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ABSTRACT

We consider, in the effective mass approximation, the problem of a hydrogenic atom in a strong static magnetic field. The ground state and the lowest lying states of angular momentum $\pm\hbar$ are calculated variationally, first for a simple parabolic conduction band and then for the nonparabolic conduction band of InSb. Both the use of improved variational trial functions and the incorporation into the theory of the nonparabolic conduction band are novel features of the present calculation. The results are compared with previous work. Nonparabolic effects are found to be significant for the energy of the lowest lying state of angular momentum $+\hbar$.

The weak-coupling polaron theory is used to derive an upper bound to the shift of the ionization energy of the ground state of the impurity due to electron-LO phonon interaction. Polaron effects on the ground state ionization energy are thereby shown to be negligible in InSb. The bound obtained may, however, prove useful in estimating polaron effects in materials with larger coupling constants.

Accepted for the Air Force
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CONTENTS

SHALLOW DONOR LEVELS OF InSb IN A MAGNETIC FIELD

I. INTRODUCTION

Cyclotron resonance[1] and Hall coefficient measurements[2] in "pure" n-type InSb at low temperatures indicate that free carriers become bound to ionized donors in moderate to strong magnetic fields.

This so-called magnetic freeze-out of conduction band electrons had been predicted by Yafet, Keyes and Adams[3] (YKA), who estimated that the application of a magnetic field of 25 kG to a hydrogenic donor in InSb would increase its binding energy by approximately a factor of four.

Wallis and Bowlden[4] (WB) extended the ground state calculation of YKA for a hydrogen atom in a strong magnetic field to a variety of excited states and showed that strong optical transitions should occur between the ground state and the lowest lying states of angular momentum ±ħ. Such transitions have recently been observed and their energies measured as a function of magnetic field.[5]

We can now inquire to what extent the model of isolated hydrogenic impurities treated in the effective mass approximation can account quantitatively for the optical and Hall effect data in InSb. The purpose of the present work is to improve previous calculations of donor energy levels by introducing the following refinements: (1) improved variational trial functions, (2) accounting for the nonparabolic nature of the conduction band, (3) estimation of the effect of electron-LO phonon interaction.

II. VARIATIONAL TREATMENT FOR PARABOLIC BAND

The energy levels of a hydrogenic impurity in a simple parabolic band subjected to a uniform magnetic field, H, are eigenvalues of the Hamiltonian (1):

$$\tilde{\mathcal{H}} = \frac{p^2}{2m} + \frac{\omega_c}{2}(xp_y - yp_x) + \frac{1}{8}\,m\omega_c^2(x^2 + y^2) + \lambda V(r) \quad , \tag{1}$$

where

$$V(r) = -\frac{e^2}{\mathcal{E}_o(x^2 + y^2 + z^2)^{1/2}} = -\frac{e^2}{\mathcal{E}_o r} \quad , \tag{2}$$

$\mathcal{E}_o$ is the static dielectric constant, m is the band mass, ω_c is the cyclotron frequency, eH/mc, and we have used the vector potential $\underline{A}$ defined by $\underline{A} = H/2(-y, x, 0)$, corresponding to a uniform magnetic field in the z-direction. We take the parameter λ equal to 1.

If our unit of length is $(\hbar/2m\omega_c)^{\frac{1}{2}} = 2^{-\frac{1}{2}} \times$ cyclotron radius, and our unit of energy, $\hbar\omega_c$, we can rewrite (1) in dimensionless form in cylindrical polar coordinates as

$$\mathcal{H} = \widetilde{\mathcal{H}}/\hbar\omega_c = \mathcal{H}_0 + \mathcal{H}_1 \quad ,$$

$$\mathcal{H}_o = -\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2} L_z + \frac{\rho^2}{16} \quad , \tag{3}$$

$$\mathcal{H}_1 = -(\gamma/2)^{-1/2}/(\rho^2 + z^2)^{1/2} \quad ,$$

where L_z is the angular momentum operator $1/i\ \partial/\partial\varphi$ with integer eigenvalues M,

$$\gamma = \frac{\hbar^2 \epsilon_o^2(\hbar\omega_c)}{me^4} \equiv \frac{\hbar\omega_c}{2R}$$

and R is the hydrogenic Rydberg.

The Schrödinger equation

$$\mathcal{H}\psi = E\psi \tag{4}$$

is not completely separable and we are forced to resort to a variational solution. YKA have pointed out that in the limit $\gamma \to \infty$ (strong field limit) the eigenfunctions of $\mathcal{H}$ take the product form

$$f(\rho)\ g(z) \tag{5}$$

and in fact $f(\rho) = \varphi_{NM}(\rho)$ where $\mathcal{H}_0\varphi_{NM} = (N + \frac{1}{2})\ \varphi_{NM}$.

Since $\varphi_{00} = e^{-\rho^2/8}$ and $\varphi_{\binom{1,\,1}{0,\,-1}} = \rho\ e^{-\rho^2/8}\ e^{\pm i\varphi}$, one is motivated to use for the ground state trial function

$$e^{-\rho^2/8a^2}\ e^{-z^2/8b^2} \tag{6a}$$

and for the lowest lying M = ±1 states:

$$\rho\ e^{-\rho^2/8a^2}\ e^{-z^2/8b^2}\ e^{i\varphi} \tag{6b}$$

$$\rho\ e^{-\rho^2/8a^2}\ e^{-z^2/8b^2}\ e^{-i\varphi} \quad . \tag{6c}$$

YKA actually took (6a) as their ground state trial function, varying both a^2 and b^2, while WB used (6a-c) as trial functions fixing $a^2 = 1$ and varying b^2 to obtain lowest energy. We remark that since M is a good quantum number of $\mathcal{H}$, a trial function which is an eigenfunction of L_z with eigenvalue M' yields an energy which is an upper bound to the energy of the lowest-lying M = M' eigenstate of $\mathcal{H}$.

The wave functions (6a-c) have two important weaknesses as variational trial functions: (1) the H = 0 eigenfunctions of $\mathcal{H}$, being hydrogenic wave functions, can not be written in the product form (5) for any choice of f and g; thus any trial function of form (5) is likely to get progressively worse as H decreases; (2) even at high fields, wave functions (6a-c) decay too rapidly with increasing z at constant ρ (because the effective potential for motion in the z-direction[6] vanishes as $z \to \infty$).

To eliminate these shortcomings we have chosen the following trial functions:

$$e^{-\rho^2/8a^2}\; e^{-\kappa(\rho^2+\alpha z^2)^{1/2}} \qquad M = 0 \quad , \tag{7a}$$

$$\rho\; e^{-\rho^2/8a^2}\; e^{-\kappa(\rho^2+\alpha z^2+\beta^2)^{1/2}}\; e^{\pm i\varphi} \qquad M = \pm 1 \quad , \tag{7h}$$

where a^2, κ, α and β^2 are variational parameters which are adjusted to optimize independently each of the above functions. Note that (7a) and (7b) become 1s and 2p hydrogenic eigenfunctions respectively as $a^2 \rightarrow \infty$, $\alpha \rightarrow 1$ and $\beta \rightarrow 0$. Further, they decay in a realistic way as $z \rightarrow \infty$ with ρ fixed. The price we pay for our improved functions is that the required integrations can no longer be performed analytically.

In Table 1 we tabulate ionization energies,* $E^{(I)}$ deduced from the variational calculations of WB, YKA (wave functions (6a-c) with a^2 and b^2 varied) and the present calculation denoted PC. All energies are tabulated in units of the hydrogenic Rydberg.

TABLE 1

γ	$E^{(I)}_{WB}(M=0)$	$E^{(I)}_{YKA}(M=0)$	$E^{(I)}_{PC}(M=0)$	$E^{(I)}_{WB}(M=1)$	$E^{(I)}_{YKA}(M=1)$	$E^{(I)}_{PC}(M=1)$
0	0.000	0.8488	1.000	0.000	0.2264	0.2500
1	1.346	1.523	1.661	0.8564	0.8919	0.9118
5	2.520	2.615	2.750	1.664	1.686	1.717
25	4.515	4.565	4.733	3.100	3.113	3.183
100	7.174	7.200	7.457	5.095	5.1030	5.261

Table 1 indicates that the wave functions (7) give lower energies than (6) over the range of γ calculated. Notice, however, that the percentage deviation of E_{YKA} from E_{PC} decreases with increasing field and is smaller at given field for the M = 1 level than for M = 0. This last result might have been anticipated from the fact that the M = 1 wave function vanishes at the Coulomb center. This means that the effect of the Coulomb field is weaker on the M = 1 state than on the M = 0. The strong field product wave function (5) should therefore be, at the same value of H, a better approximation to the M = 1 state than to the M = 0 state.

Because it can be deduced directly from cyclotron resonance experiments, the quantity $\Delta(H) = E^{(I)}(M = 0) - E^{(I)}(M = 1)$ is of particular interest. From Table 1, we calculate that $\Delta^{(H)}_{PC}$ is always greater than $\Delta^{(H)}_{YKA}$ and the percentage difference becomes particularly marked at lower fields.

Finally, we expect, as noted above, that our trial functions (7a, b) should also be quite satisfactory at $\gamma \lesssim 1$, where product functions of the form (5) are suspect. Since there is some

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*The ionization energy of an impurity level is defined as follows. Let E_{i,λ_o} be the energy of the ith eigenstate of (1) with $\lambda = \lambda_o$. Then the ionization energy of this eigenstate is $\lim_{\lambda \rightarrow 0} (E_{i,\lambda} - E_{i,1})$. Thus, in the parabolic band case for M = 0 and M = −1 states the ionization energy in Rydbergs is defined by $E^{(I)}(M = {0 \atop -1}) = \gamma - E(M = {0 \atop -1})$ while for the M = 1 level the ionization energy is $E^{(I)}(M = 1) = 3\gamma - E(M = 1)$.

experimental interest in this region of γ, we tabulate below our variational results for the hydrogenic ground state ionization energy with $\gamma \leqslant 3$.

TABLE 2

γ	0.3	0.5	0.7	1.0	1.5	2.0	2.5	3.0
$E^{(I)}_{PC}$	1.26	1.39	1.51	1.66	1.87	2.04	2.19	2.32

III. NONPARABOLIC BAND

In order to study the effects on binding energy of the nonparabolic structure of the InSb conduction bands, we turn to the model of Bowers and Yafet.[7] This model gives a simple and accurate description of the conduction band Landau level energies observed in InSb.

The BY model is defined by the 8×8 Hamiltonian matrix $H^{BY}_{nn'}$ given in the position representation by

$$H^{BY}_{nn'} = \left[\epsilon_{n'} + \frac{(p + \frac{e}{c} A)^2}{2m_v}\right] \delta_{nn'} + (p + \frac{e}{c} A) \cdot \bar{p}_{nn'} \quad , \tag{8}$$

where $\epsilon_{n'}$ is the energy of the edge of band n' in the absence of magnetic fields, m_v is the electron mass in vacuum, and $\bar{p}_{jnn'}$ is the matrix element of $1/m_v \; \hbar/i \; \nabla_j$ in the band edge functions u_n and $u_{n'}$. We use the same band-edge functions and notation as Pidgeon and Brown,[8] define our impurity Hamiltonian by the matrix

$$\bar{H}_{nn'} = H^{BY}_{nn'} + V(r)\,\delta_{nn'} \tag{9}$$

and look for conduction band solutions to the eigenvalue problem

$$\sum_{n'=1}^{8} \bar{H}_{nn'} f_{n'} = E f_n \quad . \tag{10}$$

The functions f_n in (10) are the usual envelope functions associated with the total electronic wave function given by

$$\Psi = \sum f_n u_n \quad .$$

Taking our zero of energy at the valence band edge in the absence of magnetic field we write out (10) explicitly:

$$(E_G - \lambda')\, f_1 + \bar{p}\left[\frac{K}{\sqrt{2}} f_3 + \frac{K^*}{\sqrt{6}} f_5 + \frac{k_z}{\sqrt{3}} f_8 - i\left(\frac{2}{\sqrt{6}} k_z f_6 + \frac{K^*}{\sqrt{3}} f_7\right)\right] = 0 \quad , \tag{11a}$$

$$(E_G - \lambda')\, f_2 + \bar{p}\left[\frac{K^*}{\sqrt{2}} f_4 + \frac{K}{\sqrt{6}} f_6 + \frac{k_z}{\sqrt{3}} f_7 - i\left(\frac{2}{\sqrt{6}} k_z f_5 + \frac{K}{\sqrt{3}} f_8\right)\right] = 0 \quad , \tag{11b}$$

$$\lambda' f_3 = \bar{p}\,\frac{K^*}{\sqrt{2}} f_1 \quad , \tag{11c}$$

$$\lambda' f_4 = \bar{p}\,\frac{K}{\sqrt{2}} f_2 \quad , \tag{11d}$$

$$\lambda' f_5 = \bar{p}\left(\frac{K}{\sqrt{6}}\, f_1 + \frac{2ik_z}{\sqrt{6}}\, f_2\right) \quad , \tag{11e}$$

$$\lambda' f_6 = \bar{p}\left(\frac{2i}{\sqrt{6}}\, k_z f_1 + \frac{K^*}{\sqrt{6}}\, f_2\right) \quad , \tag{11f}$$

$$(\Delta + \lambda')\, f_7 = \bar{p}\left(\frac{-i}{\sqrt{3}}\, K f_1 + \frac{k_z}{\sqrt{3}}\, f_2\right) \quad , \tag{11g}$$

$$(\Delta + \lambda')\, f_8 = \bar{p}\left(\frac{k_z}{\sqrt{3}}\, f_1 + \frac{i}{\sqrt{3}}\, K^* f_2\right) \quad , \tag{11h}$$

where $\lambda' = E - V(r)$, $K = (p_x + e/c\, A_x) + i(p_y + e/c\, A_y)$, $k_z = p_z$, E_G is the band gap, Δ is the spin-orbit splitting of the valence band and for all values of j, n and n' for which $\bar{p}_{j\,nn'}$ does not vanish, $\bar{p}_{j\,nn'} = \bar{p}$.

Left multiplying (11a) and (11b) by λ' and inserting (11c-h) into (11a) and (11b) gives a pair of coupled equations for f_1 and f_2:

$$\begin{aligned} &\Biggl\{\frac{\lambda'(E_G - \lambda')}{E_G} + \frac{\bar{p}^2}{E_G}\Biggl(\frac{1}{2}\, KK^* + \frac{1}{6}\, K^*K + \frac{2}{3}\, k_z^2 + \frac{\lambda' K^*}{3}\, \frac{1}{\Delta + \lambda'}\, K + \frac{1}{3}\, \lambda' k_z\, \frac{1}{\Delta + \lambda'}\, k_z \\ &\qquad + \frac{1}{2}\, \frac{[\lambda', K]}{\lambda'}\, K^* + \frac{1}{6}\, \frac{[\lambda', K^*]}{\lambda'}\, K + \frac{2}{3}\, \frac{[\lambda', k_z]}{\lambda'}\, k_z\Biggr)\Biggr\}\, f_1 + \bar{p}^2\, \frac{i}{3}\, \Biggl(\frac{[\lambda', K^*]}{\lambda'}\, k_z \\ &\qquad - \frac{[\lambda', k_z]}{\lambda'}\, K^*\Biggr)\, f_2 = 0 \quad , \end{aligned} \tag{12a}$$

$$\begin{aligned} &\Biggl\{\frac{\lambda'(E_G - \lambda')}{E_G} + \frac{\bar{p}^2}{E_G}\Biggl(\frac{1}{2}\, K^*K + \frac{1}{6}\, KK^* + \frac{2}{3}\, k_z^2 + \frac{\lambda' K}{3}\, \frac{1}{\Delta + \lambda'}\, K^* + \frac{\lambda' k_z}{3}\, \frac{1}{\Delta + \lambda'}\, k_z \\ &\qquad + \frac{1}{2}\, \frac{[\lambda', K^*]}{\lambda'}\, K + \frac{1}{6}\, \frac{[\lambda, K]}{\lambda'}\, K^* + \frac{2}{3}\, \frac{[\lambda', k_z]}{\lambda'}\, k_z\Biggr)\Biggr\}\, f_2 + \bar{p}^2\, \frac{i}{3}\Biggl(\frac{[\lambda', K]}{\lambda'}\, k_z \\ &\qquad - \frac{[\lambda', k_z]}{\lambda'}\, K\Biggr)\, f_1 = 0 \quad . \end{aligned} \tag{12b}$$

Within the framework of our model (12a) and (12b) are exact. Four fundamental energies occur in Eqs. (12). They are tabulated in Table 3 in units of 10^{-3} eV for InSb at experimentally interesting magnetic field strengths.

TABLE 3			
Hydrogenic Rydberg (R)	Cyclotron Energy ($\hbar\omega_c$)	E_G	Δ
0.6	10.0 – 100.0	236.0	805.0

It is easy to estimate the order of magnitude of the various terms appearing in (12a, b) by means of the following scheme, valid for conduction band eigenvalues and magnetic fields such that $\hbar\omega_c > R$:

$$\lambda' = 0(E_G + \hbar\omega_c) \quad , \quad \frac{\bar{p}^2}{E} = 0\left(\frac{1}{m^*}\right)$$

$$K \text{ or } K^* = O[(m^*\hbar\omega_c)^{1/2}]$$

$$V(r) = O[(R\hbar\omega_c)^{1/2}] \tag{13}$$

where m^* is the conduction band mass in InSb ($m^* \simeq 0.0138 m_V$).

In view of (13), Table 3 and the definition of λ' [$\lambda' = E - V(r)$], we see that to an excellent approximation we can neglect commutators of K, K^* and k_z with $(\underline{\Delta} + \lambda')^{-1}$ in (12a, b).

Introducing definitions

$$\mathcal{E} = E - E_G \quad ,$$

$$\frac{1}{2m^*(\mathcal{E})} = \left(\frac{2}{3} + \frac{1}{3}\,\frac{E}{\underline{\Delta} + E}\right)\frac{\bar{p}^2}{E_G} \text{ hence } \frac{2}{3}\,\frac{\bar{p}^2}{E_G} = C/2m^*(\mathcal{E}) \text{ where } C = \frac{2/3(\underline{\Delta} + E)}{(\frac{2}{3}\underline{\Delta} + E)} \quad ,$$

$$\omega_c(\mathcal{E}) = \frac{eH}{m^*(\mathcal{E})\,c} \quad R(\mathcal{E}) = \frac{e^4 m^*(\mathcal{E})}{\hbar^2\,\mathcal{E}_o^2} \quad ,$$

$$\gamma(\mathcal{E}) = \hbar\omega_c(\mathcal{E})/2R(\mathcal{E}) \quad , \tag{14}$$

and taking as unit of length $r_c \equiv [\hbar/2m^*(\mathcal{E})\,\omega_c(\mathcal{E})]^{1/2}$ and unit of energy $\hbar\omega_c(\mathcal{E})$, (12a, b) become

$$H_{11}f_1 + H_{12}f_2 = \left(1 + \frac{\mathcal{E}}{E_G}\right)\mathcal{E}f_1 \equiv \bar{\mathcal{E}}f_1 \quad , \tag{15a}$$

$$H_{22}f_2 + H_{21}f_1 = \left(1 + \frac{\mathcal{E}}{E_G}\right)\mathcal{E}f_2 \equiv \bar{\mathcal{E}}f_2 \quad , \tag{15b}$$

where, in the gauge of section 1, we have

$$\begin{aligned} H_{11} = {} & \left[1 + 0.5C\left(\frac{E - V(r_c r)}{\underline{\Delta} + E - V(r_c r)} - \frac{E}{\underline{\Delta} + E}\right)\right]\left(-\nabla^2 + \frac{\rho^2}{16} + \frac{1}{2}L_z\right) + \left(1 + \frac{2\mathcal{E}}{E_G}\right)\upsilon(r) \\ & - \frac{C\hbar\omega_c}{E - V(r_c r)}\,\frac{1}{r}\,\frac{d\upsilon(r)}{dr}\left\{\rho\,\frac{\partial}{\partial\rho} - \frac{i}{2}\,\frac{\partial}{\partial\varphi} + \frac{\rho^2}{8} + z\,\frac{\partial}{\partial z}\right\} - \frac{1}{4}\,C\left(\frac{\underline{\Delta}}{\underline{\Delta} + E - V(r_c r)}\right), \end{aligned} \tag{16a}$$

$$H_{22} = H_{11} + \frac{1}{2}\,C\,\frac{\underline{\Delta}}{\underline{\Delta} + E - V(r_c r)} - \frac{C\hbar\omega_c}{E - V(r_c r)}\,\frac{1}{r}\,\frac{d\upsilon(r)}{dr}\left\{i\,\frac{\partial}{\partial\varphi} - \frac{\rho^2}{4}\right\} \quad , \tag{16b}$$

$$H_{12} = -\frac{iC\hbar\omega_c}{2(E - V(r_c r))}\,\frac{1}{r}\,\frac{d\upsilon(r)}{dr}\,e^{-i\varphi}\left[-z\left(\frac{\partial}{\partial\rho} - \frac{i}{\rho}\,\frac{\partial}{\partial\varphi} + \frac{\rho}{4}\right) + \rho\,\frac{\partial}{\partial z}\right] \quad , \tag{16c}$$

$$H_{21} = H_{12}^{+} \quad ,$$

where $\upsilon(r) = V(r_c r)/\hbar\omega_c$. Decoupling (15a, b) we obtain the Schrödinger-like equations

$$[H_{11} - H_{12}(H_{22} - \bar{\mathcal{E}}_{\uparrow})^{-1}H_{21}]\,f_1 = \bar{\mathcal{E}}_{\uparrow}f_1 \tag{17a}$$

$$[H_{22} - H_{21}(H_{11} - \bar{\mathcal{E}}_{\downarrow})^{-1}H_{12}]\,f_2 = \bar{\mathcal{E}}_{\downarrow}f_2 \quad . \tag{17b}$$

Our desire to solve for $\bar{\mathcal{E}}_{\uparrow}$ and $\bar{\mathcal{E}}_{\downarrow}$ from (17a, b) by the variational method is thwarted by the difficulty of evaluating the expectation value of terms containing the inverse operators. In Appendix A we show how to evaluate, approximately, the effect of these terms. For the present we need only the result that for the eigenvalues of the lowest lying M = 0 or M = 1 states we can, to very good accuracy, write simply:

$$H_{11}f_1 = \bar{\mathcal{E}}_{\uparrow} f_1 \tag{18a}$$

$$H_{22}f_2 = \bar{\mathcal{E}}_{\downarrow} f_2 \quad . \tag{18b}$$

The reason for using variational methods for estimating eigenvalues of Schrödinger equations is, of course, that a relatively inaccurate trial wave function can produce a fairly accurate energy. In (18a, b) the Hamiltonians H_{11} and H_{22} are themselves functions of the eigenvalue $\mathcal{E}$; moreover, $\bar{\mathcal{E}}$ is not itself an eigenvalue but rather a function of the eigenvalue as indicated in (15a, b). Is it true that for (18a, b) the variational method produces a good energy from an only moderately good wave function? This question is answered affirmatively in Appendix B.

Using trial functions of the form (7a) and (7b) we have solved (18a) and (18b) variationally by computer, making sure that the final variational energy deduced is equal to the energy which was inserted into H_{11} and H_{22}, respectively. Our results for $\mathcal{E}^{I}_{\uparrow}(M = 0)$, the ionization energy associated with the spin-up impurity ground state level, are given in Table 4. Values of R, E_G and Δ employed are taken from Table 3. Energies are in meV.

TABLE 4

H(kG)	12.0	18.0	25.0	50.0	80.0	120.0
$\mathcal{E}^{I}_{\uparrow}(M = 0)$	1.97	2.27	2.54	3.23	3.80	4.40

Table 4 results are obtained using a bottom-of-the-band Rydberg of 0.6 meV for InSb. Given a different Rydberg value, R_o, where $0.5 \lesssim R_o \lesssim 0.8$, $\mathcal{E}^{I}_{\uparrow}(M = 0)$ in meV can be obtained approximately by multiplying the tabulated value by $1 + 1.1\,(R_o - 0.6)$, whereas the analogous factor for $\mathcal{E}^{I}_{\uparrow}(M = 1)$ is $1 + (R_o - 0.6)$.

We have plotted the ionization energy difference $\mathcal{E}^{I}_{\uparrow}(M = 0) - \mathcal{E}^{I}_{\uparrow}(M = 1) \equiv \Delta_{\uparrow}(H)$ in Fig. 1 both for the nonparabolic and parabolic bands with identical bottom-of-the-band mass and Rydberg. The quantity $\Delta_{\uparrow}(H)$ is, in our model, expected to be equal to the energy difference between the cyclotron resonance and impurity cyclotron resonance absorption lines at fixed magnetic field.

The striking nonparabolic band effect on $\Delta_{\uparrow}(H)$ shown in Fig. 1 can be understood qualitatively as follows. In the InSb conduction band the electronic effective mass increases with electron energy. Thus the ionization energy of the M = 1 impurity level increases markedly with magnetic field relative to the corresponding nonparabolic energy. On the other hand the M = 0 impurity level, lying always near the bottom of the band, behaves much the same for both parabolic and nonparabolic bands. At high fields the electron mass characterizing the M = 1 level in the nonparabolic band increases sufficiently rapidly that $\Delta_{\uparrow}(H)$ reaches a maximum and then begins to decrease with increasing field. This effect should be detectable experimentally.

The spatial spread of the envelope function f_1 gives a good idea of the degree of localization of the spin-up electron with respect to the Coulomb center. For the ground state (M = 0), we find that f_1 is somewhat less markedly elongated in the direction along the magnetic field than

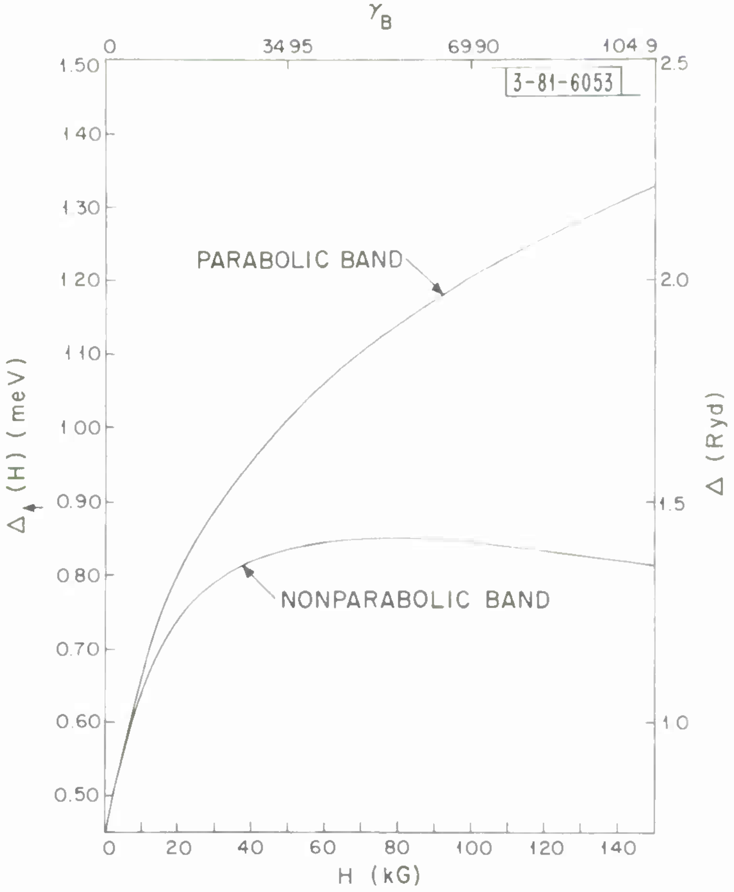

Fig. 1. Comparison of $\Delta_\uparrow(H)$ computed for the nonparabolic conduction band of InSb and for a simple parabolic band with the same bottom-of-the-band parameters. $\gamma_B = \hbar\omega_c/2R$ evaluated at the bottom of the band.

the wave function calculated by YKA. Of greater interest is the very marked elongation of the M = 1 level. If we let ρ_{max} be the radial coordinate at which $|f_1|^2$ achieves its maximum value, $|f_{1\,max}|^2$, at $z = 0$ [that is, $f_{1\,max} = f_1(\rho_{max}, 0)$], then we define the extent of $|f_1|^2$ in the z-direction by z_o where

$$|f_1(\rho_{max}, z_o)/f_1(\rho_{max}, 0)|^2 = e^{-1} \quad . \tag{19}$$

Our calculations show that z_o varies from $\sim 2 \times 10^{-5}$ cm at 12 kG to $\sim 1 \times 10^{-5}$ at 120 kG in InSb. Since the very purest samples of InSb presently available have a mean interimpurity separation not significantly smaller than 2×10^{-5} cm it seems possible that impurity overlap effects may not be entirely negligible for the M = 1 state.

Finally, we remark that, unlike the parabolic band case, the M = −1 state ionization energy is less than, rather than equal to, the M = 1 ionization energy. The energy differences are, however, never greater than a few tenths of a meV for fields up to 120 kG.

IV. POLARON EFFECTS

Because of the small conduction band mass in InSb, the kinetic energy of electrons bound to donors in InSb exceeds the longitudinal optical phonon energy, $\hbar\omega_o$, in magnetic fields of $\sim$60 kG or more. One might doubt, therefore, that the simple introduction of the static dielectric constant $\mathcal{E}_0$ into the Coulomb potential (2) would completely characterize the polarization properties of the crystal for the whole range of experimentally interesting magnetic fields (say 0 to 150 kG).

Platzman[9] has shown on the basis of the Fröhlich polaron model that the proper treatment of lattice polarization requires augmenting the Hamiltonian (1) by introducing the Fröhlich phonon energy and electron-phonon interaction terms and solving for the eigenvalues of the new Hamiltonian. Because we are interested in relatively low lying states and because the Fröhlich electron-phonon coupling constant, α, is very small ($\alpha \sim 0.02$) in InSb, we are justified in calculating corrections to our impurity levels to lowest order in α and in assuming a simple parabolic conduction band for obtaining these corrections.

Thus for our purposes it will suffice to consider the Hamiltonian $\mathcal{H}$ which is written below using units appropriate to a polaron calculation (length in units of $r_0 \equiv (\hbar/2m\omega_0)^{\frac{1}{2}}$, energy in units of $\hbar\omega_0$).

$$\mathcal{H} = \mathcal{H}_0(\lambda) + \mathcal{H}_1 \quad , \tag{20a}$$

$$\mathcal{H}_0(\lambda) = \pi^2 + U(r) + \sum b_{\underline{k}}^+ b_{\underline{k}} \quad , \tag{20b}$$

$$\mathcal{H}_1 = \sum \nu_k (e^{-i\underline{k}\cdot\underline{r}}\, b_{\underline{k}}^+ + e^{i\underline{k}\cdot\underline{r}}\, b_{\underline{k}}) \quad , \tag{20c}$$

where $\nu_k = (4\pi\alpha/S)^{\frac{1}{2}}/k$ with S = crystal volume and $\alpha = \frac{1}{2}(1/\mathcal{E}_\infty - 1/\mathcal{E}_0)\, e^2/r_0/\hbar\omega_0$,

$$U(r) = \lambda V(r_0 r)/\hbar\omega_0 \quad ,$$

$$\pi^2 = \left[\frac{1}{i}\,\underline{\nabla} + \frac{r_0 e}{\hbar c}\,\underline{A}(r_0 r)\right]^2 \quad .$$

$b_{\underline{k}}^+$ is the creation operator for a LO phonon of wave vector $\underline{k}$ and λ is a parameter introduced to facilitate the discussion of Appendix C. For present purposes we consider $\lambda = 1$.

We will confine ourselves to obtaining a rigorous upper bound to the polaron corrections to the ionization energy of the ground state of $\mathcal{H}$ in lowest order in α. Except near the polaron resonances[10] we would expect that the shift in ionization energies of the excited states would be of the same order of magnitude as that of the ground state.

In Appendix C we show that a rigorous upper bound to the shift of the ground state ionization energy due to electron-LO phonon interaction is given to lowest order in α by

$$\frac{\alpha}{6}\,\hbar\omega_0 \left(\langle 0|\pi^2|0\rangle - \frac{1}{2}\,\frac{\omega_c}{\omega_0}\right) \quad , \tag{21}$$

where $|0\rangle$ is the ground state eigenfunction of $\mathcal{H}_0(\lambda = 1)$. From (21) we can conclude that to order α the ionization energy shift of a polaron in the ground state is overestimated at all fields by replacing the band mass, m, by the polaron mass $m^* = (1 + \alpha/6)\,m$ in (1). We believe, in addition, that the replacement of m by m^* in (1) gives a quite accurate estimate of the polaron correction for the range of fields considered here.

Numerical calculation of (21) employing optimized wave functions of the form (7a) and using values of 0.6 meV for the hydrogenic Rydberg, 0.0138 for the band mass to vacuum mass ratio, and 0.02 for α shows that polaron effects shift the ground state ionization energy certainly less than 0.25% for magnetic fields from 4 kG to 120 kG.

V. CONCLUSIONS

Nonparabolic effects can not be neglected in calculating the binding energies of impurity states which lie near or above the n = 1 Landau level in magnetic fields greater than ~15 kG in InSb. The nonparabolic effects result in greater ionization energies for the higher lying states than would be expected from calculations for a simple parabolic band. These effects should be observable experimentally in cyclotron resonance.

For samples of highest attainable purity, overlap effects between adjacent impurity sites should be insignificant for the ground state. Overlap may be important for excited states, particularly those which tend to be strongly elongated along the magnetic field direction such as the $M = \pm 1$ levels.

Central cell corrections, not taken into account in the present calculation, may be important for the ground state ionization energy and will be expected to increase rapidly with magnetic field.

In the simplest possible picture we can imagine that the central cell correction is proportional to the probability of finding an electron in a small volume (dimensions of the order of the lattice spacing) around the impurity center. If we assume that the effective mass wave function is contained in a volume whose dimensions are proportional to the cyclotron radius, then the increase of the central cell correction with magnetic field should be proportional to $H^{3/2}$.

For states with $M \neq 0$ we would expect central cell corrections to be relatively very small.

Poloron effects on the ionization energies are negligible except at fields near which the polaron resonance occurs.

APPENDIX A

We consider the energy shift introduced by the presence of the perturbations H_{12} and H_{21} in (15a) and (15b), respectively. These terms have been neglected in (18a, b) and the discussion which follows in the body of the paper.

First we observe qualitatively that from (16c), H_{21} and H_{12} are small quantities, being only of order $(\hbar\omega_c R)^{\frac{1}{2}}\hbar\omega_c/E$. Further f_1 and f_2, which are coupled by the perturbation, differ in energy by an amount of the order of the conduction band spin splitting, which is small compared to E_G. Thus we have a small perturbation coupling together levels which lie relatively near each other in energy. We do not expect, therefore, any significant shift in energy due to H_{12} and H_{21}.

To make a quantitative calculation we focus for definiteness on (17a), reproduced below

$$H_{11}f_1 - [H_{12}(H_{22} - \bar{\mathcal{E}}_\uparrow)^{-1}H_{21}]\, f_1 = \bar{\mathcal{E}}_\uparrow f_1 \quad . \tag{A1}$$

From (16b) we observe that to a good approximation

$$H_{22} = H_{11} + \frac{1}{2}\, C\, \frac{\Delta}{\Delta + E} = H_{11} + \tilde{K} \quad .$$

Inserting into (A1) gives

$$(H_{11} - H'_{11})\, f_1 = \bar{\mathcal{E}}_\uparrow f_1 \quad ,$$

$$H'_{11} = H_{12}(H_{11} + \tilde{K} - \bar{\mathcal{E}}_\uparrow)^{-1}\, H_{21} \quad . \tag{A2}$$

We still cannot compute $\bar{\mathcal{E}}_\uparrow$ variationally because of the difficulty of evaluating expectation values of H'_{11}. However, by exploiting the smallness of H_{21}, we can obtain accurate values for $\bar{\mathcal{E}}_\uparrow$ by a trick. Since $H_{11} - H'_{11}$ commutes with L_z we can choose energy eigenstates which are simultaneously angular momentum eigenstates. We are interested in finding the energies of the lowest lying angular momentum eigenstates with $M = -1,\ 0,\ 1$. For each value of M we construct a new Hamiltonian H_M whose eigenvalues for given M are equal to the eigenvalues of $H_{11} - H'_{11}$ for the same M to order $|H_{21}|^2$. However H_M, unlike $H_{11} - H'_{11}$, is so constructed that it is easy to find its eigenvalues variationally.

Such a Hamiltonian is given in (A3)

$$\mathsf{H}_M = \bar{H}_M + \bar{H}'_M \quad ,$$

$$\bar{H}_M = H_{11} - \tilde{K}(\sigma_z - 1/2) \quad ,$$

$$\bar{H}'_M = (P_M H_{12} + H_{21} P_M)\, \sigma_x \quad , \tag{A3}$$

where

$$\sigma_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad ,$$

and P_M is the Hermitian operator defined by

$$P_M\, e^{im\varphi} = (1 - \delta_{m,\,M-1})\, e^{im\varphi} \quad .$$

We easily verify that H_M is Hermitian, and if h_j is an eigenfunction of H_{11} with eigenvalue $\bar{\mathcal{E}}_j^{(o)}$ then $h_j|\uparrow\rangle$ and $h_j|\downarrow\rangle$ are eigenfunctions of $\bar{H}_M$ with eigenvalues $\bar{\mathcal{E}}_j^{(o)}$ and $\bar{\mathcal{E}}_j^{(o)} + \tilde{K}$, respectively.

Treating $\overline{H}'_M$ as a perturbation on $\overline{H}_M$ we find that to order $|H_{12}|^2$ the perturbed eigenvalue of H_M is given in perturbation theory by

$$\langle H_{11} - H'_{11} \rangle \quad , \tag{A4}$$

where the expectation value is taken in the eigenstate of H_{11} of interest with angular momentum eigenvalue M. But (A4) is the expectation value we want to find. Thus if we compute the eigenvalues of H_M by an appropriate variational method we should be able to approximate (A4).

We have used the following trial functions:

$$\begin{aligned} \psi_{GS} &= a g_o \, |\uparrow\rangle + i b z g_1 \, |\downarrow\rangle \quad , \\ \psi_{M=1} &= a g_1 \, |\uparrow\rangle + i b \rho z \, e^{i\varphi} \tilde{g}_1 \, |\downarrow\rangle \quad , \\ |\uparrow\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad , \end{aligned} \tag{A5}$$

where g_o, g_1 and $\tilde{g}_1$ have the form (7a), (7b) and (7b), respectively, and both g_1 and $\tilde{g}_1$ are $M = +1$ eigenfunctions of L_z. Note that neither ψ_{GS} nor $\psi_{M=1}$ are eigenstates of L_z and that the method described here is useless for approximating the eigenfunctions of $H_{11} - H'_{11}$.

For ψ_{GS} and $\psi_{M=1}$ we have 8 and 9 independent parameters to vary respectively (b is a variational parameter). In both cases we find that the effect of H_{12} on the binding energies calculated from H_{11} alone is less than 1%.

APPENDIX B

For definiteness we consider the error in determining $\mathcal{E}_\uparrow$ by the variational method for the eigenvalue problem (18a)

$$H_{11}(\mathcal{E}_\uparrow)\, f_1 = \left(1 + \frac{\mathcal{E}_\uparrow}{E_G}\right)\mathcal{E}_\uparrow f_1 = \overline{\mathcal{E}}_\uparrow f_1 \tag{B1}$$

with $H_{11}(\mathcal{E}_\uparrow)$ given by (16a).

Assume that for the exact solution of (B1), $\mathcal{E}_{\text{exact}}$, the error in estimating the eigenvalue of $H_{11}(\mathcal{E}_{\text{exact}})$ using our variational trial function is δ_v where δ_v is small enough to allow neglect of quantities of order δ_v^2. The final result of the variational calculation will be an approximate value of $\mathcal{E}_\uparrow$, $\mathcal{E}_{\text{approx}}$. Let

$$\delta_a = \mathcal{E}_{\text{approx}} - \mathcal{E}_{\text{exact}} \quad .$$

If we can neglect terms of higher order than δ_a then the error introduced in the variational calculation by inaccuracy of $\mathcal{E}_\uparrow$ in the Hamiltonian $H_{11}(\mathcal{E}_\uparrow)$ is

$$\left\langle \left[\frac{\partial H_{11}(\mathcal{E}_\uparrow)}{\partial \mathcal{E}_\uparrow}\, \delta_a\right]_{\mathcal{E}_\uparrow = \mathcal{E}_{\text{exact}}} \right\rangle \equiv \langle \tilde{H}'_{11} \rangle\, \delta_a \quad . \tag{B2}$$

Thus, the total error introduced in $\overline{\mathcal{E}}_\uparrow$ of (B1) is

$$\delta_v + \langle \tilde{H}'_{11} \rangle\, \delta_a = \left(1 + \frac{2\,\mathcal{E}_{\text{exact}}}{E_G}\right)\delta_a$$

so that

$$\delta_a \cong \frac{\delta_v}{1 + \dfrac{2\mathcal{E}_{\text{approx}}}{E_G} - \langle \tilde{H}'_{11} \rangle} \quad . \tag{B3}$$

Note from (B2), (16a) and (13) that $\langle \tilde{H}'_{11} \rangle$ is a quantity of order $\dfrac{\mathcal{E}_{\text{exact}}}{\Delta} + \dfrac{(R\hbar\omega_c)^{\frac{1}{2}}}{E_G}$. We conclude then from (B3) that for (16a) the variational procedure leads to an estimate of $\mathcal{E}_{\text{exact}}$ whose accuracy is not worsened by the fact that the eigenvalue of $H_{11}(\mathcal{E}_\uparrow)$ is $\overline{\mathcal{E}}_\uparrow$ and not $\mathcal{E}_\uparrow$ and that H_{11} itself depends upon $\mathcal{E}_\uparrow$. The analogous remark applies, of course, to $H_{22}(\mathcal{E}_\downarrow)$.

APPENDIX C

To derive an upper bound to the shift in the ground state ionization energy due to the presence of $\mathcal{H}_1$ from (20c) in the Hamiltonian $\mathcal{H}$, we treat $\mathcal{H}_1$ as a perturbation on the eigenstates of $\mathcal{H}_0(\lambda)$. Denoting by $|0, \lambda\rangle$ and $|n, \lambda\rangle$ the ground state and n^{th} excited state, respectively, of $\mathcal{H}_0(\lambda)$ and by $E_{0\lambda}$ and $E_{n\lambda}$ the corresponding unperturbed eigenvalues, we obtain the lowest order polaron correction to the ground state of $\mathcal{H}_0(\lambda)$:

$$E_{pol} = -\frac{S}{(2\pi)^3} \sum_{n=0}^{\infty} \int d\underline{k} \frac{\nu_k^2 \,|\langle n, \lambda| e^{i\underline{k}\cdot\underline{r}} |0, \lambda\rangle|^2}{E_{n\lambda} - E_{0\lambda} + 1} \quad . \tag{C1}$$

Following Platzman[9] we iterate the identity

$$\frac{1}{E_{n\lambda} - E_{0\lambda} + 1} = \frac{1}{1 + k^2} - \frac{(E_{n\lambda} - E_{0\lambda} - k^2)}{(E_{n\lambda} - E_{0\lambda} + 1)(1 + k^2)} \quad . \tag{C2}$$

to obtain from (C1)

$$E_{pol}(\lambda) = -T_1 + T_2 - T_3(\lambda) \quad ,$$

$$T_1 = \sum_n \int d\underline{k} \frac{M_{n0}^2(\underline{k}, \lambda)}{1 + k^2} \quad , \tag{C3a}$$

$$T_2 = \sum_n \int d\underline{k} \frac{M_{n0}^2(\underline{k}, \lambda)\,(E_{n\lambda} - E_{0\lambda} - k^2)}{(1 + k^2)^2} \quad , \tag{C3b}$$

$$T_3(\lambda) = \sum_n \int d\underline{k} \frac{M_{n0}^2(\underline{k}, \lambda)\,(E_{n\lambda} - E_{0\lambda} - k^2)^2}{(1 + k^2)^2\,(E_{n\lambda} - E_{0\lambda} + 1)} \quad , \tag{C3c}$$

where $M_{n0}^2(\underline{k}, \lambda) = \frac{S}{(2\pi)^3} \nu_k^2 \,|\langle n, \lambda| e^{i\underline{k}\cdot\underline{r}} |0, \lambda\rangle|^2$. From (C3c) it is important to note that every term in T_3 is positive.

By completeness we have

$$T_1 = \frac{S}{(2\pi)^3} \int d\underline{k} \frac{\nu_k^2}{1 + k^2} = \alpha \quad .$$

Using the relation

$$\sum_n (E_n - E_0) \langle 0| e^{-i\underline{k}\cdot\underline{r}} |n\rangle \langle n| e^{i\underline{k}\cdot\underline{r}} |0\rangle = \langle 0| [e^{-i\underline{k}\cdot\underline{r}}, \mathcal{H}_0]\, e^{i\underline{k}\cdot\underline{r}} |0\rangle \quad ,$$

we obtain

$$T_2 = 0 \quad ,$$

where we have used $\langle 0, \lambda \,|\, \underline{k} \cdot \underline{\pi} \,|\, 0, \lambda\rangle = 0$, which follows from the fact that $|0, \lambda\rangle$ has definite parity.

The problem remaining is to approximate $T_3(\lambda)$ in an appropriate way. Our procedure is to replace $E_{n\lambda} - E_{0\lambda} + 1$ in the denominator of $T_3(\lambda)$ in (C3c) by some function $g(k)$ thus obtaining

$$\tilde{T}_3(\lambda) = \sum \int d\underline{k} \, \frac{M_{n0}^2(\underline{k}, \lambda)\,(E_{n\lambda} - E_{0\lambda} - k^2)^2}{(1 + k^2)^2 \, g(k)} \equiv C(g, \lambda)\, T_3(\lambda) \quad , \qquad \text{(C4)}$$

where $C(g, \lambda)$ is a number which depends upon the form of g chosen as well as λ.

We now make two very plausible assumptions. First we assume that if we denote $\lim_{\lambda \to 0+} \tilde{T}_3(\lambda)$ by $\tilde{T}_3(0+)$, then $\tilde{T}_3(0+) = \tilde{T}_3(0)$ and likewise $T_3(0+) = T_3(0)$. Second we assume that if we denote $\lim_{\lambda \to 0+} E_{n\lambda} = E_{n0+}$ then

$$E_{n0+} - E_{00+} < E_{n1} - E_{01} \quad . \qquad \text{(C5)}$$

What (C5) says is that turning on the Coulomb potential lowers the ground state energy more than it lowers the energy of any other level. This is obviously true when there is no magnetic field. It is plausible generally because the ground state is the only nodeless state and therefore can crowd itself in toward the Coulomb center with minimum cost in curvature (kinetic energy) compared to any other state.

From (C5), (C4) and (C3c) we conclude that

$$C(g, 1) > C(g, 0+) \quad . \qquad \text{(C6)}$$

The polaron correction to the ground state ionization energy is by definition

$$E_{pol}(0+) - E_{pol}(1) = T_3(1) - T_3(0) \quad . \qquad \text{(C7)}$$

The quantity $\tilde{T}_3(1) - \tilde{T}_3(0)$ will certainly be an upper bound to $T_3(1) - T_3(0)$ if

$$C(g, 0) \geqslant 1 \qquad \text{(C8)}$$

by virtue of (C4) and (C6).

We can ensure the validity of (C8) by setting $g(k) = 1$ as is obvious from (C3c) and (C4). In that case we evaluate (C4) using

$$\begin{aligned} &\sum_n (E_n - E_0)^2 \; \langle 0 | e^{-i\underline{k}\cdot\underline{r}} | n \rangle \; \langle n | e^{i\underline{k}\cdot\underline{r}} | 0 \rangle \\ &\quad = \langle 0 | \{ [e^{-i\underline{k}\cdot\underline{r}}, \mathcal{H}_0], \mathcal{H}_0 \} \, e^{i\underline{k}\cdot\underline{r}} | 0 \rangle \\ &\quad = \langle 0 | (2\underline{k} \cdot \underline{\pi} + k^2)^2 | 0 \rangle \end{aligned}$$

and

$$[e^{-i\underline{k}\cdot\underline{r}}, \mathcal{H}_0] = (2\underline{k} \cdot \underline{\pi} + k^2)\, e^{-i\underline{k}\cdot\underline{r}}$$

to obtain

$$\tilde{T}_3(1) - \tilde{T}_3(0) = \frac{2}{3}\,\alpha \left(\langle 1, 0 \mid \pi^2 \mid 0, 1 \rangle - \frac{\omega_c}{2\omega_0} \right) \quad .$$

Computer evaluation of (C1) at $\lambda = 0$ as a function of magnetic field and asymptotic forms for small and large field[11] show that (C8) is also satisfied by setting $g(k) = 1 + k^2$. With this choice of g we find

$$T_3(1) - T_3(0) < \tilde{T}_3(1) - \tilde{T}_3(0) = \frac{\alpha}{6}\left(\langle 1, 0 \mid \pi^2 \mid 0, 1\rangle - \frac{\omega_c}{2\omega_o}\right) \quad . \qquad \text{(C9)}$$

Finally, we remark that setting $g(k) = 1 + k^2$ is equivalent to applying (C2) to (C3c) and truncating the resulting series for $T_3(\lambda)$ after the first term. This procedure generates the polaron effective mass approximation for the problem of a polaron interacting with a central potential and applied magnetic field. For weak magnetic and Coulomb fields the polaron effective mass approximation and hence our bound (C9) should be excellent.

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13. ABSTRACT

We consider, in the effective mass approximation, the problem of a hydrogenic atom in a strong static magnetic field. The ground state and the lowest lying states of angular momentum $\pm\hbar$ are calculated variationally, first for a simple parabolic conduction band and then for the nonparabolic conduction band of InSb. Both the use of improved variational trial functions and the incorporation into the theory of the nonparabolic conduction band are novel features of the present calculation. The results are compared with previous work. Nonparabolic effects are found to be significant for the energy of the lowest lying state of angular momentum $+\hbar$.

The weak-coupling polaron theory is used to derive an upper bound to the shift of the ionization energy of the ground state of the impurity due to electron-LO phonon interaction. Polaron effects on the ground state ionization energy are thereby shown to be negligible in InSb. The bound obtained may, however, prove useful in estimating polaron effects in materials with larger coupling constants.

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