerate semiconductors

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We present a theoretical study of the coupled electron phonon in a degenerate polar electron gas. The ground-state energy of the many-polaron gas is determined within a dynamical screening treatment and several approximations for the dielectric function. The effect of carrier densities on the static screening correction of the electron-phonon interaction to the polaronic energy and effective mass is investigated within second-order perturbation theories. Electron self-energies are also evaluated. It is shown that the polaronic energies have lower values in the dynamical approach as compared with the static one for all electron densities. Polaron effective masses derived from different perturbative schemes show quantitative different results which are properly interpreted.

### I. INTRODUCTION

The polaron is a single-particle excitation which has been quite useful in describing the physical properties of an electron in ionic crystals and polar semiconductors.<sup>1</sup> In a broad sense, it constitutes a very interesting theoretical model of a fermion interacting with a scalar boson field. Earlier work on polarons deals with the interaction of a single charge carrier (electron or hole) and a cloud of virtual dispersionless optical phonons, described by the so-called Fröhlich Hamiltonian.<sup>2,3</sup> The original model has been generalized to include other polarization fields such as, for instance, the acoustical-phonon and exciton fields. Recently, much attention has been given to the polaron problem in low-dimensional systems such as two-dimensional (2D) and one-dimensional (1D) semiconductor heterostructures and the system of electrons deposited over the surface of liquid helium.<sup>4-11</sup> Furthermore, most of the polaron studies have essentially been theoretically done in the one-polaron limit even in systems with finite electron densities. The one-polaron approximation is very good in ionic crystals, in which the original concept was proposed, but doped polar semiconductors must be described by a degenerate many-body system in which one has to consider the electron-electron interaction along with the electron-phonon interaction on an equal footing. Consequently, the study of the many-polaron interacting system is actually a highly nontrivial problem. Screening effects are important because, by weakening the coupling between electrons and phonons, they change the polaronic self-energy with serious implications on the polaronic band-gap renormalization.<sup>12</sup> Despite the intensive investigation of these effects in 2D systems, the degeneracy and screening effects are almost neglected in bulk semiconductors, except in earlier works of Mahan.<sup>13</sup> Recently, the subject has attracted the interest of Das Sarma, Kobayashi, and Lai<sup>14</sup> who studied the influence of dynamical screening on scattering prop-

erties of semiconductors.

Our paper presents a theoretical study of the coupled electron-LO phonon in a degenerate 3D polar electron gas. From a theoretical point of view, the calculation is intractable in its full generality and approximations must be made. Even though a fully dynamical treatment is not considered here, dynamical screening effects are incorporated somewhat by a variational method. It is well known that the static approximation to the screening is probably reasonable as long as the plasma frequency is much larger than the phonon energies. Das Sarma, Kobayashi, and Lai<sup>14</sup> have shown that at high values of the electron densities the results of quasiparticle damping rates in a dynamically screening approach are quite close to the static screening results, whereas at low densities, as one expects, dynamical as well as static results are close to unscreened results.

Our main interest in this work is in studying the effect of carrier densities on screening corrections to the polaronic energy and the effective mass. The calculations are performed by using two different approaches. One is the straightforward perturbative method of evaluating the leading-order self-energy diagram with an effective electron-phonon interaction screened out by the static dielectric function of the electron gas. The other one is a variational approach<sup>15,16</sup> based on an extension of the Lee-Low-Pines transformation to the many-polaron system which leads to an expression of the polaronic energy in terms of the static structure factor  $S(k)$  of the electron gas. Since  $S(k)$  is obtained from the evaluation of the density-density response function, or its counterpart the dielectric function, for all frequencies the method can be considered as a dynamical approach in contrast with the previous one. However, as in the former case, the electron-phonon coupling is taken within the lowest-order perturbation scheme. The dielectric function and the structure factor of the electron gas, which provide the screening corrections on the electron-phonon interaction,

are evaluated in the following approximations of the many-body theory: the Hartree-Fock approximation (HFA), the Thomas-Fermi approximation (TFA), the random-phase approximation (RPA), the Hubbard approximation (HA), and the more sophisticated Singwi-Tosi-Land-Sjölander approximation (STLS).<sup>17,18</sup> It is surprising that the issue of the screened electron-phonon interaction, which has a long history, has not been addressed in detail beyond the RPA. This approximation has shown, in 3D and more pronounced in 2D, quantitative deficiencies including negative values of the pair-correlation function at small distances, overestimation of the correlation energy, and a free value of the screening length, which is essential in describing screening effects on the electron-phonon interaction. Our work fills this gap through a detailed comparison between the results of the ground-state properties of the polaron gas among several approximations. It is shown that the polaronic energies have lower values in the dynamical approach as compared with the static one for all electron densities. Polaron effective masses derived from energy expansion in the so-called "on the mass shell" Rayleigh-Schrödinger perturbation theory (RSPT) and in the Tamm-Dancoff approximation to the Wigner-Brillouin perturbation theory (TD-WBPT) show quantitative different results which are properly interpreted. For simplicity and clarity, and without loss of generality, we restrict ourselves in this paper to the zero-temperature case and to specific parameters of ZnS. In Sec. II we review the generalized canonical transformation method to calculate the variational ground-state energy of the polaron gas and discuss the static structure factor in different approximations of the many-body dielectric formalism. In Sec. III we consider the perturbative calculation in the static approximation of the lowest-order electron self-energy due to the electron-phonon interaction, the polaronic energy, and the polaron effective masses in RSPT and TD-WBPT. In Sec. IV we present numerical results for the self-energy, polaronic energies in the dynamical and static screening approaches, and effective masses as a function of electron densities within all approximations cited above. A comparison of the polaronic energies in both calculations is made and our conclusions are presented.

## II. VARIATIONAL METHOD TO THE GROUND-STATE ENERGY

The many-polaron system is described by the Hamiltonian

$$H = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar \omega_{\text{LO}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{p}'} V(\mathbf{p}') c_{\mathbf{k}+\mathbf{p}}^{\dagger} c_{\mathbf{p}-\mathbf{p}'}^{\dagger} c_{\mathbf{p}} c_{\mathbf{k}} + \sum_{\mathbf{k}, \mathbf{q}} M_{\mathbf{q}} (a_{\mathbf{q}}^{\dagger} + a_{-\mathbf{q}}) c_{\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}}, \quad (1)$$

where  $a_{\mathbf{q}}$  and  $a_{\mathbf{q}}^{\dagger}$  are the creation and annihilation operators for phonons with energy  $\hbar \omega_{\text{LO}} = \hbar^2 q^2 / 2m$  and wave number  $q$ , whereas  $c_{\mathbf{k}}^{\dagger}$  and  $c_{\mathbf{k}}$ , respectively, create and annihilate an electron with wave vector  $\mathbf{k}$ . The bare

electron-electron potential is given by  $V(k) = 4\pi e^2 / \Omega k^2$  and the prime on the summation denotes the exclusion of the  $k=0$  term which cancels the contribution from the positive background in the jellium model. The electron-phonon interaction strength is given by

$$M_{\mathbf{q}} = i \hbar \omega_{\text{LO}} \left[ \frac{4\pi\alpha}{\Omega q^2} \right]^{1/2} \left[ \frac{\hbar}{2m \omega_{\text{LO}}} \right]^{1/4}, \quad (2)$$

where  $\alpha$  is the standard Fröhlich coupling constant of the electron-phonon interaction.

Lemmens, Devreese, and Brosens<sup>15</sup> provide an interesting method to calculate the ground-state energy of the polaron gas by introducing a generalized Lee-Low-Pines canonical transformation to the many-body system. In order to clarify the differences between this and the perturbation approach we review the essentials of the method. The Hamiltonian given by Eq. (1) is subjected to the similarity transformation given by

$$U = \exp Q, \quad (3)$$

where

$$Q = \sum_{\mathbf{k}, \mathbf{q}} f_{\mathbf{q}} (a_{\mathbf{q}} - a_{-\mathbf{q}}^{\dagger}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}+\mathbf{q}}, \quad (4)$$

and  $f_{\mathbf{q}}$  are variational functions to be determined. The transformed Hamiltonian contains several terms that arise from the interactions between electrons and phonons. One assumes that the ground state can be written as

$$|\psi_{\text{g.s.}}\rangle = |\text{vac}\rangle |\psi_{\text{el}}\rangle, \quad (5)$$

where  $|\text{vac}\rangle$  represents the phonon vacuum state and  $|\psi_{\text{el}}\rangle$  is the ground-state (g.s.) wave function for the electrons. With this ansatz, one can construct a reduced Hamiltonian which operates only in the electronic ground state,

$$H_{\text{red}} = \langle \text{vac} | U^{-1} H U | \text{vac} \rangle = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{q}, \mathbf{p}, \mathbf{p}'} V_{\text{eff}}(\mathbf{q}) c_{\mathbf{p}+\mathbf{q}}^{\dagger} c_{\mathbf{p}'-\mathbf{q}}^{\dagger} c_{\mathbf{p}'} c_{\mathbf{p}} - \sum_{\mathbf{q}} (M_{\mathbf{q}}^* f_{\mathbf{q}} + M_{\mathbf{q}} f_{\mathbf{q}}^*) N + \sum_{\mathbf{q}} \left[ \hbar \omega_{\text{LO}} + \frac{\hbar^2 q^2}{2m} \right] f_{\mathbf{q}} f_{\mathbf{q}}^* N, \quad (6)$$

where  $N$  is the number operator.  $H_{\text{red}}$  has the same form as the original one, but with an effective potential between the electrons given by

$$V_{\text{eff}} = V(k) - 2(M_{\mathbf{k}} f_{\mathbf{k}}^* + M_{\mathbf{k}}^* f_{\mathbf{k}} - \hbar \omega_{\text{LO}} f_{\mathbf{k}} f_{\mathbf{k}}^*). \quad (7)$$

By minimizing the expectation value of the reduced Hamiltonian over the electronic ground state with respect to  $f_{\mathbf{k}}$ , the following expression for the total energy per particle of the polaron gas is obtained:

$$E = K + \sum_{\mathbf{k}} V(k) [S(k) - 1] + E_p. \quad (8)$$

The first two terms correspond to the total energy of the

electron gas, including exchange and correlation effects, and  $E_p$  is the correction to the ground-state energy due to the electron-phonon interaction which can be written as

$$\begin{aligned} E_p &= - \sum_{\mathbf{q}} \frac{M_{\mathbf{q}} M_{\mathbf{q}}^* S(\mathbf{q})}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 q^2}{2mS(\mathbf{q})}} \\ &= - \hbar\omega_{\text{LO}} \frac{2\alpha}{\pi} \int_0^\infty dx \frac{S^2(x)}{S(x)+x^2}, \end{aligned} \quad (9)$$

where  $x = q/q_{\text{LO}}$  and

$$S(\mathbf{q}) = \frac{1}{2} \sum_{p,p'} \langle \Psi_{\text{el}} | c_{p+\mathbf{q}}^\dagger c_{p-\mathbf{q}} c_{p'} c_{p'}^\dagger | \Psi_{\text{el}} \rangle$$

is the static structure factor of the electron gas. It is a fundamental quantity in determining the screening properties of the electron system. In the linear-response theory,  $S(\mathbf{q})$  is the integral over frequencies of the dynamical structure factor  $S(\mathbf{q}, \omega)$  which is related, via the fluctuation-dissipation theorem, to the imaginary part of the dielectric function  $\varepsilon(\mathbf{q}, \omega)$  as

$$S(\mathbf{q}, \omega) = - \frac{\hbar q^2}{4\pi^2 n e^2} \text{Im} \frac{1}{\varepsilon(\mathbf{q}, \omega)}, \quad \omega > 0 \quad (10)$$

where  $n$  is the number density. Since  $S(k)$  is different from  $S(k, 0)$  and corresponds to the evaluation of  $\text{Im} 1/\varepsilon(\mathbf{q}, \omega)$  for all frequencies, this approach can be considered as a dynamical one. As one will see in the next section, the static approximation corresponds to take  $\varepsilon(\mathbf{q}, 0)$  in the calculation. The evaluation of the dielectric function  $\varepsilon(\mathbf{q}, \omega)$  constitutes the central problem of the electron gas. Among the various methods of the linear screening theory, the dielectric function can be written in terms of an effective polarization field which takes the short-range exchange-correlation effects into account. In this approximation one has

$$\varepsilon(\mathbf{q}, \omega) = 1 - \frac{V(\mathbf{q}) \chi_0(\mathbf{q}, \omega)}{1 + V(\mathbf{q}) \chi_0(\mathbf{q}, \omega) G(\mathbf{q})}, \quad (11)$$

where  $\chi_0(\mathbf{q}, \omega)$  is the density-density response function of the free system (the Lindhard function) and  $G(\mathbf{q})$  is the local-field correction which reduces the electron-electron interaction at small distances. In the HFA, the particles respond to external perturbations as free particles, then  $G(\mathbf{q})$  is taken to be unity for all  $\mathbf{q}$ . In the HFA,  $S(\mathbf{q})$  can be analytically evaluated. In the RPA all correlations are neglected, which corresponds in the polarization field approximation to set  $G(k)$  equal to zero in Eq. (11). The first attempt to incorporate short-range correlation effects in the electron gas was made by Hubbard. In the HA, one has

$$G_H = \frac{1}{2} \frac{q^2}{q^2 + k_F^2}, \quad (12)$$

where  $k_F$  is the Fermi wave vector. Many forms of  $G(\mathbf{q})$  have been proposed in different kinds of approximations. In most self-consistent schemes,  $G(\mathbf{q})$  is expressed as a

functional of  $S(\mathbf{q})$ , which in conjunction with Eqs. (10) and (11) form a set of coupled integral equations. In the self-consistent STLS approximation, the expression of  $G(k)$  arises from an ansatz in decoupling the two-body distribution function in terms of the pair-correlation function, which is directly related to  $S(\mathbf{q})$  by a Fourier transform. The local-field correction in STLS is given as

$$G_{\text{STLS}}(\mathbf{q}) = - \frac{1}{n} \int \frac{d^3 k}{(2\pi)^3} \frac{\mathbf{q} \cdot \mathbf{k}}{k^2} [S(\mathbf{q}-\mathbf{k}) - 1]. \quad (13)$$

The Hubbard local field  $G_H(\mathbf{q})$  can be obtained from Eq. (13) by substituting  $S(\mathbf{q})$  for its HFA value. In STLS, the numerical calculation of  $S(\mathbf{q})$  by solving self-consistently Eqs. (10), (11), and (13), must be done carefully in order to extract the contribution of the plasmons which are obtained from the zeros of the dielectric function. It is worth it to emphasize that this method has only been applied to the HFA for bulk semiconductors.<sup>15</sup> In this paper we provide a systematic calculation to show the effect of electron correlations, completely absent in the HFA, and compare the final results obtained in different approximations beyond the HFA.

### III. PERTURBATIVE CALCULATION

The leading Feynman diagram contribution to the electron self-energy due to the electron-phonon interaction is given as<sup>2</sup>

$$\begin{aligned} \Sigma(\mathbf{p}, i\omega_n) &= -k_B T \sum_{i\omega_n} \int \frac{d^3 q}{(2\pi)^3} \frac{|M_{\mathbf{q}}|^2}{\varepsilon^2(\mathbf{q}, i\omega_n)} \\ &\quad \times G(\mathbf{p} + \mathbf{q}, i\omega_n + i\omega_n) \\ &\quad \times D(\mathbf{q}, i\omega_n), \end{aligned} \quad (14)$$

where  $G(\mathbf{p}, i\omega_n)$  is the bare electronic Green's function and  $D(\mathbf{q}, i\omega_n)$  is the renormalized LO-phonon propagator. The purely electronic dielectric function  $\varepsilon(\mathbf{q}, i\omega_n)$  contains all information about screening as discussed in the previous section.  $D(\mathbf{q}, i\omega_n)$  is usually written in terms of the polarizability of the electron gas in the RPA. It is responsible by the coupled plasmon-phonon process that we shall ignore in this work due to the great complexity of the problem involving three different fields, namely the electron, phonon, and plasmon, that are coupled all together. These processes are not quite important in describing the ground state of the system, which is what we are concerned with here, but play a fundamental role in describing the excitations of the system.<sup>19</sup> The effect of the renormalized phonon propagator is significant as long as LO-phonon-plasmon coupled modes are relevant and this coupling is weak when the plasma frequency  $\omega_p$  is greater than the phonon frequency  $\omega_{\text{LO}}$ . So, we neglect the plasmon-phonon coupling and assume that

$$D(\mathbf{q}, i\omega_n) = \frac{2\omega_{\text{LO}}}{(i\omega_n)^2 - \omega_{\text{LO}}^2}. \quad (15)$$

A full dynamical screening in the perturbation calculation is intractable and we are forced to make some ap-

proximations in  $\varepsilon(\mathbf{q}, i\omega_n)$ . First, a popular approximation considered in the literature is the ‘‘effective frequency’’ approximation<sup>14</sup> which consists of putting  $\varepsilon(\mathbf{q}, i\omega_n) = \varepsilon(\mathbf{q}, \omega_{\text{LO}})$ . However, when  $\omega_p \gg \omega_{\text{LO}}$ ,  $\varepsilon(\mathbf{q}, \omega_{\text{LO}})$  is well approximated by the static limit  $\varepsilon(\mathbf{q})$ . This approximation has shown good results at high densities.<sup>14</sup> So, in order to avoid a disproportionate numerical effort, we take the static screening and the electron self-energy, given by Eq. (14), which assumes the form

$$\Sigma(p, ip) = \int \frac{d^3q}{(2\pi)^3} \frac{|M_q|^2}{\varepsilon^2(\mathbf{q}, 0)} \times \left[ \frac{1 + N_q - n_{\mathbf{p}+\mathbf{q}}}{ip - \xi_{\mathbf{p}+\mathbf{q}} - \hbar\omega_{\text{LO}}} + \frac{N_q + n_{\mathbf{p}+\mathbf{q}}}{ip - \xi_{\mathbf{p}+\mathbf{q}} + \hbar\omega_{\text{LO}}} \right], \quad (16)$$

where  $N_q$  ( $n_{\mathbf{p}+\mathbf{q}}$ ) is the Bose (Fermi) occupation number and  $\xi_{\mathbf{p}+\mathbf{q}}$  is the bare electron energy measured from the Fermi energy. We shall only discuss the zero-temperature limit where we can neglect the phonon thermal occupation factor and  $n_{\mathbf{p}+\mathbf{q}} = \Theta(-\xi_{\mathbf{p}+\mathbf{q}})$ . The imaginary part of the self-energy gives the phonon emission rate which has been calculated by Das Sarma, Kobayashi, and Lai.<sup>14</sup> Calculations of the electron self-energy have been performed by Mahan and Duke,<sup>20</sup> but they restricted themselves to either TFA or RPA in the treatment of static screening. We must also point out that we have neglected the direct electron-electron interaction to the electron self-energy. The implication of this fact in the calculation of the polaron effective mass will be discussed in the next section. Here we are concerned with the dispersion relation of the polaron given by

$$E(p) = \frac{\hbar^2 p^2}{2m} + \text{Re}[\Sigma(p, E(p))]. \quad (17)$$

The calculation of the excitation spectra was done by taking a perturbative procedure which consists of solving Eqs. (16) and (17) self-consistently. This procedure is equivalent to Wigner-Brillouin perturbation theory. Since only the one-phonon term in the self-energy is considered, we are dealing with the Tamm-Dancoff approximation. From Eq. (17), we can define the effective mass as

$$\frac{m}{m_F^*} = 1 + \frac{m}{\hbar^2 k_F} \left[ \frac{\partial \text{Re}[\Sigma(p)]}{\partial p} \right]_{p=k_F}. \quad (18)$$

The so-called ‘‘on the mass shell’’ RSPT has provided better results for the energies than TD-WBPT in the one-polaron limit. So, we choose RSPT to calculate the contribution of the electron-phonon interaction to the electron energy by putting  $E = p^2/2m$  in  $\text{Re}\Sigma(p, E)$ . Then Eq. (17) becomes

$$E(p) = \frac{\hbar^2 p^2}{2m} - \hbar\omega_{\text{LO}} \frac{\alpha q_{\text{LO}}}{\pi} \times \int_0^\infty \frac{dq}{\varepsilon^2(q, 0)} \int_0^\pi \frac{\sin\theta d\theta}{p^2 + 2pq \cos\theta + q^2}. \quad (19)$$

Since we are interested in polaronic corrections to the band edge, we can take the limit of small  $p$  to get the following expressions to the polaronic binding energy:

$$E_p = \hbar\omega_{\text{LO}} \frac{2\alpha}{\pi} \int_0^\infty \frac{dx}{\varepsilon^2(x, 0)} \frac{1}{1+x^2}, \quad (20)$$

and to the effective mass

$$\frac{m}{m_R^*} = 1 - \frac{8\alpha}{3\pi} \int_0^\infty \frac{dx}{\varepsilon^2(x, 0)} \frac{x^2}{(1+x^2)^3}. \quad (21)$$

These expressions recover by taking  $\varepsilon(q, \omega) = 1$ , the previous unscreened results of  $E_p = -\alpha\hbar\omega_{\text{LO}}$  and  $m/m_R^* = (1-\alpha)/6$ .<sup>2,3</sup> Equation (20) must be compared with the similar result, Eq. (9), in the dynamical screening approach.

#### IV. NUMERICAL RESULTS AND DISCUSSIONS

In Fig. 1 we show the results of the polaronic energy  $E_p$  [Eq. (9)] in units of  $\hbar\omega_{\text{LO}}$  ( $=73.27$  meV for ZnO) calculated using the variational method as a function of the electron density in STLS, HA, RPA, and HFA. Even though our results are presented for ZnO, with  $\alpha=0.849$ , a polar semiconductor which also shows piezoelectric properties, they remain qualitatively valid for other polar semiconductors. We also have obtained similar results for ZnS. We note that the screening effects on the electron-phonon interaction increase with increasing density and  $|E_p|$  decreases as the density increases in all approximations. It is clear that the RPA (HFA overestimates (underestimates) screening effects. A gradual reduction of the screening is observed as we include short-range correlation effects beyond the RPA. At low densities, the results are quantitatively different. Note that the results in HFA,<sup>15</sup> which was the only approximation used up to now, are shifted from all those obtained in

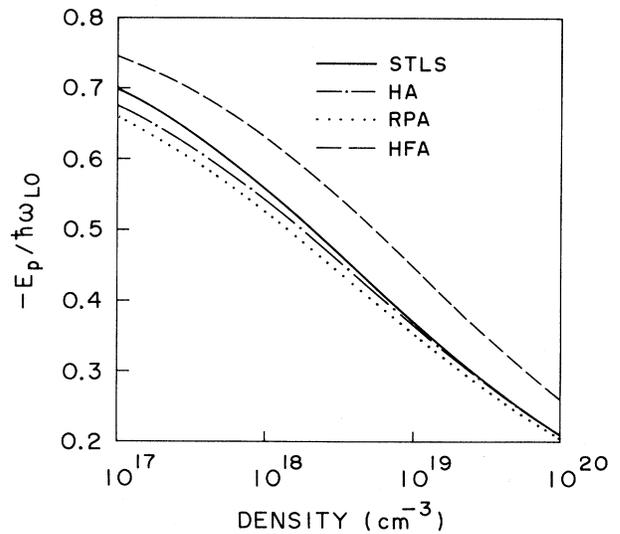


FIG. 1. Contribution of the electron-phonon interaction to the ground-state energy as a function of the electron density in the dynamical screening approach [Eq. (9)] using the static structure factor in several approximations of the electron gas.

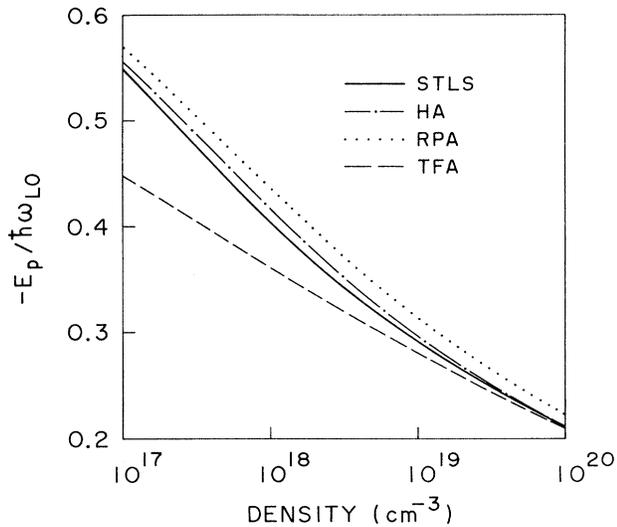


FIG. 2. Polaronic binding energy vs the electron density in the static screening approach [Eq. (20)]. The static dielectric function was evaluated in the TFA, RPA, HA, and STLS approximations.

other approximations even in the high-density limit. At high densities, STLS and HA curves approach the RPA curve. The overall physical description is the same as in low-dimensional systems previously studied and no qualitative differences are found. However, the actual magnitude of the polaronic energy, which is not an experimentally relevant quantity to GaAs heterostructures, should produce relevant shifts of band edges in more polar semiconductors, such as ZnO. In Fig. 2, the results of the polaronic energy in the screening static approach [Eq. (20)] are presented for different approximations. As one ex-

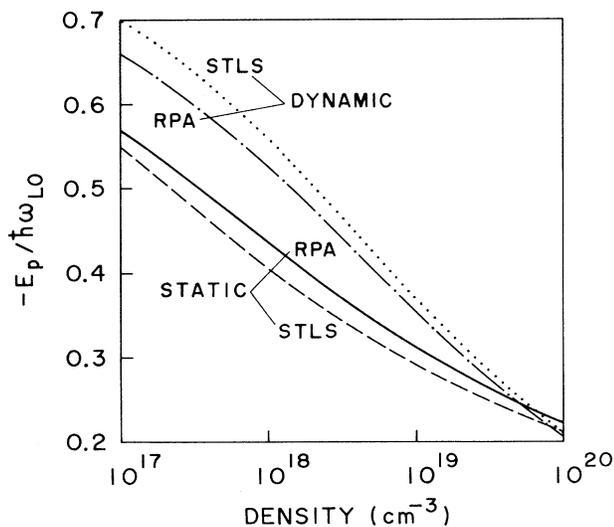


FIG. 3. Comparison of the polaronic binding energies as a function of the electron density in the static and dynamical screening approaches by using the RPA and STLS approximations.

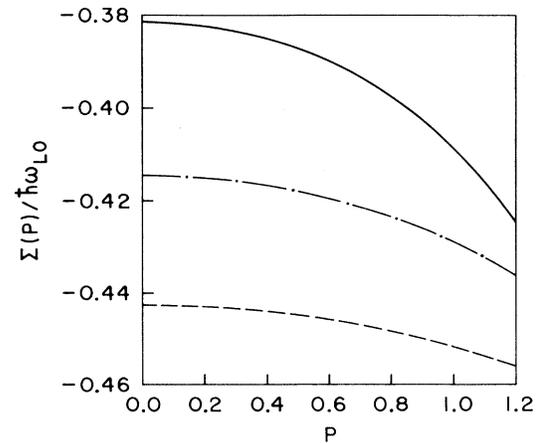


FIG. 4. The electron-phonon interaction contribution to the electron self-energy for different densities,  $n = 2.8 \times 10^{18} \text{ cm}^{-3}$  (solid curve),  $n = 1.2 \times 10^{18} \text{ cm}^{-3}$  (dashed-dotted curve), and  $n = 6.0 \times 10^{17} \text{ cm}^{-3}$  (dashed curve) as a function of the wave vector in the STLS approximation.

pects, the TFA gives the poorest results, since the correlation effects are completely neglected in this approximation. It must be noticed that the RPA result for the dielectric function equals the one in the TFA for  $k < 2k_F$ . However, we found the largest difference in the results of the RPA and the TFA. There is no significant difference (less than  $0.01\hbar\omega_{LO}$ ) in energy for all approximations in the static screening approach. In Fig. 3, we compare the results of the polaronic binding energy in the dynamical and static screening approaches within the RPA and STLS. For almost all densities ( $10^{17}$ – $10^{20} \text{ cm}^{-3}$ ), the static screening approach gives a smaller binding energy  $|E_p|$  than the dynamical screening ap-

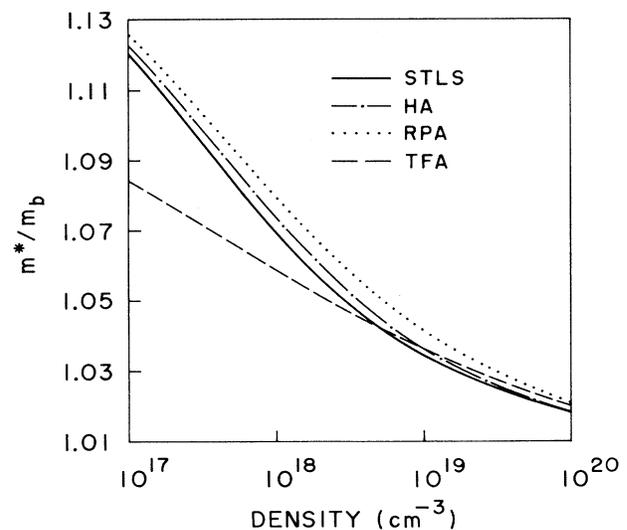


FIG. 5. The effective mass [Eq. (21)] calculated within different approximations for the dielectric function by using Rayleigh-Schrödinger perturbation theory as a function of the electron density.

proach. At higher values of the electron density, dynamical screening results are quite close to static screening results. Since no equivalent canonical transformation method has been developed to calculate the effective masses, our results are based on the static screening treatment of the many-polaron system as discussed in Sec. III. We show, in Fig. 4, the real part of the electron self-energy  $\Sigma(p)$  in TD-WBPT, from which the effective mass  $m_F^*$  is derived, in the STLS approximation for three values of the electron density. At  $p=0$ ,  $\Sigma(0)$  increases with increasing density, which is consistent with the calculation of the polaronic energy. However, as pointed out by Xiaoguang, Peeters, and Devreese,<sup>16</sup>  $\Sigma(0) \neq E_p$  because, as a consequence of the Fermi-Dirac statistics, in the ground state different electrons have different  $k$  vectors. At small densities, a weak dependence of the self-energy with  $p$  is observed. However, as one increases the density, a nonparabolic effect arises due to the electron-phonon interaction. This effect leads to an increase of the derivative of  $\Sigma(p)$  at  $p=k_F$  which becomes more negative with increasing density and consequently contributes to the increase of the effective mass. Qualitative behavior is observed in the other approximations considered. In Fig. 5, the effective mass  $m_R^*$  [Eq. (21)] is presented as a function of the density. For all approximations,  $m_R^*$  decreases monotonously as the density increases. For large densities, the curves approach the same asymptotic limit. We can observe that the TFA gives the poorest behavior for  $m_R^*$  and our study suggests that the TFA is not adequate to treat the screening of the electron-phonon interaction even in 3D. In Fig. 6, the effective mass  $m_F^*$  [Eq. (17)] in TD-WBPT is shown as a function of the electron density for all approximations. At low densities the effective mass does not depend strongly on the density in all approximations. However, we observe a sharp in-

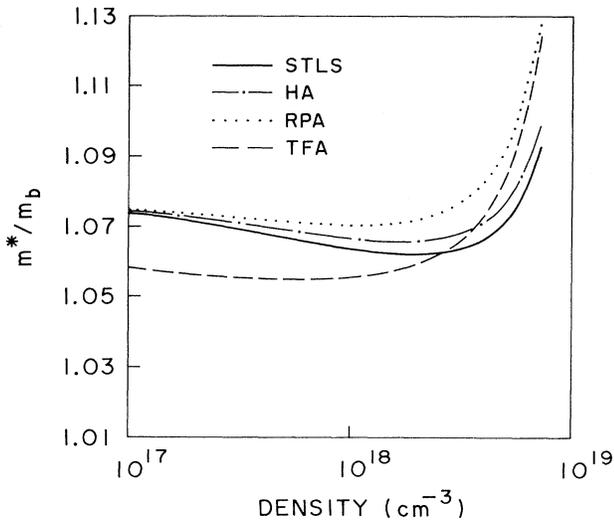


FIG. 6. The effective mass calculated within different approximations for the dielectric function by using the Tamm-Dancoff approximation to the Wigner-Brillouin perturbation theory as a function of the electron density. As discussed in the text, this result is not valid for large densities.

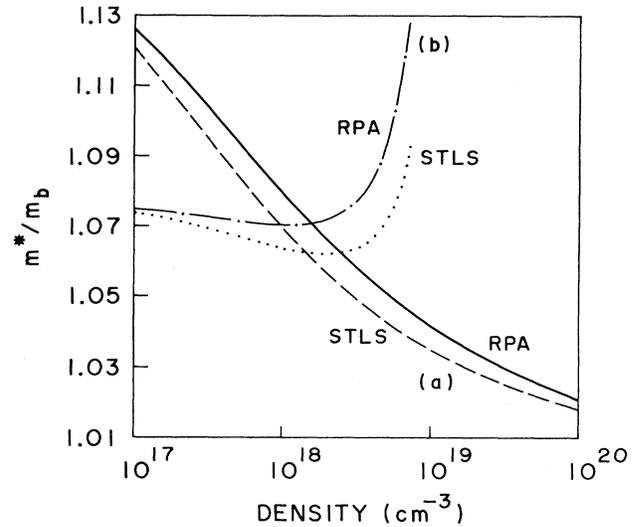


FIG. 7. Polaron effective mass as a function of the density calculated within the RPA and STLS approximations. (a) shows  $m_R^*$  and (b) shows  $m_F^*$ .

crease in the effective mass for densities near  $10^{19} \text{ cm}^{-3}$ . The behavior of  $m_F^*$  was explained by Xiaoguang, Peeters, and Devreese<sup>16</sup> in terms of two competing effects: the first one arises from the effective electron-phonon interaction which is screened out as the density increases and leads to smaller mass renormalization: the second one comes from the nonparabolic behavior of the self-energy for large  $p$  as the density increases as shown in Fig. 4. The same behavior was observed in two dimensions and was exhaustively discussed by Xiaoguang, Peeters, and Devreese.<sup>16</sup> The conclusion is that the result for  $m_F^*$  is not valid for large densities. The inclusion of the direct electron-electron interaction in the self-energy may correct this failure at high densities. Finally, we show the differences between the two calculated effective masses by plotting  $m_F^*$  and  $m_R^*$  as a function of the density (see Fig. 7). At low densities, the renormalization mass effects are much more pronounced in  $m_R^*$  as compared with  $m_F^*$ . The conclusion is that for the many-polaron interacting system, RSPT still works better than TD-WBPT, as in the one-polaron problem.

Pioneering experimental studies by Brown<sup>21</sup> have combined mobility experiments and cyclotron resonance measurements to demonstrate polaron effects. At this time one of the more used tools to study the strength of the electron phonon is the cyclotron resonance experiment. In bulk semiconductors, in the case where accurate cyclotron resonance data are available,<sup>22</sup> the electron densities are relatively small (typically of the order of  $10^{13} \text{ cm}^{-3}$  in GaAs). In this case the one-polaron theories can well describe the polaron effects. For ZnO, there is earlier experimental information about infrared reflection spectra containing various concentrations of free electrons. Collins and Kleinman<sup>23</sup> showed that the reflection spectra are quite different for electron densities below or above  $10^{17} \text{ cm}^{-3}$ . In the actual case, we have additional complications in understanding the effect of free carriers in the

polaronic properties because we have to include other types of phonons, mainly the acoustical phonon coming from the piezoelectrical deformation potential which is present in ZnO. We expect that our results may motivate experimental work in 3D polar semiconductors, as occurred in semiconductor heterostructures,<sup>24-26</sup> in order to establish the many-polaron effects in bulk semiconductors.

In summary, we have studied the effects of the screening in the interacting polaron gas, by using two different approaches: a dynamical screening method based in a generalization of the Lee-Low-Pines treatment for many-polaron systems and the usual static screening approach based on first-order perturbation theories. As in two dimensions, the dynamical treatment results in larger polaron effects for densities less than  $10^{20} \text{ cm}^{-3}$  in comparison with a static screening approach. The correlation

effects are properly taken into account in the dynamical screening method and shown to be relevant at small densities. We show that the TFA is not valid to treat screening effects and the RSPT gives more reasonable results for the polaron gas as compared with TD-WBPT.

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