



Polaizability and susceptibility in the valley orbit split states in an intense field

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Abstract

Objectives: To compute the polarizability and diamagnetic susceptibility values of a shallow donor in the valley – orbit split A_1 , T_2 , and E states of a many valley semiconductor. **Methods/ findings:** We demonstrate the enhanced values of the above quantities in the excited states, which clearly indicate a catastrophic behavior when Metal-Insulator Transition is approached. In intense magnetic fields, the polarizability values decrease as the system behaves like a harmonic oscillator. In an electric field, the magnitude of the diamagnetic susceptibility values increases.

Keywords: Many Valley Semiconductor, Si, Valley-orbit Split States, Donor Polarizability, Diamagnetic Susceptibility.

1. Introduction

Though the electronic states of a shallow donor in a many valley semiconductor has been investigated over the last six decades, certain properties like the diamagnetic susceptibility and the polarizability in the excited E and T_2 states among the valley-orbit split states in a semiconductor such as Si have not been explored [1–4]. Experimentally, these properties have been investigated to have a better knowledge of the Metal-Insulator Transition (MIT). The values of the above quantities diverge as MIT is approached [5–11]. The reason for the non-consideration of these values in the excited valley – orbit split states are (1) the absence of a proper many valley effective mass theory [12–13] and (2) the shift of interest to low-dimensional semiconductor systems in the last three decades [14–22].

The studies on MIT in doped semiconducting systems are on the increase at present especially after the observation of MIT in a two-dimensional electron gas in semiconducting systems [23–27]. Also, it has been clearly established at present that MIT is a precursor to superconductivity [11,26–28]. In the present work, we evaluate the donor polarizabilities in all the valley-orbit split states in Si as a function of magnetic field. Also,

we evaluate diamagnetic susceptibility values as a function of electric field. These results clearly demonstrate a tendency towards divergence as the electron is taken from the A_1 ground state to the excited states.

The organization of this manuscript is as follows. In section 2, we present the theoretical background. Results and discussions are provided in section 3. We summarize the important conclusions of the present work in section 4.

2. Theory

Since the site symmetry of a substitutional donor in Si, is T_d , the donor bound states should be designated according to the different irreducible representations of the T_d group [29]. Hence the 1s ground state of the hydrogenic atom should be split into A_1 , E, and T_2 states [1]. These are referred to as valley – orbit states. Considerable attention has been paid in the past to provide a many valley theory for a donor in a many valley semiconductor. At present no such theory free from criticism exists [12–13]. We follow here a one valley theory choosing the eigen functions transforming as A_1 , T_2 , and E representations.

The Hamiltonian for a donor electron in the effective mass approximation is given by

$$\left(-\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{Kr} \right) \Psi(r) = E \Psi(r) \quad (1)$$

where m^* is the effective mass pertinent to the conduction band minimum and k is the static dielectric constant. We choose the following functions for the valley – orbit split states.

$$\begin{aligned} F_{A_1}(r) &= N_1 e^{-\frac{r}{a_1}} \\ F_{T_2}(r) &= \frac{1}{\sqrt{24}} \left(\frac{1}{a_2} \right)^{\frac{5}{2}} r e^{\frac{-r}{2a_2}} \left(\frac{3}{4\pi} \right)^{\frac{1}{2}} \\ F_E(r) &= \frac{4}{81} \frac{1}{\sqrt{30}} \left(\frac{1}{a_3} \right)^{\frac{7}{2}} r^2 e^{\frac{-r}{3a_3}} \left(\frac{5}{16\pi} \right)^{\frac{1}{2}} \end{aligned} \quad (2)$$

Since these are the basic functions of the different irreducible representations, they are orthogonal. The values of a_1 , a_2 , & a_3 are taken from a many valley calculation of donor binding energies [30]. These values are given in Table 1.

TABLE 1. Donor binding energies and wave function parameters of Eq. (2) for the valley-orbit split 1s-like states

State	E^a (meV)	Values of a_i (Å)
A_1	45.47	25.7
T_2	33.74	36.7
E	32.51	133.5

^aThese values are for P donor in Si; a_i ($i = 1, 2 \& 3$).

Two of the important properties of a doped semiconductor which require the wave functions are (1) the donor polarizability and (2) the diamagnetic susceptibility. The methods of calculation of these quantities are given below.

2.1. Donor Polarizability

For a hydrogenic donor, in a spherically symmetric state, the exact value of polarizability is given by

$$\alpha = 4.5 a^{*3} \quad (3)$$

where a^* is the orbit size of the donor electron given by $a^* = \frac{K\hbar^2}{m^* e^2}$

Here we are interested in estimating the polarizability values as a function of magnetic field. In the presence of an externally applied strong field the Hamiltonian becomes [31].

$$H = \frac{1}{2m^*} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 - \frac{e^2}{kr} \quad (4)$$

Where \vec{A} is the vector potential. In cylindrical coordinates, choosing the units for energy and length as $E = \hbar\omega_c$ and $l = \left(\frac{\hbar}{2m^*\omega_c} \right)^{\frac{1}{2}}$ and defining $\gamma = \left(\frac{\hbar\omega_c}{2R_y^*} \right)$ where R_y^* is the hydrogenic Rydberg given by $R_y^* = \frac{m^* e^4}{2\hbar^2 K^2}$, we choose the following wave function for computing the energies of the ground state (A_1 state)

$$\psi(r) = Ne^{\frac{-\rho^2}{8a^2} - \frac{z^2}{8b^2}} \quad (5)$$

Treating a and b as variational, parameters, the values of the energies obtained together with the variational parameters are provided in Table 2. The value of the magnetic field corresponding $\gamma=1$ is 154.22T in Si. The trial function given in Eq. (5) corresponds to the strong field case and is not the hydrogenic ground state function. The above function has

TABLE 2. The ionization energy and variational parameters for a donor in a magnetic field

γ	a	b	R	$E_{\text{ion}} (Ry^a)$
0.2	0.4050	0.4147	0.3710	1.0314
0.5	0.6083	0.6325	0.5599	1.2502
0.8	0.7000	0.7616	0.6542	1.4242
1	0.7280	0.8246	0.6890	1.5238
5	0.9000	1.3340	0.9320	2.6150
10	0.9382	1.6278	1.0240	3.3320
25	0.9849	2.0976	1.1570	4.5700

^a R is the radius of a spherical charge distribution obtained by $R = (3/4a^2b)^{1/3}$.

been specifically chosen to take into account the spheroidal symmetry introduced in the charge distribution in a strong field [27,32].

An interesting observation from Table 2 is that as γ increases the orbit sizes a and b also increase. It is tempting to assume that as the magnetic field increases the orbit sizes in the direction of magnetic field increases while that in the xy -plane decreases due to strong localization Table 2 reveals a different trend. This can be explained as below. In a strong field, the coulomb energy is only a small perturbation and the electron behaves almost like a free particle. As the intensity of the magnetic field increases the freedom for the donor electron from coulomb potential enhances. Hence, in the computation of polarizability for various magnetic fields one should not use the hydrogenic formula; instead treat the system as a harmonic oscillator and use the corresponding expression for polarizabilities. A simple text book exercise [31] for the polarizability of a harmonic oscillator leads to $\alpha = \frac{e^2}{mc^2}$. In the above expression $\omega = \frac{eB}{m^*c}$, the cyclotron frequency, where m^* is the effective mass of electron. Hence the polarizability of a harmonic oscillator in a Magnetic field becomes.

$$\alpha = \frac{mc^2}{B^2} \quad (6)$$

The computed values of polarizability for different values of B are given in Figures 1 and 2.

2.2. Diamagnetic Susceptibility

The diamagnetic susceptibility of a hydrogenic donor is given by the Langevin formula [33]

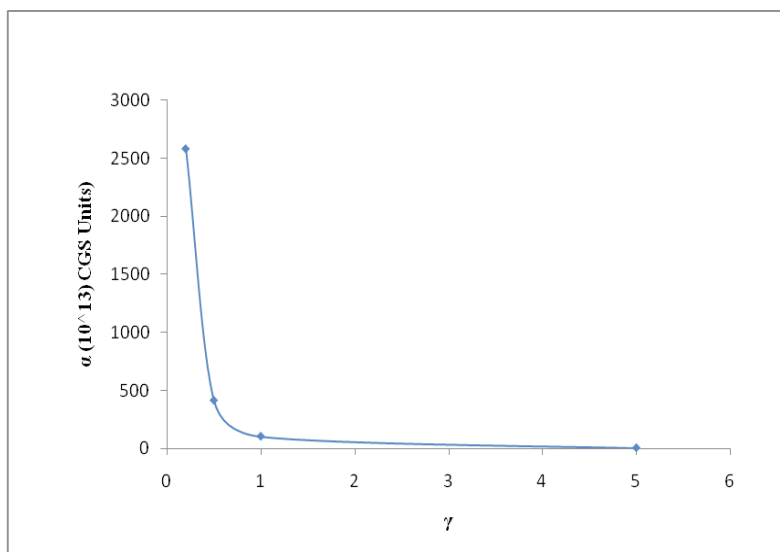


FIGURE 1. Donor polarizability versus magnetic field.

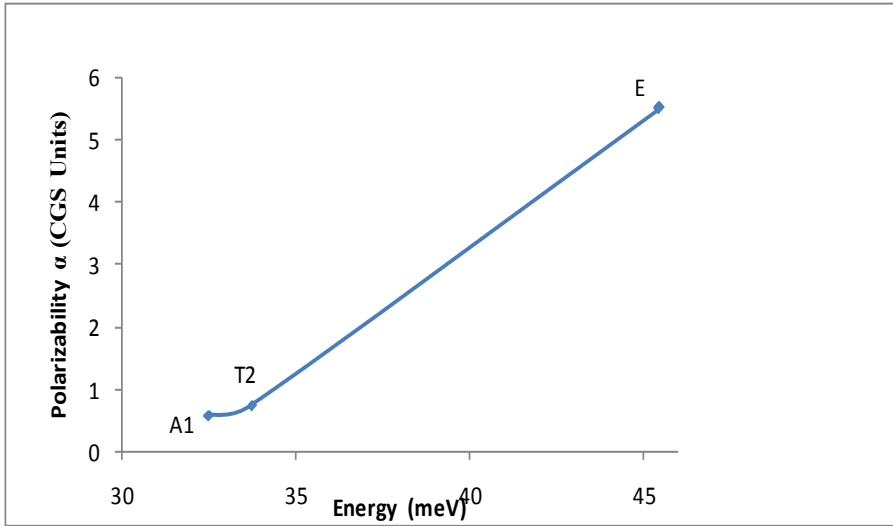


FIGURE 2. Polarizability of a shallow donor in Si in A₁, T₂, and E states.

$$\chi_{dia} = \frac{-e^2}{4m^*c^2} \langle \rho^2 \rangle$$

where $\rho^2 = x^2 + y^2$. For a spherically symmetric state $\langle \rho^2 \rangle$ may be replaced by $\frac{2}{3} \langle r^2 \rangle$. In this work, we are interested in computing the diamagnetic susceptibility in the different valley – orbit split states as a function of electric field.

We choose the following wave functions for the different states.

$$\begin{aligned} \psi_{A1} &= F_{A1} \left(1 - \frac{E}{e} a_1 r \cos \theta \right) \\ \psi_{T1} &= F_{T2} \left(1 - \frac{E}{e} a_2 r \cos \theta \right) \\ \psi_E &= F_E \left(1 - \frac{E}{e} a_3 r \cos \theta \right) \end{aligned} \quad (7)$$

In the expressions obtained for energy coefficients of the E^2 term give. The results obtained are given in Figures 3 and 4.

3. Results and Discussion

From Figure 1, we find that the donor polarizability decreases as the magnetic field increases. Physically, this corresponds to the situation where the localization is enhanced in a magnetic field. The result for $\gamma = 0$ does not follow from Figure 1.

This is because the wave function used in the magnetic field case (Eq. (5)) does not reduce to the hydrogenic case when γ approaches zero. On the other hand, if we replace a

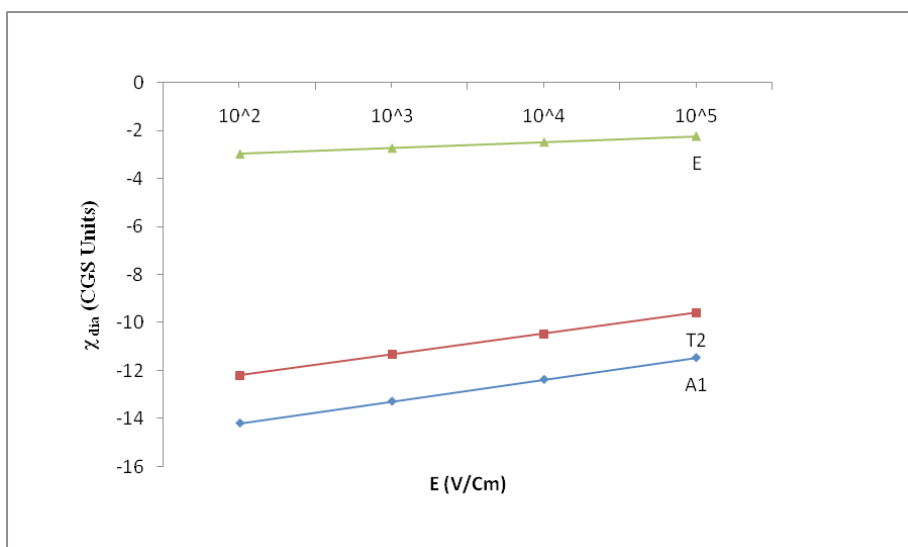


FIGURE 3. Variation of χ_{dia} of a shallow donor in Si with applied electric field.

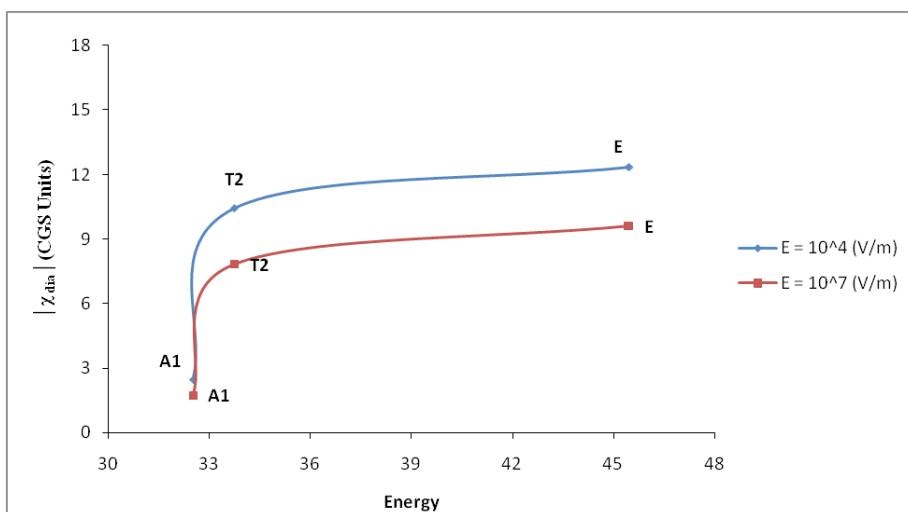


FIGURE 4. Variation of $|\chi_{\text{dia}}|$ of a shallow donor in Si with energy. The three points correspond to A_1 , T_2 , and E states.

spheroidal charge distribution in a magnetic field to an effective spherical charge distribution such that $a^2b = a^{*3}$, the magnetic field increase a^* values also increase indicating enhanced polarizability in a magnetic field which is in contradiction to expectations. In Figure 2, we have given this value of α for the three states. The enhancement of polarizability values is evident

Figure 3 gives the variation of χ_{dia} with electric field. We find that χ_{dia} values increase with electric field linearly. As expected the susceptibility values increase for any electric field as we go from the ground state of A_1 symmetry to the excited states.

In Figure 4, we have plotted the magnitude of χ_{dia} for the three states in two different electric fields. Appreciable enhancement of the susceptibility values in the excited states is obvious. Experimentally, χ_{dia} and α are shown to diverge at MIT [7,34] is approached under heavy doping. We have not considered the effect of different donors on the ionization energy. Instead, we have demonstrated that as the donor electron is taken to the different excited states. The enhancement in χ_{dia} and α values occur. Actually, in the presence of either an electric field (or) a magnetic field the symmetry of the donor system reduces to D_3 point group from the original T_d . In such a case, the 3-fold degenerate triplet state (T_3) should be split into A_1 and E states. In such a situation, the above results for T_3 states become unphysical.

An electric dipole transition from A_1 to E state is forbidden. However, a transition is from A_1 to T_2 and T_2 to E are allowed. Hence, in any physical process such as photo ionization or MIT, the electron may be thought of taken from A_1 to T_2 and from T_2 to E states, before entering into other excited states such as $2P_0, 2P_{\pm}$, etc. Hence the demonstration of divergences in α and χ_{dia} values in the excited states is justified.

4. Conclusions

The electric field dependent diamagnetic susceptibilities and magnetic field dependent electronic polarizabilities of a shallow donor in the different valley-orbit split states of Si have been computed. The values of these two physical quantities have been shown to enhance appreciably as the donor electron is taken away from the ground state of A_1 symmetry to the excited states T_2 and E. These results clearly lend support to the observation of divergences at Metal-Insulator transition, widely studied under heavy doping.

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