Polaron Landau levels in InSb: A study of the influence of band nonparabolicity

Serge Huant and Khaled Karraï
Service National des Champs Intenses, Centre National de la Recherche Scientifique, Boîte Postale 166X, 38042 Grenoble Cédex, France

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Polaron Landau levels in a nonparabolic conduction band are calculated within second-order perturbation theory restricted to the conduction-band eigenstates using a three-level band structure for the unperturbed states. In the limit of a vanishing magnetic field, the results of Fröhlich are recovered, showing that the nonparabolicity itself does not affect the polaronic properties of the bottom of the band. In the limit of resonant magnetic fields (cyclotron energy close to the LO-phonon energy), resonant polarons are found to be shifted to a higher field and the coupling only slightly modified by the band nonparabolicity. The calculations are in good agreement with the experimental data available on InSb using the physical parameters of the material found in the literature.

I. INTRODUCTION

Polaron coupling in weakly polar bulk three-dimensional (3D) semiconductors has been extensively studied since the pioneer work of Fröhlich.[1] Much theoretical work has been devoted to the calculation of polaron Landau levels[2–5] (PLL) in arbitrary magnetic fields and special attention was paid to the resonant case $n\hbar\omega_c=\hbar\omega_{\rm LO}$ ($\hbar\omega_c=\hbar eB/m^*$, B is the magnetic field, and m^* the band-edge effective mass) where the energy separation between the level n and the level 0 is resonant with the LO-phonon energy, leading to the so-called resonant polaron effect.[2] Polarons have recently gained revitalizing interest because of the ability to form two-dimensional (2D) electron gases in semiconducting heterostructures. Two-dimensional PLL have been calculated by several authors.[6–8] Recently, Peeters and Devreese[5] extended previous theoretical works to arbitrary magnetic field strength and arbitrary quantum number n, both in three and two dimensions.

From the experimental point of view, 3D and 2D polarons have been observed in several materials, including, for instance, the narrow-gap semiconductors InSb (Refs. 3 and 9–13) and $Ga_{1-x}In_xAs$.[14–16]

Most of the calculations mentioned so far have been restricted to a parabolic conduction band with equally spaced Landau levels in a magnetic field. Deviation from this simple parabolic law, however, occurs in semiconductors in a magnetic field such that $\hbar\omega_c$ is comparable to the gap width E_g. In this case, resonant polarons should be affected in narrow gap materials (where typically $\hbar\omega_{\rm LO}=E_g/10$). In fact, they are shifted to a higher field due to the increase of the effective mass with energy. However, as far as the magnitude of the effects (e.g., the splitting of PLL at the resonance[5]) is concerned, one generally expects polaron effect and band nonparabolicity to be simply "additive" since both are small. Such an intuitive procedure was justified in simple terms by Larsen[2] for weak magnetic fields and essentially confirmed by Zawadzki[17] in resonant fields. Recently, Das Sarma and Mason[18] developed a new calculation of the polaron binding energy and mass renormalization taking into account the band nonparabolicity (within a two-band $\mathbf{k}\cdot\mathbf{p}$ model) and found a modification of the above quantities. They suggest that resonant polarons should be strongly influenced by band nonparabolicity[18] (enhanced by almost 50% in InSb). In a very recent comment of this work, Larsen predicts smaller corrections.[19]

We develop in this paper a calculation of PLL taking into account the band nonparabolicity within the three-band model of Bowers and Yafet,[20] and we apply it to InSb. We restrict our discussion to the 3D case and we essentially follow the method outlined by Peeters and Devreese in Ref. 5. In Sec. II, we derive a general expression for the polaronic shift of any Landau level in an arbitrary field (for energies below $\hbar\omega_{\rm LO}$). In Sec. III, we focus on the limiting cases of weak and resonant fields where the calculated quantities are easy to compare to the parabolic case. In Sec. IV, we compare our results with the available experimental data on InSb. The conclusions appear in Sec. V.

II. CALCULATION OF POLARON LANDAU LEVELS IN A NONPARABOLIC CONDUCTION BAND

A fairly good description of the Landau states in zinc-blende semiconductors may be obtained from the simple model of Bowers and Yafet[20] which treats exactly the interaction between the close-lying Γ_6 conduction band, Γ_8 heavy- and light-hole bands, and Γ_7 spin-orbit splitoff valence band, while the interaction with all other bands is neglected. The effective-mass Hamiltonian $\mathcal{H}_0$ for the Landau states is a 8×8 matrix operator acting on eight components slowly varying envelope wave functions (see Ref. 20 and for instance Appendix C of Ref. 21 where all details can be found) which should be multiplied by the corresponding Bloch functions from the Γ point of the Brillouin zone and summed up to obtain the total wave function. The envelope wave function of the Landau state n with the wave vector k (in the direction of $\mathbf{B}$) and

spin up (only this spin state will be considered here[22]) will be denoted by ψ_{nk}. The corresponding energy $\mathcal{E}_n(k)$ is the positive root of the cubic equation:[20,21]

$$\mathcal{E}(\mathcal{E}+E_g)(\mathcal{E}+E_g+\Delta) - C\left[\left[\frac{\lambda^2}{2}(2n+1)+k^2\right](3\mathcal{E}+3E_g+2\Delta) - \frac{\lambda^2}{2}\Delta\right]=0 . \quad (1)$$

In Eq. (1), Δ is the spin-orbit splitting of the valence band, $C=E_g(E_g+\Delta)/(2\Delta+3E_g)$, and $\lambda^2=\hbar\omega_c/\hbar\omega_{\mathrm{LO}}$ is the dimensionless magnetic field. Throughout the paper we use polaron units where the energies are expressed in units of $\hbar\omega_{\mathrm{LO}}$ and lengths in polaron radius $r_0=[\hbar/(2m^*\omega_{\mathrm{LO}})]^{1/2}$.

Within the multiband effective-mass approximation[23] (EMA), the Hamiltonian of our problem—namely the Hamiltonian of a slow electron interacting with its LO-phonon cloud in a weakly polar zinc-blende semiconductor—reads

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{\mathrm{ph}}+\mathcal{H}_F , \quad (2)$$

where $\mathcal{H}_{\mathrm{ph}}$ is the phonon matrix operator and $\mathcal{H}_F$ is a diagonal 8×8 matrix operator, with all diagonal components being the standard Fröhlich Hamiltonian H_F.[1] In writing (2), we assume H_F to be slowly varying in space over the unit cell a, i.e., $r_0 \gg a$. As already stated by Larsen,[2] this requirement is also necessary to comply with the basic assumption of Fröhlich,[1] that the crystal be treated in the continuum approximation.

The polaronic shift of the nth Landau level (with $k=0$ and zero phonons) within second-order perturbation theory[5] is

$$\Delta\mathcal{E}_n=-\sum_{m,k}\sum_{\mathbf{q}}\frac{\langle\psi_{mk};\mathbf{q}\,|\,\mathcal{H}_F\,|\,\psi_{n0};\mathbf{0}\rangle^2}{\mathcal{E}_m(k)+1-\mathcal{E}_n(0)-\Delta_n} , \quad (3)$$

where the summations run over all valence and conduction states and over all phonon wave vectors $\mathbf{q}$, respectively. In Eq. (3), Δ_n depends upon the exact perturbative scheme employed.[5] Following the approach of Peeters and Devreese (we are thus limiting ourselves to energies below $\hbar\omega_{\mathrm{LO}}$), Eq. (3) is rewritten as

$$\Delta\mathcal{E}_n=-\frac{\alpha}{2\pi^2}\int_{-\infty}^{+\infty}\frac{d^3q}{q^2}\int_0^{\infty}du\,e^{-(1-\Delta_n)u}\langle\psi_{n0}\,|\,e^{i\mathbf{q}\cdot\mathbf{r}(u)}e^{-i\mathbf{q}\cdot\mathbf{r}(0)}\,|\,\psi_{n0}\rangle , \quad (4)$$

where the summation over $\mathbf{q}$ has already been converted into an integral, $\mathbf{r}(u)$ is the electron position operator at imaginary time $u=it$,[5] and α is the Fröhlich constant. Knowing the expression of $\mathbf{r}$ restricted to the subspace of parabolic Landau states,[5] we obtain those restricted to the subspace of Landau states in the nonparabolic conduction band (see Appendix A). Intermediate states in the valence band are now excluded which means that the weak Fröhlich interaction cannot excite a hole in the valence band: this is a reasonable assumption (unless $\hbar\omega_{\mathrm{LO}}\ll E_g$) for the materials considered here [note that in Eq. (4), the valence-band states as well as spin-down states[24,25] are included in the matrix element]. The intermediate states which we omit should contribute to the order α/E_g as was recently shown by Larsen.[19] This allows us to calculate the matrix element appearing in Eq. (4) and to perform the $\mathbf{q}$ integral (see Appendix B where some details of the calculation are given). The nonequidistance of Landau levels makes the calculation of $\Delta\mathcal{E}_n$ here more tedious and leads to a final expression including an infinite sum, while—due to the equal spacing of Landau levels in the parabolic case—the results of Peeters and Devreese have only finite sums [Eqs. (12)–(14) of Ref. 5]. $\Delta\mathcal{E}_n$ is obtained as

$$\Delta\mathcal{E}_n=-\frac{\alpha}{\lambda\sqrt{\pi}}\int_0^{\infty}\frac{du}{\sqrt{u}}e^{-[(1-\Delta_n)/\lambda^2]u}\mathcal{I}_n(u,\lambda^2) , \quad (5)$$

where

$$\mathcal{I}_n(u,\lambda^2)=\sum_{p=0}^{n}\sum_{m=0}^{n}\sum_{l=\max(p,m)}^{\infty}A_{npml}(u,\lambda^2)J_{npml}(u,\lambda^2) , \quad (6)$$

with

$$A_{npml}(u,\lambda^2)=(-1)^{p+m}\frac{n!\,l!\,(H_n^2H_l^2/H_m^2/H_p^2)(V_l)^{1/2}e^{u(\mathcal{E}_n-\mathcal{E}_l)/\lambda^2}}{(n-m)!(n-p)!(l-m)!(l-p)!p!\,m!} , \quad (7a)$$

$$J_{npml}(u,\lambda^2)=\frac{p'!}{2p'+1}\left[\frac{V_l}{u}\right]^{p'}{}_2F_1(p'+\tfrac{1}{2},p'+1,p'+\tfrac{3}{2};(u-V_lB_{nl})/u) , \quad (7b)$$

$$p'=n+l-m-p , \quad (7c)$$

$$B_{nl}=\tfrac{1}{2}[(n+1)K_{n+1}^2-nK_n^2+(l+1)K_{l+1}^2-lK_l^2] , \quad (7d)$$

$$H_n=\prod_{i=0}^{n}K_i , \quad (7e)$$

$$K_n(n\geq 1)=\left[1+C\lambda^2\left[\frac{2n-1}{(\mathcal{E}_{n-1}+E_g)(\mathcal{E}_n+E_g)}+\frac{n+1}{(\mathcal{E}_{n-1}+E_g+\Delta)(\mathcal{E}_n+E_g+\Delta)}\right]\right]\Big/(N_{n-1}N_n)^{1/2}\,, \tag{7f}$$

$$K_0=1\,, \tag{7g}$$

$$N_n=1+C\lambda^2\left[\frac{2n+\frac{1}{2}}{(\mathcal{E}_n+E_g)^2}+\frac{n+1}{(\mathcal{E}_n+E_g+\Delta)^2}\right]\,, \tag{7h}$$

$$V_n=\frac{(\mathcal{E}_n+E_g+\Delta)(2\mathcal{E}_n+E_g)+\mathcal{E}_n(\mathcal{E}_n+E_g)-\frac{3}{2}C\lambda^2(2n+1)}{C(3\mathcal{E}_n+3E_g+2\Delta)}\,. \tag{7i}$$

In Eq. (6), the index l numbers the intermediate Landau states with one phonon. Note that for each intermediate state, the q integral is already performed. In Eq. (7), K_n is related to the annihilation and creation operators of Landau states in the nonparabolic conduction band (see Appendix A); N_n is the square modulus of ψ_{n0} (see Appendix C of Ref. 21); V_n represents the increase of the effective mass at the bottom of the nth Landau subband: this is immediately seen by considering the limit $\Delta\to\infty$ which leads to the well-known two-band result $V_n=1+2\mathcal{E}_n/E_g$; ${}_2F_1(a,b,c;z)$ are the hypergeometric functions.[26] It is worthwhile noting in Eq. (7) that in the limit $\Delta\to\infty$ and $E_g\to\infty$ (i.e., in the parabolic approximation), one has $B_{nl}=K_n=N_n=H_n=V_n=1$ for any n and λ^2, so that $\Delta\mathcal{E}_n$ tends to its parabolic value ΔE_n as given in Ref. 5.

III. DISCUSSION OF THE LIMITING CASES

A. Weak magnetic field $\lambda^2\ll 1$

The first limit we consider is that of the weak magnetic field $\lambda^2\ll 1$, in order to point out some qualitative ideas on the effect of the band nonparabolicity on the polaronic properties at the band edge.

$\Delta\mathcal{E}_n$ is obtained by expanding $\mathcal{G}_n(u,\lambda^2)$ in powers of u.[27] By inspection of Eq. (7), it is seen that the coefficients K_n, H_n, B_{nl}, and V_l tend towards one for small λ^2 and that $\mathcal{E}_n$ tends to its parabolic value $\mathcal{E}_n=\lambda^2[n+\frac{1}{2}-\Delta/2(2\Delta+3E_g)]$, so that for any u, one has

$$\lim_{\lambda^2\to 0}\mathcal{G}_n(u,\lambda^2)=G_n(u)\,, \tag{8}$$

where $G_n(u)$ is the function of Peeters and Devreese[5] which enters Eq. (5) in the parabolic case. Since one has for small u

$$G_n(u)=1+\frac{2n+1}{6}u+\frac{18n^2+18n-1}{180}u^2+\cdots\,, \tag{9}$$

Eq. (8) gives, in our case, the following equation:

$$\mathcal{G}_n(u,\lambda^2)=1+\frac{2n+1}{6}u(1+a\lambda^2+\cdots)+\frac{18n^2+18n-1}{180}u^2(1+b\lambda^2+\cdots)+\cdots\,, \tag{10}$$

with a and b being some coefficients whose analytical determinations are tedious and of no fundamental interest for our purpose. We will numerically show below that a is nonzero. After integration over u, $\Delta\mathcal{E}_n$ is rewritten as[27]

$$\Delta\mathcal{E}_n=-\alpha\left[1+\frac{2n+1}{12}\lambda^2+\left[\frac{18n^2+18n-1}{240}+\frac{2n+1}{12}a\right]\lambda^4+\cdots\right]\,. \tag{11}$$

The important result quoted in Eq. (11) is that, up to the term λ^2, $\Delta\mathcal{E}_n$ is identical to its parabolic counterpart[5] and in the limit $\lambda^2\to 0$ (i.e., at the bottom of the band) the standard results[1] are recovered for the polaron binding energy $E_p=-\alpha$ and polaron effective mass $m^{**}=m^*(1+\alpha/6)$ when the small contributions of the intermediate states in the valence band are neglected. Larsen has recently shown[19] that the inclusion of these far-lying states changes the expressions for E_p and m^{**} (see below). Since the bottom of the band remains parabolic within the three-band model (e.g., for $\lambda^2\ll 1$, one has the following in the limit $\Delta\to\infty$: $\mathcal{E}_n=(n+\frac{1}{4})\lambda^2-1/E_g(n+\frac{1}{4})^2\lambda^4$ to second order in the magnetic field) and the above quantities are governed by the dispersion law for small wave vectors,[1] our result is quite reasonable from the physical point of view. Das Sarma and Mason[18] recently predicted the expressions $E_p=-\alpha(1-3/2E_g)$ and $m^{**}=m^*[1+(\alpha/6)\ (1+11/2E_g)]$ within a two-band $\mathbf{k}\cdot\mathbf{p}$ model, which respectively lead to a reduction of 14% and an enhancement of 57% of the polaron binding energy and polaron correction to the effective mass in InSb. The summation over intermediate states was restricted to the conduction band as was done here. It is, however, worthwhile pointing out that not only the unperturbed energies enter the second-order perturbation calculation, but also the unperturbed wave functions do [see Eq. (3)]. This latter point was ignored in Ref. 18.

In a recent comment[19] on the paper of Das Sarma and Mason, Larsen found smaller but finite corrections, namely $E_p=-\alpha(1-1/2E_g)$ and $m^{**}=m^*[1+(\alpha/6)\ (1+5/2E_g)]$, respectively. These results are obtained through an approximate diagonalization of the multiband (4×4 matrix) $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian including Fröhlich's interaction and intermediate states in the light-hole valence

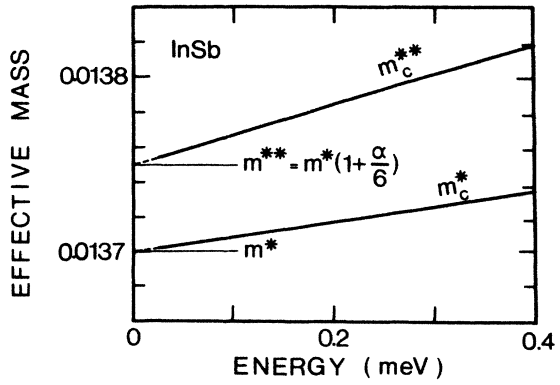

FIG. 1. Cyclotron mass (m_c^*) and polaron cyclotron mass (m_c^{**}) in InSb vs the cyclotron resonance energy in the limit $\lambda^2 \ll 1$. Note the amplified vertical scale. The masses are in units of m_e.

band. The terms in order α/E_g given by Larsen which we do not find in our calculation are thus a direct contribution of the valence band, i.e., they reveal a further small mixing of neighboring bands due to Fröhlich's interaction. It is shown in Sec. IV that they are not quantitatively important for InSb.

In Fig. 1, we have plotted for the real case of InSb the bare cyclotron effective mass m^* versus the cyclotron energy in the region $\lambda^2 \lesssim 0.05$ together with the polaron cyclotron mass deduced from the standard definition:

$$m_c^{**}=2\lambda^2/(\mathcal{E}_1+\Delta\mathcal{E}_1-\mathcal{E}_0-\Delta\mathcal{E}_0) . \tag{12}$$

The band parameters ($\mathcal{E}_g=235.2$ meV, $\Delta=803$ meV, $m^*=0.0137m_e$) are taken from Ref. 28. The low-frequency dielectric constant $\epsilon_0=16.8$ was measured in Ref. 29 and we use the Lyddane-Sachs-Teller relation together with the phonon energies of Ref. 30 to obtain the high-frequency dielectric constant. This leads to $\alpha=0.022$. $\Delta\mathcal{E}_0$ and $\Delta\mathcal{E}_1$ are calculated using Eqs. (5)–(7) with the computational cutoff $l_{\max}=74$ for the maximum value of l in Eq. (6). It is confirmed that m_c^{**} extrapolates to $m^*(1+\alpha/6)$ at zero field and it is seen that the increase of m_c^{**} with energy is slightly higher than that of m_c^*. This means that the coefficient a in Eqs. (10) and (11) does not vanish and that there is some interference between polaron-induced and band nonparabolicity (i.e., this interference acts only from the term λ^4, thus leading to unchanged E_p and m^{**}). Let us remember that the inclusion of the light-hole intermediate states changes E_p and m^{**} in the order α/E_g.

B. Resonant polarons

The second limiting case of interest, which can directly be related to the experiment, is the resonant one where the Landau level n is degenerate with the virtual level at the energy of the level 0 plus one LO phonon. The unperturbed levels cross at a field such as $\mathcal{E}_n-\mathcal{E}_0=1$ (for the real case of InSb and for $n=1$, this corresponds to $\lambda^2=1.16$) and not $n\lambda^2=1$ as in the parabolic case. One may obtain information on the splitting of the interacting levels at the resonance by replacing $\varphi_n(u,\lambda^2)$ in Eq. (5) by its asymptotical expression for large u.[5,31] This form is obtained for $p=m=l=0$ and we see that the asymptotical form of $\Delta\mathcal{E}_n$ will then be identical to that obtained within the so-called two-level model[2] where only the resonant part to $\Delta\mathcal{E}_n$ is retained. We obtain[31]

$$\Delta\mathcal{E}_n=-\frac{\alpha}{2n}(V_0)^{1/2}\frac{H_n^2}{B_{n0}^n}\frac{1}{(1-\Delta\mathcal{E}_n+\mathcal{E}_0-\mathcal{E}_n)^{1/2}} . \tag{13}$$

The splitting between $\mathcal{E}_n$ and $\mathcal{E}_0+1$ is then

$$|\Delta\mathcal{E}_n|=\left[\frac{\alpha}{2n}\right]^{2/3}\left[\frac{H_n^2}{B_{n0}^n}\right]^{2/3}V_0^{1/3} . \tag{14}$$

Since H_n, V_0, and B_{n0} are close to 1 (in InSb), the splitting is only slightly modified (enhanced by 2%) relative to the parabolic case where $|\Delta E_n|=(\alpha/2n)^{2/3}$. The term $V_0^{1/3}$ gives the main contribution in Eq. (14) so that a good approximation consists in replacing the mass m^* by the increased mass m^*V_0 in the definition of α [α is proportional to $m^{*1/2}$ (Ref. 1)].

IV. COMPARISON WITH AVAILABLE EXPERIMENTAL DATA ON InSb

In order to discuss in more detail the effect of band nonparabolicity on the polaron effects, one has to deal with the whole expression of Eqs. (5)–(7), using the so-called improved Wigner-Brillouin perturbation theory (IWBPT),[4] where $\Delta_n=\Delta\mathcal{E}_n-\Delta\mathcal{E}_0^{\mathrm{RSPT}}$, with $\Delta\mathcal{E}_0^{\mathrm{RSPT}}$ the polaronic shift of the zeroth Landau level calculated within the Rayleigh-Schrödinger perturbation theory. IWBPT gives here the best results for $\alpha<0.1$.[32] This is done in Figs. 2 and 3 where we have plotted the polaron-cyclotron mass versus the cyclotron resonance energy $\mathcal{E}_1+\Delta\mathcal{E}_1-\mathcal{E}_0-\Delta\mathcal{E}_0$ for the real case of InSb and for two values of the hydrostatic pressure. The high hydrostatic pressure increases E_g (and thus m^*) in an amount of 140 meV/GPa (Ref. 33) (the phonon energies remain un-

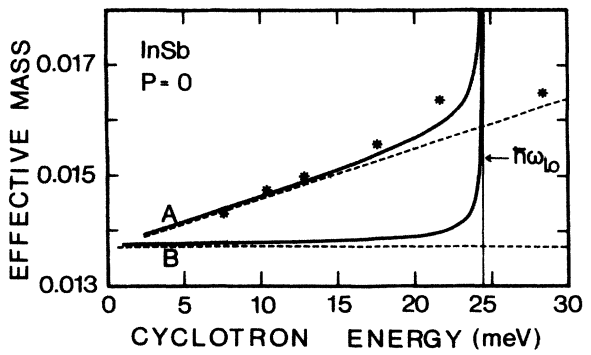

FIG. 2. Cyclotron mass (dashed curves) and polaron cyclotron mass (solid curves) in InSb vs the cyclotron resonance energy. Curves A are calculated within the nonparabolic model while curves B are calculated within the parabolic approximation. The asterisks are experimental points at zero pressure taken from Ref. 33. The masses are in units for m_e.

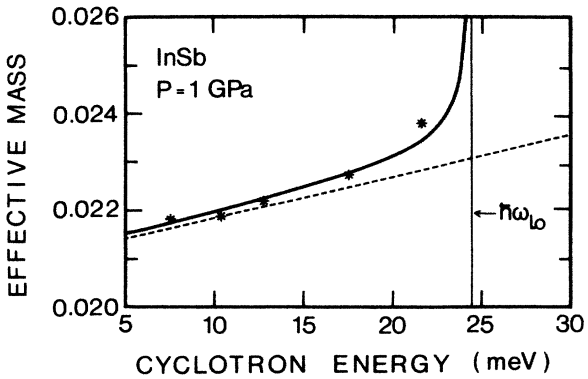

FIG. 3. Same as Fig. 2 for the hydrostatic pressure of 1 GPa. Only the nonparabolic curves are shown.

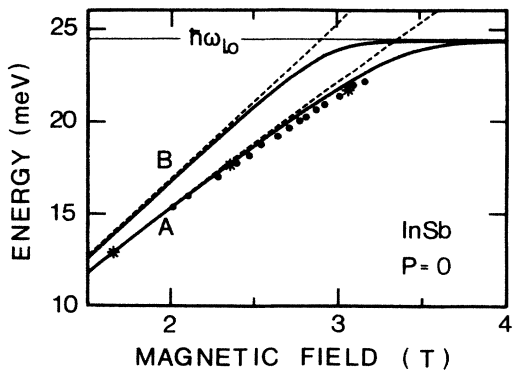

FIG. 4. Cyclotron resonance energy vs the magnetic field for InSb at zero pressure. Solid curves show the polaron cyclotron resonance, and dashed curves the unperturbed cyclotron resonance. *A* nonparabolic; *B* parabolic. The asterisks and the solid circles are experimental points taken from Ref. 33 and Ref. 10, respectively.

changed in the pressure range considered here) and decreases the dielectric constants,[34] so that one has $\alpha=0.029$ at a pressure of 1 GPa. We show the results for the maximum value $l_{\max}=15$ of the index l in Eq. (6). The calculated curves for $1<l_{\max}<20$ are almost the same as those for $l_{\max}=15$. This, together with the satisfactory agreement between calculation and experiment, indicates that the energy region of experimental interest—close to the LO-phonon energy—is very well described by a few intermediate states in the calculation of $\Delta\mathcal{E}_1$ (and $\Delta\mathcal{E}_0$). In fact, increasing $l_{\max}$ first increases $\Delta\mathcal{E}_0$ and $\Delta\mathcal{E}_1$ by the same small quantity thus leaving the cyclotron resonance energy almost unchanged. The contribution of the nonresonant and far-lying (as compared to the phonon energy) intermediate states in the valence band should further improve this agreement. This contribution is expected to be of the order of that given by Larsen at zero field, i.e., it should thus be much smaller than the resonant renormalization. One would rather expect this agreement to be more improved by the inclusion of higher-order phonon corrections as demonstrated by Becker *et al.*[35]

The results shown in Figs. 2 and 3 lead us to formulate the main limitation of our model. If one further increases $l_{\max}$ from a higher value, $\Delta\mathcal{E}_1$ is found to diverge (the divergence first occurs around $\lambda^2\approx 0.1$ and for $l_{\max}>40$). This is an artifact of the three-band model of Bowers and Yafet which gives unperturbed energies going like $\sqrt{n}$ for large n (and like k for large k), leading to the same logarithmic divergence of the final result as discussed by Das Sarma and Mason in Ref. 18. As stated in Ref. 18, this divergence does not affect the results in a crucial way since they rapidly converge in a wide range of the $l_{\max}$ value. Note that no such problems arise in the parabolic case or at zero field in the nonparabolic case since all integrals [or infinite sums like that of Eq. (6)] converge very rapidly.[1,5]

Before concluding, we would like to point out more precisely the differences between the parabolic case and the nonparabolic one. In Fig. 4, we have plotted in both cases the energy of the cyclotron resonance versus the magnetic field. The nonparabolicity strongly bends downward the PLL to lower energies so that the crossing between the $n=1$ and $n=0+\hbar\omega_0$ occurs at a higher field as mentioned in the preceding section. In such a graph as that of Fig. 4, nonparabolicity and polaron effects are thus obviously nonadditive. However, in a graph such as that in Fig. 2, namely of the cyclotron effective mass versus the cyclotron energy, (i.e., on a graph which eliminates the parameter λ^2), nonparabolicity and polaron effects are found to be essentially additive, even in the resonant case. They are additive in the sense that at a given energy, the polaronic contribution to the cyclotron mass is almost the same in the parabolic case and in the nonparabolic one, as seen on Fig. 2. The latter point is in accordance with the simple limiting case discussed in Sec. III [Eq. (14)].

It would be interesting to extend the present calculation to the 2D case. Up to now, the nonparabolicity has only been included in the resonant part of $\Delta\mathcal{E}_n$ (Refs. 8 and 36) which leads to unphysical results in the limit $\lambda^2\ll 1$ (Ref. 37) or in the resonant part, but within a local parabolic approximation.[37] Since electric subbands in semiconducting heterostructures are located relatively high in the band (typically 100 meV) where the effective mass already increases (for instance, the ground-subband effective mas in accumulation layers in HgCdTe can be seven times higher than the bulk band-edge mass[38]), one may expect polaronic effects to be enhanced by nonparabolicity. A rough estimate of this is to replace the band-edge effective mass by the subband effective mass at the Fermi energy in the definition of α,[38] which is supported by Eq. (14). The spatial confinement is also expected to allow resonant polaron coupling between states with different spin as the k terms in the 3D case do.[25] The presence of k-linear[39] terms in band structure of 2D electron gases might well also affect the band-edge quantities E_p and m^{**} since the electron energy possesses a ring of parabolic minima[39] rather than a simple parabolic edge.

V. CONCLUSIONS

We have calculated the energies of PLL within a second-order perturbation theory using a three-band model to describe the unperturbed conduction states of a (3D) weakly polar zinc-blende semiconductor. We have

demonstrated that in the limit of vanishing magnetic fields, there is no change of the polaron-binding energy and mass renormalization due to nonparabolicity of the conduction band itself. This is in accordance with the intuitive physical picture that the conduction band still remains parabolic at its bottom. The small terms in α/E_g given by Larsen are due to a direct mixing of valence and conduction bands through the Fröhlich interaction. In nonvanishing magnetic fields (e.g., in resonant fields), the polaronic shifts of the Landau levels are found to be slightly enhanced by the nonparabolicity in such a way that the polaronic correction to the energy difference between two successive Landau levels (e.g., the fundamental cyclotron resonance) remains almost unaffected. We thus conclude that the main effect of the nonparabolicity in 3D systems is to shift the resonant polarons to a higher field. Our results are important not only because they compare favorably with the experiment (within IWBPT) but also because the effect of nonparabolicity on the weak coupling polarons was still controversial[2,17–19] and partially enigmatic up to now, thus requiring a more rigorous treatment. They can also give us some insight into the case of 2D systems which are currently the subject of considerable debate.[12,13,15,16,36–38]

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APPENDIX A: ELECTRON POSITION IN THE THREE-BAND MODEL OF BOWERS AND YAFET

In this appendix, an expression for the conduction-electron position is calculated from its matrix elements in the subspace of the Γ_6 electron states $|\psi_{nk}\rangle$. The $|\psi_{nk}\rangle$ vectors are given in the symmetric gauge by Eqs. (C3) and (C4) of Ref. 21. Using Eq. (6) of the same reference, the $\langle\psi_{mk'}|X|\psi_{nk}\rangle$ and $\langle\psi_{mk'}|Y|\psi_{nk}\rangle$ matrix elements are calculated within the effective-mass approximation. By inspection of these matrix elements, expressions for X and Y operators are given by

$$X=X_0-\frac{1}{\lambda}(CK+KC^\dagger)+F\ , \tag{A1a}$$

$$Y=Y_0-\frac{i}{\lambda}(CK-KC^\dagger)+iF\ . \tag{A1b}$$

X_0 and Y_0 are the center of orbit coordinate operators which have the commutation relation $[X_0,Y_0]=2i/\lambda^2$. C and $C^\dagger$ are lowering and raising operators in the $|\psi_{nk}\rangle$ ladder. In these equations, K and F are two new operators dealing with nonparabolicity, their action on the $|\psi_{nk}\rangle$ states is given by the following equations;

$$K|\psi_{nk}^{\pm}\rangle=K_n^{\pm}|\psi_{nk}^{\pm}\rangle\ , \tag{A2a}$$

where + and − mean spin-up and spin-down state, respectively (for the sake of clarity, only the spin-up state was considered in the text, and the signs were removed),

$$K_n^{\pm}=\frac{1}{N_{n-1}^{\pm}N_n^{\pm}}\left[1+C\left[\frac{\lambda^2(2n\mp1)+2k^2}{(\mathcal{E}_{n-1}^{\pm}+E_g)(\mathcal{E}_n^{\pm}+E_g)}+\frac{\lambda^2(n\pm1)}{(\mathcal{E}_{n-1}^{\pm}+E_g+\Delta)(\mathcal{E}_n^{\pm}+E_g+\Delta)}\right]\right]\ , \tag{A2b}$$

$N_n^{\pm}$ is the norm of $|\psi_{nk}^{\pm}\rangle$ states [see Eq. (C5) of Ref. 21 or Eq. (7) here];

$$F|\psi_{nk}^{\pm}\rangle=F_n|\psi_{nk}^{\mp}\rangle\ , \tag{A3a}$$

$$F_n=\frac{iCk\lambda}{N_n^-N_n^+}\left[\frac{1}{(\mathcal{E}_n^++E_g)(\mathcal{E}_n^-+E_g)}-\frac{1}{(\mathcal{E}_n^-+\Delta+E_g)(\mathcal{E}_n^++\Delta+E_g)}\right]\ . \tag{A3b}$$

Here the operator F flips the spin, and its action vanishes in the parabolic case. However, it will be ignored in the following since the electronic states on which perturbative calculation is made have a zero k momentum (i.e., $F_n=0$).

The electron position operators at imaginary time $u=it$ are

$$X(u)=X_0-\frac{1}{\lambda}U^\dagger(CK+KC^\dagger)U\ , \tag{A4a}$$

$$Y(u)=Y_0-\frac{i}{\lambda}U^\dagger(CK-KC^\dagger)U\ , \tag{A4b}$$

$$Z(u)=Z_0+\int_0^u[Z,\mathcal{H}_0]d\tau\ , \tag{A4c}$$

where U is the evolution operator. Using the Bowers and Yafet equation [see Eq. (1)] the $Z(u)$ operator is calculated:

$$Z(u)-Z_0=\frac{2C(3\mathcal{H}_0+3E_g+2\Delta)P_zu}{(\mathcal{H}_0+E_g+\Delta)(2\mathcal{H}_0+E_g)+\mathcal{H}_0(\mathcal{H}_0+E_g)-\frac{3}{2}C[\lambda^2(2n+1)+2P_z^2]}\ . \tag{A5}$$

In the calculation of $\langle\psi_{n0}|e^{i\mathbf{q}\cdot\mathbf{r}(u)}e^{-i\mathbf{q}\cdot\mathbf{r}(0)}|\psi_{n0}\rangle$, we made use of $[\dot{Z}(u),Z_0]$ which is

$$[Z(u),Z_0]\,|\,\psi_{n0}\rangle=-\frac{u}{V_n}\,|\,\psi_{n0}\rangle\ , \tag{A6}$$

where V_n represents the increase of the effective mass at the bottom of the nth Landau level and is defined in the text by Eq. (7i).

APPENDIX B: DEVELOPMENT OF MATRIX ELEMENT

In this appendix, the matrix element $\langle\psi_{n0}\,|\,e^{i\mathbf{q}\cdot\mathbf{r}(u)}e^{-i\mathbf{q}\cdot\mathbf{r}(0)}\,|\,\psi_{n0}\rangle$ is developed. Using Eq. (A1), the operator $e^{-i\mathbf{q}\cdot\mathbf{r}(0)}$ is written as follows:

$$e^{-i\mathbf{q}\cdot\mathbf{r}(0)}=e^{-i(q_xX_0+q_yY_0)}e^{-iq_zZ}e^{-i(q_-/\lambda)KC^\dagger}e^{-i(q_+/\lambda)CK}e^{\{-(q_\perp^2/\lambda^2)[CK,KC^\dagger]/2\}}\ , \tag{B1}$$

where $q_\pm=q_x\pm iq_y$ and $q_\perp^2=q_x^2+q_y^2$. Here, the assumption was made that $(1/3!)[KC^\dagger,[KC^\dagger,CK]]\approx 0$, which is reasonable since K_n is close to unity for a wide range of n and λ^2 (e.g., $K_{10}=0.98$ in InSb for $\lambda^2=1.16$). All exponential terms dealing with the C and $C^\dagger$ operators are expanded into infinite series. The matrix element is then

$$\langle\psi_{n0}\,|\,e^{i\mathbf{q}\cdot\mathbf{r}(u)}e^{-i\mathbf{q}\cdot\mathbf{r}(0)}\,|\,\psi_{n0}\rangle=\sum_{m=0}^{n}\sum_{p=0}^{n}\sum_{l=\max(m,p)}^{a}\frac{n!l!H_n^2H_l^2(-1)^{p+m}e^{-u(\mathcal{E}_e-\mathcal{E}_n)}}{m!p!H_m^2H_p^2(n-m)!(l-m)!(l-p)!(n-p)!}$$
$$\times\left[\frac{q_\perp^2}{\lambda^2}\right]^{(n+l-m-p)}\exp\left[-\frac{uq_z^2}{V_l}\right]\exp\left[-\frac{q_\perp^2B_{nl}}{\lambda^2}\right]\ , \tag{B2}$$

where H_n, B_{nl}, and V_l are defined in Eq. (7).

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