Acceptor excitation spectra in germanium in a uniform magnetic field

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The irreducible-spherical-tensor form of the effective-mass Hamiltonians for acceptors in cubic semiconductors in a homogeneous magnetic field parallel to a ⟨001⟩ direction or to a ⟨111⟩ direction has been derived. The Hamiltonians take into account the full structure of the $\Gamma_8^+ \oplus \Gamma_7^+$ valence-band edge, and they contain a point-charge potential with spherically symmetric q-dependent dielectric screening. The eigenstates have been calculated variationally for the case of acceptors in germanium. For both orientations, the computations have been performed as a function of the magnetic-field strength, in the range from 0 to 5 T. The binding energies of the first 36 odd-parity excited states and of the first 4 even-parity states (which form the ground-state multiplet) are obtained. The oscillator strengths of the electric-dipole transitions from the ground-state sublevels to the excited states are also calculated, and the results are used to simulate theoretical acceptor excitation spectra, which are in excellent agreement with the available experimental far-infrared-absorption and photothermal-ionization-spectroscopy spectra. For the ground state and for the final states of the G and D lines, theoretical g factors are obtained which are very close to the experimental ones. In particular, the values $g_1' = -0.45$ and $g_2' = +0.22$ are computed for the acceptor ground state. It is found also that for the ground state and for the excited $\Gamma_8(\bar{T}_d)$ final states of the G, D, and B spectral lines, the ratio $r = g_2/4g_1$ is always very close to the special value $-\frac{5}{41}$, which corresponds to a linear Zeeman splitting of the Γ_8 states into a degenerate doublet for $\mathbf{B} \| \langle 111 \rangle$ and into an equally spaced quartet for $\mathbf{B} \| \langle 001 \rangle$.

I. INTRODUCTION

Angular-momentum theory and the irreducible-spherical-tensor method[1] have been introduced into the effective-mass description of shallow acceptors in cubic semiconductors by Baldereschi and Lipari.[2–4] Their method has been used by several authors to compute accurate energy levels and electric-dipole transition probabilities[5–7] for acceptors in Ge and Si with no external perturbations present. In a recent paper[8] we have extended that method to the case of acceptors in uniaxially stressed cubic semiconductors, and similar results have been obtained independently by Buczko.[9] The problem of acceptors and excitons in a homogeneous magnetic field was briefly touched on in a paper by Lipari and Altarelli,[10] but to our knowledge no explicit Hamiltonians nor any application to the energy levels of acceptors in Ge and Si have ever been published. It is the purpose of this paper to present schematically our derivation of the irreducible-spherical-tensor form of the effective-mass acceptor Hamiltonians when a homogeneous magnetic field is present, parallel to a ⟨001⟩ or to a ⟨111⟩ crystallographic direction, and to comment briefly on our computed results for the Zeeman effect on acceptors in Ge. A more elaborate discussion of the theory, and full details of the calculations, will be published later.

II. THEORY

We start from the Luttinger effective-mass Hamiltonian with spin-orbit coupling and with an external magnetic field.[11,12] The Hamiltonian is a 6×6 matrix operator, referred to a coordinate system whose axes coincide with the cubic symmetry axes of the crystal:

$$\mathcal{H} = \frac{\hbar^2}{2m_0}(\gamma_1 k^2 - 6\gamma_2[(I_x^2 - \tfrac{1}{3}I^2)k_x^2 + \text{c.p.}] - 12\gamma_3(\{I_y, I_z\}\{k_y, k_z\} + \text{c.p.}))$$
$$+ \tfrac{2}{3}(\tfrac{1}{2} - \mathbf{I}\cdot\mathbf{S})\Delta_0 + \mu_B[(3\kappa + \tfrac{1}{2}g_s)\mathbf{I}\cdot\mathbf{B} - g_s\mathbf{S}\cdot\mathbf{B}] - \frac{1}{4\pi\epsilon_0}\frac{e^2}{\epsilon(r)r} .$$

In this Hamiltonian $\hbar\mathbf{k} = \mathbf{p} + e\,\mathbf{A} = -i\hbar\nabla + e\,\mathbf{A}$, and we will always use the gauge $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$; c.p. denotes cyclic permutation of the indices x,y,z; and $\{a,b\} \equiv \frac{1}{2}(ab + ba)$.

The expression contains the spin matrix operators $\mathbf{I}$ and $\mathbf{S}$ for spin $I = 1$ and $S = \frac{1}{2}$ (defined without the factor $\hbar$); $\epsilon(r)$ is the (isotropic) dielectric function, with the static dielectric constant ϵ_∞ as its limit for $r \to \infty$. The scalar constants in the Hamiltonian are the free-electron mass m_0 and g factor g_s, the Bohr magneton μ_B, the valence-band spin-orbit splitting Δ_0, and the Luttinger valence-band parameters[11] γ_1, γ_2, γ_3, and κ. The Luttinger parameter q has been taken to be

zero, because it is associated with higher-order spin-orbit interactions in the valence band,[12] and because it is negligibly small[13,14] compared with κ in both Si and Ge.

The Hamiltonian is made "dimensionless" by introducing the energy unit $\mathcal{R}_0^*$, the unit of length a_0^*, the constant $\Delta_0^*=\Delta_0/\mathcal{R}_0^*$, and the factor β as a measure for the magnetic-field strength:

$$\mathcal{R}_0^*=\frac{1}{(4\pi\epsilon_0)^2}\frac{m_0e^4}{2\hbar^2\gamma_1\epsilon_\infty^2},\quad a_0^*=4\pi\epsilon_0\frac{\hbar^2\gamma_1\epsilon_\infty}{m_0e^2},\quad \beta=\frac{\gamma_1\mu_B B}{R_0^*}\ .$$

For $\mathbf{B}\|\langle 001\rangle$ the substitution $\mathbf{B}=(0,0,B)$ is made directly in the above expression, while for $\mathbf{B}\|\langle 111\rangle$ the coordinate system is first rotated over the Euler angles $(+\pi/4, \arccos(1/\sqrt{3}), 0)$ to make the quantization axis coincide with the direction of the magnetic field, whereafter the same substitution is made in the new coordinate system. The transformation to irreducible-tensor form starts by introducing the first-order spherical tensors $I^{(1)}$, $S^{(1)}$, and $L^{(1)}$, corresponding to the vector operators **I**, **S**, and $\mathbf{L}=\hbar^{-1}\mathbf{r}\times\mathbf{p}$, and by defining the following four symmetric and traceless second-rank Cartesion tensor operators:

$$I_{\mu\nu}=\tfrac{3}{2}(I_\mu I_\nu+I_\nu I_\mu)-\delta_{\mu\nu}I^2\ ,$$

$$P_{\mu\nu}=\frac{1}{\hbar^2}(3p_\mu p_\nu-\delta_{\mu\nu}p^2)\ ,$$

$$M_{\mu\nu}=\frac{i}{\hbar}[\tfrac{3}{2}(r_\mu p_\nu+r_\nu p_\mu)-\delta_{\mu\nu}\mathbf{r}\cdot\mathbf{p}]\ ,$$

$$X_{\mu\nu}=3r_\mu r_\nu-\delta_{\mu\nu}r^2\ ,$$

which decompose into second-order spherical tensors $I^{(2)}$, $P^{(2)}$, $M^{(2)}$, and $X^{(2)}$ only. After straightforward but very long algebraic manipulations, an acceptor Hamiltonian of the following general form is obtained for both orientations:

$$\mathcal{H}^{\mathbf{B}\|\langle hkl\rangle}=\mathcal{H}_0^{\langle hkl\rangle}+\beta\mathcal{H}_{LZ}^{\langle hkl\rangle}+\beta^2\mathcal{H}_{QZ}^{\langle hkl\rangle}\ ,$$

with, for $\mathbf{B}\|\langle 001\rangle$,

$$\mathcal{H}_0^{\langle 001\rangle}=\frac{p^2}{\hbar^2}+\tfrac{2}{3}(\tfrac{1}{2}-\mathbf{I}\cdot\mathbf{S})\Delta_0^*-\frac{\epsilon_\infty}{\epsilon(r)}\frac{2}{r}-\tfrac{1}{3}\mu(P^{(2)}\cdot I^{(2)})+\tfrac{1}{3}\delta[(P^{(2)}\times I^{(2)})^{(4)}_{-4}+(\sqrt{70}/5)(P^{(2)}\times I^{(2)})^{(4)}_{0}+(P^{(2)}\times I^{(2)})^{(4)}_{+4}]\ ,$$

$$\mathcal{H}_{LZ}^{\langle 001\rangle}=\frac{1}{\gamma_1}[(3\kappa+\tfrac{1}{2}g_s)I_0^{(1)}-g_sS_0^{(1)}]+L_0^{(1)}-\tfrac{1}{3}\delta[(M^{(2)}\times I^{(2)})^{(4)}_{-4}-(M^{(2)}\times I^{(2)})^{(4)}_{+4}]$$
$$-\tfrac{1}{2}(\tfrac{5}{3})^{1/2}\mu[(L^{(1)}\times I^{(2)})^{(1)}_0+(\tfrac{2}{3})^{1/2}(M^{(2)}\times I^{(2)})^{(1)}_0]-(\tfrac{2}{5})^{1/2}\delta[(L^{(1)}\times I^{(2)})^{(3)}_0-\tfrac{1}{3}(M^{(2)}\times I^{(2)})^{(3)}_0]\ ,$$

$$\mathcal{H}_{QZ}^{\langle 001\rangle}=\tfrac{1}{12}\{2r^2-(\tfrac{2}{3})^{1/2}X_0^{(2)}+(\mu-\tfrac{6}{5}\delta)(\tfrac{2}{3})^{1/2}r^2I_0^{(2)}+\tfrac{1}{3}\mu(X^{(2)}\cdot I^{(2)})$$
$$+(\mu-\tfrac{12}{35}\delta)(\sqrt{14}/3)(X^{(2)}\times I^{(2)})^{(2)}_0-\delta[(X^{(2)}\times I^{(2)})^{(4)}_{-4}-(2/\sqrt{70})(X^{(2)}\times I^{(2)})^{(4)}_0+(X^{(2)}\times I^{(2)})^{(4)}_{+4}]\}\ ,$$

and, for $\mathbf{B}\|\langle 111\rangle$,

$$\mathcal{H}_0^{\langle 111\rangle}=\frac{p^2}{\hbar^2}+\tfrac{2}{3}(\tfrac{1}{2}-\mathbf{I}\cdot\mathbf{S})\Delta_0^*-\frac{\epsilon_\infty}{\epsilon(r)}\frac{2}{r}-\tfrac{1}{3}\mu(P^{(2)}\cdot I^{(2)})$$
$$-\tfrac{2}{9}\delta[2(P^{(2)}\times I^{(2)})^{(4)}_{-3}+(\sqrt{70}/5)(P^{(2)}\times I^{(2)})^{(4)}_0-2(P^{(2)}\times I^{(2)})^{(4)}_{+3}]\ ,$$

$$\mathcal{H}_{LZ}^{\langle 111\rangle}=\frac{1}{\gamma_1}[(3\kappa+\tfrac{1}{2}g_s)I_0^{(1)}-g_sS_0^{(1)}]+L_0^{(1)}+\tfrac{1}{3}\delta[(M^{(2)}\times I^{(2)})^{(4)}_{-3}+(M^{(2)}\times I^{(2)})^{(4)}_{+3}]$$
$$-\tfrac{1}{6}\mu[\sqrt{15}(L^{(1)}\times I^{(2)})^{(1)}_0+\sqrt{10}(M^{(2)}\times I^{(2)})^{(1)}_0]$$
$$+\tfrac{1}{3}\delta[(L^{(1)}\times I^{(2)})^{(3)}_{-3}+(2\sqrt{10}/5)(L^{(1)}\times I^{(2)})^{(3)}_0-(L^{(1)}\times I^{(2)})^{(3)}_{+3}]$$
$$-\tfrac{1}{9}\delta[(M^{(2)}\times I^{(2)})^{(3)}_{-3}+(2\sqrt{10}/5)(M^{(2)}\times I^{(2)})^{(3)}_0-(M^{(2)}\times I^{(2)})^{(3)}_{+3}]\ ,$$

$$\mathcal{H}_{QZ}^{\langle 111\rangle}=\tfrac{1}{12}\{2r^2-(\tfrac{2}{3})^{1/2}X_0^{(2)}+(\mu+\tfrac{4}{5}\delta)(\tfrac{2}{3})^{1/2}r^2I_0^{(2)}+\tfrac{1}{3}\mu(X^{(2)}\cdot I^{(2)})$$
$$+(\mu+\tfrac{8}{35}\delta)(\sqrt{14}/3)(X^{(2)}\times I^{(2)})^{(2)}_0-\tfrac{2}{3}\delta[(X^{(2)}\times I^{(2)})^{(3)}_{-3}+(X^{(2)}\times I^{(2)})^{(3)}_{+3}]$$
$$+\tfrac{2}{3}\delta[(X^{(2)}\times I^{(2)})^{(4)}_{-3}-(2/\sqrt{70})(X^{(2)}\times I^{(2)})^{(4)}_0-(X^{(2)}\times I^{(2)})^{(4)}_{+3}]\}\ .$$

In the above expressions, μ and δ are the valence-band parameters defined by Baldereschi and Lipari:[2-4]

$$\mu=\frac{4\gamma_2+6\gamma_3}{5\gamma_1}, \quad \delta=\frac{\gamma_3-\gamma_2}{\gamma_1} .$$

Due to the spherical symmetry of the impurity potential employed, the symmetry group of the zero-field acceptor Hamiltonian is $\bar{O}_h$; with a homogeneous magnetic field parallel to $\langle 001 \rangle$ or to $\langle 111 \rangle$, the symmetry group then becomes $\bar{C}_{4h}$ or $\bar{C}_{3i}$, respectively. The effective-mass theory (EMT) equation with $\mathcal{H}^{\mathbf{B}\|\langle 001 \rangle}$ or $\mathcal{H}^{\mathbf{B}\|\langle 111 \rangle}$ has been solved variationally. The eigenfunctions transforming like basis functions for a given (one-dimensional) representation $\Gamma_R^{\pm}$ of $\bar{C}_{4h}$ or $\bar{C}_{3i}$ are expanded into an orthogonal series of angular basis functions belonging to $\Gamma_R^{\pm}$, with undetermined radial functions as the coefficients. The angular basis functions are six-component spinors, constructed as linear combinations with different F_z of the angular-momentum eigenfunctions $|L,(I,S)J,F,F_z\rangle$ in the LJ-coupled scheme. **L** is the angular momentum associated with the space coordinates (θ,ϕ), **J** is the pseudospin of a hole near the top of the $\Gamma_8^+(J=\frac{3}{2})$ or $\Gamma_7^+(J=\frac{1}{2})$ valence bands, and $\mathbf{F}=\mathbf{L}+\mathbf{J}$. The series has been truncated by the criterion $L \leq 7$, which guarantees good convergence of the computed energies. The angular matrix elements were evaluated numerically by a computer program with the reduced-matrix-element technique.[1] The resulting set of coupled differential equations for the radial functions was solved variationally by expanding each function into a number of exponentials with fixed exponents, multiplied by an appropriate power of r.

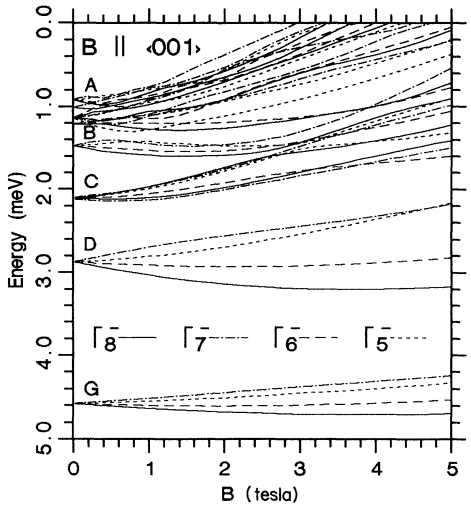

FIG. 1. Magnetic-field dependence of the computed binding energies of the first 36 odd-parity excited states of acceptors in Ge with $\mathbf{B}\|\langle 001 \rangle$. The energy scale has been inverted in order to make the more tightly bound states appear lower in the figure; zero energy lies at the zero-field $\Gamma_8^+(\bar{O}_h)$ band edge. The symmetry assignment refers to the irreducible representations of $\bar{C}_{4h}$. The labels at the left correspond to the unperturbed far-infrared spectrum.

III. RESULTS

Throughout our calculations we used the following valence-band parameters[13] and g factors:[14] $\gamma_1=13.38$, $\gamma_2=4.24$, $\gamma_3=5.69$, $\Delta_0=0.290$ eV, $\kappa=3.41$. We employed a point-charge potential, in which the dielectric function $\epsilon(r)$ was derived from $\epsilon(q)$ as given by Richardson and Vinsome,[15] but adjusted to the low-temperature $\epsilon_\infty=15.36$ for germanium.[16] Therefore the calculations apply to the so-called *point-charge acceptor*. When comparing the computed results with experimental data, the chemical differences between real acceptors must be accounted for by adding a constant and supposedly field-independent *chemical shift* to all computed binding energies of the ground-state sublevels. As usual, we expect that the odd-parity excited states remain unaffected by the chemical differences, and will therefore be well described by the model.

Figures 1 and 2 show the computed binding energies as a function of the magnetic-field strength for all 36 odd-parity excited states involved as final states in the Zeeman-split G, D, C, B, A_4, A_3, A_2, and A_1 spectral lines observed by far-infrared spectroscopy. For the irreducible representations of all double groups mentioned we employ the notation of Koster *et al.*[17,18] which has become the *de facto* standard in effective-mass theory. When comparing our results with the group-theoretical model of Bhattacharjee and Rodriguez,[19] it is important to notice that a different nonstandard labeling is used by them. From the figures it is seen that all states experience a quadratic as well as a linear Zeeman effect. A diamagnetic shift towards lower energies is present in all multiplets, becoming more important for the more loosely bound states. But the most obvious feature is that the whole energy spectrum is dominated by interactions between states of like symmetry. For the C, B, and A multiplets, this leads to an intricate pattern with many *avoided crossings*. Such a behavior as a function of the

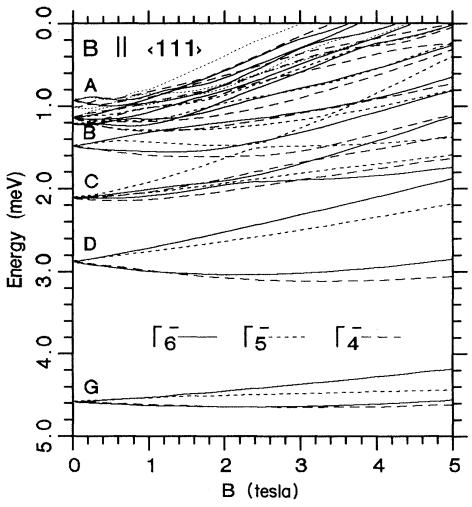

FIG. 2. Same as Fig. 1 but with $\mathbf{B}\|\langle 111 \rangle$. The symmetry assignment refers to the irreducible representations of $\bar{C}_{3i}$.

TABLE I. Compatibility relations for the split sublevels of an even-parity $\Gamma_8^+(\bar{O}_h)$ or an odd-parity $\Gamma_8^-(\bar{O}_h)$ state with $\mathbf{B}\|\langle 001\rangle$. The m_J values to be used for computing g_1 and g_2 in the model of Bhattacharjee and Rodriguez (Ref. 19) are the row indexes in $\Gamma_8(\bar{T}_d)$.

$\bar{C}_{4h}$	Γ_7^+	Γ_6^+	Γ_5^+	Γ_8^+	Γ_7^-	Γ_6^-	Γ_5^-	Γ_8^-
$\bar{O}_h$	$\Gamma^+_{8,-3/2}$	$\Gamma^+_{8,-1/2}$	$\Gamma^+_{8,+1/2}$	$\Gamma^+_{8,+3/2}$	$\Gamma^-_{8,-3/2}$	$\Gamma^-_{8,-1/2}$	$\Gamma^-_{8,+1/2}$	$\Gamma^-_{8,+3/2}$
$\bar{T}_d$	$\Gamma_{8,-3/2}$	$\Gamma_{8,-1/2}$	$\Gamma_{8,+1/2}$	$\Gamma_{8,+3/2}$	$\Gamma_{8,+1/2}$	$\Gamma_{8,+3/2}$	$\Gamma_{8,-3/2}$	$\Gamma_{8,-1/2}$

magnetic-field strength could not possibly be deduced from perturbation-theory models, which are based on noninteracting unperturbed states.[19] On the other hand, the sublevels in the *G* and *D* multiplets remain rather well separated from the other energy levels over the whole range of fields concerned. We expect therefore that the model of Bhattacharjee and Rodriguez[19] for the splitting of isolated $\Gamma_8(\bar{T}_d)$ states in a magnetic field, should be approximately applicable to these two multiplets, certainly as far as the *linear Zeeman effect* only is concerned. To a lesser extent, the same conclusion holds true for the *B* multiplet in fields up to only 1 T. In order to estimate the *g* factors governing the linear Zeeman effect, we have fitted quadratic polynomials to the computed level energies as a function of the field strength. From the coefficients of the linear terms, and with the help of the compatibility relations in Table I, we obtained the *g* factors given in the first column of Table II. One finds excellent agreement with the experimental values[20–23] in the next columns. Most often the differences fall within the experimental uncertainties. The agreement is obviously many times better than for the theoretical values from Lin-Chung and Wallis[24] quoted in the last column.

In Table II we have included also the data for the acceptor ground state in germanium. Our theoretical results for g_1' and g_2' apply to the point-charge acceptor. They have been obtained from the computed energy levels between 0 and 5 T, which are shown in Fig. 3. The only available experimental *g* factors for the ground state are for the isocoric Ga acceptor. They have been deduced by Tokumoto and Ishiguro[25] from magnetoacoustic-resonance-attenuation experiments. The smallness of the ground-state *g* factors found by them is verified by the absence of any noticeable effects due to the ground-state splitting in the far-infrared spectra of acceptors in germanium[20,21,23] in magnetic fields up to 5 T. Our computed *g* values have the same sign and the same order of magnitude as the experimental ones for

TABLE II. *g* factors for the final $\Gamma_8(\bar{T}_d)$ states of the *G*, *D*, and *B* spectral lines of acceptors in germanium, and for the acceptor ground state.

	Present theory	Gallium	Boron	Aluminum	LCW[c] theory
g_1^G	−2.57	$\mp 2.05\pm 0.49$[a]	∓ 2.49[b]		−3.38
g_2^G	+1.15	$\pm 1.10\pm 0.15$[a]			+1.61
r^G	−0.122	−0.134[a]			−0.119
g_1^D	−7.00	$\mp 7.41\pm 0.53$[a]	$\mp 6.97\pm 0.16$[d]	$+8.4\pm 0.4$[e]	−4.11
g_2^D	+3.41	$\pm 3.62\pm 0.11$[a]	$\pm 3.33\pm 0.11$[d]	-4.1 ± 0.4[e]	+1.79
r^D	−0.122	−0.122[a]	−0.119[d]	−0.121[e]	−0.109
g_1^B	−8.27				
g_2^B	+4.03				
r^B	−0.122				
g_1'	−0.45	-0.16 ± 0.08[f]			−1.13
g_2'	+0.22	$+0.08\pm 0.04$[f]			+0.63
r'	−0.122	−0.125[f]			−0.139

[a]Reference 20.
[b]Obtained from the data in Ref. 21 with our hypothesis that $r=-\frac{5}{41}$; the value $|g_1|=1.4$ given in Ref. 21 was based on $r=-\frac{1}{13}$.
[c]Reference 24.
[d]Reinterpretation given in Ref. 20 of the experimental data from Ref. 22.
[e]Reference 23. The signs of g_1 and g_2 were based on an earlier model calculation, and obviously they should be reversed.
[f]Reference 25.

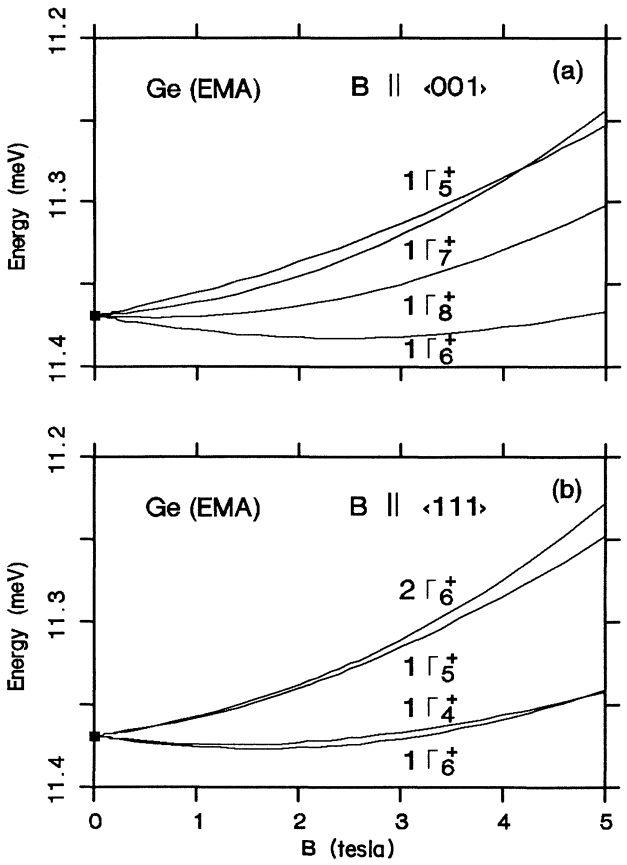

FIG. 3. Computed energies of the ground-state sublevels of the *point-charge acceptor* in Ge with magnetic fields from 0 to 5 T. (a) $\mathbf{B}\|\langle 001\rangle$: double group $\bar{C}_{4h}$; (b) $\mathbf{B}\|\langle 111\rangle$: double group $\bar{C}_{3i}$.

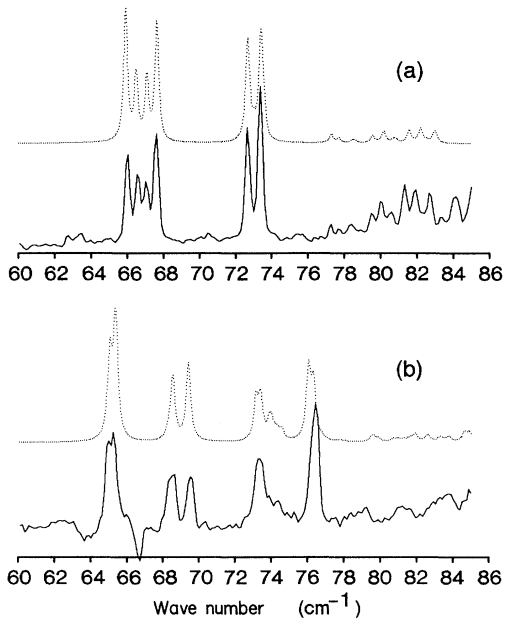

FIG. 4. Comparison between far-infrared photothermal-ionization-spectroscopy spectra of Al acceptors in germanium (solid lines), and numerically simulated excitation spectra with chemical shift −0.218 meV (dashed lines). (a) $\mathbf{B}\|\langle 001\rangle$: experimental, $B=0.50$ T, res.$=0.13$ cm^{-1}; simulation, $B=0.60$ T, FWHM$=0.13$ cm^{-1}. (b) $\mathbf{B}\|\langle 111\rangle$: experimental; $B=1.86$ T res.$=0.25$ cm^{-1}; simulation; $B=1.80$ T, FWHM$=0.25$ cm^{-1}.

Ge(Ga), but they are about three times as big. Apparently the agreement is not perfect yet, although much better than it was for the theoretical results by Lin-Chung and Wallis.[24] For the moment, we have no clear explanation for the remaining discrepancy. Chemical effects, which are known to be important on the acceptor ground-state wave functions, could perhaps be responsible for it. Further numerical experiments with different screening parameters in the impurity potential[6] should be done to explore this possibility. Other experimental determinations of the ground-state g factors for different group-III acceptors in germanium would be desirable as well. High-resolution far-infrared transmission measurements in magnetic fields around or above 5 T should in principle allow one to resolve the small ground-state splittings of the order of 0.12 meV according to our present calculation, or about 0.05 meV according to the parameters taken from Ref. 25.

We have also computed the oscillator strengths for all the allowed electric-dipole transitions from the four Zeeman-split sublevels of the $1\Gamma_8^+(\bar{O}_h)$ acceptor ground state to the 36 calculated odd-parity excited states. Together with the transition energies, this information has allowed us to plot the simulated absorption spectra, using a Lorentzian line shape of given full width at half maximum (FWHM). The simulated spectra are the most direct means of comparing the results from our computational model with experimental far-infrared data. An example is shown in Fig. 4, and it illustrates the astonishing similarity between the theoretical and experimental curves, which is found in almost every instance. Space does not permit us to go into any more details of this comparison.

A final remark has to be made about the computed g factors for the $\Gamma_8(\bar{T}_d)$ states. From Table II, it is seen that in all four cases considered, the ratio $r=g_2/4g_1$ is found to be equal to -0.122, or about $-\frac{5}{41}$. This "*magic value*" characterizes[23] a linear Zeeman splitting into degenerate doublet when $\mathbf{B}\|\langle 111\rangle$, and into four equally spaced sublevels when $\mathbf{B}\|\langle 001\rangle$. Although pure coincidence cannot be ruled out, that possibility seems to us highly unlikely. We therefore suggest that the Hamiltonian might contain an additional "*hidden symmetry*" which has hitherto escaped attention and which, for $\mathbf{B}\|\langle 111\rangle$, forces the $m_J=\pm\frac{3}{2}$ doublet to be degenerate with the $m_J=\pm\frac{1}{2}$ doublet when only the linear Zeeman effect is considered.

[1]A. R. Admonds, *Angular Momentum in Quantum Mechanics* (Princeton University, Princeton, NJ, 1974).
[2]A. Baldereschi and N. O. Lipari, Phys. Rev. B **8**, 2697 (1973).
[3]A. Baldereschi and N. O. Lipari, Phys. Rev. B **9**, 1525 (1974).
[4]A. Baldereschi and N. O. Lipari, in *Proceedings of the 13th International Conference on the Physics of Semiconductors, Rome, 1976,* edited by F. G. Fumi (North-Holland, Amsterdam, 1976), pp. 595–598.
[5]N. Binggeli and A. Baldereschi, Solid State Commun. **66**, 323 (1988).
[6]P. Clauws, J. Broeckx, E. Rotsaert, and J. Vennik, Phys. Rev. B **38**, 12 377 (1988).
[7]I. L. Beinikhes, Sh. M. Kogan, M. G. Novak, and A. F. Polupanov, in Proceedings of the 4th International Conference on Shallow Impurities in Semiconductors, London, 1990 (unpublished).
[8]J. Broeckx and J. Vennik, Phys. Rev. B **35**, 6165 (1987).
[9]R. Buczko, Nuovo Cimento **9**, 669 (1987).
[10]N. O. Lipari and M. Altarelli, Solid State Commun. **33**, 47 (1980).
[11]J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[12]K. Suzuki and J. C. Hensel, Phys. Rev. B **9**, 4184 (1974).
[13]J. C. Hensel and K. Suzuki, Phys. Rev. B **9**, 4219 (1974).
[14]J. C. Hensel and K. Suzuki, Phys. Rev. Lett. **22**, 838 (1969).
[15]D. Richardson and P. K. W. Vinsome, Phys. Lett. **36A**, 3 (1971).
[16]R. A. Faulkner, Phys. Rev. **184**, 713 (1969).
[17]G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (MIT, Cambridge, MA, 1965).
[18]Note, however, that in Ref. 17 the last column of the character table for $\bar{S}_4$ contains some typographical errors, which are easily corrected by comparison with the character table for $\bar{C}_{4h}$, which is correct in the same reference.
[19]A. K. Bhattacharjee and S. O. Rodriguez, Phys. Rev. B **6**, 3836 (1972).
[20]C. A. Freeth, P. Fisher, and P. E. Simmonds, Solid State Commun. **60**, 175 (1986).
[21]G. Jungwirt and W. Prettl, J. Infrared Millimeter Waves **10**, 1033 (1989).
[22]H. P. Soepangkat and P. Fisher, Phys. Rev. B **8**, 870 (1973).
[23]J. Broeckx, P. Clauws, K. Van den Steen, and J. Vennik, J. Phys. C **12**, 4061 (1979).
[24]P. J. Lin-Chung and R. F. Wallis, J. Phys. Chem. Solids **30**, 1453 (1969).
[25]H. Tokumoto and T. Ishiguro, Phys. Rev. B **15**, 2099 (1977).