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Energy and polarizability of atoms in a weak magnetic field: Hydrogenic atoms

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The ground-state wave function of a hydrogenic atom is approximated by $\psi_0(\mathrm{H}) = \exp\{-[k(x^2 + y^2 + sz^2)^{1/2}]^{1/p}\}$, and the expectation value of the Hamiltonian, including diamagnetic and spin-orbit terms in a magnetic field H_z, is minimized with respect to k, s, and p so as to determine these H_z-dependent parameters, and the energy is evaluated. In the presence of an infinitesimal electric field $\mathcal{E}_t$, in the t direction, the wave function is taken to be $\psi_0(\mathrm{H})(1 + bt + c\rho t)$, where $\rho = (x^2 + y^2 + sz^2)^{1/2}$. The energy is minimized with respect to b and c, and the coefficient of $\mathcal{E}_t^2$ is identified as $-(1/2)\alpha_t$, the polarizability component, which contains diamagnetic and weakly spin-dependent terms. Comparison with experiments of Castner and Lee on donors in Si is briefly discussed.

I. INTRODUCTION

Increasing the concentration of donor impurities (N_D) in Si leads to a semiconductor-metal transition at $N_D \sim 10^{18}$ donors per cm^3. Castner *et al.*[1] measured the low-frequency dielectric constant in these samples on the low-N_D side of the transition, and observed onset of a "dielectric catastrophe" attributed to the large polarizability α of these spatially extended donors. This observation led them to perform low-frequency magneto-capacitance measurements at low temperatures in low-N_D samples, in analogy to magneto-resistance studies on the high-N_D side, which they have interpreted as indicating a reduction in $\alpha(\mathrm{H})$ of weakly interacting donors by a static magnetic field.[2]

A great deal of theoretical work has been done on the energies of atoms and donor impurities[3] in the effective-mass approximation (EMA) in the presence of a magnetic field. Much of this work in recent years has dealt with the high-field regime, i.e., where the magnetic energy is large compared with the Coulomb energy, and where transport properties are strongly affected by the field. Very little theory exists for optical properties such as dipole matrix elements, oscillator strengths, etc.[4]; surprisingly, a calculation of the magnetic field dependence of α even for the hydrogen atom does not seem to have been reported for weak field.

Section II contains a calculation of the ground-state energy and polarizability for a hydrogenic impurity atom in the EMA by means of variational methods. In the weak-field limit the calculation is done analytically; it is extended approximately by numerical methods into the intermediate-field regime. A brief discussion is given in Sec. III.

II. THE HYDROGENIC ATOM

An approximate Hamiltonian[5] for the ground-state hydrogenic impurity in a constant magnetic field H_z can be expressed in the EMA as

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

Here ϵ is the dielectric constant, $a^* \equiv \epsilon\hbar^2/m^*e^2$, m^* is the scalar effective mass, $\hat{h}^2 \equiv \epsilon a^{*3}H_z^2/m^*c^2$, and $\beta \equiv \mu_B H_z/m^*c^2$, where μ_B is the Bohr magneton, $e\hbar/2mc$. The intermediate-field regime is that for which $\hat{h} \simeq 1$. The third term, the diamagnetic energy, tends to compress the wave function. The last term arises from the spin-orbit interaction; it would couple the ground state to excited s and d states in perturbation theory, and gives rise to a spin-dependent polarizability. Its effect is expected to be small. Other spin-dependent terms are decoupled from the spatial part of the wave function and are ignored.

We expect the size, shape, and "hardness" of the wave function to be modified by H_z, i.e., it becomes compressed, relatively elongated, and approaches a Gaussian for large H_z, and accordingly we choose a trial wave function of the form

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

where $k \equiv 1+\kappa$, $p \equiv 1+\lambda$, $s \equiv 1-\sigma$ are expected to be close to unity and dependent on H_z. Calculating the expectation value of H_0 and normalizing, we obtain

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

where

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

$$\cong 1-\sigma/10+\cdots\ . \tag{4a}$$

For small H_z we may expand Eq. (3) through terms of second order in β, $\hat{h}^2$, λ, σ, κ, and their products, and obtain

$$\frac{E_0}{e^2/2\epsilon a^*}=-1+\frac{\hat{h}^2}{2}\pm\frac{2\beta}{3}-\sigma\frac{\kappa}{3}+q\kappa\lambda-\frac{q\sigma\lambda}{6}+j\lambda\hat{h}^2$$
$$+\kappa^2+\tfrac{11}{60}\sigma^2+\mu\lambda^2-\kappa\hat{h}^2\pm\tfrac{2}{3}\beta\kappa$$
$$\mp\frac{\beta\sigma}{15}\mp\tfrac{2}{3}\beta\lambda(C+\ln 2-\tfrac{5}{2})\,, \tag{4b}$$

where $q=2C-5+2\ln 2$, $\mu=5-5\ln 2+\ln^2 2+C^2+C(2\ln 2-5)+\frac{1}{6}\pi^2$, $j=\frac{71}{24}-C-\ln 2$, and C is Euler's constant, $0.577\cdots$. We may now minimize the energy with respect to variations in λ, σ, and κ.

It is instructive to perform the variation one, two, and three parameters at a time. When only λ is varied (the most sensitive one, as noted earlier by Halbo[3e]), we find

$$\lambda=-\frac{j}{2\mu}\hat{h}^2\pm\left(\frac{C+\ln 2-5/2}{3\mu}\right)\beta$$

$$=-0.4426\hat{h}^2\mp 0.2149\beta\,, \tag{5a}$$

and E_0 is equal to $-(e^2/2\epsilon a^*)(1-\frac{1}{2}\hat{h}^2\mp\frac{2}{3}\beta+0.3735\hat{h}^4)$. As will be seen, for H_z sufficiently large that an effect on α can be measured, the diamagnetic term dominates the $\pm\beta$ term, and here and in the following the contributions of β^2 and $\beta\hat{h}^2$ to the energy will be ignored. When both λ and σ are varied, we obtain

$$\lambda=-0.5030\hat{h}^2\mp 0.2665\beta\,,$$
$$\sigma=0.5623\hat{h}^2\mp 0.1682\beta\,, \tag{5b}$$

and E_0 is equal to $-(e^2/2\epsilon a^*)(1-\frac{1}{2}\hat{h}^2\mp\frac{2}{3}\beta+0.4245\hat{h}^4)$, a 15% improvement in the "redistribution" energy proportional to $\hat{h}^4$. When all three parameters vary, we obtain

$$\lambda=-0.5803\hat{h}^2\mp 2.0757\beta,$$
$$\sigma=\tfrac{15}{28}\hat{h}^2\mp\tfrac{1}{7}\beta\,, \tag{5c}$$
$$\kappa=-0.1242\hat{h}^2\mp 2.9095\beta\,,$$

and E_0 is $-(e^2/2\epsilon a^*)(1-\frac{1}{2}\hat{h}^2\mp\frac{2}{3}\beta+0.4258\hat{h}^4)$, another 0.3% improvement. The smallness of the last correction gives some confidence in the wave function for small $\hat{h}^2$. For somewhat larger values of $\hat{h}^2$, where the quadratic expansion is inadequate, Eq. (3) was numerically minimized with respect to variations in p and s, and κ was ignored. The results are shown in Fig. 1 in the solid lines. These energies are comparable to or lower than those calculated elsewhere by numerical methods, often with a large number of parameters.

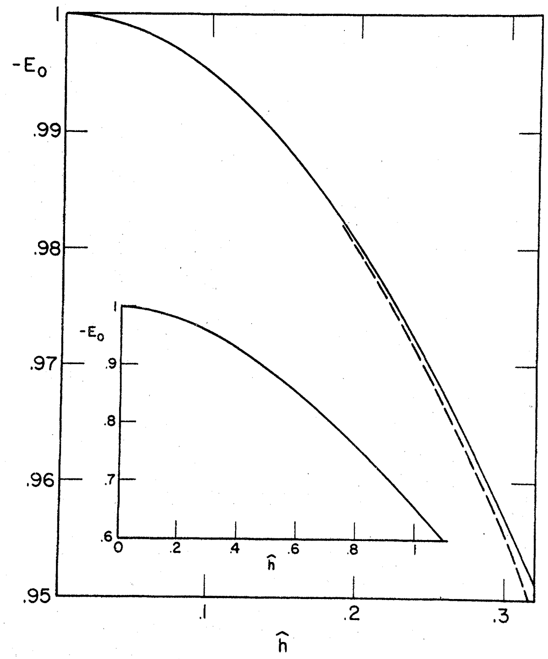

FIG. 1. Lowest atomic energy level (in rydbergs) in a magnetic field. The solid line is the minimum calculated from Eq. (3) upon minimizing with respect to p and s. The dashed line includes the diamagnetic energy only, calculated with an unperturbed wave function. Equation (4b) fits the solid line closely for $\hat{h}\lesssim 0.2$, and then falls off slightly less rapidly.

To calculate the polarizability we follow the variational method used by Hassé.[6] We introduce an additional term $-e\mathcal{E}_t t$ into the Hamiltonian, where t stands for x or z and where $\mathcal{E}_t$ is an *infinitesimal* electric field. We select a trial wave function

$$\psi_t(\vec{r})=\psi_0(H_z)(1+bt+c\rho t)\,, \tag{6}$$

where $\rho\equiv(x^2+y^2+sz^2)^{1/2}$ and where b and c are infinitesimal parameters to be determined variationally. The resulting expression for the energy is given by Eq. (3) plus a term proportional to $\mathcal{E}_t^2$, the coefficient of which is identified as $-\frac{1}{2}\alpha_t$. In the absence of H_z this method gives the exact result, $\frac{9}{2}a_0^3$, for the hydrogen atom. The usefulness for the present purpose is the elimination of need for excited-state wave functions. Accordingly we compute the expectation value of $H_0-e\mathcal{E}_z z$ with the perturbed wave function Eq. (6), normalize, and obtain

$$\alpha^{\parallel}=\frac{9}{2}\frac{a^{*3}\epsilon}{s}\frac{(\frac{4}{9})^2}{(k2^p)^4\Gamma(3p)}$$
$$\times\left(\frac{\Gamma^2(6p)J_{BZ}+\Gamma^2(5p)J_{CZ}-\Gamma(5p)\Gamma(6p)J_{DZ}}{4J_{BZ}J_{CZ}-J_{DZ}^2}\right), \tag{7a}$$

where

$$J_{BZ}=\frac{(3p+1)(2+3s)\Gamma(3p)}{40p}-\frac{g_Z(s)\Gamma(4p)}{3k2^p}$$
$$-\frac{E_0\Gamma(5p)}{6(k2^p)^2}+\frac{\hat{h}^2\Gamma(7p)}{60(k2^p)^4}$$
$$\pm\frac{\beta\Gamma(4p)}{15k2^p}(1-\tfrac{3}{14}\sigma+\cdots), \tag{7b}$$

$$J_{CZ}=\frac{(9p+5)(2+3s)\Gamma(5p)}{120p}-\frac{g_Z(s)\Gamma(6p)}{3k2^p}$$
$$-\frac{E_0\Gamma(7p)}{6(k2^p)^2}+\frac{\hat{h}^2\Gamma(9p)}{60(k2^p)^4}$$
$$\pm\frac{\beta}{15}\frac{\Gamma(6p)}{k2^p}(1-\tfrac{3}{14}\sigma+\cdots), \tag{7c}$$

$$J_{DZ}=\frac{(2p+1)(2+3s)\Gamma(4p)}{15p}-\frac{2g_Z(s)\Gamma(5p)}{3k2^p}$$
$$-\frac{E_0\Gamma(6p)}{3(k2^p)^2}+\frac{\hat{h}^2\Gamma(8p)}{30(k2^p)^4}$$
$$\pm\frac{2\beta}{15}\frac{\Gamma(5p)}{2^pk}(1-\tfrac{3}{14}\sigma+\cdots). \tag{7d}$$

Here $|E_0|\sim 1$ is the energy in the magnetic field, Eq. (3) expressed in rydbergs, and

$$g_Z(s)=\frac{3}{2(1-s)}\left[s^{1/2}-\frac{s^{3/2}}{(1-s)^{1/2}}\sinh^{-1}\left(\frac{1-s}{s}\right)^{1/2}\right]$$
$$\cong 1-\frac{3\sigma}{10}+\cdots. \tag{8}$$

Similar expressions ensue for $\vec{\mathcal{E}}\perp\vec{\mathrm{H}}$, in which case α becomes $\alpha^{\perp}$,

$$\alpha^{\perp}=\tfrac{9}{2}\epsilon a^{*3}\frac{(\frac{4}{9})^2}{(k2^p)^4\Gamma(3p)}$$
$$\times\left(\frac{\Gamma^2(6p)J_{BX}+\Gamma^2(5p)J_{CX}-\Gamma(5p)\Gamma(6p)J_{DX}}{4J_{BX}J_{CX}-J_{DX}^2}\right), \tag{9a}$$

where

$$J_{BX}=\frac{(3p+1)(4+s)\Gamma(3p)}{40p}-\frac{g_X(s)\Gamma(4p)}{3k2^p}$$
$$-\frac{E_0\Gamma(5p)}{6(k2^p)^2}+\frac{\hat{h}^2\Gamma(7p)}{30(k2^p)^4}$$
$$\pm\frac{2\beta\Gamma(4p)}{15k2^p}(1-\tfrac{1}{14}\sigma+\cdots), \tag{9b}$$

$$J_{CX}=\frac{(9p+5)(4+s)\Gamma(5p)}{120p}-\frac{g_X(s)\Gamma(6p)}{3k2^p}$$
$$-\frac{E_0\Gamma(7p)}{6(k2^p)^2}+\frac{\hat{h}^2\Gamma(9p)}{30(k2^p)^4}$$
$$\pm\frac{2\beta\Gamma(6p)}{15k2^p}(1-\tfrac{1}{14}\sigma+\cdots), \tag{9c}$$

$$J_{DX}=\frac{(2p+1)(4+s)\Gamma(4p)}{15p}-\frac{2g_X(s)\Gamma(5p)}{3k2^p},$$
$$-\frac{E_0\Gamma(6p)}{3(k2^p)^2}+\frac{\hat{h}^2\Gamma(8p)}{15(k2^p)^4}$$
$$\pm\frac{4\beta\Gamma(5p)}{15k2^p}(1-\tfrac{1}{14}\sigma+\cdots), \tag{9d}$$

in which

$$g_X(s)=\frac{3}{2}\left(\frac{s}{1-s}\right)^{1/2}$$
$$\times\left\{\sinh^{-1}\left(\frac{1-s}{s}\right)^{1/2}\right.$$
$$\left.-\frac{1}{2}\left[(1-s)^{-1/2}-\frac{s}{1-s}\sinh^{-1}\left(\frac{1-s}{s}\right)^{1/2}\right]\right\}$$
$$\cong 1-\frac{\sigma}{10}+\cdots. \tag{10}$$

The approximate expressions $(1-\frac{3}{14}\sigma+\cdots)$ and $(1-\frac{1}{14}\sigma+\cdots)$ are expansions of $\sinh^{-1}[(1-s)/s]^{1/2}$ and powers of s and $1-s$ in the two cases.

In the limit of small field we may expand to terms in $\hat{h}^2$ and β, and obtain

$$\alpha^{\parallel}\cong(\tfrac{9}{2}\epsilon a^{*3})\left[1+\frac{7\sigma}{6}-\frac{23\kappa}{9}+\lambda\left(\frac{209}{27}-\frac{23}{9}(C+\ln 2)\right)\right.$$
$$\left.-\frac{53}{72}\hat{h}^2\pm\frac{14}{45}\beta\right],$$
$$\alpha^{\perp}\cong(\tfrac{9}{2}\epsilon a^{*3})\left[1+\frac{\sigma}{18}-\frac{23\kappa}{9}+\lambda\left(\frac{209}{27}-\frac{23}{9}(C+\ln 2)\right)\right.$$
$$\left.-\frac{149}{72}\hat{h}^2\pm\frac{113}{270}\beta\right], \tag{11}$$
$$\frac{\alpha^{\parallel}}{\alpha^{\perp}}\cong 1+\frac{10\sigma}{9}+\frac{4}{3}\hat{h}^2\mp\frac{29}{270}\beta.$$

Inserting the best values for λ, σ, κ from Eq. (5c), we obtain

$$\alpha^{\parallel}\cong(\tfrac{9}{2}\epsilon a^{*3})(1-2.402\hat{h}^2\mp 1.749\beta),$$
$$\alpha^{\perp}\cong(\tfrac{9}{2}\epsilon a^{*3})(1-4.3303\hat{h}^2\mp 1.483\beta), \tag{12}$$
$$\alpha^{\parallel}/\alpha^{\perp}\cong 1-1.928\hat{h}^2\mp 0.266\beta.$$

For larger values of $\hat{h}^2$, where the analytic expansions are not adequate, the complete equations and the numerical results leading to Fig. 1 were evaluated, leading to Fig. 2. The units on the ordinate scale are ϵa^{*3}, and the effect of the $\pm\beta$ terms was not included.

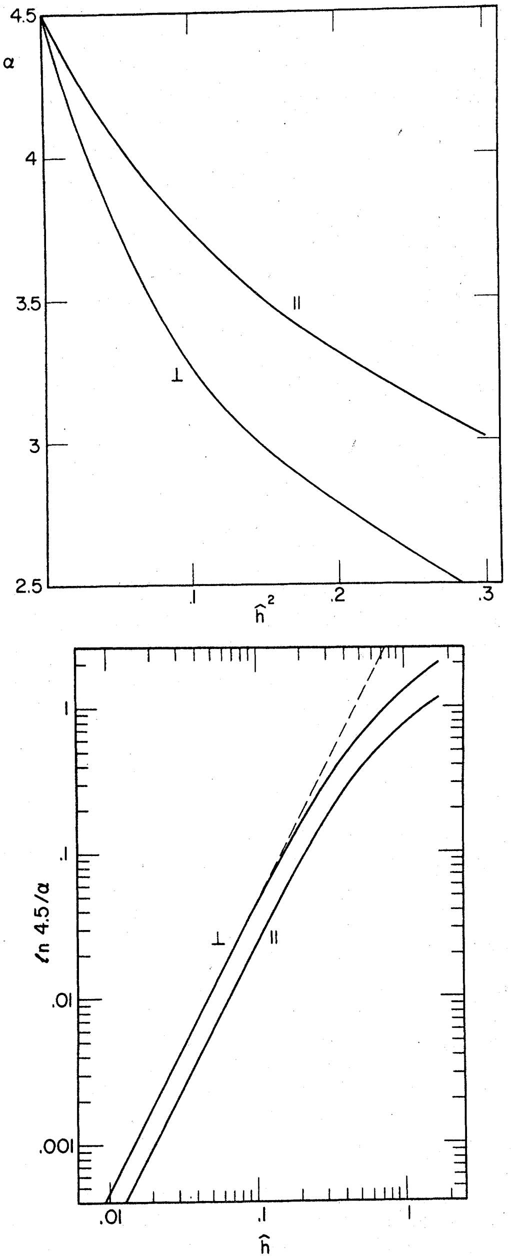

FIG. 2. Polarizability of hydrogen calculated parallel and perpendicular to a magnetic field $\hat{h}$. A deviation from $\hat{h}^2$ dependence is barely detectable for $\hat{h} \sim 0.1$. Units for α are ϵa^{*3}.

Several points are to be noted. First, α varies as $\epsilon^4(m/m^*)^3$, and can easily be 10^6 greater than for a real hydrogen atom. Second, α decreases with increasing field, as one's intuition would suggest from the consideration that $\hat{h}^2(x^2+y^2)$ acts to compress the wave function. This result is not apparent from the standpoint of perturbation theory; one could argue that the excited-state wave functions are compressed more than for the ground state, hence the overlap is improved, and the dipole matrix elements increase. Indeed, Aldrich and Green found[3] that the $1s$-$2p$ and $1s$-$3p$ matrix elements do increase with $\hat{h}^2$ for small $\hat{h}^2$. However, the energy denominators increase also, and much of the total oscillator strength is in the continuum so that this counter argument is inconclusive. Third, α decreases much more rapidly than does $|E_0|$ for small $\hat{h}^2$, that is

$$\frac{d\ln}{d\hat{h}^2}|E_0|\bigg|_{\hat{h}^2=0}=-\frac{1}{2},$$

$$\frac{d\ln}{d\hat{h}^2}\alpha^{\parallel,\perp}\bigg|_{\hat{h}^2=0}=-2.4 \text{ or } -4.3.$$

Fourth, the wave function becomes nonspherical, with $[\langle z^2\rangle/\langle x^2\rangle]^{1/2}=(1/s)^{1/2}=1+\frac{15}{56}\hat{h}^2\mp\frac{1}{14}\beta$. The polarizability is substantially more anisotropic than this, with $\alpha^{\perp}/\alpha^{\parallel}=1-1.93\hat{h}^2\pm0.27\beta$ for small H_z, thus raising interesting possibilities for the dielectric behavior upon rotating the magnetic field. Fifth, the magnetic field required to produce a measurable effect is much reduced from that required for the hydrogen atom. $\hat{h}=1$ for the free atom means $H_z=2.35\times10^9$ G, but for the hydrogenic atom it is reduced by a factor $(m^*/m)^2/\epsilon^2$. An effect on α can readily be seen in Si for $H_z=10^4$ G. Sixth, the spin-dependent term is

$$\alpha^{\parallel}(\uparrow)-\alpha^{\parallel}(\downarrow)=\frac{9}{2}a_0^3\left(\frac{\epsilon m}{m^*}\right)^4 3.50\,\frac{\mu_B H_z}{mc^2}\,.$$

This is much larger in the solid than for the pure atom, but much smaller than the change caused by the diamagnetic term in realistic cases where the latter can be conveniently measured. That is, $\beta=\frac{1}{2}(m^*/m\epsilon^2)(e^2/\hbar c)^2\hat{h}$; a value of 10^{-2} for $\hat{h}^2$ produces a -4% change in $\alpha^{\perp}$ from the diamagnetic term but, if $\epsilon^2 m/m^*=500$, less than $\pm10^{-6}\%$ from β.

III. DISCUSSION

There are certain similarities between these results and those of Castner and Lee[2] in Si doped with As, P, and Sb. In both cases α decreases quadratically with H for small H and then falls off less rapidly. Also the magnitude of $\alpha(H=0)$ is of the general magnitude of those observed by Castner *et al.*,[7] namely, $6.7\times10^5 a_0^3$ for As donors in Si, 16.2×10^5 for P, and 20.9×10^5 for Sb. If one approximates Si by a dielectric constant[8] of $\epsilon=11.4$ and a spherical effective mass[9] of $m^*=0.3m$, one obtains a zero field polarizability of $28\times10^5 a_0^3$. Clearly this procedure is inadequate, since there does exist an important donor dependence unaccounted for in the simple $e/\epsilon r$ potential.

Even so, the predicted magnetic field dependence might have turned out to be reasonably correct, but the rate of decrease with H^2 predicted here turns out to be a factor of 16–23 smaller than that observed by Castner and Lee[2] for $\vec{H} \parallel \vec{\mathcal{E}}$ along $\langle 111 \rangle$. The agreement with experiment is not improved with the use of the Ning and Sah[9b] approximation to the wave functions, since the predicted polarizabilities are substantially too low.

It is unfortunate that there are no experimental data for α for the hydrogen atom in a magnetic field, but considerable experimental ingenuity and/or larger fields than are now available in terrestrial laboratories will be required. Failing such results, one would like to have data on donors in single valley semiconductors where this simple version of EMA might be deemed applicable. In this context, it should be noted that even if a donor in such a system might be well approximated by an EMA wave function in the absence of $\vec{H}$, it is possible, and in the author's view probable that it will not be well approximated by EMA in the presence of $\vec{H}$ (with the possible exception of "isocoric" impurities[10]). That is, even if the amount of central cell wave function is small enough to exhibit only a negligible effect on energies, the amount of central cell wave function may change with $\vec{H}$ at a rate large enough that the renormalization of the extended EMA wave function will have a greater effect on the polarizability than will the diamagnetically induced shrinkage of the EMA part of the wave function considered here.

Consideration of this point, and others connected with donors in many-valley semiconductors are now under investigation by N. Lipari and the author.

Note added in proof. The results proportional to the small parameter β are in error. Since they are negligibly small it does not seem worthwhile to correct them here. They will be corrected in a subsequent publication. All of the major conclusions are unaffected.

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