

Carrier-concentration-dependent polaron cyclotron resonance in GaAs heterostructures

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A detailed theoretical analysis is made of the experimental results on the polaron cyclotron-resonance mass in GaAs/Al_xGa_{1-x}As heterostructures of Langerak *et al.* [Phys. Rev. B **38**, 13 133 (1988)], with emphasis on the electron-density dependence. We found that (1) coupling to bulk GaAs LO phonons is responsible for the observed resonant polaron cyclotron-resonance effects, and (2) the occupation effect with inclusion of spin splitting is mainly responsible for the electron-density dependence of the polaron-mass renormalization.

Cyclotron-resonance experiments have been used to determine the effective mass of electrons in materials through the relation $m^* = eB / c\omega_c^*$, where e is the electron charge, c the velocity of light, B the magnetic field, and ω_c^* the cyclotron-resonance frequency. In polar semiconductors one observes¹ that the mass determined in this way depends on the magnetic field. Two main effects are responsible for this, (1) band nonparabolicity which leads to an almost linear increase of the cyclotron mass with magnetic field, and (2) the electron-phonon interaction which for small magnetic fields results in a linear increase of m^* with B but for higher fields a strong non-linear component is present which is strongest at resonance $\omega_c^* = \omega_{LO}$, where ω_{LO} is the longitudinal-optical phonon frequency. Thus a cyclotron-resonance experiment can provide us with detailed information on the strength of the polaron interaction and on the frequency

of the relevant LO phonon responsible for this interaction.

The aim of this paper is to present a quantitative comparison between theoretical and experimental results on the polaron cyclotron-resonance position. A theoretical analysis with *no* adjustable parameters will be made of the far-infrared (FIR) reflectivity measurements of Langerak *et al.*² Two main questions of interest to us are, (1) which are the relevant phonons responsible for the electron-phonon interaction which determine the polaron cyclotron mass? Do we have to invoke an interaction with a lower frequency phonon mode than the bulk LO phonon as was suggested by magnetophonon resonance experiments³ and some experiments on bound two-dimensional (2D) polarons?⁴ (2) How important is the dependence of the electron-phonon interaction on the electron density? This density dependence is an effect

specific to 2D systems which is not encountered in bulk systems⁵ that have relative low electron densities such that one-electron theories are able to describe the experimental results.

At present there does not exist a systematic comparison between experimental and theoretical results on the polaron cyclotron-resonance mass. Previous theoretical work, (1) did not compare⁶⁻⁹ with experiments because of the unavailability of such results, or (2) compared¹⁰ only with results from low density samples where many-particle effects are only of minor importance. Only recently has a systematic experimental investigation of polaron effects in heterostructures become available for comparison with theoretical work.

The effect of band nonparabolicity is well known and will be described by using Kane's theory. In the following we will concentrate on the polaron effect. In the initial calculations⁶⁻⁸ on the polaron-mass renormalization of electrons in 2D systems polaron effects were predicted which were a factor 2 to 3 times larger than for corresponding 3D systems. Experimentally no such large enhancements were found and, in general, the 2D polaron-mass renormalizations¹⁰ are even smaller than for bulk systems. These theories were one-polaron theories, where the polaron was assumed to have no extension in the z-direction, which is taken perpendicular to the 2D layer.

Three major corrections must be included in the original ideal 2D calculations in order to describe realistic structures.

(1) Finite-size effect: the nonzero width of the two-dimensional electron gas (2D EG) reduces the polaron interaction considerably. It leads to a quasi-two-dimensional (Q2D) polaron-mass renormalization which lies between the ideal 2D and the 3D result. This correction is a consequence of the fact that the polaron diameter in GaAs, which is about 20 Å, is of the same order or even smaller than the width of the 2D layer (typically 50 Å in GaAs heterostructures). Consequently as far as polaron effects are concerned the system is not a strict 2D system. In the calculation this amounts to replacing⁹ the interaction coefficient $|V_k|^2$ by $|V_k|^2 |\langle \phi_0 | e^{ik_z z} | \phi_0 \rangle|^2$, which for the Fang-Howard wave function¹¹ results in the effective 2D-interaction coefficient $|V_k|^2 f(k, b)$. $f(k, b) = (8b^3 + 9kb^2 + 3k^2b) / 8(k+b)^3$ is called the form factor and is smaller than one (b is a measure of the inverse width of the 2D electron layer). It turns out that for low-electron density heterostructures this is the major correction to the one-polaron calculation [see Figs. 1(a) and 1(b)].

(2) Landau-level occupancy effect. For typical 2D densities of $n_e = 10^{11} \text{ cm}^{-2}$ the Fermi energy $E_F = 3.6 \text{ meV} \gg k_B T \approx 4.2 \text{ K}$ is much larger than the thermal energy at which the experiments are performed. The Boltzmann statistics of the one-polaron theories have to be corrected in order to include the exclusion principle as described by Fermi-Dirac statistics. This implies that the electron can only make a transition from an occupied state with energy E_i and occupancy probability $f(E_i)$ to an unoccupied state E_f with nonoccupancy probability $[1 - f(E_f)]$. This effect strongly depends on the electron

density, as was shown in Ref. 12, and can reduce the polaron-mass renormalization appreciably. In addition the splitting of the cyclotron-resonance peak at resonance is reduced with increasing electron density. Furthermore this effect has the property that at complete filling the mass renormalization is minimal and equals the $B=0$ result. As a consequence the cyclotron-mass renormalization is an oscillating function of the filling factor. Unfortunately in practical experimental situations the latter effect is difficult to observe because (1) except for extremely high-electron densities these oscillations occur away from resonance where the polaron effect is small, and (2) there is a competing effect resulting from band nonparabolicity. When the filling factor ν moves through complete filling, due to increasing magnetic field, the transition $n \rightarrow n+1$ is no longer allowed and the cyclotron-resonance transition will be between the Landau levels $n-1 \rightarrow n$. This is between different states which have different band nonparabolicity [$n = \text{int}(\nu/2)$]. As a consequence the band nonparabolicity contribution to the cyclotron mass shows a jump. This effect is much larger than the oscillatory contributions due to polaron effects in the present day GaAs heterostructures.

(3) Screening of the electron-phonon interaction. The electron-phonon interaction is an interaction between the electric field of the electron and the polarization field of the lattice. This interaction will be screened by the presence of many electrons. We have treated this type of screening and used two different approximations (i) static screening, this in essence amounts to replacing the bare electron-phonon interaction $|V_k|^2$ by $|V_k|^2 / \epsilon^2(k, 0)$, where the static dielectric function is calculated within the random-phase approximation (RPA); (ii) dynamic screening, here the full frequency dependence of the dielectric function $\epsilon(k, \omega)$ is included. Numerical calculations¹³ have shown that dynamical screening of the electron-phonon interaction does not lead to appreciable differences from the static screening result. Therefore it suffices to limit ourselves to a calculation with the much more simple static screening approximation.

Recently we presented a theory¹⁴ for the cyclotron-resonance absorption spectrum from which the position of the cyclotron-resonance peak ($\omega_c^* = \omega$) was determined by the nonlinear equation

$$\omega = \omega_c + \text{Re}\Sigma(\omega; \omega_c), \quad (1)$$

where $\text{Re}\Sigma(\omega; \omega_c) < 0$ is the real part of the memory function which is responsible for the polaron shift of the cyclotron-resonance frequency towards lower frequencies. The difference from standard theories for the polaron cyclotron-resonance frequency is that in Eq. (1) we calculate directly the quantity which is experimentally measured while in previous theories the position of the Landau levels (E_n) are calculated. The resonance frequency is then determined by $\omega_c^* = (E_1 - E_0) / \hbar$.

The work of Ref. 14 has been generalized^{12,13} to the many-particle case. The memory function, which in essence is a force-force correlation function, where the time evolution is restricted to the Liouville space which is orthogonal to the velocity operator $\dot{x} + i\dot{y}$ must be calculated. In the evaluation of the memory function we made

the following approximations: (1) the temperature is taken to be equal to zero (the typical LO-phonon temperatures are of the order of 400 K while the experiments are done at 1.3 K); (2) the nonzero width of the 2D layer is described by the Fang-Howard variational wave function;¹¹ (3) the many-particle aspects of the system are included by a probability function for the occupation of the Landau levels which is governed by Fermi-Dirac statistics, and (4) the electrons are taken to be in a parabolic energy band. However, in order to incorporate band nonparabolicity we replace ω_c by $(\omega_c)_{NP}$ where $(\omega_c)_{NP}$ is obtained from a three-band calculation¹⁵ without polaron effects. This approach corresponds to a local parabolic approximation. We checked that this approach is justified by verifying that such an approach gives (within 1%) the same polaron correction as a calculation where

the intermediate Landau energies are replaced by the nonparabolic expression. The latter approach has been shown by Larsen¹⁶ to give very accurate results. For the numerical calculation we used the following material parameters for GaAs: band gap $E_g=1520$ meV, $\hbar\omega_{LO}=36.75$ meV, $\alpha=0.068$, and the band mass $m_b/m_e=0.0665$ was determined earlier⁹ from a theoretical analysis of the cyclotron-resonance data of Hopkins *et al.*¹⁷ To calculate the band nonparabolicity we take the energy of the Landau level n of the following form:

$$E_n = \frac{E_g}{2} (-1 + \sqrt{1 + 4E_n^0/E_g}), \quad (2)$$

with $E_n^0 = \hbar\omega_c(n + \frac{1}{2}) + \langle T \rangle$ where $\langle T \rangle = \hbar^2 b^2 / 8m_b$ with $b = (48\pi N m_b e^2 / \hbar^2 \epsilon_0)^{1/3}$ and $N = n_d + \frac{11}{32} n_e$. A constant

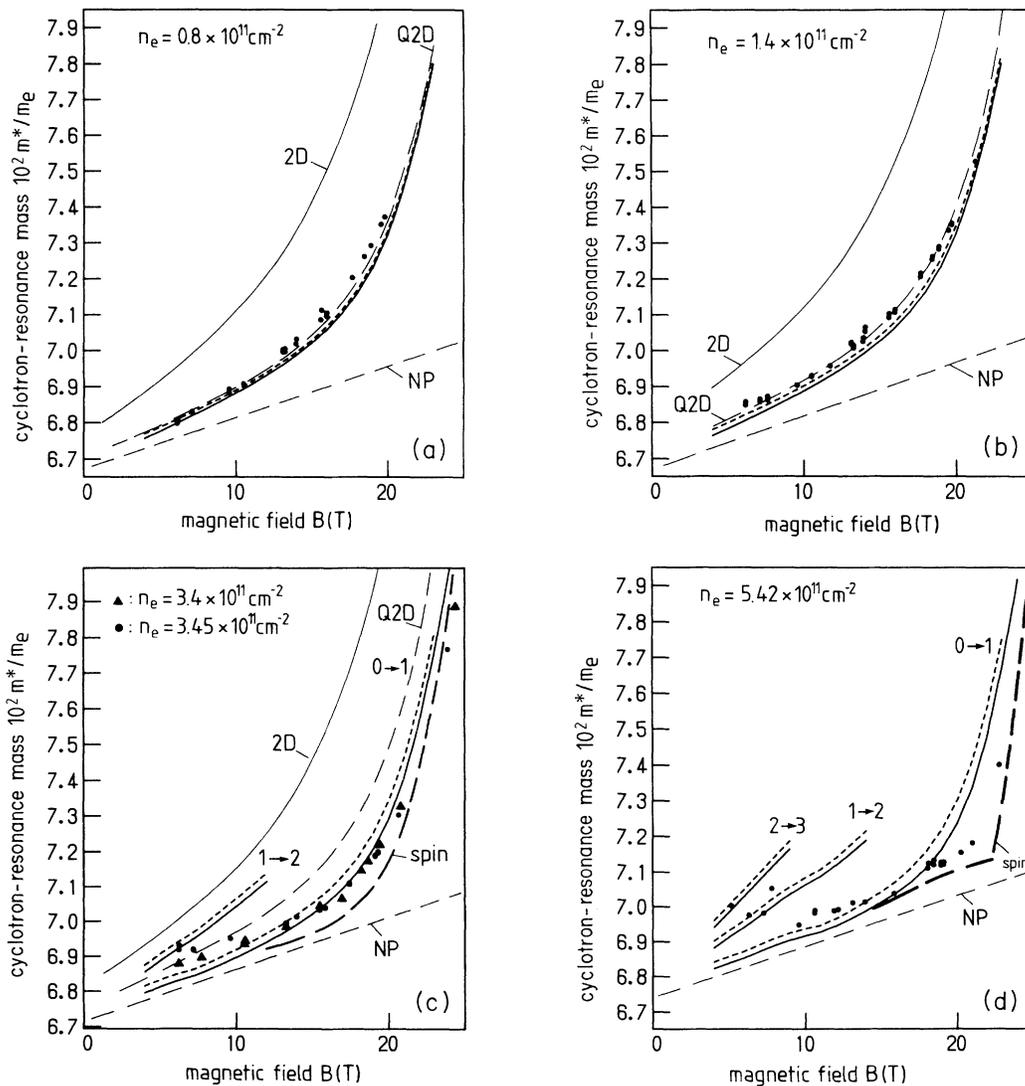


FIG. 1. Cyclotron-resonance mass as a function of the magnetic field for different electron densities: (a) $n_e = 0.8 \times 10^{11} \text{ cm}^{-2}$, (b) $n_e = 1.4 \times 10^{11} \text{ cm}^{-2}$, (c) $n_e = 3.4 \times 10^{11} \text{ cm}^{-2}$, and (d) $n_e = 5.4 \times 10^{11} \text{ cm}^{-2}$. The full dots are the experimental results. The different curves are the present theoretical results for different approximations.

shift of the energy levels with the average potential $\langle U \rangle$ is not important for our purposes. In case of a large band gap we can expand this expression into

$$E_n = E_n^0 \left[1 - \delta \frac{E_n^0}{E_g} \right], \quad (3)$$

with $\delta=1$ (some authors have used the notation $K_2 = -\delta$). Note that taking $\delta \neq 1$ has the same effect as taking a different band gap. In previous work people have taken $\delta=1.4$ which implies an effective band gap of $E_g = 1086$ meV.

In Figs. 1(a)–1(d) a comparison is made between the experimental results of Langerak *et al.*,² which are represented by the dots in the figure, and our theoretical results for four different electron densities. Theoretical results are given for the mass renormalization in order of increasing complexity, and thus also fuller inclusion of the different corrections: (1) the thin-dashed curve, indicated by “NP,” is the result without electron-phonon interaction but with inclusion of band nonparabolicity for the $n=0 \rightarrow n=1$ transition, (2) inclusion of the one-polaron effect for a 2D EG of zero width results in the thin full curve, indicated by “2D,” (3) taking the finite-size effect into account leads to the curve indicated by “Q2D,” (4) if we also include the occupancy effect we obtain the thick dashed curve, and (5) the solid curve represents the results where static screening was also included.

Note that for the low density samples [Figs. 1(a) and (b)] very good agreement between our theoretical results and the experimental results of Langerak *et al.*² is obtained. The effect of screening is negligible in this case. For the sample with $n_e = 3.4(5) \times 10^{11} \text{ cm}^{-2}$ [Fig. 1(c)] again good agreement is obtained in the magnetic-field range $B=10\text{--}20$ T. For $B < 10$ T the second Landau level ($n=1$) can be partially occupied and two transitions are possible: $0 \rightarrow 1$ and $1 \rightarrow 2$. Due to band nonparabolicity both transitions lead to a different cyclotron mass and two peaks in the cyclotron-resonance spectrum are expected. Experimentally this splitting of the cyclotron peak is not resolved and only one broad peak is observed which, as seen from Fig. 1(c), is situated between the theoretical $0 \rightarrow 1$ and $1 \rightarrow 2$ results. With decreasing magnetic fields the weight corresponding to the $0 \rightarrow 1$ transition decreases because the Landau state $n=1$ starts to become filled and the $1 \rightarrow 2$ transition starts to dominate. This agrees with the experimental observation where we see that with decreasing magnetic field the experimental results approach the $1 \rightarrow 2$ results. For $B > 20$ T the theoretical results overestimate the polaron contribution to the cyclotron mass slightly. This effect is even more pronounced for the highest density sample as shown in Fig. 1(d). Note that screening of the electron-phonon interaction is more important with increasing density but it is not able to lower the polaron contribution sufficiently in the two highest density samples in the $B > 20$ T region.

For the high-density samples multiple Landau levels are occupied at low magnetic field. During a cyclotron-resonance experiment spin is conserved and the electron makes a transition from $|n, s\rangle$ to $|n+1, s\rangle$ with $s \uparrow \downarrow$.

Only a small shift is expected from band nonparabolicity. The electron-phonon interaction is independent of the spin state. However, in the many-particle case the electrons will be distributed over spin-up and spin-down states and when these levels are well separated they can have a significant influence on the occupancy effect. The splitting of the spin-up and spin-down state is $\Delta = g^* \mu_B B = 0.06g^* B(T)$ meV which for $g^* = 0.44$ (bulk GaAs value) and $B=22$ T gives $\Delta = 0.6$ meV. In heterostructures exchange enhancements^{18,19} of the electron g factor with factors of 10 have been observed which would give $\Delta = 6$ meV. This value should be compared with the Landau-level width Γ . A typical value is $\Gamma \sim 1$ meV $\sqrt{B(T)}$ which gives for $B=22$ T the value $\Gamma \sim 4.7$ meV. We have calculated the polaron correction to the cyclotron mass in the extreme case of well-separated spin-split levels, i.e., $\Delta \gg \Gamma$. Such a calculation leads to an upper bound on the effect of spin splitting. Broadening of the Landau levels will diminish this correction. We have given the results of such a calculation for the two highest density samples [Figs. 1(c) and (d)] by the curves indicated by “spin.” The cusp in the curve occurs at complete filling of the $n=1$ lowest spin state. Note that the experimental results are above the theoretical curve as expected with the exception of the two points at the highest magnetic fields of the $n_e = [3.4(5)] \times 10^{11} \text{ cm}^{-2}$ samples, which are slightly below the theoretical curve.

In Fig. 2 the density dependence of cyclotron mass is plotted for four different values of the cyclotron frequency $\omega = \omega_c^*$. Notice that the experimental results for the polaron cyclotron mass decreases with increasing density. From band nonparabolicity alone (the curves indicated by NP) one obtains an increasing mass with increasing electron density. Increasing the density decreases the

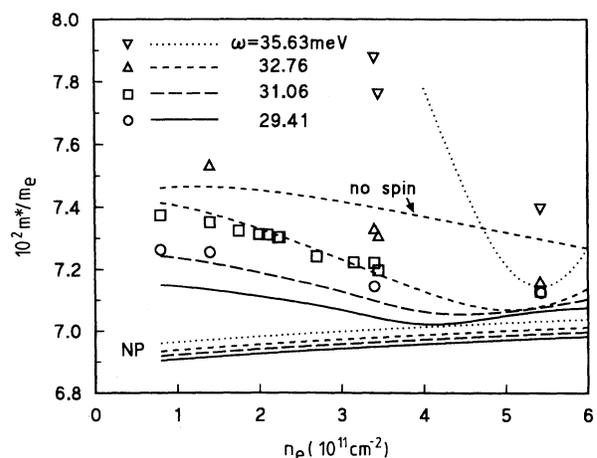


FIG. 2. Cyclotron-resonance mass vs the electron density for fixed cyclotron-resonance frequencies $\omega = \omega_c^*$. Theoretical results are given for (1) band nonparabolicity alone (curves indicated by NP), (2) including the effects of finite size, many-particle effects, and spin, and (3) in the case of $\omega = 32.76$ meV our theoretical results are also given neglecting the spin effect on the occupancy effect.

width of the 2D EG layer which will lead to an increase of the single polaron-mass renormalization. Thus the many-particle effects, i.e., the occupancy effect and screening, should be sufficiently strong to overcome the above two increasing trends and must lead to an overall decreasing cyclotron mass with increasing n_e . This is also what we have found theoretically up to a certain electron density (see Fig. 2) above which m^* increases again. For the $\omega=32.76$ meV case we have also included a curve where we did not include the spin effect. Notice that the theoretical curves are at least able to describe the qualitative trends seen in the experiment: (1) the decrease of m^* with increasing n_e . There are no experimental points to check the increase of m^* for $n_e > (4-5) \times 10^{11} \text{ cm}^{-2}$. (2) At the highest density ($n_e \sim 5.4 \times 10^{11} \text{ cm}^{-2}$) m^* has almost no ω dependence. Notice that for the $\omega < 35$ meV results the present theoretical calculation underestimates the polaron cyclotron resonance mass especially at low-electron density. This is also seen in Figs. 1(a) and 1(b) in the $B=10-20$ T region. An increase in the nonparabolicity as mentioned in Eq. (3) would lead to an improved agreement but worse at smaller frequencies.

In conclusion we made a detailed comparison between the experimental cyclotron-resonance data of Langerak *et al.*² and our theoretical calculation which is based on a direct calculation of the magneto-optical absorption spectrum. It was found that the experimental results are consistent with an interaction of the electrons with the bulk LO-phonon mode of GaAs. Furthermore with increasing

electron density the polaron contribution to the cyclotron mass decreases, primarily as a consequence of the blocking effect due to the Landau-level occupation. This effect is nonzero even when the magnetic fields are so high that only the lowest Landau level is occupied; in this case the effect of spin splitting should be included. Screening of the electron-phonon interaction slightly lowers the polaron effect and its effect increases with increasing electron density. For the low density samples we found that our theoretical results underestimate the polaron correction in the region $B=10-20$ T which is substantially below the resonant magnetic field. The interaction of the electron with a phonon of frequency lower than the bulk LO-phonon mode of GaAs (e.g., interface phonons) would be able to increase the polaron effect. But then the theoretical results near the resonant magnetic field would be increased above the experimental result [see, e.g., the points at the highest magnetic fields in Figs. 1(b) and 1(c)] and therefore we can rule out this possibility. A larger band nonparabolicity as given by Eq. (3) would improve the agreement for $B=10-20$ T but for $B > 20$ T the theoretical results would overestimate the cyclotron-resonance mass.

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