CHAPTER 2

CENTRAL-CELL EFFECTS ON DONOR BINDING ENERGIES

Abstract

Ionization energies and the central cell corrections have been worked out for a few shallow donors in Si, GaP and GaAs. A short range potential with two parameters (one for the strength and another for the range) for each donor, representing the central—cell effects have been assumed. These parameters are fixed using the experimentally available ionization energies for each donor in a semiconductor. In the presence of a magnetic field the donor ionization energies are estimated using a variational procedure. The results show that the ionization energies and the central —cell corrections increase with magnetic field.
I. Introduction

The Kohn-Luttinger effective mass theory [KLEMT] provides a simple model for estimating shallow donor binding energies in a semiconductor [1]. This model considers a hydrogenic atom embedded in a dielectric medium with a mass renormalization (effective mass) for the donor electron. While the excited states are described accurately, there are large deviations for the ionization energies from the predicted values based on this model. These deviations are also impurity dependent (chemical shift). In general all these deviations are referred to as central-cell corrections [2]. It is well known that these central-cell corrections are small for a direct band gap semiconductor like GaAs. For indirect gap semiconductors like Si, Ge and GaP a major central-cell correction arises due to the presence of equivalent conduction band minima in the band structure of these semiconductors. This correction is accounted for using inter-valley mixing and leads to valley-orbit splitting [3]. Several authors have attempted to include this inter-valley mixing while attempting to provide an effective mass theory in its general form [4,5]. Unfortunately none of these investigations is free from criticism and a better theory is yet to be worked out. Also use of KLEMT for a narrow gap semiconductor like InSb is questionable.

The magnitude and species dependence of the central-cell corrections arise due to deviations from a Coulombic potential, $-\frac{e^2}{\varepsilon_0 r}$ assumed in the KLEMT. This potential is not valid at the donor site ($r \rightarrow 0$) since the concept of the static dielectric constant breaks down there. This can be corrected by
using proper screening functions \( \varepsilon(r) \), which approach the value \( \varepsilon_0 \) as \( r \to \infty \). This modification cannot reflect the chemical shift since the screening function is a host property. This correction is less than 10% of the donor ionization energies in most semiconductors [6].

One contribution to this central-cell correction, which reflects the donor dependence, is the size effect. This arises due to the fractional oversize (or undersize) of the donor ion. Some attempts have been made to estimate this contribution [7]. Unfortunately, no rigorous theory explaining the deformation of the lattice as a function of distance is available. When the potential seen by the donor electron is worked out using the available atomic functions, the size effect is not considered separately [8].

In a recent work, Heron et al.[9] have estimated the central-cell corrections for Si and S donors in GaAs in strong magnetic fields. From their experimental data and using a simple model provided by Fetterman et al.[10], they have shown that the central-cell corrections increase with magnetic field. While the general behavior of the variation is the same for both these donors, the variation with magnetic field is a little faster for S than Si. They also suggest that the difference in the central-cell correction between these two species arises due to the difference in atomic volume (size effect).

In the present work, it is shown that their results follow from a more detailed variation calculation using a model potential to represent the central-cell effects. The results are given for a few impurities in GaAs, GaP, and Si and the polaronic shifts of the donor ionization energies in GaAs and GaP are estimated. The theory is outlined in section II and the results and discussion are provided in section III.
II. Theory

A. Central-cell potential

The model potential of the form

\[ V(r) = \frac{-e^2}{\varepsilon_0 r} \left[ 1 + V_0 \exp\left( -\frac{\lambda r^2}{2} \right) \right] \]  

(1)
is employed where \( \varepsilon_0 \) is the static dielectric constant of the host semiconductor, \( V_0 \) and \( \lambda \) are parameters representing the strength and the range of the potential in the central-cell region. Note that as \( r \to \infty \), \( V(r) \) approaches a simple screened Coulomb potential. Only donor states like the ground state which have an appreciable amplitude at the donor site will be affected by the central-cell effects. For GaP and Si the valley-orbit split states with \( A_1 \) symmetry (irreducible representation of \( T_d \) symmetry) will be affected by the central-cell term.

To fix the potential parameters, available donor ionization energies in Si, GaAs and GaP semiconductors are used. In the present work, P, Si, Ge and S donors in Si, GaAs, and GaP are investigated.

The Hamiltonian for the donor electron in the absence of the magnetic field is given by,

\[ H = \frac{-\hbar^2 \nabla^2}{2m^*} + V(r) \]  

(2)

where \( m^* \) is the effective-mass of the electron at the bottom of the conduction band. Actually, one should have used the longitudinal and transverse effective-masses for Si and GaP. Instead, an average value that is commonly employed in the spherical band approximation [11] is used. These values are given in Table 1.

Using the trial wave function

\[ \Psi_0(r) = N \exp\left(-\beta r^2\right) \]  

(3)
### TABLE 1 Physical constants of semiconductors

<table>
<thead>
<tr>
<th>Host</th>
<th>$m^\ast$ (a.u)</th>
<th>$\varepsilon_0$</th>
<th>$R^\ast$ (meV)</th>
<th>$\alpha$</th>
<th>$\hbar\omega_{LO}$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>0.3$^a$</td>
<td>11.7$^a$</td>
<td>29.805</td>
<td>-</td>
<td>65.135</td>
</tr>
<tr>
<td>GaP</td>
<td>0.369$^b$</td>
<td>10.86$^c$</td>
<td>42.55</td>
<td>0.201$^c$</td>
<td>49.96$^e$</td>
</tr>
<tr>
<td>GaAs</td>
<td>0.0665$^d$</td>
<td>12.56$^d$</td>
<td>5.72</td>
<td>0.068$^e$</td>
<td>39.75$^e$</td>
</tr>
</tbody>
</table>

$m^\ast$: effective mass; $\varepsilon_0$: static dielectric constant; $R^\ast$: effective Rydberg; $\alpha$: Fröhlich coupling constant; $\hbar\omega_{LO}$: zone center LO phonon energy.

$^a$Ref. 6; $^b$Ref. 15; $^c$Ref. 12; $^d$Ref. 9; $^e$Ref. 14
where $\beta$ is the variation parameter and $N$, the normalization constant, the expectation value is obtained as

$$<H> = \frac{3h^2 \beta}{2m^*} - \frac{2e^2}{\varepsilon_0} \sqrt{\frac{2\beta}{\pi}} - \frac{2V_0e^2\pi(2\beta)^{\frac{3}{2}}}{\varepsilon_0(2\beta + \lambda)}$$  \hspace{1cm} (4)

The variation parameter can be obtained by demanding that $\partial<H>/\partial \beta = 0$. Assuming $\lambda^{-1/2}$ as the range of the potential whose value is chosen to be ten times the difference between the ionic radii of host and impurity atoms in each semiconductor, $\beta$ is adjusted for each value of $V_0$ so as to reproduce the experimental ionization energy for each donor in a given semiconductor. This value of $\beta$ should also satisfy the expression for $\partial<H>/\partial \beta = 0$. The values obtained by this numerical procedure are given in Table 2.

B. Donor electron in a magnetic field

Choosing the unit of length $l_0 = \sqrt{\frac{\hbar}{2m^*\omega_c}}$, the cyclotron radius where $\omega_c$ is the cyclotron frequency and the unit of energy $\hbar\omega_c$, the Hamiltonian in dimensionless form can be written as

$$H = \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{L_z^2}{2} + \frac{\rho^2}{16} - \frac{2}{\sqrt{\rho^2 + z^2}}(1 + \exp(-\lambda^2(\rho^2 + z^2)))$$  \hspace{1cm} (5)

where $\gamma = \hbar\omega_c/2R^*$ with $R^* = \frac{m^*e^4}{2\hbar^2\varepsilon_0^4}$. In Eq.(5) cylindrical coordinates are employed. Again following the variational procedure the ionization energy is obtained. Following Yafet et al.[13],
<table>
<thead>
<tr>
<th>Host(impurity)</th>
<th>Magnetic field in Tesla when $\gamma=1$</th>
<th>$V_0$</th>
<th>$\lambda$ (a.u)</th>
<th>$\beta$ (a.u)</th>
<th>$E_{\text{ion}}^a$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si (P)</td>
<td>154.49</td>
<td>37.25</td>
<td>0.573</td>
<td>0.257</td>
<td>45.58</td>
</tr>
<tr>
<td>GaP(S)</td>
<td>271.29</td>
<td>32.59</td>
<td>0.78</td>
<td>0.346</td>
<td>107.0</td>
</tr>
<tr>
<td>GaAs(Ge)</td>
<td>6.57</td>
<td>330.67</td>
<td>1.756</td>
<td>0.867</td>
<td>5.88</td>
</tr>
<tr>
<td>GaAs(S)</td>
<td>6.57</td>
<td>93.04</td>
<td>0.143</td>
<td>0.069</td>
<td>5.83(6.87)</td>
</tr>
<tr>
<td>GaAs(Si)</td>
<td>6.57</td>
<td>145.85</td>
<td>0.347</td>
<td>0.169</td>
<td>5.78(5.84)</td>
</tr>
</tbody>
</table>

$^a$Numbers given within parentheses refer to O. Madelung [12]
\[ \Psi = N \exp \left( -\frac{\rho^2}{8a^2} \right) \exp \left( -\frac{z^2}{8b^2} \right) \]  
(6)

with \( N = (8\pi^{3/2} \, a^2 \, b) \,^{-1/2} \) and \( a \) and \( b \) are parameters. The expectation value of the Hamiltonian becomes,

\[
<H> = \frac{1}{8} \left[ \frac{2}{a^2} + \frac{1}{b^2} + 2a^2 - \frac{4}{\gamma \sqrt{\pi}} \ln \left( \frac{b + d}{b - d} \right) \right] - \frac{2b}{\gamma \sqrt{2cd\sqrt{\pi}}} \ln \left( \frac{b + d}{b - d} \right)
\]  
(7)

where \( c = b(1 + 4a^2 \lambda)^{1/2} \) and \( d = (b^2 - a^2)^{1/2} \).

Minimizing \( <H> \) with respect to \( a \) and \( b \) the ionization energies for various magnetic fields can be calculated. The ionization energy is given by

\[ E_{\text{ion}} = \gamma - <H_{\text{min}}>, \]  
where \( <H_{\text{min}}> \) is expressed in \( R^* \).

The ionization energies thus obtained with and without \( (V_0 = 0) \), the central-cell effects along with the variation parameters are given in Table 3.

C. Polaronic shifts

In a compound semiconductor, the donor spectrum is complicated due to interaction of the electron with the LO phonon. One uses the terminology 'dielectric polaron' for the donor electron. The consequences of such an interaction are (i) the electron mass becomes heavier (ii) a uniform shift of the entire donor spectrum by an amount \( -\alpha \hbar \omega_{LO} \), where \( \alpha \) is the Fröhlich coupling constant and \( \omega_{LO} \) the zone center LO phonon frequency, and (iii) the splitting of some of the excited states which is termed as phonon Lamb shift.

Since the coupling is weaker in semiconductors, a perturbation method is adequate. Based on the theory developed by Bajaj et al.,

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TABLE 3 Variational parameters for different Magnetic fields

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>Si(P)</th>
<th>GaP(S)</th>
<th>GaAs(Ge)</th>
<th>V_{cc}=0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>a</td>
<td>b</td>
<td>a</td>
<td>b</td>
</tr>
<tr>
<td>0.5</td>
<td>0.56</td>
<td>0.58</td>
<td>0.55</td>
<td>0.57</td>
</tr>
<tr>
<td>0.8</td>
<td>0.65</td>
<td>0.7</td>
<td>0.65</td>
<td>0.67</td>
</tr>
<tr>
<td>1.0</td>
<td>0.68</td>
<td>0.75</td>
<td>0.68</td>
<td>0.74</td>
</tr>
<tr>
<td>2.0</td>
<td>0.78</td>
<td>0.93</td>
<td>0.77</td>
<td>0.91</td>
</tr>
<tr>
<td>3.0</td>
<td>0.82</td>
<td>1.03</td>
<td>0.82</td>
<td>1.0</td>
</tr>
<tr>
<td>4.0</td>
<td>0.84</td>
<td>1.10</td>
<td>0.83</td>
<td>1.09</td>
</tr>
<tr>
<td>5.0</td>
<td>0.85</td>
<td>1.14</td>
<td>0.85</td>
<td>1.12</td>
</tr>
<tr>
<td>10.0</td>
<td>0.88</td>
<td>1.27</td>
<td>0.87</td>
<td>1.2</td>
</tr>
<tr>
<td>25.0</td>
<td>0.88</td>
<td>1.31</td>
<td>0.88</td>
<td>1.44</td>
</tr>
</tbody>
</table>

The parameters $a$ and $b$ are expressed in L.U., wherein

\[ 1 \text{ L.U. of length} = \frac{\varepsilon}{m \sqrt{2\gamma}} \text{ a.u. of length.} \]
Balasubramanian and Navaneethakrishnan [14] have obtained shallow donor ionization energies in the presence of the electron–phonon coupling in strong magnetic fields. The polaronic shift in a magnetic field can be estimated by using

$$\Delta E = -\frac{m^* u^2 a^2}{\hbar^2 b \sqrt{\pi}} \exp(-4b^2/\beta^2)$$

(8)

as obtained in Ref.[14] where ‘a’ and ‘b’ are the variational parameters mentioned earlier. In Eq.(8)

$$u^2 = 4\pi \alpha \beta (\hbar \omega_{LO})^2$$

where

$$\beta^2 = \frac{\hbar}{2m \omega_{LO}}$$

and $\alpha$ is the Fröhlich coupling constant.

III. Results and discussions

Using the values of $m^*$ and $\varepsilon_0$, the variation of ionization energy with magnetic field has been determined for shallow donors in GaAs, GaP and Si. The results for GaAs are presented in Fig.1. In all these cases ionization energy increases with magnetic field as obtained by several authors [15,16]. The central-cell corrections are separately presented in Fig.2 for S and Si donors in GaAs. The central-cell corrections increase with magnetic field. On the same figure, the results of Heron et al. are also presented. While the variations are similar, the results of Heron et al. are lower for both the impurities. The deviations are more for larger magnetic fields. These deviations are attributed to the choice of the trial function chosen in the present work in contrast to the numerical values chosen by...
Fig. 1 Variation of ionization energy with magnetic field for donors in GaAs
Fig. 2 Central-cell corrections for donors in GaAs
Heron et al. Unlike the present work, Heron et al. also use the model suggested earlier by Fetterman et al.[10] namely, the central-cell correction for a donor species \( j \) is given by

\[
\Delta E_j = k_j |\varphi(0)|^2
\]

(9)

where \( \varphi(0) \) is the wavefunction evaluated at the origin (donor site) and \( k_j \) is a constant independent of the magnetic field.

A check on the trial wave function is to see how well it reproduces the \( |\varphi(0)|^2 \) values as a function of magnetic field for a donor. Usually, such data comes from EPR or ENDOR experiments. Such a result, except for zero magnetic field, does not exist for any semiconductor. The values of \( |\varphi(0)|^2 \) as a function of magnetic field can be directly obtained from the wavefunction we have used (Eq.3). These values are plotted in Fig.3 for both Si and S donors in GaAs. It is not possible to show the difference between these two donors in the plot for low magnetic fields. This result is the same as that obtained by Heron et al. in Fig.2 of their paper. It is also observed that the present values are lower approximately by a factor of 2 for all values of the magnetic field. This difference is also attributed to the choice of the wave function. Heron et al. have used experimental data of \( \Delta E_j \) as input.

Central-cell effects have been estimated for a few isocoric impurities in Si, GaP and GaAs and the results are plotted in Fig.4. In the same plot, the polaronic shifts for the donor ionization energies for GaP are also displayed. It is observed that the polaronic shifts are not only small (smaller than the central-cell corrections), but also become insignificant for intense magnetic fields. This amounts to a softening of the electron-LO phonon coupling as observed by other investigators [14]. The variation of the
Fig. 3 $\frac{|\psi(0)|^2}{|\phi(0)|^2}$ values for different magnetic fields
Fig. 4 Central-cell corrections and polaronic shifts in a magnetic field
central-cell corrections with the magnetic field in the case of GaAs is found to be slow when compared to Si or GaP. Also the central-cell corrections are large for these semiconductors. This behaviour is attributed to the multivalley nature in the conduction band minimum in Si and GaP.

The variation of donor ionization energy as a function of magnetic field has been obtained earlier by Sukumar and Navaneethakrishnan [15] for donors in Si and GaP. These authors have employed a central—cell potential of the form

\[ V_{cc} = -V_0 \exp\left(-\frac{r}{w}\right) \]  \hspace{1cm} (10)

similar to a Yukawa potential or Thomas Fermi potential in contrast to a form used in the present work (see Eq.1). The actual values of the central—cell corrections depend upon the choice of the central-cell potential representing the central-cell effects. In Fig.5, the present results for P donors in Si and S donor in GaP are compared with those obtained in Ref.[15]. From this Fig.5, it is noticed that for the case of S donor in GaP these two results differ by a factor of 2 for large magnetic fields. However, for the case of P donor in Si or for small magnetic fields (\(\gamma<1\)), the results are similar.

Fig.6 displays the plot of the Fermi contact term, viz. \(|\phi(0)|^2\) values for isocoric impurities in the three semiconductors. These results are similar to the variation observed earlier in Fig.3.

Heron et al. suggest that the difference in central-cell corrections between Si and S in GaAs reflects the difference in the atomic volume. They have not done any detailed calculation in support of this conjecture. Even though no rigorous theory exists to take into account this so-called
Fig. 5 Central-cell corrections for different model potentials
Fig. 6 Probability ratio for isocoric impurities as a function of magnetic field.
deformation correction, there exist some rough estimates in literature [7,17].

The ionic radii of few elements are given in Table 4. Based on the theory of Weinreich [7], Schechter [17] has given the following expression for the deformation corrections due to the difference in ionic radii (between an impurity and the host atom)

$$\Delta E = -4 \Xi_d r_0 \Delta r/\alpha_0^2$$

(11)

where $\Xi_d$ is the deformation potential constant, $r_0$ the tetrahedral covalent radius of the donor atom, $\alpha_0$ is the radius of the impurity ground state, and $\Delta r$ the difference between the tetrahedral covalent radii of the impurity and the host atoms. The results obtained by Schechter are presented in Table 5 for different donors in the three semiconductors. While these corrections are small, usually <10% of the ionization energies, for certain impurities like Te in GaP and Sb in Si, they are about 50% of the donor ionization energy values. As Schechter has pointed out, a better theory is yet to be worked out.

It is interesting to note that these deformation corrections may also be worked out in the following way. The change in energy due to forcing an impurity atom of a different radius into a substitutional site in a semiconductor will result in an additional energy

$$\Delta E = (V_h^2 - V_1^2)/KV_h$$

(12)

where $K$ is the compressibility of the host, $V_h$ and $V_1$ are the volume occupied by the host and impurity atoms respectively. If $N_d$ is the number of donor atoms available per unit volume, a fraction equal to $4\pi a_0^3 N_d/3$ is the number effective in deciding the central-cell correction due to the deformation of the lattice. Taking $N_d = 10^{14}$ cm$^{-3}$, the deformation corrections are worked out and presented in Table 5. These corrections are found to be
TABLE 4 Ionic radii of atoms in tetrahedral coordination

<table>
<thead>
<tr>
<th>Element</th>
<th>Ionic radius (Å)</th>
<th>Element</th>
<th>Ionic radius (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>1.17</td>
<td>As</td>
<td>1.18</td>
</tr>
<tr>
<td>Ge</td>
<td>1.22</td>
<td>Sb</td>
<td>1.36</td>
</tr>
<tr>
<td>Ga</td>
<td>1.26</td>
<td>S</td>
<td>1.04</td>
</tr>
<tr>
<td>P</td>
<td>1.1</td>
<td>Te</td>
<td>1.32</td>
</tr>
</tbody>
</table>

\[\textsuperscript{a} \text{Ref. 21}\]
TABLE 5 Deformation corrections due to difference in ionic radii between host and impurity atoms

<table>
<thead>
<tr>
<th></th>
<th>Donors in GaAs</th>
<th>Donors in GaP</th>
<th>Donors in Si</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Si  S  Ge</td>
<td>Si  Te  Ge  S</td>
<td>P  As  Sb</td>
</tr>
<tr>
<td>ΔE(meV)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Schechter@</td>
<td>0.311 0.43 0.144</td>
<td>10.73 -29.59 0.974 6.36</td>
<td>6.13 -9.39 -20.56</td>
</tr>
<tr>
<td>ΔE (meV)a</td>
<td>0.593 0.72 0.29</td>
<td>0.26 -0.97 0.13 0.14</td>
<td>0.47 -0.08 -2.24</td>
</tr>
<tr>
<td>Present work</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* For GaAs, $N_d$ is chosen to be $10^{14}$ cm$^{-3}$; for GaP and Si, $N_d$ is $10^{16}$ cm$^{-3}$.

@ Ref.[17]
one or two orders smaller than those obtained by Schechter. In a few cases, the corrections are negative as in the work of Schechter. Only in the case of GaAs, these corrections are appreciable, namely, about 10% of the donor ionization energies. Also for this case the present results are approximately twice the results obtained by Schechter. Hence it follows that the conjecture by Heron et al. is correct. However, for Si and GaP the corrections are too small and deformation correction can completely be dropped in estimating the central-cell correction. As mentioned earlier, in these indirect bandgap semiconductors, the major cause of the central-cell correction is the presence of equivalent conduction band minima. Since the inter-valley separation is of the order of $2\pi/a$, where ‘$a$’ is the lattice constant, the spatial extent of this separation is of the order of $10^{-8}$ cm. Hence the inter-valley effects may also be termed as a component of central-cell correction. Since the symmetry becomes lower, this central-cell effect will split up hydrogenic states into states of $A_1$, $E$ and $T_2$ symmetries of the $T_d$ group (site symmetry of the donor).

To see the merit of the trial function (Eq.6) used, the above calculations are repeated with another function $\psi=N(1+\beta r^2)e^{-\alpha r}$ with $\alpha$ and $\beta$ as variational parameters. This wave function is an approximate form of $\exp[-\alpha r-\beta(x^2+y^2)]$ originally used by Pokatilov and Rusanove [18]. In an earlier work, Cabib et al.[19] have compared the results obtained using reference [18] and the one used by Larsen [20]. Their results show that for $\gamma>1$, the results obtained using Eq.(6) are in good agreement with the results obtained using the other two functions. As expected, Eq.(6) gives a poor estimate of the ionization energy for $\gamma<1$, the maximum deviation being 15%.
In the present calculations, an approximate form given above has been used as it leads to minimum numerical work. For central cell potential, the form given in Eq.(10) is used and the model potential parameters for S and Si in GaAs, P in Si and S in GaP are given in Table 6. The ionization energies obtained are for GaP using YKA (Ref.13), PR[18] and an approximate form given above [PR(M)] are presented in Fig.7. For lower fields ($\gamma<1$) PR and PR(M) functions give better results than YKA function whereas for higher fields ($\gamma>1$) the results of YKA are closer to PR(M) function. The corresponding oscillator strengths are plotted in Fig.8. While the results obtained by PR and YKA give similar variations with $\gamma$, PR(M) function gives larger oscillator strengths. The variational parameters in the case of PR(M) function are given in Table 7.

The ionization energies obtained using the central-cell effects for S donor in GaP and P donor in Si are given in Fig.9 using YKA and PR(M) functions. This figure shows that for larger fields ($\gamma>1$), the YKA function gives larger values. For the same system, the oscillator strengths for various magnetic fields are plotted in Fig.10. From this figure it follows that the PR(M) function gives larger values than the corresponding YKA function.

The central-cell corrections for various magnetic fields are plotted in Fig.11 for S and Si donors in GaAs. It follows from this figure that the YKA function gives larger central-cell effects when compared to the PR(M) function. The central-cell corrections are more for S donor than for Si donor, a result similar to Fig.2. The oscillator strengths for S donors in GaAs obtained using two different trial functions are given in Fig.12. For comparison, the experimental results of Heron et al. are also plotted and the experimental results lie in between the results obtained using these two trial
TABLE 6  Potential parameters for a few donors using

\[ V_{cc} = \frac{-2V_0 \exp(-\lambda r)}{\lambda r} \]

<table>
<thead>
<tr>
<th>Host (Impurity)</th>
<th>( V_0 ) (a.u)</th>
<th>( \lambda ) (a.u.)</th>
<th>( \beta ) (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si(P)</td>
<td>47.45</td>
<td>29.53</td>
<td>1.1</td>
</tr>
<tr>
<td>GaP(S)</td>
<td>43.43</td>
<td>26.0</td>
<td>1.6</td>
</tr>
<tr>
<td>GaAs(S)</td>
<td>37.57</td>
<td>71.5</td>
<td>0.86</td>
</tr>
<tr>
<td>GaAs(Si)</td>
<td>38.84</td>
<td>111.23</td>
<td>0.9</td>
</tr>
</tbody>
</table>
TABLE 7 Variational parameters for different magnetic fields using PR(M) function with $V_{cc} = -\frac{2V_0 \exp(-\lambda r)}{\lambda r}$

(The parameters $\alpha$ and $\beta$ are expressed in L.U.)

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>GaP (S)</th>
<th>Si(P)</th>
<th>GaAs(S)</th>
<th>GaAs(Si)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\alpha$</td>
<td>$\beta$</td>
<td>$\alpha$</td>
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Fig. 7 Variation of Ionization energy with magnetic field for GaP(S)
Fig. 8 Variation of oscillator strength with magnetic field
Fig. 9 Variation of ionization energy with magnetic field with central-cell effect
Fig. 10 Variation of probability ratio with magnetic field

PR(M)-GaP(S)  
PR(M)-Si(P)  
YKA-GaP(S)  
YKA-Si(P)
Fig. 11 Variation of central cell correction with magnetic field
Fig. 12 Variation of probability ratio with magnetic field for S donors in GaAs
wave functions. As observed earlier, the PR(M) function gives larger values for oscillator strength.

In Fig. 13 the central-cell corrections for various magnetic fields for P donor in Si and S donor in GaP are plotted. The results obtained by Sukumar et al. [15] using YKA function yield larger central-cell corrections for all magnetic fields (γ > 1).

To conclude, for weaker fields (γ < 1) YKA function gives a poor estimate of donor ionization energies. This can be easily seen that as γ → 0, this function does not reduce to the hydrogenic form. However, for strong fields, since there is a reduction in the orbital size in the transverse plane and due to the fact that the free particle behaviour is harmonic oscillator like, the product Gaussian leads to better results.
Fig. 13 Variation of central-cell correction with magnetic field
References