

Spin-dependent polarizabilities of hydrogenic atoms in magnetic fields of arbitrary strength

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Utilizing the magnetic field-dependent spin-orbit interaction, the relativistic correction to the Zeeman energy, and the usual diamagnetic interaction, we have calculated spin-dependent electrical polarizabilities of hydrogenic atoms using the Hassé variational approach. The polarizabilities $\alpha(\uparrow)$ and $\alpha(\downarrow)$ for the two spin directions have been obtained for the electric field both parallel and perpendicular to the magnetic field H_z in the weak-field ($\gamma \ll 1$), intermediate-field ($\gamma \sim 1$), and strong-field ($\gamma \gg 1$) limits, where $\gamma = (\epsilon^2 \hbar^3 H_z / m^* e^3 c)$, with ϵ a static dielectric constant and m^* an isotropic effective mass. The results for hydrogen atoms ($\epsilon = 1$ and $m^* = m$) in the weak-field limit yield $[\alpha(\downarrow) - \alpha(\uparrow)]/\alpha(0) \approx 2.31\alpha_f^2 \gamma$ ($\alpha_f = 1/137$) with a negligible anisotropy. In the strong-field limit $[\alpha_\perp(\downarrow) - \alpha_\perp(\uparrow)]$ falls precipitously while $[\alpha_\parallel(\downarrow) - \alpha_\parallel(\uparrow)]$ continues to increase up to at least $\gamma = 10^4$, but more slowly than linearly with γ . The spin-independent quantities $[\alpha_\parallel(\downarrow) + \alpha_\parallel(\uparrow)]$ and $[\alpha_\perp(\downarrow) + \alpha_\perp(\uparrow)]$ are discussed in the intermediate- and high-field limits and represent an extension of the earlier low-field results obtained by Dexter. The implications of these results for shallow-donor impurity atoms in semiconductors and for hydrogen-atom atmospheres of magnetic white dwarfs and neutron stars are briefly considered. The effects of the dramatic shrinkage of the electron's wave function on the spin Zeeman energy and the electron-proton hyperfine interaction are also discussed.

I. INTRODUCTION

Interest in the effect of very large magnetic fields on the energy levels of atoms and on atomic spectroscopy has been revived in recent years by spectroscopic measurements on highly excited atoms (for example, barium) and by the discovery of very large magnetic fields associated with white dwarf stars and neutron stars. This topic has recently been reviewed by Garstang.¹ Since the pioneering work of Yafet, Keyes, and Adams² there has been substantial interest in the effect of large magnetic fields on transport properties in semiconductors³ and on the energy levels of shallow donors and excitons and magnetic field-induced shifts of various spectroscopic transitions.⁴ There have been many calculations⁵⁻¹⁶ of energies of hydrogenic systems (applicable to H atoms, shallow donors, and excitons) in both weak and strong magnetic fields. More recently there has been a number of calculations^{17,18} made for arbitrary magnetic field strength which address the more difficult intermediate-field regime. Despite substantial interest in the effect of large magnetic fields on spectroscopy and also on transport properties in semiconductors there has been surprising little work done on the effect of a magnetic field H_z on the electrical polarizability of atoms (in their ground state). Since the magnetic field effect on ground states is much less than on excited states this may simply reflect the fact that magnetic fields available to date in terrestrial laboratories have been too small to make pertinent measurements feasible. However, sev-

eral calculations of the polarizability $\alpha(H_z)$ for hydrogenic^{19,20} and nearly hydrogenic^{21,22} atoms have recently been carried out utilizing variational and numerical approaches.

In connection with studies of the dielectric anomaly^{23,24} in n -type semiconductors doped below the critical concentration N_c for the insulator-metal transition, we have made magnetocapacitance measurements²⁵ on n -type Si and Ge samples in the liquid He temperature range in magnetic fields up to 18 T. In the past the shrinkage of shallow-donor impurity wave functions in large magnetic fields has been inferred from magnetoresistance results.²⁶ On the insulating side ($N < N_c$) of the insulator-metal transition the magnetic field reduces the hopping matrix elements (because of decreased overlap resulting from shrinkage of the wave function), but can also increase the hopping activation energy.²⁷ On the other hand, at sufficiently low temperatures that hopping processes make a negligible contribution to the dielectric constant of the sample, the magnetocapacitance data²⁵ lead to a determination of the shallow-donor polarizability $\alpha_D(H_z)$ and a direct measure of the shrinkage of the donor ground-state wave function with increasing magnetic field. The experimental results exhibit an unexplained, somewhat Curie-type, temperature dependence of the effective donor polarizability $\alpha_{D,\text{eff}}(N_D, H_z, T)$ in the temperature range 4.2 to 1.1 K. This temperature dependence has led us to consider the possible spin dependence of the electrical polarizability of hydrogenic atoms.

A variational calculation of $\alpha(H_z)$ performed by one of us²⁰ (DLD) utilizing the Hassé approach²⁸ has been carried out in the weak-field limit, where the calculation can be performed analytically. The weak-field limit is that for which the diamagnetic energy is much less than the Coulomb energy, i.e., $\gamma^2 \ll 1$, where

$$\gamma = \frac{\epsilon^2 \hbar^3 H_z}{m^{*2} c e^3}. \quad (1)$$

Here ϵ is the (assumed scalar) static dielectric constant and m^* is the (assumed scalar) effective mass of the electron (in Ref. 20 γ was denoted by \tilde{h}). For $\gamma=1$ the diamagnetic energy is twice the hydrogenic atom Rydberg, which corresponds to a magnetic field of 2.35×10^5 T for a free hydrogen atom. A numerical calculation²¹ has also been carried out for donor impurities in Si from the weak-field regime up to $\gamma=1$. In this donor calculation a semiphenomenological potential was used in an attempt to take into account the "chemical shifts" of donor impurities, i.e., the different binding energies of the P, As, and Sb impurities. This is a much more difficult problem in principle because of the many-valley band structure and anisotropic mass tensor.²²

In the present paper we attempt to calculate $\alpha(H_z)$ for hydrogenic atoms from the weak-field limit up to $\gamma=10^4$. Those terms in the "nonrelativistic" Hamiltonian coupling the electron spin and the orbital motion (diagonal contribution) lead to spin-dependent polarizabilities $\alpha(H_z, \uparrow)$ and $\alpha(H_z, \downarrow)$. Although the spin dependence $\alpha(H_z, \uparrow) - \alpha(H_z, \downarrow)$ is expected to be small, a major purpose of this work is to determine reliably its magnitude. The spin dependence was included in Ref. 20, where it was shown to be negligibly small for weak fields ($\gamma \ll 1$); however a relativistic correction to the Zeeman energy,²⁹ frequently ignored in many treatises, of the same order of magnitude as the field-dependent spin-orbit interaction considered, was combined with the latter in a way which is inadequate for large γ . Not only do we obtain the spin dependence of $\alpha(H_z)$, but in the process we determine approxi-

mate spin-dependent ground-state eigenvalues and eigenfunctions of a convenient analytic form. The variational calculation is performed numerically to high precision and leads to reliable results for $\alpha(H_z, \downarrow)$ and $\alpha(H_z, \uparrow)$ for the electric field applied both parallel and perpendicular to the magnetic field.

II. SPIN-DEPENDENT NONRELATIVISTIC HAMILTONIAN AND WAVE FUNCTION

The one-electron atomic nonrelativistic Hamiltonian with magnetic field and electron spin effects included (however with nuclear spin effects neglected), obtained utilizing the canonical transformation of Foldy and Wouthuysen³⁰ is frequently given by (see, for example Zeiger and Pratt,³¹ Eq. 1.48a)

$$H = \frac{1}{2m} \left(\vec{p} + \frac{e\vec{A}}{c} \right)^2 - eV - \frac{e\hbar}{2m^2 c^2} \vec{S} \cdot \vec{\nabla} V \times \left(\vec{p} + \frac{e\vec{A}}{c} \right) + \frac{g_e e \hbar}{2m c} \vec{S} \cdot (\vec{\nabla} \times \vec{A}) - \frac{e \hbar^2}{8m^2 c^2} \nabla^2 V, \quad (2)$$

where we have omitted a relativistic p^4 term because it generally makes no significant contribution to magnetic field effects (see the discussion in Sec. 1.13 by Zeiger and Pratt³¹). In Eq. (2) $V(\vec{r})$ is the electrostatic potential seen by the atomic electron, \vec{S} is the electron spin, g_e is the free-electron g value [$g_e \simeq 2(1 + \alpha_{fs}/2\pi + \dots)$, $\alpha_{fs} = 1/137$], and \vec{A} is the vector potential due to an external magnetic field. Equation (2) does not include a frequently omitted relativistic correction to the Zeeman energy of the form $-H_{\text{Zeeman}}(p^2/2m)/(mc^2)$ which is considered by Abragam and Van Vleck²⁹ and has been discussed by Hegstrom.³² The last term in Eq. (2) will be identically zero at the electron position for a Coulombic potential ($\propto 1/r$), but can contribute a correction for a non-Coulombic portion of $V(\vec{r})$ resulting from a central-cell correction. Here we utilize the Coulombic potential $V = e/\epsilon r$, a vector potential $\vec{A} = \frac{1}{2} \vec{H} \times \vec{r} = \frac{1}{2} H_z (x\hat{j} - y\hat{i})$, the Bohr magneton $\mu_B = e\hbar/2mc$, and replace the mass elsewhere by an isotropic effective mass m^* to obtain

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\epsilon r} + \frac{e^2 H_z^2}{8m^* c^2} (x^2 + y^2) + \mu_B (L_z + g_e S_z) H_z \left(1 - \frac{p^2}{2m^* c^2} \right) + \frac{\mu_B e}{m^* c \epsilon r^3} \vec{L} \cdot \vec{S} + \frac{\mu_B H_z e}{m^* c^2 \epsilon r^3} \left(S_z (x^2 + y^2) - \frac{z}{2} [S_+ (x - iy) + S_- (x + iy)] \right), \quad (3)$$

where the frequently omitted relativistic correction to the Zeeman energy, $[-\mu_B H_z (L_z + g_e S_z) p^2 / 2m^* c^2]$, which is the same order of magnitude ($\alpha_{fs}^2 \mu_B H_z$) as the field-dependent spin-orbit inter-

action [last term in Eq. (3)], has now been explicitly included. Only those terms in H which couple the spatial coordinates to the magnetic field and to the spin are important for the calculation of

spin-dependent polarizabilities. When one neglects the higher order off-diagonal field-dependent spin-orbit terms $S_{+z}(x-iy)$ and $S_{-z}(x+iy)$ which couple to the excited d states $m_l = -1$ and $m_l = +1$, respectively, the spin-orbit interaction $(\vec{L} \cdot \vec{S})$ and the orbital Zeeman interaction $H_z L_z$ are identically zero for the hydrogenic atom ground state. The new spin-dependent terms which couple to the orbital motion are exactly those terms that lead to the Breit-Margenau correction^{33,34} for the g shift ($g - g_e$) of the H atom ($\Delta g_{BM} = -g_e \alpha_{fs}^2/3$). It is these very same terms that lead to the different polarizabilities $\alpha(H_z, \uparrow)$ and $\alpha(H_z, \downarrow)$.

It is convenient to deal with this Hamiltonian in reduced units, to wit

$$H_0 = -\frac{e^2}{2\epsilon a^*} \left[(1 \mp \beta) \nabla^2 + \frac{2}{r} - \frac{\gamma^2}{4} (x^2 + y^2) \mp \frac{\beta}{2} \left(\frac{x^2 + y^2}{r^3} \right) \right]. \quad (4)$$

Here $a^* \equiv \epsilon \hbar^2 / (m^* e^2)$ and $\beta \equiv \mu_B H_z / (m^* c^2)$, and we have omitted those terms dismissed in the preceding paragraph and also the spin Zeeman term

which cannot contribute to the polarizability, though certainly to the energy. The negative sign in front of β means that the spin is parallel to the static magnetic field H_z .

Eigenfunctions and eigenvalues of H_0 cannot be obtained exactly. Qualitatively, we expect H_z to have three main effects: (1) It will shrink the wave function through the diamagnetic term; (2) it will shrink it less parallel to H_z than perpendicular to H_z , so that the wave function will become elongated, like a cigar; and (3) the wave function will become more rigid—from an exponential at $H_z = 0$ it will become a Gaussian as $H_z \rightarrow \infty$. Accordingly we select a trial ground-state wave function of the form

$$\psi_0(H_z) = \exp\{-[k(x^2 + y^2 + sz^2)^{1/2}]^{1/p}\}, \quad (5)$$

where $k > 1$ represents the shrinkage, $s < 1$ the elongation, and $p < 1$ the "hardness". This trial function has the advantages that $\langle H_0 \rangle$ can be evaluated exactly, and that it shows the correct qualitative behavior for all fields. Normalizing and calculating the expectation value of Eq. (4), we obtain

$$E_0 = \frac{e^2}{2\epsilon a^*} \left(\frac{(k2^p)^3}{4p\Gamma(3p)} \left[\frac{\Gamma(p)}{k2^p} \left(\frac{2+s}{3} \right) (p+1)(1 \mp \beta) - \frac{8p\Gamma(2p)}{(k2^p)^2} \left(\frac{s}{1-s} \right)^{1/2} \sinh^{-1} \left(\frac{1-s}{s} \right)^{1/2} + \frac{2\gamma^2 p \Gamma(5p)}{3(k2^p)^5} \pm 4\beta \frac{p\Gamma(2p)}{3(k2^p)^2} f(s) \right] \right), \quad (6)$$

where

$$f(s) = \frac{3}{4} \left(\frac{s}{1-s} \right)^{1/2} \left[\left(\frac{2-s}{1-s} \right) \sinh^{-1} \left(\frac{1-s}{s} \right)^{1/2} - (1-s)^{-1/2} \right]. \quad (7)$$

The parameters k , s , and p are of course dependent on magnetic field and spin orientation.

Equation (6) was minimized to high precision by numerical means with respect to k , s , and p for each spin for γ ranging from 10^{-3} to 10^4 . Table I shows the energies in rydbergs and the wave-function parameters for $\psi_0(H_z)$ for some of the calculated points in this range. It is reemphasized that the spin Zeeman term is not included here. It would have an effect in a real situation in determining which spin states are occupied, because of the Boltzmann factor, and hence in determining the net polarizability.

III. CALCULATION OF THE POLARIZABILITY

We now follow the variational method of Hassé,²⁸ known to be exact for $H_z = 0$. We select a trial wave function of the form

$$\psi_t(\vec{r}) = \psi_0(H_z)(1 + bt + cpt), \quad (8)$$

in the presence of an infinitesimal electric field \mathcal{E}_t . Here b and c are undetermined, infinitesimal parameters,

$$\rho \equiv (x^2 + y^2 + sz^2)^{1/2}, \quad (9)$$

and t equals z or x depending on whether \mathcal{E}_t is parallel or perpendicular to H_z . We now re-evaluate analytically the expectation value of $H_0 - e\mathcal{E}_t t$ with renormalized wave functions but containing the undetermined parameters b and c . We minimize analytically with respect to b and c and obtain E_0 as in Eq. (6) plus a term proportional to \mathcal{E}_t^2 , the coefficient of which is $-\frac{1}{2}$ the desired polarizability, α . There are four such quantities, $\vec{\mathcal{E}} \parallel$ and $\perp \vec{H}$ and for parallel and anti-parallel spins. For $\mathcal{E}_t = \mathcal{E}_z \parallel H_z$, we obtain

$$\alpha_{\parallel} = \frac{9}{2} \frac{\alpha^{*3} \epsilon}{s} \frac{\left(\frac{4}{3}\right)^2}{(k2^p)^4 \Gamma(3p)} \left(\frac{\Gamma^2(6p)J_{Bz} + \Gamma^2(5p)J_{Cz} - \Gamma(5p)\Gamma(6p)J_{Dz}}{4J_{Bz}J_{Cz} - J_{Dz}^2} \right), \quad (10)$$

TABLE I. Wave-function parameters^a and energies.

γ	$\frac{\kappa(t)+\kappa(t)}{2}$	$\frac{\sigma(t)+\sigma(t)}{2}$	$-\left(\frac{\lambda(t)+\lambda(t)}{2}\right)$	$\frac{E(t)+E(t)}{2}$
	$\frac{\kappa(t)-\kappa(t)}{2}$	$\frac{\sigma(t)-\sigma(t)}{2}$	$\frac{\lambda(t)-\lambda(t)}{2}$	$E(t)-E(t)$
1(-3)	-1.330(-7)	5.357(-7)	5.874(-7)	[5.00(-7)]-1
	2.188(-8)	1.903(-9)	<1(-12)	3.55(-8)
10 ^{1/2} (-3)	-1.242(-6)	5.349(-6)	5.795(-6)	[4.99(-6)]-1
	6.915(-8)	6.014(-9)	<1(-12)	1.12(-7)
1(-2)	-1.241(-5)	5.356(-5)	5.801(-5)	[5.00(-5)]-1
	2.188(-7)	1.906(-8)	<1(-12)	3.558(-7)
10 ^{1/2} (-2)	-1.231(-4)	5.335(-4)	5.775(-4)	[4.99(-4)]-1
	6.903(-7)	6.113(-8)	<1(-12)	1.12(-6)
1(-1)	-1.150(-3)	5.215(-3)	5.614(-3)	[4.958(-3)]-1
	2.175(-6)	2.202(-7)	3.920(-8)	3.59(-6)
10 ^{1/2} (-1)	-6.072(-3)	4.287(-2)	4.421(-2)	[4.647(-2)]-1
	6.916(-6)	1.270(-6)	6.755(-7)	1.243(-5)
1(0)	2.627(-2)	1.943(-1)	1.717(-1)	[3.455(-1)]-1
	1.977(-5)	7.255(-6)	4.230(-6)	5.708(-5)
10 ^{1/2} (0)	2.613(-1)	0.4393	0.3163	8.229(-1)
	5.452(-5)	2.368(-5)	1.012(-5)	3.778(-4)
1(1)	8.595(-1)	0.6589	0.4071	6.585
	1.852(-4)	5.365(-5)	1.739(-5)	3.139(-3)
10 ^{1/2} (1)	2.028	0.8076	0.4545	2.660(1)
	7.826(-4)	1.033(-4)	2.760(-5)	2.879(-2)
1(2)	4.173	0.8977	0.4782	9.275(1)
	3.805(-3)	1.841(-4)	4.270(-5)	2.767(-1)
10 ^{1/2} (2)	8.024	0.9474	0.4898	3.059(2)
	1.989(-2)	3.105(-4)	6.455(-5)	2.709
1(3)	1.492(1)	0.9742	0.4954	9.856(2)
	1.083(-1)	5.004(-4)	9.512(-5)	2.687(1)
10 ^{1/2} (3)	2.722(1)	0.9878	0.4979	3.138(3)
	6.007(-1)	7.757(-4)	1.368(-4)	2.673(2)
1(4)	4.964(1)	0.9942	0.4991	9.883(3)
	3.465	1.225(-3)	2.040(-4)	2.693(3)

^aNote that $\kappa \equiv k-1$, $\lambda \equiv p-1$, and $\sigma \equiv 1-s$. The numbers in parentheses indicate the power of ten.

where

$$J_{Bz} = \frac{(3p+1)(2+3s)\Gamma(3p)(1-\beta)}{40p} - \frac{g_z(s)\Gamma(4p)}{3k2^p} - \frac{E_0\Gamma(5p)}{6(k2^p)^2} + \frac{\gamma^2\Gamma(7p)}{60(k2^p)^4} + \frac{\beta\Gamma(4p)}{30k2^p} G_z, \quad (11a)$$

$$J_{Cz} = \frac{(9p+5)(2+3s)\Gamma(5p)(1-\beta)}{120p} - \frac{g_z(s)\Gamma(6p)}{3k2^p} - \frac{E_0\Gamma(7p)}{6(k2^p)^2} + \frac{\gamma^2\Gamma(9p)}{60(k2^p)^4} + \frac{\beta}{30} \frac{\Gamma(6p)}{k2^p} G_z, \quad (11b)$$

$$J_{Dz} = \frac{(2p+1)(2+3s)\Gamma(4p)(1-\beta)}{15p} - \frac{2g_z(s)\Gamma(5p)}{3k2^p} - \frac{E_0\Gamma(6p)}{3(k2^p)^2} + \frac{\gamma^2\Gamma(8p)}{30(k2^p)^4} + \frac{\beta}{15} \frac{\Gamma(5p)}{2^p k} G_z. \quad (11c)$$

The functions g_z and G_z are defined as

$$g_z(s) = \frac{3}{2} [d(1+d^2)^{1/2} - d^3 \sinh^{-1}(1/d)], \quad (12)$$

and

$$G_z(s) = \frac{15}{16} d[(3d^2+2)(1+d^2)^{1/2} - d^2(3d^2+4) \sinh^{-1}(1/d)], \quad (13)$$

where $d \equiv [s/(1-s)]^{1/2}$.

Similarly, for $\delta_z = \delta_x \perp H_z$, we obtain

$$\alpha_1 = \frac{9}{2} \epsilon \alpha^{*3} \frac{\left(\frac{4}{3}\right)^2}{(k2^p)^4 \Gamma(3p)} \left(\frac{\Gamma^2(6p)J_{Bx} + \Gamma^2(5p)J_{Cx} - \Gamma(5p)\Gamma(6p)J_{Dx}}{4J_{Bx}J_{Cx} - J_{Dx}^2} \right), \quad (14)$$

where

$$J_{Bx} = \frac{(3p+1)(4+s)\Gamma(3p)(1-\beta)}{40p} - \frac{g_x(s)\Gamma(4p)}{3k2^p} - \frac{E_0\Gamma(5p)}{6(k2^p)^2} + \frac{\gamma^2\Gamma(7p)}{30(k2^p)^4} + \frac{\beta\Gamma(4p)}{15k2^p} G_x, \quad (15a)$$

$$J_{Cx} = \frac{(9p+5)(4+s)\Gamma(5p)(1-\beta)}{120p} - \frac{g_x(s)\Gamma(6p)}{3k2^p} - \frac{E_0\Gamma(7p)}{6(k2^p)^2} + \frac{\gamma^2\Gamma(9p)}{30(k2^p)^4} + \frac{\beta\Gamma(6p)}{15k2^p} G_x, \quad (15b)$$

$$J_{Dx} = \frac{(2p+1)(4+s)\Gamma(4p)(1-\beta)}{15p} - \frac{2g_x(s)\Gamma(5p)}{3k2^p} - \frac{E_0\Gamma(6p)}{3(k2^p)^2} + \frac{\gamma^2\Gamma(8p)}{15(k2^p)^4} + \frac{2\beta\Gamma(5p)}{15k2^p} G_x, \quad (15c)$$

where

$$g_x(s) = \frac{3}{2}d[(1-d^2/2)\sinh^{-1}(1-d) - \frac{1}{2}(1+d^2)^{1/2}], \quad (16)$$

and

$$G_x(s) = \frac{15}{8}d[(1+d^2 + \frac{3}{8}d^4)\sinh^{-1}(1/d) - \frac{3}{8}(d^2+2)(1+d^2)^{1/2}]. \quad (17)$$

In all twelve places where β appears in these equations the sign corresponds to the case of the spin parallel to the magnetic field. The sign of β in every term is to be changed for the spin-antiparallel case. The main reason for the use of high (quadruple) precision for small γ comes from the functions of s , which appear to diverge as $s \rightarrow 1$ but which actually vary as

$$\begin{aligned} f(s) &\cong 1 - (1-s)/10, \\ g_x(s) &\cong 1 - 3(1-s)/10, \\ g_y(s) &\cong 1 - (1-s)/10, \\ G_x(s) &\cong 1 - 3(1-s)/14, \\ G_y(s) &\cong 1 - (1-s)/14, \end{aligned} \quad (18)$$

for s close to unity. For example, ten terms in the expansion of the \sinh^{-1} function in $G_x(s)$ are required to obtain this result.

The minimization procedure for the energy itself was an unsophisticated "brute force" method, made particularly tractable because of the circumstance that E is monotonic in s , p , and k . A $3 \times 3 \times 3$ volume element in s , p , k space was created so as to include the point of minimum energy, and the expectation value of the energy, Eq. (6), was evaluated at the center of each of the 27 volume subelements. The origin of a new $3 \times 3 \times 3$ cube was shifted to this point of lowest energy, and the linear cube size was reduced by a factor of 0.6. This procedure was repeated until convergence to 16 significant figures was achieved. The quadruple precision referred to above did not apply to the Γ functions, for which only double precision is available, but this deficiency is immaterial. The quadruple precision was not necessary for $\gamma > 0.1$ even for the parameter s , and was dropped at this point, the energy, k , s , p , and the G and g functions for the larger

γ values being evaluated with double precision by the same methods throughout.

IV. RESULTS AND DISCUSSION

Before discussing the polarizability results we discuss spin-dependent wave-function parameters and energies versus the magnetic field strength (γ) as given in Table I. In Table I we introduce the new parameters $\kappa \equiv k - 1$, $\lambda \equiv p - 1$, and $\sigma \equiv 1 - s$ which are particularly useful for $\gamma \ll 1$ where k , p , and s are all close to unity. In addition, a word about the mathematical notation in Table I is in order. The first line means that $\gamma = 1 \times 10^{-3}$, that $[\kappa(\dagger) + \kappa(\ddagger)]/2 = -1.330 \times 10^{-7}$, ..., $[E(\dagger) + E(\ddagger)]/2 = 5.00 \times 10^{-7} - 1$; the second line means $\gamma = 1 \times 10^{-3}$, $[\kappa(\dagger) - \kappa(\ddagger)]/2 = 2.188 \times 10^{-8}$, etc. The individual values $\kappa(\dagger)$, $\kappa(\ddagger)$, $\sigma(\dagger)$, etc. can be deduced by addition and subtraction. The quantities $[\kappa(\dagger) + \kappa(\ddagger)]$, $[\sigma(\dagger) + \sigma(\ddagger)]$, and $[\lambda(\dagger) + \lambda(\ddagger)]$ in the low-field limit ($\gamma \ll 1$) are all proportional to γ^2 with proportionality coefficients identical to those given in Ref. 20. In the high-field limit $[\kappa(\dagger) + \kappa(\ddagger)]$ is closely proportional to $\gamma^{1/2}$ while $[\sigma(\dagger) + \sigma(\ddagger)]/2$ and $[\lambda(\dagger) + \lambda(\ddagger)]/2$ approach 1 and $-\frac{1}{2}$, respectively, as $\gamma \rightarrow \infty$. This in turn means that $s_{av}\{s_{av} = [s(\dagger) + s(\ddagger)]/2\}$ approaches zero while $p_{av}\{p_{av} = [p(\dagger) + p(\ddagger)]/2\}$ approaches $\frac{1}{2}$. This is precisely the usual high-field limit behavior² characterized by a Gaussian wave function strongly elongated (in comparison with the x, y plane) along the z direction. The spin-difference quantities $[\kappa(\dagger) - \kappa(\ddagger)]$ and $[\sigma(\dagger) - \sigma(\ddagger)]$ in the low-field limit are both proportional to γ while $\lambda(\dagger) - \lambda(\ddagger)$ is negligible in the low-field limit. In this limit the proportionality coefficients for $[\kappa(\dagger) - \kappa(\ddagger)]$, and $\sigma(\dagger) - \sigma(\ddagger)$ are slightly different from those given in Ref. 20 (see the note added in proof therein). The reason that λ , the "hardness" parameter in the wave function, has a negligible spin dependence in the low-field limit is that the spin-dependent term, $\beta(x^2 + y^2)/2r^3$, in Eq.

(4) has the same $1/r$ radial dependence as the Coulomb interaction, unlike the spin-independent diamagnetic term. In the high-field limit the behavior is more complex with $[\kappa(\uparrow) - \kappa(\downarrow)]$ increasing more rapidly than linearly with γ while $[\sigma(\uparrow) - \sigma(\downarrow)]$ and $[\lambda(\uparrow) - \lambda(\downarrow)]$ are both increasing less rapidly than $\gamma^{1/2}$. In the entire field range ($10^{-3} < \gamma < 10^4$) $[\kappa(\uparrow) - \kappa(\downarrow)]$ is always much larger than $[\sigma(\uparrow) - \sigma(\downarrow)]$ and $[\lambda(\uparrow) - \lambda(\downarrow)]$. Thus, the most important effect of the spin-dependent terms in Eq. (4) is the difference in the size of the wave function for the $|\uparrow\rangle$ and $|\downarrow\rangle$ states.

The energy dependences of $[E(\uparrow) + E(\downarrow)]/2$ and $E(\downarrow) - E(\uparrow)$ (recall that $[E(\uparrow) - E(\downarrow)]$ does not include the normal spin Zeeman contribution) are also shown in Table I. $[E(\uparrow) + E(\downarrow)]$ varies quadratically with γ in the $\gamma \ll 1$ limit and varies nearly linearly with γ in the $\gamma \gg 1$ limit. On the other hand $E(\downarrow) - E(\uparrow)$ varies linearly with γ in the $\gamma \ll 1$ limit and quadratically with γ in the $\gamma \gg 1$ limit. The deviation of $E(\downarrow) - E(\uparrow)$ from linear behavior in the high-field limit results not only from the spin-dependent term in Eq. (4), but also from the other spin-independent terms in Eq. (4) because of the different values of $k(\uparrow)$ and $k(\downarrow)$, $s(\uparrow)$ and $s(\downarrow)$, and $p(\uparrow)$ and $p(\downarrow)$. Finally we note that the energy $[E(\uparrow) + E(\downarrow)]/2$ is not the ionization energy quoted in many papers on high magnetic fields. The ionization energy is obtained by subtracting $[E(\uparrow) + E(\downarrow)]/2$ from the lowest Landau energy level for $\hbar k_z = 0$.

Figures 1 and 2 show the normalized spin-independent field-dependent polarizabilities $[\alpha(\uparrow) + \alpha(\downarrow)]/2\alpha(0)$ vs γ . $[\alpha(0)]$ means α evaluated at $\gamma = 0$. Figure 1 best illustrates the high-field behavior showing the perpendicular case ($\vec{\mathcal{E}} \perp \vec{H}$) falling as γ^{-2} for $\gamma \gg 1$. For the parallel case ($\vec{\mathcal{E}} \parallel \vec{H}$) the falloff of $[\alpha(\uparrow) + \alpha(\downarrow)]/2\alpha(0)$ is much slower and is less than γ^{-1} . Furthermore, the parallel case is more complex, not being characterized by a single exponent. The slope of the decrease is decreasing as γ increases. Figure 1 does not do justice to the low-field ($\gamma \ll 1$) variation of $[\alpha(\uparrow) + \alpha(\downarrow)]/2\alpha(0)$. Figure 2 shows a plot of $\log \log \{2\alpha(0)/[\alpha(\uparrow) + \alpha(\downarrow)]\}$ vs γ for both the parallel and perpendicular cases. The low-field results (identical to those in Fig. 2 in Ref. 20) show that $\alpha(\gamma)/\alpha(0) = 1 - \eta\gamma^2$ and that $\eta_{\perp} \approx 1.8\eta_{\parallel}$. Figure 2 clearly shows the quadratic behavior for $\gamma \ll 1$ with deviations from quadratic behavior showing up for $\gamma > 10^{-1}$ as discussed by Dexter.²⁰

The spin-dependent polarization quantity $\log \{[\alpha(\uparrow) - \alpha(\downarrow)]/\alpha(0)\}$ vs γ is plotted in Figure 3. In the low field limit $[\alpha(\uparrow) - \alpha(\downarrow)]/\alpha(0)$ is linear in γ and virtually identical for the parallel and perpendicular cases ($[\alpha_{\perp}(\uparrow) - \alpha_{\perp}(\downarrow)] \approx 1.006[\alpha_{\parallel}(\uparrow) - \alpha_{\parallel}(\downarrow)]$). The two cases diverge as γ approaches

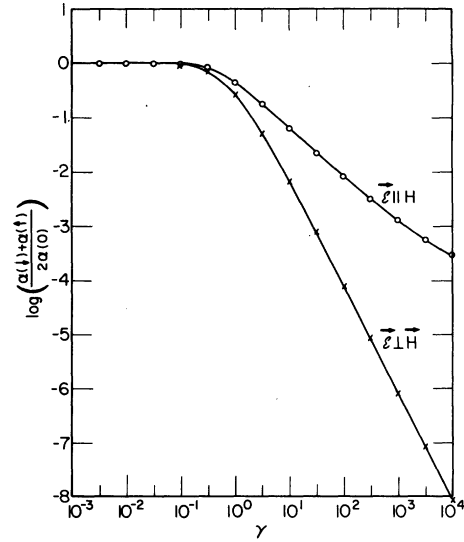


FIG. 1. \log of the average fractional polarizability $[\alpha(\uparrow) + \alpha(\downarrow)]/2\alpha(0)$ versus the dimensionless magnetic field parameter γ . At $\gamma=1$ the diamagnetic energy term in Eq. (4) is twice the hydrogenic Rydberg. In the high-field limit ($\gamma \gg 1$) $[\alpha_{\perp}(\uparrow) + \alpha_{\perp}(\downarrow)]$ falls off as γ^{-2} while for the parallel geometry case $[\alpha_{\parallel}(\uparrow) + \alpha_{\parallel}(\downarrow)]$ falls off more slowly with a slope that decreases with increasing γ .

unity and $\alpha_{\perp}(\uparrow) - \alpha_{\perp}(\downarrow)$ falls very rapidly for $\gamma \gg 1$ with a $\gamma^{-1.75}$ dependence. For the parallel case $\alpha_{\parallel}(\uparrow) - \alpha_{\parallel}(\downarrow)$ flattens out above $\gamma \sim 1$, but then starts to increase again as γ increases. The slope keeps increasing above $\gamma \sim 100$ and $\alpha_{\parallel}(\uparrow) - \alpha_{\parallel}(\downarrow)$ does not seem to fit a simple power law in the high-field region. In the $\gamma \gg 1$ region the anisotropy of $\alpha(\uparrow) - \alpha(\downarrow)$ becomes enormous, e.g., being about 3×10^5 at $\gamma = 10^3$ and 4×10^7 at $\gamma = 10^4$.

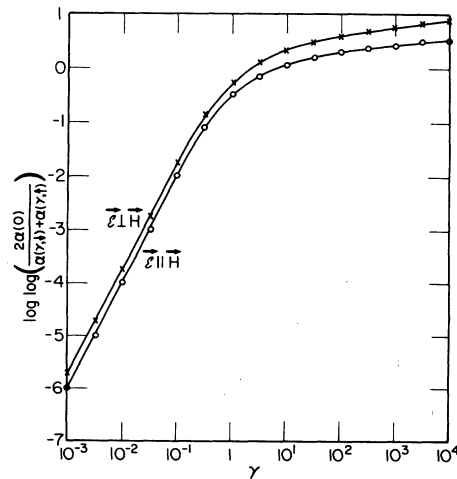


FIG. 2. $\log \log 2\alpha(0)/[\alpha(\uparrow) + \alpha(\downarrow)]$ vs γ . In the low-field limit ($\gamma \ll 1$), $\alpha(\uparrow) + \alpha(\downarrow) = 2\alpha(0)(1 - \eta\gamma^2)$, thus leading to a slope of two. The anisotropy is such that $\eta_{\perp} \approx 1.8\eta_{\parallel}$ in the low-field limit.

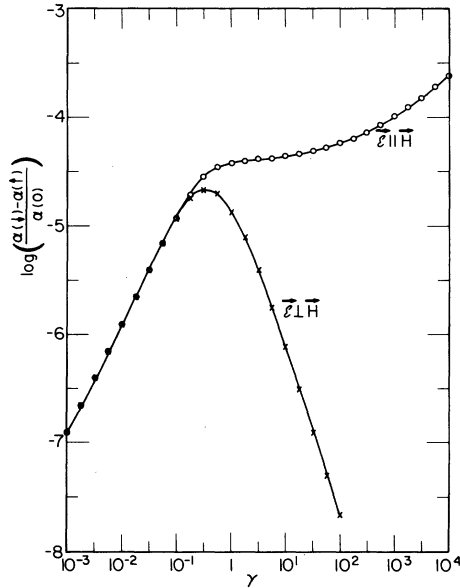


FIG. 3. \log of the fractional spin-difference polarizability $[\alpha_{\parallel}(\dagger) - \alpha_{\perp}(\dagger)]/\alpha(0)$ vs γ . In the low-field limit ($\gamma \ll 1$) $[\alpha_{\parallel}(\dagger) - \alpha_{\perp}(\dagger)]$ is proportional to γ and the anisotropy is negligible. In the extreme high-field limit ($\gamma > 10^2$), $[\alpha_{\perp}(\dagger) - \alpha_{\parallel}(\dagger)] \propto \gamma^{-1.75}$. In the same limit the slope of $[\alpha_{\parallel}(\dagger) - \alpha_{\perp}(\dagger)]$ vs γ is slowly increasing with γ .

An alternative way of showing the same results is shown in Fig. 4 where the polarization of the spin-dependent polarizability (PSP) is shown versus γ . This shows the relative importance of the spin-dependent difference $\alpha(\gamma, \uparrow) - \alpha(\gamma, \downarrow)$ to the diamagnetic contribution to $\alpha(\gamma, \uparrow) + \alpha(\gamma, \downarrow)$. Both

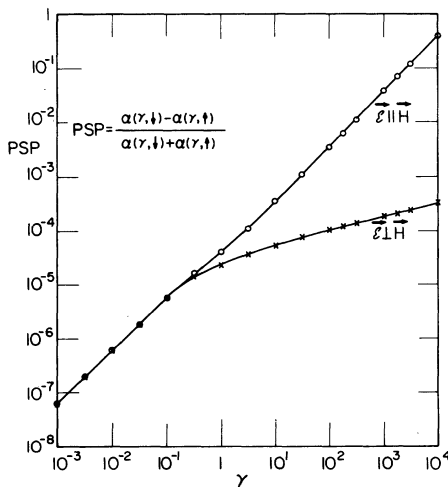


FIG. 4. Polarization of the spin-dependent polarizability (PSP) $[\alpha(\gamma, \uparrow) - \alpha(\gamma, \downarrow)]/[\alpha(\gamma, \uparrow) + \alpha(\gamma, \downarrow)]$ vs γ . The low-field limit is similar to the results in Fig. 3. In the high-field limit ($\gamma > 10^2$) PSP for the parallel geometry increases slightly more rapidly than linearly and for the perpendicular case increases as $\gamma^{0.25}$.

the parallel and perpendicular case show virtually identical linear behavior in the $\gamma \ll 1$ regime while the parallel case is increasing very slightly greater than linearly ($\gamma^{1.028}$) in the $\gamma \gg 1$ regime. For the perpendicular case PSP is increasing as $\gamma^{1/4}$ for $10^2 < \gamma < 10^4$. These results show that the fractional spin-dependent polarizability can indeed approach unity in the super high-field regime ($\gamma > 10^4$). The anisotropy in PSP is slightly greater than 10^3 at $\gamma = 10^4$.

In the very high-field range ($\gamma \gg 1$) the results presented above are expected not to be as reliable because of the neglect of the proton spreading effect considered by Virtamo and Simola.³⁵ These authors demonstrate that field-induced proton spreading can reduce the binding energy of the electron by about 10% at $\gamma = 2 \times 10^3$ and by 20% at $\gamma = 2 \times 10^4$, and they also state a rule that the correct binding energy, E_B , in the extreme field limit ($\gamma > 10^4$) is given by the binding energy at half the field calculated neglecting the proton spread. It is not easy to say how the proton spread will affect the polarizabilities $\alpha(\gamma, \uparrow)$ and $\alpha(\gamma, \downarrow)$, which depend on the parameters $k(\dagger)$, $s(\dagger)$, $p(\dagger)$ and $k(\dagger)$, $s(\dagger)$, $p(\dagger)$, respectively. In the low-field limit ($\gamma \ll 1$) $\alpha \propto E_B^{-3}$; however this result may be modified in the extreme high-field limit. Qualitatively the proton spread at a fixed γ should increase $[\alpha(\dagger) + \alpha(\dagger)]$ and decrease $\alpha(\dagger) - \alpha(\dagger)$. We estimate our calculated values are probably accurate to within 60% at $\gamma = 10^4$, improving rapidly in accuracy as γ decreases. There may also be small changes in the power law dependences of $\alpha(\dagger) + \alpha(\dagger)$ and $\alpha(\dagger) - \alpha(\dagger)$ in the range $10^2 < \gamma < 10^4$ but these changes will alter only slightly the results shown in Fig. 1–4 in the region $\gamma > 10^2$.

Unfortunately, we can envisage no experiment at present that could readily measure $[\alpha(\dagger) - \alpha(\dagger)]$ for free hydrogen atoms employing currently available steady terrestrial magnetic fields, which are limited to γ values well below 10^{-3} . At $\gamma = 10^{-3}$ the field-dependent change in $\alpha(\gamma)$, namely $[\alpha(\gamma) - \alpha(0)]/\alpha(0)$, is of order 10^{-6} while $[\alpha(\dagger) - \alpha(\dagger)]/\alpha(0)$ is of order 10^{-7} . (For $H = 24.0$ T $\gamma \sim 10^{-4}$ and $[\alpha(\gamma) - \alpha(0)]/\alpha(0) \sim 10^{-8}$ and $[\alpha(\dagger) - \alpha(\dagger)]/\alpha(0) \sim 10^{-8}$.) We shall briefly consider below extra-terrestrial H atoms in the atmosphere of neutron stars or magnetic white dwarfs.

Considerably higher values of γ for a fixed magnetic field strength can be obtained for shallow donors in doped semiconductors where the unpaired electron is orbiting the donor nucleus with a much larger Bohr radius, given in the effective-mass approximation (EMA) by $a^* = \epsilon(m/m^*)a_B$ ($a_B = \hbar^2/m_e^2$). Thus γ_{EMA} is given by

$$\gamma_{\text{EMA}} = (a^* \lambda_m)^2 = (a_B / \lambda_m)^2 (\epsilon m / m^*)^2, \quad (19)$$

where λ_m is the characteristic magnetic field length $\lambda_m = (\hbar c / eH)^{1/2}$. For Si ($\epsilon = 11.4$, $m^*/m = 0.299$) $\gamma_{\text{EMA}} = 1455\gamma_H$ while for Ge ($\epsilon = 15.36$, $m^*/m = 0.12$) $\gamma_{\text{EMA}} = 1.6 \times 10^4 \gamma_H$. In a magnetic field of 10 T one obtains $\gamma_{\text{EMA}} = 0.084$ and $\gamma_{\text{EMA}} = 0.66$ for Si and Ge, respectively. Thus it is possible barely to reach the intermediate field region ($\gamma \sim 0.1$) for donors in Si, while for Ge values of γ slightly larger than unity can be obtained. However, the spin-dependent terms in Eq. (4) proportional to β scale differently from γ . β is given by

$$\beta_{\text{EMA}} = \mu_B H_z / m^* c^2 = \beta_H (m/m^*). \quad (20)$$

β_{EMA} is enhanced only by the mass ratio, and therefore by a very much smaller amount than γ_{EMA} . As a result the scaled spin-dependent quantity $[\alpha(\uparrow) - \alpha(\downarrow)]_{\text{EMA}}$ will be very much smaller for a given γ_{EMA} than the calculated H-atom results given in Figs. 3 and 4. The much larger Bohr radius of EMA donors does not enhance the quantity $[\alpha(\uparrow) - \alpha(\downarrow)]$. On the other hand, actual donors (P, As, or Sb) have an additional central-cell correction contribution to the attractive potential that can in principle enhance the effect of the field-dependent spin-orbit interaction in Eq. (2). A reliable estimate of this enhancement requires not only a detailed knowledge of the central-cell correction potential, but also of how the wave function peaks at small r where it can no longer be characterized by a single Bohr radius (see, e.g., Ref. 21). Furthermore, for the many-valley semiconductors like Si and Ge one should also include mass anisotropy effects^{21,36} and intervalley coupling effects. The latter intervalley coupling effects make a negligible contribution to the matrix elements [with the exception of $E_0(H_z)$] contributing to the donor polarizability $\alpha_D(H_z)$. At present there is no direct experimental information on the quantity $[\alpha_D(\uparrow) - \alpha_D(\downarrow)]$ for an isolated donor and it is doubtful whether $[\alpha_D(\uparrow) - \alpha_D(\downarrow)]$ could be determined from experiments sufficiently dilute in donor doping that most of the donors are effectively isolated from each other.

The magnetocapacitance data²⁵ were obtained for n -type Si samples ($N_D > 10^{17}/\text{cm}^3$) where the exchange interaction between donors is important. The exchange interaction between a donor and its neighbors also provides a spin-dependent interaction potential that can lead to a spin-dependent polarizability and to an effective quantity $\langle \alpha_D(\uparrow) - \alpha_D(\downarrow) \rangle$. We need only recall the single atom of ion (e.g., Mn^{2+}) case of the exchange interaction between a half-filled d shell (d^5 , $S = \frac{5}{2}$) and the filled s -shell core electrons. In this case $\psi_{1s}(\vec{r} = 0, \uparrow)$ and $\psi_{1s}(\vec{r} = 0, \downarrow)$ have different values, thus leading to an isotropic Fermi contact term

hyperfine interaction from the "closed" $1s$ shell. This core polarization³⁷ effect resulting from the exchange interaction is a well known example of a spin orbital-motion effect. For the present case of one-electron donors the spin orbital motion interaction can arise from, in addition to the hydrogenic atom terms in Eq. (4), the exchange interaction between neighboring donors. A new experiment is now underway here (UR) to attempt a direct measurement of $\langle \alpha_D(\uparrow) - \alpha_D(\downarrow) \rangle$ for P-doped Si.

For H atoms present in the atmosphere of neutron stars one might readily expect to have $\gamma_H \sim 10^3$. In this field regime the quantity $\tilde{n} - 1$ [$\tilde{n}(\gamma)$ being the tensor index of refraction of the H-atom atmosphere] will be highly anisotropic with $(\tilde{n} - 1)_{\parallel} \sim 10^3$ orders of magnitude smaller than $(\tilde{n} - 1)_{\perp} \sim 10^3$. On the other hand the extremely small depth of the atmosphere (~ 1 cm) makes it difficult to imagine how this large anisotropy in $(\tilde{n} - 1)$ might be measured, particularly since $(\tilde{n} - 1)$ itself will be such a small quantity. While the dielectric properties of the H-atom atmosphere of a neutron star represent an interesting question no experimental data exists which is relevant to this question. For magnetic white dwarf stars γ_H will be very much smaller, perhaps in the range $10^{-2} < \gamma < 10^{-1}$; however this is counterbalanced by a much thicker H-atom atmosphere. For the magnetic white dwarf case the anisotropy in $(\tilde{n} - 1)$ will be many orders of magnitude smaller than for neutron stars and will probably be unobservable despite the much larger volume of the H-atom atmosphere surrounding the magnetic white dwarf. For both the neutron star and magnetic white dwarf we cannot presently envisage any experiment that could directly measure the quantity $[\alpha_H(\uparrow) - \alpha_H(\downarrow)]$.

The electron Zeeman effect for H atoms in the high-field limit will occur in the x-ray portion of the electromagnetic spectrum (at $\gamma_H = 10^3$, $\Delta E_{\text{Zeeman}}^0 = 2\mu_B H = 27.2$ kev); however, a second-order correction to the Zeeman energy [$E_{1s}(\uparrow) - E_{1s}(\downarrow)$] resulting from the field-dependent spin-orbit term and the spin-dependent relativistic kinetic-energy term varies as γ^2 in the high-field limit ($\gamma \gg 1$). This correction to ΔE_{Zeeman} is 183 eV at $\gamma = 10^3$, or about 0.7% of the first-order Zeeman effect. Thus it is doubtful that this second-order Zeeman effect could be detected.

In the present work we have neglected nuclear spin effects (nuclear Zeeman effect, hyperfine interaction between the electron and nuclear spins) in our treatment of the H atom. It is worth pointing out that in the strong-field limit the dramatic shrinkage of the electron wave function will produce a corresponding dramatic enhancement of

the electron-proton Fermi contact hyperfine interaction and the high field will also induce a large dipole-dipole contribution to the hyperfine interaction. The Fermi contact contribution will be proportional to $|\psi_{1s}(\vec{r}=0)|^2 \propto \sqrt{s} k^3$ and will contain a spin dependence as well. At $\gamma = 10^2$, $|\psi_{1s}(0)|^2$ can be enhanced by three orders of magnitude, thus leading to a hyperfine frequency of order 10^{12} Hz. Once again, this effect will be masked by the much larger nuclear Zeeman effect for the proton, which will now exhibit a resonant frequency in the ultraviolet (~ 5 eV) for $\gamma = 10^2$. Any accurate determination of both these higher-order effects, the quadratic electron Zeeman effect and the electron-proton hyperfine interaction enhancement in the high-field limit would

have to take into account the proton spreading effect.³⁵

To summarize, we have shown the dramatic effect of very large magnetic fields on the electrical polarizability of hydrogenic atoms and we have calculated the magnitude of the very small spin-dependent contribution $[\alpha(\uparrow) - \alpha(\downarrow)]$ for isolated H atoms. The best chance for observing the spin-dependent contribution at present would appear to be in the doped semiconductors.

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