Effect of Tilted Electric Field and Magnetic Field on the Energy Levels, Binding Energies and Heat Capacity of Donor Impurity in GaAs Quantum Dot

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The Hamiltonian of an electron confined in a parabolic quantum dot in the presence of perpendicular magnetic field, donor impurity, and tilted electric field, has been solved by employing an exact diagonalization method. All the energy matrix elements have been derived in analytical forms. We have displayed the variation of the computed energy levels, binding energy and heat capacity of the quantum dot with the physical Hamiltonian parameters like: external magnetic and electric fields, confining strength, tilt angle and temperature. It’s found that the binding energy increases as the magnetic field increases. However, it decreases as the electric field increases. The dependence of the heat capacity on the electric field and magnetic fields and impurity has also been investigated. The calculated results show that heat capacity increases as the electric field increases, while it decreases with the enhancement of the magnetic field. In addition, the presence of the donor impurity is found to enhance the heat capacity. The present results are consistent with those reported in the literature.

Keywords: Heat capacity, Quantum Dot, Binding energy

1 Introduction

Technological advancement necessitates smaller and faster machines. As a result, nanoscience has become a fertile ground for researchers, to investigate the properties of low-dimensional heterostructures. Among these structures, quantum dots (QDs) have attracted the attention of many researchers due to their tunable properties and ability to be fabricated in a variety of shapes and sizes. Several experimental and theoretical studies have been made out to explore the effects of applied magnetic and electric fields, pressure, temperature, impurity, and Rashba interaction on the electronic and thermomagnetic properties of QDs.

The study of hydrogenic impurity in the low dimensional structure has a great influence on the electron’s mobility, electronic, magnetic and optical properties. Rezaei et al. had studied the effects of external fields on the spectral properties of the donor impurity by direct numerical integration method, where the energy matrix elements had been performed numerically. In this work, we will implement the Exact Diagonalization Method (EDM) to investigate the system of the donor impurity in a QD in the presence of external fields and then use the computed spectra to calculate the thermal quantities like heat capacity ($C_v$). All the matrix elements in the QD Hamiltonian are produced and given in a closed analytic form which greatly simplified the process of computing the numerical results.

We consider a QD which is made from Gallium Arsenide (GaAs) encircled by a semiconductor hetero structure made of Aluminum Gallium Arsenide (AlGaAs) with a parabolic confinement potential. We consider a confined electron in the XY-plane with a uniform magnetic field $B$ applied along $Z$ direction, and a tilted electric field ($F$) with angles $\theta$ and $\phi$ as illustrated in Fig. 1 with the presence of lateral parabolic confinement potential and hydrogenic impurity.

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2 Theory

The required steps which lead to computation of the desired QD spectra are discussed in this section which are: (i) QD Hamiltonian of donor impurity in presence of external fields (ii) calculation of the energy matrix expressions, (iii) statistical average energy and (iv) heat capacity.

The Hamiltonian of a QD in two-dimensions (2D), is given by:

$$\hat{H} = \frac{\mathbf{p}^2}{2m^*} + V_c(r)$$  \hspace{1cm} (1)

$m^*$ and $\mathbf{p}$ is the electron’s effective mass and its kinetic momentum, respectively, $V_c(r)$ is the confinement potential, in present work, the confinement takes the parabolic form with frequency $\omega_0$ as:

$$V_c(r) = \frac{1}{2} m^* \omega_0^2 r^2$$  \hspace{1cm} (2)

In this study, we looked at several physical parameters such as magnetic field, titled electric field, and impurity, all of which have a significant impact on the Hamiltonian of the system.

The vector potential $\mathbf{A}$ includes the effect of a magnetic field, as:

$$\mathbf{A} = \frac{\mathbf{B} \times \mathbf{r}}{2}$$  \hspace{1cm} (3)

Where, $\mathbf{r}$ denotes the electron’s radial position, and $\mathbf{B}$ denotes for the magnetic field strength. The effect of the donor impurity arises in the Hamiltonian as a new attractive coulomb type term $(-\frac{e^2}{\mathbf{A}})$, where, $e$, $\mathbf{A}$ is the electron’s charge and the GaAs dielectric constant, respectively. We used effective Bohr radius $a^*$ (effective Rydberg $R^*$) as a unit for length (energy) in our calculations.

The effect of electric field can be seen in the Hamiltonian as $\mathbf{F} \cdot \mathbf{r} = -e F \sin \theta \cos \phi$. Where, $F$ is the electric field strength, $\theta$ and $\phi$ are angles illustrated in Fig. 1, $\mathbf{F}$ and $\mathbf{r}$ are the polar coordinates, while the tunable parameter $\theta$ describes the angle between $\mathbf{F}$ and the Z-direction.

The total Hamiltonian using the polar coordinate $(r, \phi)$ is given by

$$\hat{H} = \frac{\mathbf{p}^2}{2m^*} + \frac{e^2}{r} + e \mathbf{F} \cdot \mathbf{r} + \frac{1}{2} m^* \omega_0^2 r^2$$  \hspace{1cm} (4)

Choosing the symmetric gauge for vector potential, $\mathbf{A} = B (-y, x, 0)$, the QD Hamiltonian can be written as:

$$H = \frac{\mathbf{p}^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 r^2 + \frac{1}{8} m^* \omega_2^2 r^2 - \frac{e^2}{e r} + e F r \sin \theta \cos \phi + \frac{1}{2} h \omega_c L_z$$  \hspace{1cm} (5)

Where, $s(L_z)$ denotes the electron spin (z-component of angular momentum)

The total Hamiltonian given by Eq.5 can be separate for two Hamiltonians as:

$$H = H_0 + H_1$$  \hspace{1cm} (6)

Where,

$$H_0 = -\frac{\hbar^2}{2m^*} \nabla_r^2 + \frac{1}{2} m^* r^2 \left( \frac{1}{2} \omega_c^2 + \omega_0^2 \right)$$  \hspace{1cm} (7)

and,

$$H_1 = -\frac{e^2}{e r} + e F r \sin \theta \cos \phi + \frac{1}{2} h \omega_c L_z$$  \hspace{1cm} (8)

Where, $\omega_c$ is magnetic field cyclotron frequency given by:

$$\omega_c = \frac{e B}{m^*}$$  \hspace{1cm} (9)

$H_0$ is a Hamiltonian for harmonic oscillator with effective frequency $\omega_{eff}$.

$$\omega_{eff}^2 = \frac{1}{4} \omega_c^2 + \omega_0^2$$  \hspace{1cm} (10)

with well-known eigen energy $E_{nm}$ and eigen function $\Psi_{nm}$, given by Fock-Darwin states:

$$\Psi_{nm}(r, \phi) = N_{nm} \frac{e^{im\phi}}{\sqrt{2\pi}} \left( \beta r \right)^{|m|} e^{-\frac{\beta^2 r^2}{2}} L^{|m|}_n \left( \beta^2 r^2 \right)$$  \hspace{1cm} (11)

and,

$$E_{nm} = (2n + |m| + 1) h \omega_{eff}$$  \hspace{1cm} (12)

$L^{|m|}_n$, referred to the Laguerre polynomial, $n$ and $m$ is the radial and magnetic quantum numbers, respectively, where the constant $N_{nm}$ is obtained from normalization condition to be:

$$N_{nm} = \frac{1}{\sqrt{\left( 2n + |m| \right)!}}$$  \hspace{1cm} (13)

with

$$\beta = \left( \frac{m^2 \omega_{eff}}{\hbar} \right)^{1/2}$$  \hspace{1cm} (14)
The fact that the presence of second part in Eq. 6, makes it impossible to achieve the analytical solution. As an effective technique, we use EDM to solve the QD system. In order to reach our goal, we aim to construct a Hamiltonian matrix as:

\[ H_{mm,\nu m} = \langle \Psi_{nm} | \hat{H} | \Psi_{nm} \rangle \]  

(15)

The QD eigen values are then computed by diagonalizing the matrix \( H_{mm,\nu m} \). An important step, in this work, was to produce the integrals of the energy matrix elements \( H_{mm,\nu m} \) in the simplest closed form in order to reduce the computational amount of time required for the diagonalization process.

The Hamiltonian matrix elements are derived in the following form:

\[ \langle \Psi_{nm} | H_0 | \Psi_{nm} \rangle = (2n + |m| + 1) \alpha \delta_{nm} \]  

(16)

\[ \langle \Psi_{nm} | \frac{1}{2} \hbar \omega_c L_z | \Psi_{nm} \rangle = \left( \frac{1}{2} \right) m \omega_c \delta_{nm} \delta_{\nu m} \]  

(17)

\[ \langle \Psi_{nm} | - \frac{e^2}{\epsilon r} | \Psi_{nm} \rangle = -2 \frac{e^2}{\epsilon} \int_0^{\infty} \Psi_{nm}^* \Psi_{nm} \frac{1}{r} \Psi_{nm} r dr d\phi \]  

(18)

To perform the integral for radial part, we use of the Laguerre’s polynomial relation \[ e^{-x} e^{\alpha x} L_n(x) L_m(x) = \sum_k \frac{(-1)^k}{k!} \frac{\Gamma(n+\alpha)(\alpha)_k}{(n+\alpha)_k} \frac{\Gamma(n+\alpha+1)}{(n+\alpha+1)_k} \frac{\Gamma(n+\alpha+2)}{(n+\alpha+2)_k} \]  

(19)

So, the impurity matrix term in Eq. 19, is derived to be:

\[ \langle \Psi_{nm} | - \frac{e^2}{\epsilon r} | \Psi_{nm} \rangle = \]  

\[ \frac{2 \Gamma(n+\alpha+1)(\alpha)_k}{n! \alpha!} \sum_{j=1}^{\infty} (-n)(n+1)j^2 \sum_{k=1}^{\infty} (-n)(n+1)k^2 \]  

(20)

Now, to simplify the matrix element of the electric field term, reads as:

\[ \langle \Psi_{nm} | eF r \sin \theta \cos \phi | \Psi_{nm} \rangle = \]  

\[ \sqrt{2F} \sin \theta \int_0^{\infty} 2\pi \Psi_{nm}^* \Psi_{nm} r^2 dr \cos \phi d\phi \]  

\[ \]  

(21)

In the last equation, the integration over \( \phi \) isn’t (2\pi), due to the presence of (cos \( \phi \)), so to evaluate the integral, one can write \( \cos \phi \) to be equals \( e^{-\phi} + e^{i\phi} \).

After using the relation in Eq. (19) we had two terms, \( e^{-\phi} \) and \( e^{i\phi} \) multiplied by \( \Psi_{nm}^* \); and these terms shifts \( m \) to \( m-1 \) (\( m \) to \( m+1 \)), respectively, yielding selection rules as \( \delta_{m,m-1} \delta_{m,m+1} \). the complete expression of Eq. 21 can be given as,

\[ \langle \Psi_{nm} | eFr \sin \theta \cos \phi | \Psi_{nm} \rangle = \]  

\[ \frac{\sqrt{2F} \sin \theta}{4} \]  

\[ \frac{\Gamma(m+1)(m+1) \sum_{j=1}^{\infty} (-n)(m+1)j^2 \sum_{k=1}^{\infty} (-n)(m+1)k^2}{\Gamma(m+1)(m+1) \sum_{j=1}^{\infty} (-n)(m+2)j^2 \sum_{k=1}^{\infty} (-n)(m+2)k^2} \]  

(22)

Now, after calculating all the energy matrix elements, our Hamiltonian matrix \( H_{mm} \) is ready, for diagonalization and obtaining the desired energy. These obtained QD energy spectra are used to investigate the dependence of \( (C_v) \) of QD on parameters \( (\theta, B, F, T \) and \( \omega_0) \) in addition to donor impurity. \( C_v \) is defined as the amount of heat required to change the temperature of that substance by one degree, and it can be computed using the temperature derivative of the statistical energy \[ 40]:

\[ C_v = \frac{\partial (E(B, F, \theta, \omega_0, T))}{\partial T} \]  

(23)

3 Results and Discussion

In this work, all energy values are measured in units of effective Rydberg, as mentioned earlier. The computational work began with the first step which is to make sure that the computed energies by EDM are very accurate results. In our calculations, we changed the number of basis until convergent energy was achieved for various: \( \omega_c, \omega_0 \) and \( F \) listed in Tables (1-3). Furthermore, in Fig. 2 we have presented the number of basis effect on the ground state energy \( (E_g) \).Based on these convergency test, in our calculations, we have used a Hamiltonian matrix with dimensions: \( 72 \times 72 \), where we have obtained

<table>
<thead>
<tr>
<th>No. of basis</th>
<th>( E_g ) (meV)</th>
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</thead>
<tbody>
<tr>
<td>0</td>
<td>-14.9319</td>
</tr>
<tr>
<td>18</td>
<td>-19.7069</td>
</tr>
<tr>
<td>30</td>
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<tr>
<td>42</td>
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<tr>
<td>54</td>
<td>-20.2154</td>
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<tr>
<td>66</td>
<td>-20.2155</td>
</tr>
<tr>
<td>78</td>
<td>-20.2155</td>
</tr>
<tr>
<td>90</td>
<td>-20.2155</td>
</tr>
</tbody>
</table>

Table 1 — \( E_g \) vs. the basis of the matrix, at \( \omega_0 = 3R^* \), \( \omega_c = 2R^*, F = 5 R^* \).
numerical stable energy results listed in Table 3. Tables (1-3) and Fig. 2 show clearly the numerical stability of the energy matrix Hamiltonian. For example, \( E_g \), in Table 1, is converged to -15.65 although the number of basis increases from 66 to 90. After achieving the desired convergency, we calculate the binding energy \( B.E \) of impurity in QD and present the results of the donor impurity under several QD physical parameters. In Fig. 3, we have plotted \( B.E \) against the magnetic field cyclotron frequency \( \omega_c \). The Figure shows that \( B.E \) increases as \( \omega_c \) increases. This \( B.E \) behavior is expected due to presence of a magnetic field which adds new parabolic confinement term for the electron as can be seen from Eq. 10 and that rises \( B.E \). We have also shown the dependence of \( B.E \), on the magnetic field for various confinements, \( \omega_0 = 4R^*, 6R^*, \) and \( 8R^* \). The qualitative comparisons show that as the confinement frequency increases, the binding of the impurity enhances, as shown clearly in Fig. 3.

In addition, we have examined, in Fig. 4, the effect of electric field on the \( B.E \) for different values of \( \omega_0 \). As shown in the figure; \( B.E \) decreases, as \( F \) increases, since the field appears to detach the electron from the nucleus and drive it further, which leads to less Coulomb interaction energy, and in this case, \( B.E \) decreases. The numerical \( B.E \) results are also presented in Table 4.

Figure 5 shows the change in \( B.E \) due to the change of the tilted angle of the electric field \( \theta \). In that figure, as \( \theta \) increases, the component of electric
field increases, having the same effect on $B.E$ as $F$ increases, and the figure also shows the dependence of $B.E$ on the electric field. All the results shown in the figures mentioned above are in good qualitative agreement with the reported results in 37,43.

As an essential quantity to achieve the desired results for the QD's thermal properties, we calculated the statistical energy $<E>$, from which one can find $C_v$, as defined in Eq. (23). The electric field effect on $<E>$ is plotted in Fig. 6. The figure shows that, for fixed $\omega_e$-values, as the electric field strength gets higher, $<E>$ decreases due to larger separation distance between electron and impurity.

In Fig. 7, for fixed values of temperature, as $B$ increases, so does $<E>$, which is a result of the extra confinement by the magnetic field, and by changing the temperature, the figure shows that for higher temperatures, $<E>$ is greater as the electron gains more thermal energy, and this behavior is consistent with the results reported in 41. The effect of $\omega_0$ on $<E>$ of the donor impurity is presented in Fig. 8, where we can see that, for fixed values of $\omega_e$, $<E>$ enhances significantly as the $\omega_0$ increases.

This result is in qualitative agreement with 41. In addition, Fig. 9 shows the changing of the tilt angle $\theta$ affects $<E>$, since as $\theta$ increases, the electric field term increases. In this case, $B.E$ of the impurity decreases since the Coulomb energy reduces, ($\sim 1/r$) also, as we explained earlier in the discussion. The
presence of impurity on $<E>$ of the electron is very important and is found to reduce $<E>$ as shown in Fig. 10 due to the negative coulomb energy contribution. This in turn affects the thermal properties of the QD.

Furthermore, we have investigated $C_v$ of the electron confined in a QD taking into account various physical QD parameters. The variation of $C_v$ as a function of temperature for different strength of electric field are shown in Fig. 11. The figure shows that the as the temperature increases $C_v$ reaches a 2D limit, $C_v = 2 k_B$. This limit behavior for $C_v$ is also in agreement with $^{37,43-44}$. In this case, for high values of $F$, $C_v$ is large, but at certain $T$ (about 90 K) there is intersection and a flip in the $C_v$-behavior, so at high $T(T > 90 K)$, $C_v$ is smaller for high electric fields. As $F$ increases, $B, E$ of the donor impurity decreases, and in this case, $C_v$ decreases as shown in Fig. 11. The effect of the presence of impurity on the $C_v$ is illustrated in Fig. 12 where, we can notice that for low temperature values ($T < 90 K$), $C_v$ is larger without impurity, but when the temperature gets higher, the situation is reversed, and $C_v$ is larger when there is an impurity.

Finally, the magnetic field effect on $C_v$ is presented in Fig. 13, where it shows that the effect of the magnetic field appears at high temperature ($T > 70 K$) where $C_v$ is larger as the magnetic field is smaller.
4 Conclusion

Using diagonalization method, The Hamiltonian of donor impurity in quantum dot had solved in presence of magnetic and tilted electric fields, as well as a parabolic confinement potential. We have investigated the dependence of $B,E$ onelectric field parameters (strength, tilt angle), and confinement strength. The results are in good agreement with previously published studies. Moreover, $B,E$ were investigated as a function of system tunable parameters ($\omega_c, \omega_0, F, T$). It was found that rising either $F$ or $\theta$ decreases $\langle E \rangle$. The temperature has also an important effect on $\langle E \rangle$.

As a final step, the effect of electric field on ($C_v$) was discussed. The current study shows that, at low temperature, $C_v$ is higher for higher $F$, while for higher temperatures, the situation is reversed.

References