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Field-Dependent Central-Cell Corrections in GaAs by Laser Spectroscopy*

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We report the first definite observations of the magnetic field dependence of central-cell corrections in shallow donors. Exploiting the extreme resolution inherent in magnetospectroscopy employing infrared gas laser sources, we have observed previously unresolved transitions arising from four distinct "hydrogenic" donor species occurring in high-purity epitaxial GaAs. We show that the species-dependent differences in transition energies are directly proportional to the probability of finding an electron at the donor site to which it is loosely bound. This probability increases with increasing magnetic field because of magnetic squeezing of the wave function of the bound electron.

Recent magneto-optical studies[1,2] of the $1s$-$2p$ donor[3] transitions in epitaxial n-GaAs demonstrate that the donor states involved are hydrogenic to within experimental accuracy. We have re-examined some of these transitions both in photoconductivity and transmission in experiments of much higher resolution and with very precise magnetic-field measuring capability in order to check critically the limits of validity of the effective-mass–hydrogenic-atom model for GaAs donors. We find that under high resolution the absorption and photoconductivty previously ascribed to a single donor is actually made up of four, closely spaced, previously unresolved transitions, each arising from a different donor species. The existence of these hyperfine separations (hfs) (of the order of 0.5 cm^{-1}) in the $1s$-$2p$ transition cannot be understood from the hydrogenic isolated-donor model even when corrections for band nonparabolicity are introduced. Thus splittings offer a unique opportunity for investigating perturbations on the simple hydrogenic-donor impurity model.

The most direct evidence for our claim that the hfs arises from small variations in the $1s$-$2p$ transition energies for different donor species[4] present in our samples comes from the observation that the hyperfine peaks change in relative intensity but not in energy from sample to sample. Study of the hyperfine separations in different optical transitions shows that these spacings are attributable to differences among donor *ground-state* energies. Analysis of the field dependence of the hyperfine separations indicates that the perturbations giving rise to the observed relative shifts in the ground-state energy are (1) of short range compared to the hydrogenic Bohr radius a_0 and are (2) centered either at or very near to the donor site. The observed behavior with magnetic field of the hyperfine sepa-

rations must therefore be understood as reflecting the field dependence of differences of central-cell corrections in shallow donors. This is a new experimental effect, although the quantitative theoretical explanation proposed here has already been roughly sketched out.[5]

Experiment.—Samples with leads attached were placed in the center of a 100-kG superconducting solenoid, immersed in liquid He, and illuminated by laser radiation emerging from a tubular, brass light pipe. A magnetically shielded GaAs extrinsic photodetector positioned below the solenoid permitted observations of sample transmission simultaneously with the photoconductivity measurements. Precision magnetic field determinations were made using a small NMR coil containing ^{1}H, ^{27}Al, or ^{19}F in close proximity to the sample. Modulation coils required for the NMR device also allowed derivative spectra of the impurity transitions to be obtained. The combination of derivative spectroscopy and NMR permitted determination of fields for either relative minima in transmisson or relative maxima in photoconductivity to ±0.015 kG (for the strongest peaks) in the range 12.9 to 66.9 kG. For all transitions investigated no differences in transition fields were found between data taken in photoconductivity and transmission.

Figure 1 shows the experimental traces of donor spectra as functions of magnetic field for GaAs illuminated with 118.6-μm laser radiation. The 1*s* to 2*p* ($M=+1$) transition appears in both transmission [Fig. 1(a)] and in photoconductivity [Fig. 1(c)][7] and was identified on the basis of previous work.[1,2] It is evident from Fig. 1(b) (and Fig. 2) that the "hydrogenic" transitions have a hyperfine structure and that the transitions associated with the shallow donors are extremely narrow (0.08 to 0.18 cm^{-1} half-width at half-maximum—perhaps the sharpest shallow-donor lines yet reported in a semiconductor). Figure 1(b) illustrates the clarity with which the closely spaced donor lines can be resolved using derivative techniques.

Donor photoconductivity spectra for the 1*s*-2*p* ($M=+1$) transition for two different samples are shown in Fig. 2. Notice that the two traces differ only in the relative intensities of the hyperfine structure. We attribute this difference to variations from sample to sample of the relative concentrations of the donor species present.

Using various laser lines and different Zeeman components of the 2*p* final states of the donor transition, we have observed spectra similar to Fig. 1(b) for a wide range of magnetic fields. Measured values of the field separations ΔH_{AC} corresponding to hyperfine energy splittings between peaks *A* and *C* in sample 2 offered the best quantitative data and are tabulated in Table I. ($\Delta H_{CB}/\Delta H_{CA} \approx \frac{1}{3}$ for all transitions studied. ΔH_{CD}

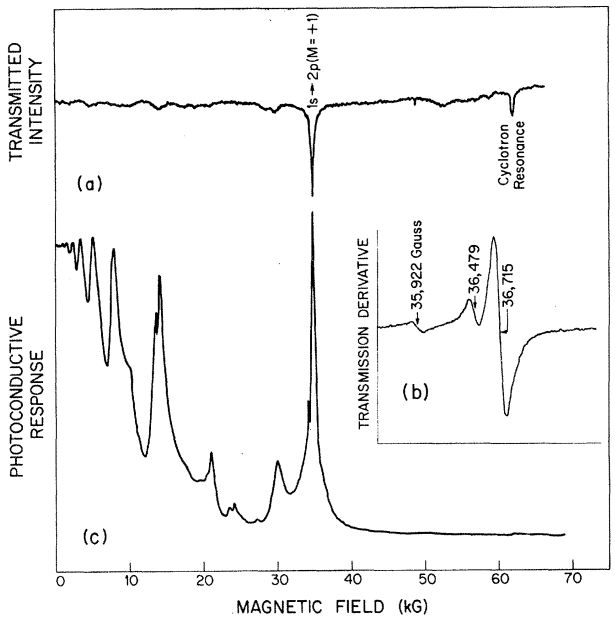

FIG. 1. Recorder traces in GaAs (sample 2) at 4.2°K and 118.6 μm as a function of magnetic field. (a) Transmission spectrum, (b) derivative of $1s \rightarrow 2p$ ($M=+1$) transitions, and (c) photoconductivity spectrum.

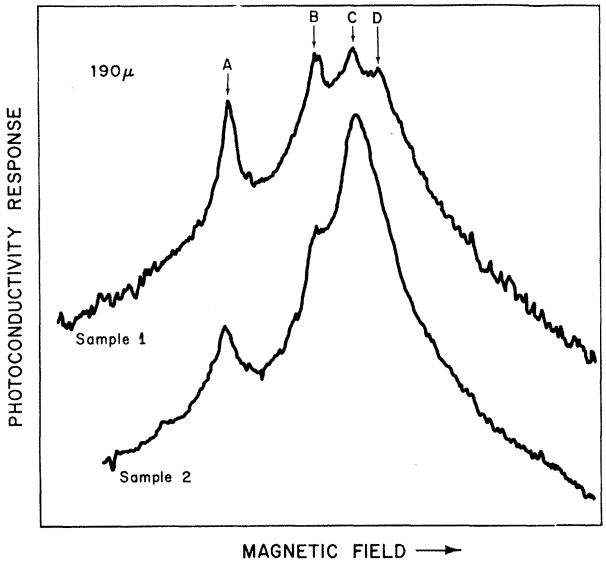

FIG. 2. The $1s \rightarrow 2p$ ($M=+1$) transition shown in photoconductivity for two different samples. N_D for sample 1 is 2.0×10^{14} cm^{-3}; N_D for sample 2 is 4.3×10^{13} cm^{-3}; $\mu_{77°}=153\,000$ and 186 000 cm^2/V sec, respectively. N_A for samples 1 and 2 are 4×10^{13} cm^{-3} and 2.5×10^{13} cm^{-3}, respectively.

Table I. Experimental and theoretical values used to study central-cell corrections in GaAs donors. $\bar{K}_{AC} = 10^4 K_{AC}/\sqrt{2}$ where K_{AC} is defined in the text (see also Ref. 10).

M of final state	Laser line (cm^{-1})	Laser line (μm)	Field (kG)	ΔH_{CA} (kG)	ΔE_{AC} (cm^{-1})	$\bar{K}_{AC}/\pi a_0^3$ (Ry)[a]	D_C (%)
1	51.36	195	13.69	0.73	1.0	146 ± 4	0.01
1	52.65	190	14.63	0.73	1.0	146 ± 4	−0.004
1	84.32	119	36.715	0.79	1.15	145 ± 4	0.08
0	51.36	195	56.655	4.61	1.28	141.4 ± 1.5	0.21
0	52.65	190	61.54	4.86	1.32	141.2 ± 1.5	0.24
1	127.48	78.4	66.805	0.99	1.42	148 ± 5	−0.18

[a]Note that this is the Rydberg in GaAs, 5.8407 meV.

could not be measured reliably.)

Theory.—Since our data suggest that all four central-cell corrections are very small compared to $\mathcal{R}$ ($\mathcal{R} \cong 47\ cm^{-1}$ in GaAs), it is natural to attempt to calculate these corrections in lowest order perturbation theory. To understand the field dependence of weak central-cell corrections, we assume that the forces acting on a donor electron can be derived from a scalar potential[8] which we write as the sum $-e^2/\epsilon_0 r + v_j(\vec{r})$, where $v_j(\vec{r})$ denotes the central-cell correction potential appropriate for the donor of species j. Although the general effective-mass wave function ψ_{em} is quite complicated, we can write $\psi_{em} = \varphi_1(\vec{r}) u_1(\vec{r})$ for the donor ground state in GaAs, where $u_1(\vec{r})$ is the spin-up or spin-down conduction-band-edge Bloch function and $\varphi_1(\vec{r})$ is the normalized, slowly varying envelope function appropriate to the parabolic-band ground state of a hydrogenic donor in a magnetic field.

Assuming that $v_j(\vec{r})$ is (1) of short range, (2) weak, and (3) spin independent, we obtain for the central-cell energy correction

$$\langle \psi_{em} | v_j(\vec{r}) | \psi_{em} \rangle = \kappa_j |\varphi_1(0)|^2, \quad (1)$$

where κ_j is simply $\langle u_1(\vec{r}) | v_j(\vec{r}) | u_1(\vec{r}) \rangle$.

We do not attempt here to calculate κ_j for various possible donors, but we emphasize that κ_j, unlike $|\varphi_1(0)|^2$, is independent of magnetic field.

In principle the difference between the central-cell corrections for the donors j and i in the field H can be measured directly by simply measuring the hyperfine energy differences $\Delta E_{ji}(H)$ in the hydrogenic transitions. These energy differences are given, from (1), by

$$\Delta E_{ji}(H) \equiv E_j - E_i = (\kappa_j - \kappa_i) |\varphi_1(0)|^2 \equiv K_{ji} |\varphi_1(0)|^2, \quad (2)$$

where E_j is the energy of the transition associated with donor j. Note that in (2), $\Delta E_{ji}(H)$ is independent of which of the hydrogenic excited states is reached in the optical transition. This is true because only odd-parity states are reached optically from the ground state and odd-parity states, vanishing at the donor site, have no central-cell correction of their own in our model.

Parabolic-band ground-state wave functions of Ref. 5, variationally optimized at each field of interest, were employed in computing $|\varphi_1(0)|^2$. Estimated computational uncertainty is ~1% for the three lowest fields in Table I and 0.5% for the others.

Results.—In order to test our model for the field dependence of the central-cell corrections, we must convert our measurements of field separations to energy increments ΔE_{AC} at constant field strength. This requires knowing slopes of transition energies as functions of magnetic field; we have used experimental values rather than calculated for the slopes wherever possible.

The bottom-of-the-band effective mass m^* was determined from cyclotron-resonance transmission measurements at 337, 311, 195, and 190 μm, the two highest frequency transitions requiring application of bias to the sample. These measurements were fit to within 0.1% by an approximate eight-band Kane model using an energy gap of 1420 meV and a spin-orbit splitting parameter Δ of 330 meV.[9] The mass obtained, $m^* = 0.066\,50m$, was used in all donor calculations. By fitting only the two lowest field transitions in Table I and assuming that donor C is hydrogenic, we find that $\mathcal{R} = 5.8407$ meV (47.114 cm^{-1}). We believe that the actual hydrogenic Rydberg is somewhat smaller than this because it appears that the central-cell potential for donor C is negative.

The essential task remaining is to compare our experimental findings with Eq. (3). To do this we express ΔE_{AC} in units of $\mathcal{R}$ and $|\varphi_1(0)|^2$ in units

of $|\varphi_1(0)|^2$ at zero field[10] (at 13.7 and 66.8 kG, $|\varphi_1(0)|^2$ in these units is 1.03 and 1.44, respectively). Numerical values of K_{AC} are obtained by dividing the values measured for ΔE_{AC} by $|\varphi_1(0)|^2$ for the appropriate magnetic field. It is clear from the near constancy of K_{AC} shown in column 6 of Table I that our theory accounts quite well for the increase of central-cell corrections with magnetic field.

Obtaining a value of K_{AC} which remains almost constant over a magnetic field variation of close to a factor of 6 in ΔH_{CA} confirms our model of magnetic field dependence. In particular it verifies that the hfs we have observed are caused by short-range interactions located either near or on the donor center.

Summers, Dingle, and Hill[12] have studied GaAs doped with Ge, Si, Se, and S. Their narrowest lines for the 1s-2p transitions are about 10 times broader than the broadest we observe, and most lines show marked asymmetry (our lines are only very slightly asymmetric). Thus we believe that the reported central-cell shifts of these authors are not directly revelant to the behavior of isolated donors in GaAs.

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[3]By 1s or 2p states in a magnetic field in this paper we refer to hydrogenic states which, as the magnetic field goes to zero, approach the named zero-field exact states.

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[10]From (1) it is clear that κ_j has dimensions energy times volume. Effectively we are choosing to write K_{AC} in units of the GaAs Rydberg times πa_0^3 where a_0 is the hydrogenic Bohr radius in GaAs.

[11]Two laser lines separated by approximately 0.2 cm^{-1} were observed in the photoconductivity traces near the 78.4-μm wavelength. We have identified the wavelength of the stronger line as 78.45 μm (this is a known strong H_2O-laser wavelength). The relevant data in Table I are tabulated accordingly.

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Calculation of Isospin Mixing in Be^8 with Correlated Wave Functions*

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Isospin mixing in the 2^+, 1^+, and 3^+ states of Be^8 has been calculated with correlated radial wave functions obtained from reference-spectrum solutions of the Bethe-Goldstone equation. The off-diagonal matrix elements are approximately a factor of 2 larger than those calculated with oscillator wave functions and provide a very reasonable interpretation of the experimental data.

Isobaric spin is generally regarded as a fairly good quantum number for most light nuclei. A notable exception occurs in the 2^+ (16.63, 16.93 MeV), 1^+ (17.64, 18.15 MeV), and 3^+ (19.05, 19.22 MeV) levels of Be^8 for which considerable isospin mixing is known to exist.[1-3] Barker[4] has computed the mixing for these states with oscillator wave functions and has found that the Coulomb perturbation accounted for less than half of the required magnitude of the off-diagonal matrix elements.

It is well known that oscillator radial functions