

Dispersion theory for the two-dimensional polaron

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(Received 1 December 1986; revised manuscript received 15 December 1987)

By using dispersion theory, the ground-state energy and the effective mass of a polaron in two-dimensional and quasi-two-dimensional space are calculated. In this theory the effect of screening on the phonon frequencies, as well as on the electron-phonon interaction, is included. The results of our calculations are applied to $\text{Ga}_{1-x}\text{Al}_x\text{As}$ and $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ heterostructures.

I. INTRODUCTION

There has been considerable interest in the two-dimensional (2D) systems recently. This is partly due to the technological advances in the technique of molecular-beam epitaxy by which almost pure two-dimensional electron gas with variable electron densities is realizable.^{1,2} The materials where 2D systems are obtained are often polar semiconductors where an electron is coupled to longitudinal-optical modes of the lattice and the polaron is a resultant elementary excitation. The polaron theory was originally developed by Landau and by Fröhlich for three-dimensional (3D) crystals a long time ago.^{3,4} Observation of polaronic effects in two-dimensional systems such as the $\text{GaAs}/\text{Ga}_{1-x}\text{Al}_x\text{As}$ superlattice and GaAs inversion layer through cyclotron resonance experiments is a topic of extensive research activity.^{5,7}

If the assumption of a pure 2D nature of electrons trapped in the inversion layer is made then it is expected that change in the 2D polaronic mass should be larger by a factor of $3\pi/4$ over the 3D polaronic mass.^{8,9} Experimentally, however, the polaronic correction to the mass in 2D GaAs heterostructure is found to be much smaller than the theoretically expected value.⁵⁻¹⁰ Even though the importance of electronic screening of the electron-phonon interaction was well known for a long time,¹¹ its importance in the 2D polaron problem was first recognized by Das Sarma.^{12,13} He showed that, by taking the screening into account and by considering the spread of the electronic wave function in the direction normal to the 2D plane, the polaron mass is smaller in two dimensions than in three dimensions for GaAs heterostructures.

The standard way of finding the effect of electronic screening on the electron-phonon interaction is thoroughly discussed by Mahan.¹⁴ He writes the dielectric constant

$$\epsilon_{\text{total}}(\mathbf{q}, \omega) = \epsilon_{\infty} + \frac{\epsilon_0 - \epsilon_{\infty}}{1 - (\omega/\omega_t)^2} - v(\mathbf{q})\Pi(\mathbf{q}, \omega), \quad (1)$$

where ω_t is the frequency of the transverse-optic mode of

the lattice, ϵ_0 and ϵ_{∞} are, respectively, the zero- and high-frequency dielectric constant, $v(\mathbf{q})$ is the Fourier transform of the Coulomb potential, and $\Pi(\mathbf{q})$ is the polarization propagator for the electron gas. Using the above definition for $\epsilon_{\text{total}}(\mathbf{q}, \omega)$, Mahan writes the effective interaction as $V_{\text{eff}}(\mathbf{q}, \omega) = v(\mathbf{q}, \omega)/\epsilon_{\text{total}}(\mathbf{q}, \omega)$. By considering the effect of electronic screening first, using Eq. (1), it is possible to separate the effect of screened electron-phonon interaction on $V_{\text{eff}}(\mathbf{q}, \omega)$. The self-energy of the electron as affected by the screened electron-phonon interaction can then be obtained. In this procedure two effects occur. The phonon frequencies are altered by the electron screening and the electron-phonon interaction is weakened by the electron screening directly and in addition through the modification of phonon frequencies. The latter effect is relevant but is usually neglected. This method for calculating the electron self-energy is somewhat complicated. An alternate method for calculating the electron self-energy is presented in this paper. Our method is considerably simpler and is based on the semiclassical dispersion theory.¹⁵ In this theory the electron self-energy is given by the change in the zero-point energy of the radiation field when the interaction between the electron and lattice is present and when it is not. The theory is ideally suited to treat problems in which more than one interaction is present as is the case with the present problem. The most crucial quantity needed in this theory is the dielectric constant $\epsilon_{\text{total}}(\mathbf{q}, \omega)$. The accuracy of the theory is limited by the correctness of the expression used for the dielectric constant. The theory was used to discuss the polaron in three dimensions by Hawton and Paranjape¹⁶ and by Hawton *et al.*¹⁷ In the present paper the theory is extended to the polaron in the 2D system in which the effect of screening is included through the use of Eq. (1). We believe our approach is much simpler and provides a direct method for calculating the polaronic effects. In our method the effect of screening on phonon frequencies is included in a natural way while such effects are excluded in the earlier works of Das Sarma^{12,13,18} and of Wu, Peeters and Devreese.¹⁹

Using the dispersion theory approach we evaluate, in this paper, 2D polaron mass and the ground-state energy of the polaron 2D and quasi-2D situations. We use the random-phase approximation to express the electronic

part of $\epsilon_{\text{total}}(\mathbf{q}, \omega)$. Although it is tempting to use the Thomas-Fermi approximation because of the simplicity it provides in the calculations, it has been shown by Wu, Peeters, and Devreese,¹⁸ and later on by Das Sarma¹⁹, that Thomas-Fermi approximation is too drastic an assumption to give meaningful results for the 2D polaron problem. The principal aim of this paper is to provide the application of the dispersion theory to the 2D polaron problem. Our calculations use the random-phase approximation (RPA).

The dispersion theory approach is given in the following section. The effective mass and the ground-state energy for the 2D polaron is obtained for the GaAs/Ga_{1-x}Al_xAs system and for Hg_{1-x}Cd_xTe using parameters given by Dornhaus and Nimtz.²⁰ These materials are selected for the contrast they provide, since the screening effect is expected to be strong in the former case and relatively weak in the later case. The results of our theory are discussed in the last section.

II. METHOD

In the dispersion theory approach we calculate the difference between the zero point energies of the radiation field when the interaction between the electron and the medium is present and when it is not. If we consider the macroscopic electric field $\mathbf{E}(\mathbf{r}', \omega)$ at point \mathbf{r}' in the medium, then the electric field $\mathbf{E}(\mathbf{r}, \omega)$ at \mathbf{r} is related to $\mathbf{E}(\mathbf{r}', \omega)$ by the relation

$$\mathbf{E}(\mathbf{r}, \omega) = \int \tilde{F}(\mathbf{r}, \mathbf{r}', \omega) \mathbf{E}(\mathbf{r}', \omega) d^3r', \quad (2)$$

where the nonlocal tensor $\tilde{F}(\mathbf{r}, \mathbf{r}', \omega)$ depends on the elec-

trical properties of the medium and of the electron. In the absence of the medium and the electron, obviously, \tilde{F} becomes $\delta(\mathbf{r} - \mathbf{r}')$. For a medium consisting of a polar lattice and 2D electron gas, the appropriate form of \tilde{F} must be found. Upon Fourier transformation, Eq. (2) becomes

$$\mathbf{E}(\mathbf{k}, \omega) = \sum_{\mathbf{k}'} \tilde{F}(\mathbf{k}, \mathbf{k}', \omega) \mathbf{E}(\mathbf{k}', \omega). \quad (3)$$

Equation (3) provides the eigenmodes of the system. The zero-point energy of these modes is given by¹⁵

$$E = \frac{\hbar}{4\pi i} \oint_C d\omega \text{Tr} \sum_{g=1}^{g=\infty} [F(\mathbf{k}, \mathbf{k}', \omega)]^g / (g), \quad (4)$$

where g is the summation index and the contour C encloses the positive real axis of the complex ω plane. To get the linear result in the coupling between the electron and the medium it is sufficient to consider the $g=1$ term in Eq. (4). Furthermore, if we neglect the coupling between the electron and the medium, the zero-point energy is given by Eq. (4) provided \tilde{F} is replaced by another tensor \tilde{F}_0 . The change in the zero-point energy in the linear approximation can now be written as

$$\Delta E = \frac{\hbar}{4\pi i} \oint_C d\omega \text{Tr} \tilde{G}(\mathbf{k}, \mathbf{k}', \omega), \quad (5)$$

where $\tilde{G}(\mathbf{k}, \mathbf{k}', \omega)$ is the difference between \tilde{F} and \tilde{F}_0 .

The expression for $\tilde{G}(\mathbf{k}, \mathbf{k}', \omega)$ appropriate to a three-dimensional crystal was obtained previously using the second-order perturbation theory by Hawton and Paranjape.¹⁶

$$\begin{aligned} \tilde{G}(\mathbf{k}, \mathbf{k}', \omega) = & \left[\frac{2\pi}{L} \right]^3 \frac{e^2}{\hbar(2\pi)^2} \sum_{\mathbf{k}''} \frac{\mathbf{k}\mathbf{k}'}{k^2(k'')^2} \left[\frac{1}{\epsilon_{\text{total}}(\mathbf{k}, \omega)} - \frac{1}{\epsilon_{\text{total}}(\mathbf{k}, \infty)} \right] \\ & \times \left[\frac{\langle \mathbf{k}_0, z | \exp(-i\mathbf{k}' \cdot \mathbf{r}) | \mathbf{k}'', z \rangle \langle \mathbf{k}'', z | \exp(i\mathbf{k} \cdot \mathbf{r}) | \mathbf{k}_0, z \rangle}{\omega_{\mathbf{k}'', \mathbf{k}_0} - \omega} \right. \\ & \left. + \frac{\langle \mathbf{k}_0, z | \exp(i\mathbf{k} \cdot \mathbf{r}) | \mathbf{k}'', z \rangle \langle \mathbf{k}'', z | \exp(-i\mathbf{k}' \cdot \mathbf{r}) | \mathbf{k}_0, z \rangle}{\omega_{\mathbf{k}'', \mathbf{k}_0} + \omega} \right], \quad (6) \end{aligned}$$

where the first and second terms in the second set of large parentheses, when multiplied by the remaining terms of Eq. (6), correspond to \tilde{F} and \tilde{F}_0 , respectively; $|\mathbf{k}_0, z\rangle$ is the unperturbed electron state, \mathbf{k}_0 describing its plane-wave character in two dimensions, and z its spread in direction normal to the 2D plane; $|\mathbf{k}'', z\rangle$ represents the remaining intermediate states of the electron; and $\omega_{\mathbf{k}'', \mathbf{k}_0} = \hbar[(k'')^2 - k_0^2]/2m$. We have neglected the excited states which are normal to the 2D plane. The form of the electronic state in the coordinate representation is given by

$$\langle \mathbf{r} | \mathbf{k}_0, z \rangle = [\psi(x)/L] \exp(i\mathbf{k}_0 \cdot \mathbf{r}), \quad (7)$$

where L is the periodic length, \mathbf{k}_0 is the wave vector of the electron in the 2D plane, and $\psi(z)$ is the variational wave function normal to the 2D plane. The suitable form for $\psi(z)$ is given by Stern and Howard²¹ as

$$\psi(z) = \begin{cases} (b^3/2)^{1/2} \exp(-bz/2)z & \text{for } z > 0 \\ 0 & \text{for } z < 0, \end{cases} \quad (8)$$

where b is the variational parameter which depends on the electron density N and the depletion charge density N_d according to

$$b = (48\pi m e^2 / \hbar^2)^{1/3} (N_d + N)^{1/3}.$$

In Eq. (6), both vectors \mathbf{k}_0 and \mathbf{k}' representing the electronic states are two dimensional while vectors \mathbf{k} and \mathbf{k}' are three dimensional.

For convenience we write Eq. (1) in the following form:

$$\frac{1}{\epsilon_{\text{total}}(\mathbf{k}, \omega)} = \frac{\omega_i^2 - \omega^2}{\epsilon_{\infty} \mu_{\infty}(\mathbf{k})(\omega_1^2 - \omega^2)}, \tag{9}$$

where

$$\mu_{\infty}(\mathbf{k}) = 1 - \frac{v(\mathbf{k})\Pi(\mathbf{k})}{\epsilon_{\infty}}, \quad \mu_0(\mathbf{k}) = 1 - \frac{v(\mathbf{k})\Pi(\mathbf{k})}{\epsilon_0}, \tag{10}$$

and

$$\omega_1^2 = \omega_0^2 \frac{\mu_0(\mathbf{k})}{\mu_{\infty}(\mathbf{k})}. \tag{11}$$

In the definitions of μ 's we have neglected in π its frequency dependence. This is a reasonable assumption¹⁴ when $\omega_0 \ll \omega_p$ — the plasma frequency. We now write the 3D vectors in terms of their components parallel and perpendicular to the 2D plane according to $\mathbf{k} = (\mathbf{k}_{\parallel}, k_{\perp})$ and $\mathbf{k}' = (\mathbf{k}'_{\parallel}, k'_{\perp})$. The matrix elements in Eq. (6) can be evaluated using Eqs. (7) and (8) to yield

$$\begin{aligned} & \langle \mathbf{k}_0, z | \exp(-i\mathbf{k}' \cdot \mathbf{r}) | \mathbf{k}', z \rangle \langle \mathbf{k}'', z | \exp(i\mathbf{k} \cdot \mathbf{r}) | \mathbf{k}_0, z \rangle \\ &= \frac{b^6}{(b + ik'_{\perp})^3 (b - ik_{\perp})^3} \delta_{\mathbf{k}'', \mathbf{k}_0 + \mathbf{k}'_{\parallel}} \delta_{\mathbf{k}', \mathbf{k}_0 + \mathbf{k}_{\parallel}}. \end{aligned} \tag{12}$$

Hence the frequency in the energy denominator of Eq. (6) becomes

$$\omega_{\mathbf{k}'', \mathbf{k}_0} = \frac{\hbar}{2m} (k_{\parallel}^2 + 2k_0 k_{\parallel} \cos\phi) = \Omega_{k_{\parallel}},$$

where ϕ is the angle between \mathbf{k}_0 and \mathbf{k}_{\parallel} . Substituting these in Eq. (6) and setting $\mathbf{k} = \mathbf{k}'$ we get

$$\begin{aligned} \tilde{G}(\mathbf{k}, \mathbf{k}, \omega) &= \frac{4\pi e^2 b^6}{L^3 \hbar \epsilon_{\text{total}}(k_{\parallel}, \omega)} \frac{1}{(k_{\parallel}^2 + k_{\perp}^2)(b^2 + k_{\perp}^2)^3} \\ &\times \frac{2\Omega_{k_{\parallel}}}{\Omega_{k_{\parallel}}^2 - \omega^2}, \end{aligned} \tag{13}$$

where wave-vector dependence of ϵ , the dielectric constant, is considered in the 2D plane.

We also make use of the random-phase approximation²² to write

$$\mu_i(k_{\parallel}) = \begin{cases} 1 + \frac{2me^2}{\hbar^2 \epsilon_i k_{\parallel}} & \text{for } k_{\parallel}^2 < (8\pi N) \\ 1 + \frac{2me^2}{\hbar^2 \epsilon_i k_{\parallel}} \{1 - [1 - (8\pi N/k_{\parallel}^2)]^{1/2}\} & \text{for } k_{\parallel}^2 > (8\pi N), \end{cases} \tag{14}$$

where i is either 0 or ∞ and N is the 2D electron (hole) density. Under the Thomas-Fermi approximation Eqs. (14) and (15) become simply

$$\mu_i = 1 + \frac{\gamma_i}{k_{\parallel}}, \tag{16}$$

where $\gamma_i = 2me^2/\hbar^2 \epsilon_i$. The use of Thomas-Fermi approximation, i.e., Eq. (16), in the calculations to follow would result, as has been pointed out,^{18,19} in polaron energy and mass significantly different from their more reliable values obtainable from using the RPA results based on Eqs. (14) and (15). Our calculations are based on RPA and are therefore more accurate than some results obtained earlier¹² using Thomas-Fermi approximation.

We now substitute Eq. (13) into Eq. (5). In the process of obtaining the trace in Eq. (5), we first sum over k_{\perp} by changing to integration; the summation over k_{\parallel} is achieved later by numerical integration. To complete the ω integration in Eq. (5) we take the residue at the poles occurring at $\omega = \omega_1$ and at $\omega = \Omega_k$. The former pole occurs at the lattice frequency as modified by the electron screening. The result of the contour integration over ω in Eq. (5) leaves the integration over k_{\parallel} . We now rescale the variable k_{\parallel} , and β in terms of the polaron radius $q_0 = (2m\omega_0/\hbar)$, and write $(k_{\parallel}/q_0) = x$ and $(b/q_0) = \beta$. Equation (5) can now be written as

$$\Delta E = \frac{\alpha \hbar \omega_0}{16\pi} \int dx \int d\phi \frac{(3s^2\beta + 8\beta^3 + 9x\beta^2)f(\mu_0, \mu_{\infty}, x)}{(x + \beta)^3 [\mu_0(x)\mu_{\infty}(x)]}, \tag{17}$$

where α the Fröhlich constant is given by

$$\alpha = \frac{e^2}{2} \left[\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_0} \right] \left[\frac{2m\omega_0}{\hbar} \right]^{1/2} \left[\frac{1}{\hbar\omega_0} \right],$$

$$x_0 = (k_0/q_0),$$

and

$$f(\mu_0, \mu_{\infty}, x) = [1 + (\mu_{\infty}/\mu_0)^{1/2}(x^2 + 2xx_0 \cos\phi)]^{-1}.$$

For a slow moving polaron (i.e., small x_0), $f(\mu_0, \mu_{inf}, x)$ can be developed in powers of x_0 . The term independent of x_0 in Eq. (17) provides the value of the ground-state energy $\Delta E^{(0)}$ of the polaron. It is given by

$$\Delta E^{(0)} = \frac{\alpha \hbar \omega_0}{8} \int_0^{\infty} dx \frac{(3x^2\beta + 8\beta^3 + 9x\beta^2)}{(x + \beta)^3 \mu_0 \mu_{\infty} [(\mu_{\infty}/\mu_0)^{1/2} x^2 + 1]}. \tag{18}$$

Similarly the energy term, $\Delta E^{(1)}$, proportional to x_0^2 is given by

$$\Delta E^{(1)} = \frac{\alpha \hbar \omega_0}{4} x_0^2 \times \int_0^\infty dx \frac{(3x^2\beta + 9x\beta^2 + 8\beta^3)x^2(\mu_\infty/\mu_0)}{(x+\beta)^3 \mu_0 \mu_\infty [(\mu_\infty/\mu_0)^{1/2} x^2 + 1]^3} . \quad (19)$$

It is possible to calculate the change in the electron mass due to electron-phonon interaction from Eq. (19). If we define m_p as the polaron mass and m_b as the band mass of the electron then

$$\frac{\hbar^2 k_0^2}{2m_p} = \frac{\hbar^2 k_0^2}{2m_b} - \frac{d^2}{\hbar^2 dk_0^2} \Delta E^{(1)} . \quad (20)$$

Following Das Sarma¹⁹ we define the change in the electron mass due to its interaction with the lattice in terms of the band mass according to

$$\Delta m = (m_p - m_b) / m_b . \quad (21)$$

Using Eqs. (19)–(21) we write

$$\Delta m = \frac{\alpha}{4} \int \frac{(3x^2\beta + 8\beta^3 + 9x\beta^2)x^2(\mu_\infty/\mu_0)}{(\mu_0\mu_\infty)(x+\beta)^3[(\mu_\infty/\mu_0)^{1/2}x^2+1]^3} dx . \quad (22)$$

Equations (18) and (22) are the principal results of this paper. The numerical estimates of ΔE^0 and Δm and the conclusions arising from these estimates are discussed in the following section.

III. CONCLUSIONS

In this paper we have applied the dispersion theory to the problem of the 2D polaron in heterojunctions and have calculated the ground-state energy and mass of the polaron. We have used the RPA to describe the proper-

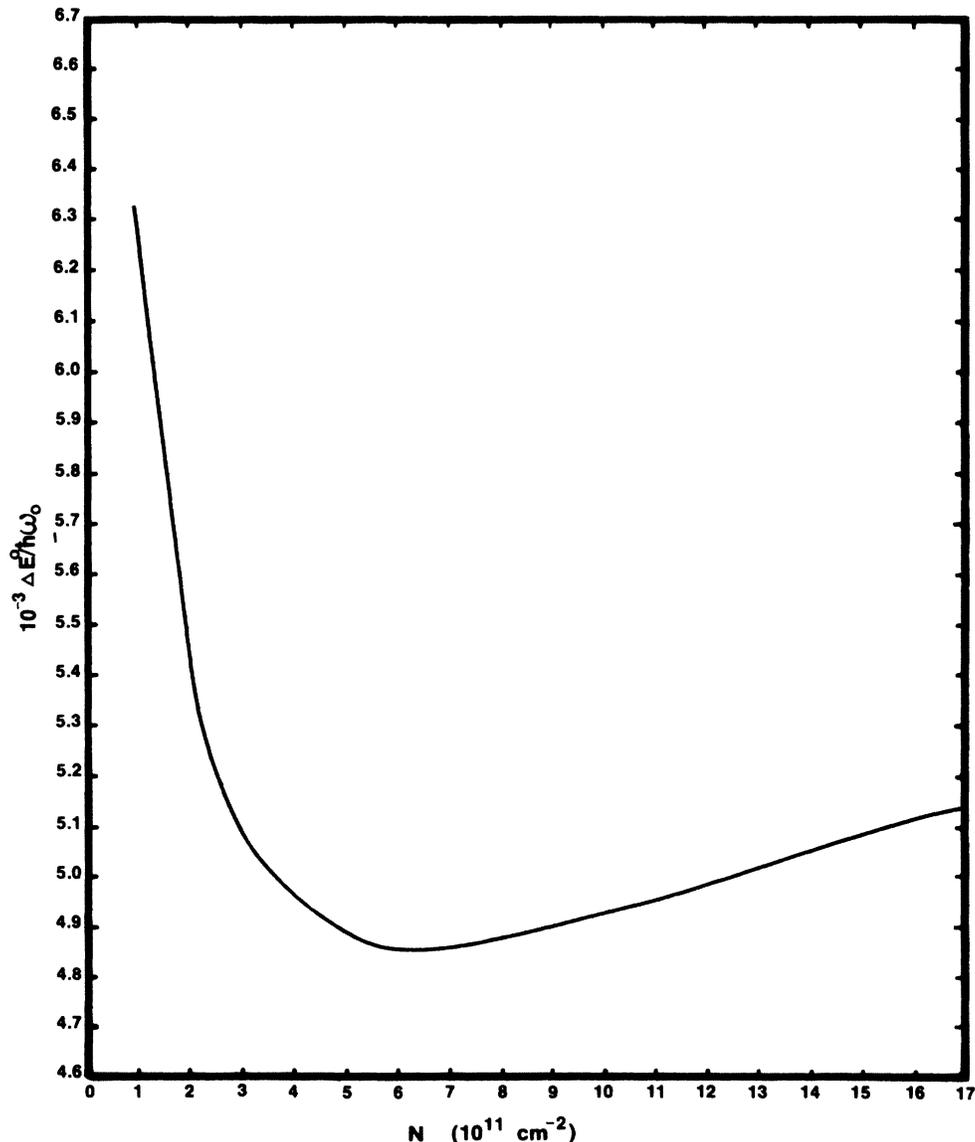


FIG. 1. Shows the polaron ground-state energy ΔE^0 (in units of $\hbar\omega_0=35$ meV) for a $\text{Ga}_{1-x}\text{Al}_x\text{As}$ heterostructure (purely 2D and 3D unscreened values for ΔE^0 are, respectively, 0.11 and 0.07).

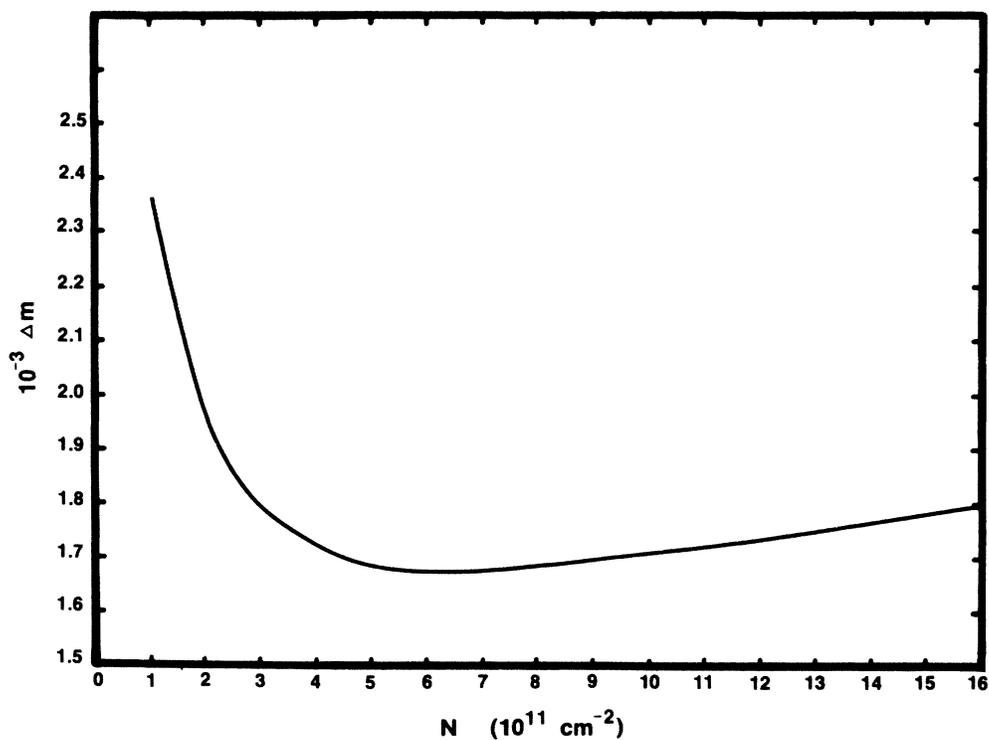


FIG. 2. Shows the variation of Δm as a function of N in a $\text{Ga}_{1-x}\text{Al}_x\text{As}$ heterostructure (purely 2D and 3D unscreened values for Δm are, respectively, 0.027 and 0.012).

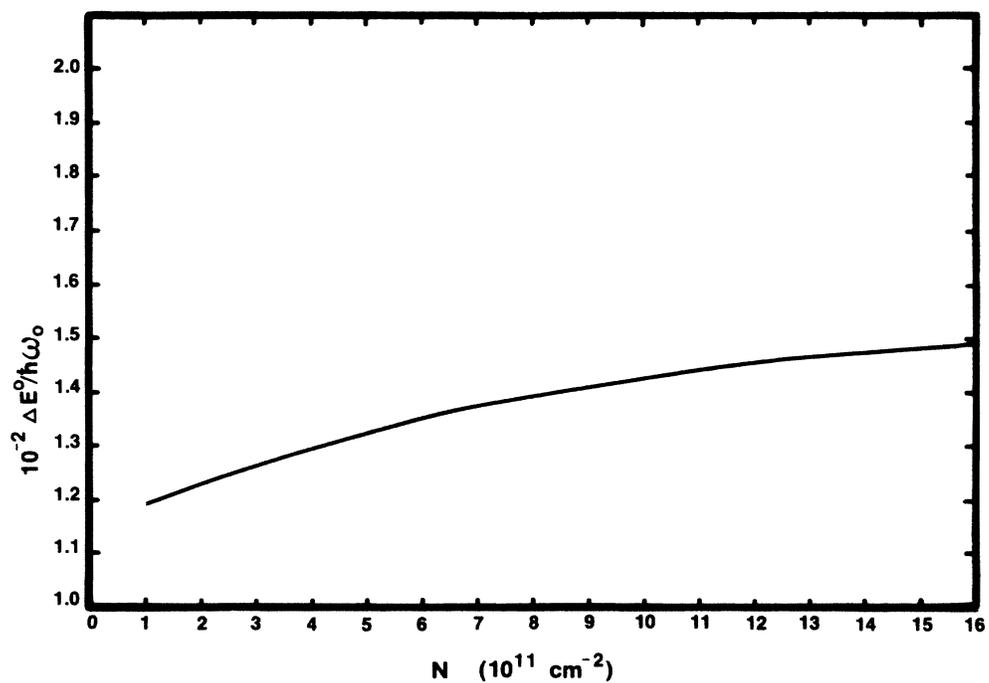


FIG. 3. Shows the polaron ground-state energy ΔE^0 (in units of $\hbar\omega_0=17.1$ meV) for a $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ ($x=0.2$) heterostructure (purely 2D and 3D unscreened values of ΔE^0 are, respectively, 0.058 and 0.03).

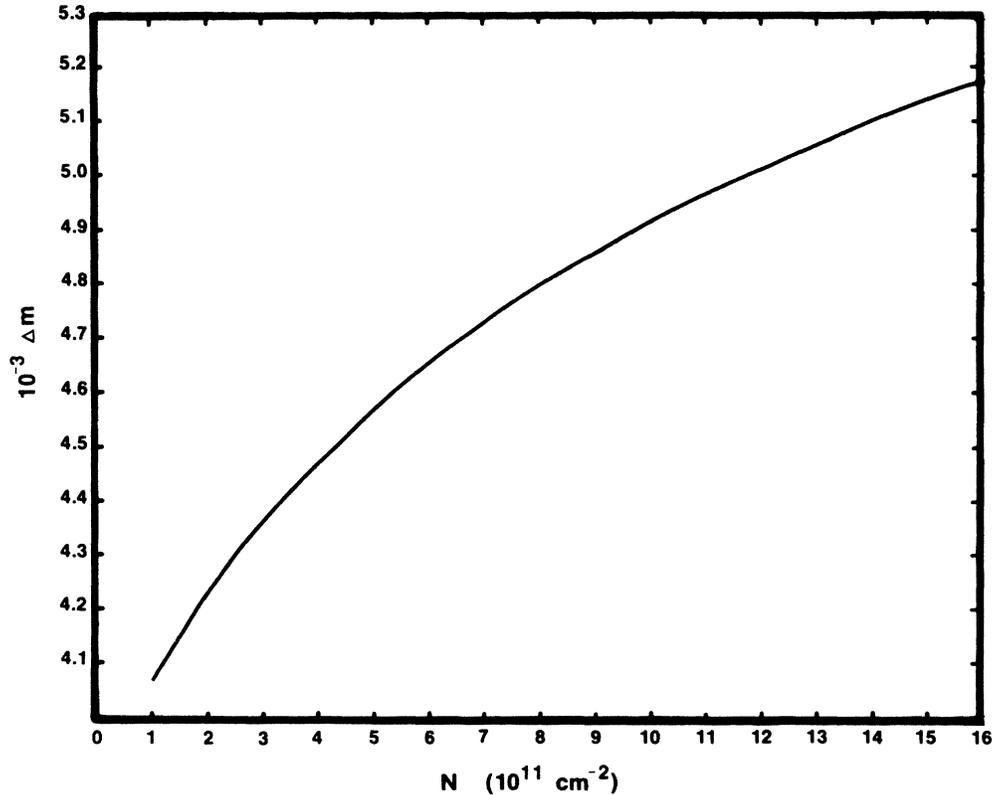


FIG. 4. Shows the variation of Δm as a function of N in a $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$ heterostructure (purely 2D and 3D unscreened values for Δm are, respectively, 0.013 and 0.005).

ties of the 2D electron gas. Our results are in quantitative agreement with the results of the ground-state energy and effective mass of the polaron in the $\text{Ga}_{1-x}\text{Al}_x\text{As}$ system as obtained by the earlier authors.^{18,19} We have obtained numerical estimates for the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ system also. As expected, the electron screening is much weaker in the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ system than in $\text{Ga}_{1-x}\text{Al}_x\text{As}$. Hence, the mass enhancement of the polaron arising from the 2D or quasi-2D confinement is most likely to be observed in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$.

Figure 1 shows the variation of the ground-state energy of the polaron with the 2D electron density, N , for the $\text{Ga}_{1-x}\text{Al}_x\text{As}$ system. We select the following parameters: $N_d = 10^{11} \text{ cm}^{-2}$, $\epsilon_\infty = 10.9$, $\epsilon_0 = 12.82$, $(m_b/m) = 0.0665$, and $\alpha = 0.07$. As N increases the ground-state energy is affected by two opposing effects. On one hand the increase in N reduces the electron-phonon interaction due to the increase in the screening while, on the other hand, the binding energy is enhanced due to the fact that increasing N makes the electron gas increasingly two dimensional. The influence of the two effects on ΔE^0 is seen in Fig. 1 where the ground-state energy decreases with N initially due to increased screening, but as N is increased further the 2D effects predominate over the screening effects resulting in the enhanced energy. In Fig. 2 the effect of N on Δm in $\text{Ga}_{1-x}\text{Al}_x\text{As}$ follows the same pattern as for ΔE^0 .

In Figs. 3 and 4 the variations of ΔE^0 and Δm with N

are shown for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. The parameters for this material are not precisely known. Dornhaus and Nimitz²⁰ have provided the estimates for the needed parameters as follows: $(m/m_0) = 0.005$, $\epsilon_0 = 17.0$, $\epsilon_\infty = 12.5$, and $\hbar\omega_0 = 17.1 \text{ meV}$. The results for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ (with $x = 0.2$), shown in Figs. 3 and 4, are in sharp contrast with those of $\text{Ga}_{1-x}\text{Al}_x\text{As}$. In the case of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ it is expected that the screening effect would be weaker than the effect due to the 2D nature of the electron gas. For the N values considered in the numerical calculations, both ΔE and Δm increase with N , indicating that the 2D effect is dominant. Conversely, the absence of a decrease in the values of ΔE^0 and Δm with increasing N clearly shows that the screening is negligible for this material. The increase in the polaron mass due to the 2D nature of the electron gas is most likely to be observed experimentally in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$.

Although our results for the variations of ΔE^0 and Δm with N in $\text{Ga}_{1-x}\text{Al}_x\text{As}$ are in qualitative agreement with those of the RPA-based results of Das Sarma¹⁹ and Wu Xiaoguang,¹⁸ they differ quantitatively with the results of both these authors. The difference can be attributed to the dissimilarity between our method and the methods used by the earlier authors.^{18,19} Our method is based on dispersion theory which takes into account the changes in the phonon frequencies due to the electron screening, an effect which is neglected by the earlier authors.^{18,19}

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