

Effect of screening on the optical absorption of a two-dimensional electron gas in GaAs-Al_xGa_{1-x}As heterostructures

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The optical-absorption spectrum is calculated for a quasi-two-dimensional electron gas interacting with polar optical phonons in a GaAs-Al_xGa_{1-x}As heterostructure. The importance of *dynamical screening*, the effect of the finite width of the two-dimensional electron layer, and the temperature dependence are investigated. The polaron mass is derived and is found to decrease with increasing electron density. For electron densities around 10¹² cm⁻² the absorption spectrum shows in addition to the usual structure a shoulder at energy $E_F + \hbar\omega_{LO}$ with E_F the Fermi energy and $\hbar\omega_{LO}$ the optical-phonon energy.

I. INTRODUCTION

In recent studies¹⁻⁵ it has been found that in semiconductor heterostructures the screening of the electron-polar-optical-phonon interaction (polaron effects) is important because of the relatively large electron densities. Most of the studies have been devoted to the calculation of the electron-phonon interaction correction to the self-energy,^{1,2} the subband energy,³ the plasmon-phonon-model coupling,⁴ and the polar-optical-phonon limited mobility.⁵ From the self-energy calculation it is found that the electron screening substantially reduces the electron-phonon interaction. The purpose of the present paper is to investigate the effects of screening on the polar optical-absorption spectrum and on the polaron mass.

To calculate the optical absorption of interacting polarons, we will use the memory-function formalism.^{6,7} The electron screening is treated within the random-phase approximation (RPA).^{8,9} The electron-phonon interaction is treated as a perturbation and the memory function is expanded to first order in the electron-phonon coupling constant α (see, e.g., Ref. 6). For simplicity, we only consider the effect of the lowest subband and a variational wave function for the subband is used⁸ (see also Ref. 2). In the present study we also neglect the plasmon-phonon-mode coupling and the nonparabolicity of the electron energy band.

The present paper is organized as follows: In Sec. II the optical absorption is expressed in terms of a memory function which is calculated (for a similar discussion for the three-dimensional (3D) polaron we refer to Refs. 6 and 10). Section III contains the numerical results and the discussion. Our conclusion is presented in the last section.

II. FORMULATION AND CALCULATION

The electron-phonon system is described by the Hamiltonian

$$H = \sum_j \frac{p_j^2}{2m_b} + \sum_{\mathbf{k}} \hbar\omega_{LO} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{i < j} V(\mathbf{r}_i - \mathbf{r}_j) + \sum_j \sum_{\mathbf{k}} (V_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} + V_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}_j}), \quad (1)$$

where $\mathbf{p}(\mathbf{r})$ is the momentum (position) operator of an electron. $a_{\mathbf{k}}^\dagger$ ($a_{\mathbf{k}}$) is the creation (annihilation) operator of a phonon with wave vector \mathbf{k} and energy $\hbar\omega_{LO}$. In Eq. (1) $V_{\mathbf{k}}$ is given by

$$V_{\mathbf{k}} = i\hbar\omega_{LO} \left[\frac{4\pi\alpha}{V k^2} \right]^{1/2} \left[\frac{\hbar}{2m_b\omega_{LO}} \right]^{1/4} \langle \psi_0 | e^{i\mathbf{k}_z z} | \psi_0 \rangle. \quad (2)$$

Here $\psi_0(z) = (b^3/2)^{1/2} z e^{-bz/2}$ is the variational wave function of the electron in the z direction which is normal to the electron layer. b is a known function of the electron density, of the depletion charge density of the system, and of the effective mass of the electron: $b = (48\pi m_b N e^2 / \hbar^2 \epsilon_0)^{1/3}$, where $N = n_d + \frac{11}{32} n_e$ with n_d and n_e the depletion and carrier densities, respectively.⁸ $V(\mathbf{r} - \mathbf{r}')$ represents the Coulomb interaction between two electrons in the quasi-two-dimensional (Q2D) electron layer. The Fourier transform of $V(\mathbf{r})$ is

$$V(k_{||}) = (2\pi e^2 / k_{||} \epsilon_\infty) f(k_{||}, b)$$

with

$$f(k, b) = (8b^3 + 9b^2k + 3bk^2) / [8(b+k)^3]$$

the form factor. For a two-dimensional (2D) electron layer with zero width one has $f(k, b = \infty) = 1$.

To calculate the optical absorption (the ac conductivity) we use the memory-function approach⁷ (see also Ref. 6). We can express the dynamic conductivity in the presence of a magnetic field as

$$\sigma_{\pm}(\omega) = \frac{in_e e^2 / m_b}{\omega \pm \omega_c - \Sigma(\omega)}, \quad (3) \quad F(t) = - \sum_{\mathbf{k}} \frac{k_{\parallel}^2}{n_e m_b \hbar} |V_{\mathbf{k}}|^2$$

where $\Sigma(\omega)$ is the memory function, n_e is the electron density, and m_b the electron band mass. The memory function $\Sigma(\omega)$ as a function of frequency ω has the form (see also Refs. 6 and 10)

$$\Sigma(\omega) = \frac{1}{\omega} \int_0^{\infty} dt (1 - e^{i\omega t}) \text{Im}F(t), \quad (4a)$$

$$\times [iD(k_{\parallel}, t) + in(\omega_{\text{LO}})D^R(K_{\parallel}, t)] e^{-i\omega_{\text{LO}}t}, \quad (4b)$$

where $n(x) = (e^{\hbar\beta x} - 1)^{-1}$ is the occupation number and $D(k_{\parallel}, t)$ [$D^R(k_{\parallel}, t)$] is the electron (retarded) density-density correlation function calculated without electron-phonon interaction.¹¹ More explicitly we have for the real part of the memory function

$$\begin{aligned} \text{Re}\Sigma(\omega) = & - \sum_{\mathbf{k}} \frac{k_{\parallel}^2}{n_e m_b \omega} \frac{|V_{\mathbf{k}}|^2}{V(k_{\parallel})} \frac{\omega^2}{\pi} \int_{-\infty}^{+\infty} dx \frac{[1+n(x)]S(k_{\parallel}, x)}{[(x+\omega_{\text{LO}})^2 - \omega^2](x+\omega_{\text{LO}})} \\ & + n(\omega_{\text{LO}}) \sum_{\mathbf{k}} \frac{k_{\parallel}^2}{n_e m_b \omega} \frac{|V_{\mathbf{k}}|^2}{V(k_{\parallel})} \frac{1}{2} \text{Re} \left[\frac{1}{\epsilon(k_{\parallel}, \omega + \omega_{\text{LO}})} + \frac{1}{\epsilon(k_{\parallel}, \omega - \omega_{\text{LO}})} - \frac{2}{\epsilon(k_{\parallel}, \omega_{\text{LO}})} \right], \end{aligned} \quad (5a)$$

and for the imaginary part

$$\text{Im}\Sigma(\omega) = \sum_{\mathbf{k}} \frac{k_{\parallel}^2}{n_e m_b \omega} \frac{|V_{\mathbf{k}}|^2}{V(k_{\parallel})} \frac{1}{2} \{ [n(\omega + \omega_{\text{LO}}) - n(\omega_{\text{LO}})] S(k_{\parallel}, \omega + \omega_{\text{LO}}) - [1 + n(\omega - \omega_{\text{LO}}) + n(\omega_{\text{LO}})] S(k_{\parallel}, \omega - \omega_{\text{LO}}) \}, \quad (5b)$$

with $S(k, \omega) = -\text{Im}\epsilon^{-1}(k, \omega)$ the electron energy loss function of the 2D electron gas and $\epsilon(k, \omega)$ the dielectric function. The real and imaginary part of the memory function are related to each other by the Kramers-Kronig relation. In the zero magnetic field limit the dielectric function has been calculated within the RPA with wave vector, frequency, and temperature dependence.^{8,9}

In the following we will concentrate on the zero magnetic field case where the dielectric function is known and leave the more difficult case of nonzero magnetic field for future study. In order to make our results more transparent we follow Ref. 12 and compare Eq. (3) with the Drude form for the conductivity (see also Ref. 6)

$$\sigma(\omega) = \frac{in_e e^2}{(m_b + \Delta m)(\omega + i\nu)}. \quad (6)$$

We may identify Δm as the mass renormalization with

$$\frac{\Delta m}{m_b} = - \frac{\text{Re}\Sigma(\omega)}{\omega}, \quad (7a)$$

and ν the collision frequency

$$\nu = - \frac{\text{Im}\Sigma(\omega)}{1 + \Delta m / m_b}, \quad (7b)$$

which are now both frequency dependent.

In the absence of a magnetic field a formal expansion of Eq. (3) can be made for high frequencies and after a lengthy calculation one finds the results of Tzoar.¹² In Ref. 12 a diagrammatic approach was used to obtain the high-frequency conductivity and numerical results were given for the imaginary part of the memory function of the 2D electron layer with zero width in the limit of zero temperature. Here (in the next section) we will present re-

sults for the optical-absorption spectrum which not only involves the imaginary part of the memory function but also the real part of the memory function. The temperature will also be taken different from zero and furthermore the effect of the finite width of the 2D electron layer on the optical-absorption spectrum will be investigated.

III. RESULTS AND DISCUSSION

We have calculated the optical-absorption spectrum which is defined as

$$\frac{-\text{Im}\Sigma(\omega)}{[\omega - \text{Re}\Sigma(\omega)]^2 + [\text{Im}\Sigma(\omega)]^2}. \quad (8)$$

Physical parameters are taken which correspond to the GaAs-AlGaAs heterostructure, i.e., $\hbar\omega_{\text{LO}} = 36.77$ meV, dielectric constants $\epsilon_0 = 12.83$, $\epsilon_{\infty} = 10.9$, band mass $m_b = 0.0657m_e$, and electron-phonon coupling constant $\alpha = 0.068$. The depletion charge density is taken to be $n_d = 8 \times 10^{10} \text{ cm}^{-2}$.

In Fig. 1 we show the optical-absorption spectrum of an ideal 2D electron system (zero layer width) at zero temperature for different values of the electron density. The zero-density absorption spectrum corresponds to the 2D equivalent of the 3D results of Ref. 10 (see also Ref. 6) in which the two Feynman parameters v and w are taken as $v = w$. This corresponds to a calculation of the memory function within second-order perturbation theory. Figure 1 shows that the electron screening reduces the intensity of the absorption spectrum appreciably.

At zero temperature there are no real phonons. The electron can only emit phonons but no phonon absorption processes are possible. This is the reason why the absorp-

tion is zero for frequencies below the LO-phonon frequency. There is a delta function peak¹³ at the origin with weight π/m^* where m^* is the polaron mass. For frequencies above the LO-phonon frequency the absorption first increases, it reaches a maximum after which it decreases. In the limit of high frequencies the absorption spectrum behaves as $\omega^{-5/2}$ and is independent of the electron density. Note that Tzoar¹² finds that $\text{Im}\Sigma(\omega) \sim \omega^{-3/2}$ for large frequencies. We found for large frequencies $\text{Im}\Sigma(\omega) \sim \omega^{-1/2}$ which results in the $\omega^{-5/2}$ behavior of the absorption spectrum [see Eq. (8)].

For electron densities around 10^{12} cm^{-2} (see Fig. 1 and its insert) the absorption spectrum shows besides a peak also a shoulder structure. The shoulder is around $\omega = \omega_{\text{LO}} + E_F/\hbar$, with E_F the Fermi energy. This frequency is indicated by arrows in the insert of Fig. 1. At lower electron densities the shoulder structure is no longer present because it is mixed with the maximum of the absorption spectrum. For higher electron densities the shoulder disappears in the tail of the absorption spectrum and becomes very hard to resolve.

The real and the imaginary parts of the memory function of the ideal 2D electron system at zero temperature are plotted in Fig. 2 for different values of the electron density. The zero electron-density results are the 2D equivalent of the 3D results of Refs. 6 and 10. The electron screening smoothes and reduces the memory function which results in the reduction of the absorption spectrum.

We also calculated the absorption spectrum within the Hartree-Fock (HF) approximation. In this approximation

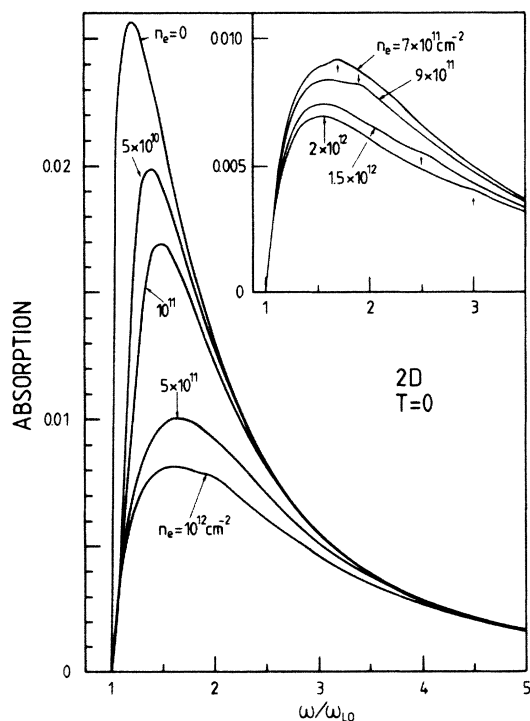


FIG. 1. Optical-absorption spectrum of an ideal two-dimensional electron gas interacting with polar optical phonons at zero temperature is plotted for different values of the electron density. In the insert the arrows indicate the position of the frequency $\omega_{\text{LO}} + E_F/\hbar$.

the screening is neglected but the occupation effect, resulting from Fermi-Dirac statistics, is included. In Fig. 3 the optical-absorption spectrum of the ideal 2D system in the HF approximation at zero temperature is plotted for different values of the electron density. We notice that no shoulder structure appears in the absorption spectrum in the HF approximation. The extra structure at $\omega = \omega_{\text{LO}} + E_F/\hbar$ in the absorption spectrum for the RPA approximation is replaced by an abrupt decrease of the absorption at $\omega = \omega_{\text{LO}} + E_F/\hbar$. In the insert of Fig. 3 we plotted the imaginary part of the memory function calculated within the HF approximation. The imaginary part of the memory function has a cusp at $\omega = \omega_{\text{LO}} + E_F/\hbar$ which is the origin of the abrupt decrease of the absorption spectrum. Comparing Fig. 2 and the insert of Fig. 3 we notice that the electron screening included in the RPA smoothes the cusp structure of the memory function.

The physical origin of the structure in the absorption around $\omega = \omega_{\text{LO}} + E_F/\hbar$ will now be discussed. For convenience we will limit ourselves to the zero-temperature case where only emission processes are possible. Consider an electron with energy E_i which absorbs a photon with energy $\hbar\omega$. The electron, as a consequence, will emit a LO-phonon and will be scattered to a state with energy E_f . Conservation of energy requires that $E_i + \hbar\omega = E_f + \hbar\omega_{\text{LO}}$ and therefore $E_i = E_f + \hbar\omega_{\text{LO}} - \hbar\omega$. At zero temperature Fermi-Dirac statistics lead to the following bounds, $E_i \leq E_F$ and $E_f \geq E_F$. This sets the following limits to the range of electron energies for participation in the scattering process $E_F \geq E_i \geq E_F + \hbar\omega_{\text{LO}} - \hbar\omega$. A maximum energy range is obtained when $E_F + \hbar\omega_{\text{LO}} - \hbar\omega = 0$. For a photon energy $\hbar\omega = \hbar\omega_{\text{LO}} + E_F$ a maximum number of electrons in the Fermi sea can participate in the scattering process. For larger frequencies the number of elec-

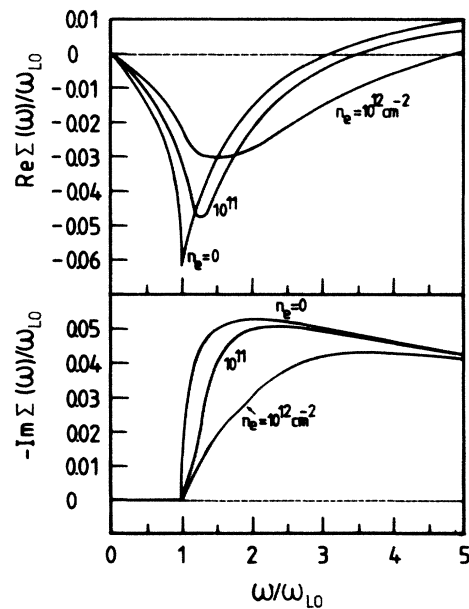


FIG. 2. Real part and the imaginary part of the memory function of an ideal two-dimensional electron system at zero temperature are plotted for different values of the electron density.

trons which can contribute to the absorption of light no longer increases. This is the underlying physical reason for the appearance of the shoulder structure at $\omega = \omega_{LO} + E_F/\hbar$. The exact frequency dependence of the absorption spectrum also strongly depends on the efficiency with which the electron interacts with the LO-phonons. For example for high frequencies the absorption strength decreases due to the decreasing efficiency with which the electron interacts with the LO-phonons.

The effect of the finite width of the 2D electron layer on the optical-absorption spectrum is investigated in Fig. 4 for the zero-temperature case. The Q2D character of the system reduces the intensity of the absorption spectrum considerably. The reduction is about a factor of 2 around the maximum of the absorption but increases to a factor of 3 for larger frequencies. Note also that the shoulder structure of the absorption spectrum still exists for the electron densities around 10^{12} cm^{-2} .

In the present study we only considered the lowest subband. This approximation breaks down for larger electron densities because higher subbands will then also be occupied. In Ref. 3 the subband separation is calculated and shown to depend on the electron density. For the electron densities in the present study ($n_e = 10^{10} \text{ cm}^{-2} \sim 10^{12} \text{ cm}^{-2}$) the Fermi energy is smaller than the separation between the first two subbands.³ We also neglected the phonon assisted intersubband transition which will contribute to the optical absorption at high frequencies. In Ref. 14 the effect of the intersubband transition on the

optical absorption has been studied for the quantum-well structure and results in additional peaks in the absorption spectrum which corresponds to the different thresholds for transitions to the different subbands. In Ref. 14 only one electron is involved with Boltzmann statistics and consequently no screening has been considered. In contrast, in the present paper many electrons are considered. The limitation to the lowest subband is introduced for convenience because it severely reduces numerical work.

The effect of the temperature on the optical-absorption spectrum is shown in Fig. 5 for the ideal 2D electron system for different values of the lattice temperature and the electron density. At low temperature (i.e., the $T = 20 \text{ K}$ result for $n_e = 10^{11} \text{ cm}^{-2}$) the absorption spectrum is very close to the zero-temperature result since the LO-phonon frequency is rather large, i.e., $T_0 = \hbar\omega_{LO}/k_B = 427 \text{ K}$. For $T = 20 \text{ K}$ the relevant quantity $T/T_0 = 0.047$ is very small. For nonzero temperature LO-phonons are present in the semiconductor and contribute to the scattering processes. Consequently the absorption becomes nonzero for frequencies below the LO-phonon frequency. The shoulder structure of the absorption spectrum for electron densities around 10^{12} cm^{-2} still exists, but is less pronounced. The delta-function peak at the origin broadens with increasing temperature.^{6,10}

Screening also affects the mass renormalization which is given by Eq. (7a). In Fig. 6 the mass shift at zero temperature and zero frequency is shown as a function of the electron density. For the ideal 2D system the mass decreases as the electron density increases. The reason is that screening increases with increasing electron density.

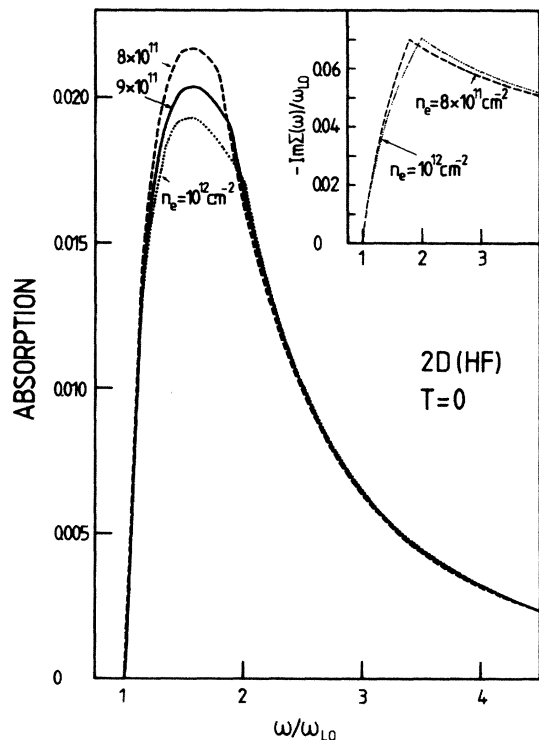


FIG. 3. Zero-temperature absorption spectrum of an ideal two-dimensional electron gas calculated within the Hartree-Fock (HF) approximation is plotted for different values of the electron density. The insert shows the imaginary part of the memory function in the HF approximation.

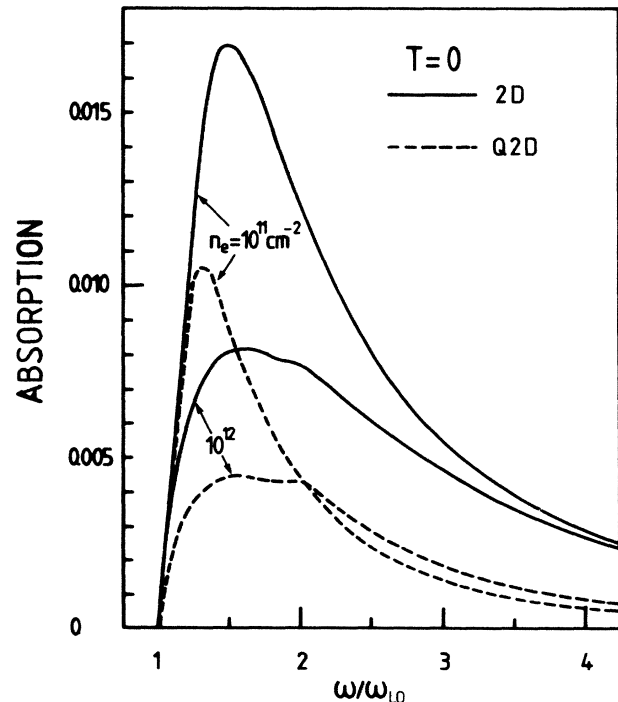


FIG. 4. Zero-temperature absorption spectrum is shown for an ideal two-dimensional and a quasi-two-dimensional electron system.

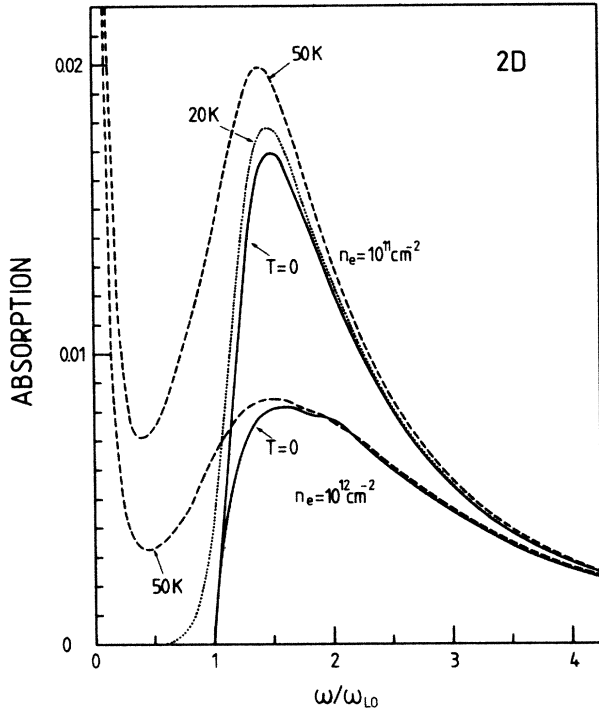


FIG. 5. Optical-absorption spectrum of an ideal two-dimensional interacting electron gas is shown for different values of the lattice temperature and the electron density.

In the zero-density limit the well-known result $\pi\alpha/8$ is obtained. For the Q2D system, the subband effect, i.e., the finite width of the electron layer, reduces the mass shift over the whole electron-density region with a factor of about 3 for $n_e = 10^{11} \text{ cm}^{-2}$ and a factor of 2.5 for

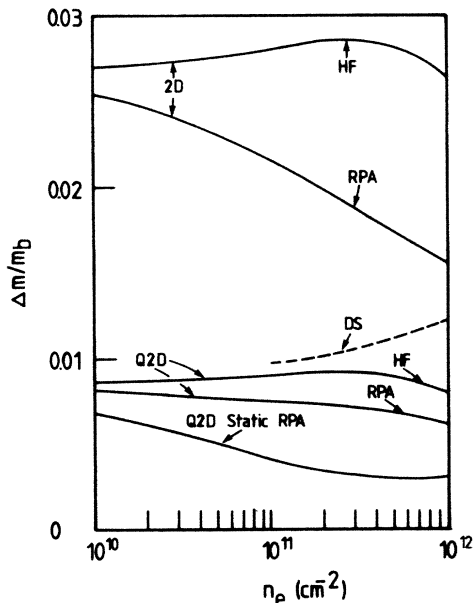


FIG. 6. Mass renormalization at zero temperature is plotted as a function of the electron density for both the ideal two-dimensional (two upper curves) and the quasi-two-dimensional (lower part of the figure) electron system. The results from different approximations are shown.

$n_e = 10^{12} \text{ cm}^{-2}$. However with increasing electron density the mass decreases more slowly than for the ideal 2D case. The screening effect seems to be compensated by the subband effect. The reason is that the subband width depends on the electron density and at higher electron density the electron layer is squeezed and becomes closer to the ideal 2D system. While the screening reduces the mass shift, the subband effect tends to enhance the mass renormalization. As a result the mass decreases slowly as a function of the electron density.

In Fig. 6 the mass shift corresponding to the HF approximation is also plotted. In the HF approximation only the Fermi-Dirac distribution function affects the mass shift. There is no screening effect, i.e., no electron-electron interaction is incorporated in the dielectric function. The results are also compared with the polaron mass renormalization found recently by Das Sarma¹ (indicated by the symbol DS in Fig. 6) who found that the mass shift is an increasing function of the electron density. In Das Sarma's approach the subband effect seems to be strong enough to compensate the screening effect. Although we find a different electron-density dependence, our mass renormalization is only a factor of 1.3 smaller for $n_e = 10^{11} \text{ cm}^{-2}$ but increases to a factor of 2 for $n_e = 10^{12} \text{ cm}^{-2}$ in comparison with the result of Ref. 1. A static RPA screening (see, e.g., Ref. 2) overestimates the effect of screening as shown in Fig. 6.

IV. CONCLUSION

In conclusion we have calculated the optical-absorption spectrum of a two-dimensional electron gas interacting with polar optical phonons. We found that the optical-absorption spectrum shows a shoulder structure for electron densities around 10^{12} cm^{-2} . The screening of the electron-phonon interaction reduces the intensity of the absorption spectrum and the correction to the electron effective mass. The subband effect, i.e., the finite width of the electron layer, also reduces the intensity of the absorption spectrum and the mass renormalization. The combined effect of screening and finite width of the two-dimensional electron layer results in a slow decrease of the mass renormalization as a function of the electron density.

We also want to point out that screening has been incorporated *dynamically*, i.e., the dielectric function for nonzero frequency appears in the memory function. For the imaginary part of the memory function at frequency ω only the imaginary part of the inverse dielectric function at frequencies $\omega \pm \omega_{LO}$ is important. This is in contrast with the real part of the memory function which contains both the real and imaginary part of the inverse dielectric function. In $\text{Re}\Sigma(\omega) \text{Im}\epsilon^{-1}(k, x)$ is needed for all frequencies but $\text{Re}\epsilon^{-1}(k, x)$ is needed only for the frequencies $x = \omega_{LO}$ and $x = \omega \pm \omega_{LO}$. Consequently the mass renormalization at zero temperature involves an integration over all positive frequencies of a function which contains $\text{Im}\epsilon^{-1}(k, x)$. This is analogous to the ground-state energy where we also found² that all frequencies of $\text{Im}\epsilon^{-1}(k, x)$ were important.

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