Effect of dielectric screening function on binding energy and diamagnetic susceptibility of impurity doped in GaAs conical quantum dots.

E Iqraoun 1, A Salı 1 and K El – Bakkari 1

1 Department of Physics, Sidi Mohamed Ben Abdellah University, Faculty of Science, B.P.1796. Dhar El Mahraz, Fez, Morocco.

Corresponding author. elhassaniqra@gmail.com

Abstract. In this study, we have investigated the effect of the impurity dependent dielectric screening function on the diamagnetic susceptibility and the binding energy of a shallow-donor impurity confined in a GaAs conical quantum dot (CQD). The calculations have been made within the effective mass approximation, variational method and considering an infinite confining potential. Our results suggest that the effects of the variation of geometrical parameters of CQD are playing a pronounce influence on the diamagnetic susceptibility and the binding energy. The results show that the diamagnetic susceptibility depends strongly on the impurity position and it severely affected by the geometrical parameters of CQD.

Keywords: Diamagnetic susceptibility; binding energy; conical quantum dot; impurity dependent dielectric screening function.

1. Introduction

In the last decades, semiconductors of low-dimensional (nanostructures) stay one of the most intensely studied objects because of their peculiarity with the development of new techniques for nanofabrication like laser beam, Stranski Krastanov, chemical lithography and molecular beam epitaxy. [1-3]. Among these nanostructures we find, quantum dots (QDs) with various geometrical such as spherical, cylindrical, ellipsoidal, pyramid-like, lens-shaped and cone-like and other nanostructures which have received lots of attention due to their particular electronic and optical properties. These properties can be modified by different factors such as hydrostatic pressure, temperature, the position of impurity atoms, the geometry of the structure and the effects of static magnetic or electric fields, etc. This low-dimensional quantum dot has been used in a various modern technological application [4-8].
In low dimensional semiconductor systems, the spatial dependent screening of an impurity ion caused by the valence electrons and the effect of dielectric mismatch at the interfaces play a very important role [9-13]. A. John Peter et al. [14] calculated the effects of impurity position-dependent effective mass and dielectric function of a hydrogenic donor in a quantum dot. Their results indicated that the inclusion of the spatially varying mass and dielectric function results to an increment of the binding energy. S. Rajashabala et al. [15] have investigated the effects of dielectric screening and position dependent effective mass on the donor binding energy and the diamagnetic susceptibility in a quantum well. They found that the incorporation of the effect of the impurity position dependent effective mass on the donor binding energy is more significant for systems with thin well dimensions.

In the present work, we have investigated the effect of impurity dependent of dielectric screening function on the binding energy and diamagnetic susceptibility of a hydrogenic donor impurity located in a GaAs conical semiconductor quantum dot. The results have been presented as a function of the geometrical dimensions. For this purpose, the binding energy and corresponding wave functions of an electron confined in conical QDs have been calculated by employing a variational method. The paper is constituted as follows: Section 2 contains the theoretical framework. In Section 3, we present the results and their discussion. Finally, the conclusions are given in Section 4.

2. Theoretical framework

We consider an impurity donor confined in a GaAs conical quantum dot. The Hamiltonian describing this impurity is treated in the effective mass and the parabolic band approximations:

\[
H_0 = -\frac{\hbar^2}{2m^*}\Delta + V_{\text{conf}}(x,y,z) - \frac{e^2}{\varepsilon(r)}r, \tag{1}
\]

where \(m^*\) and \(\varepsilon(r)\) are the electron effective mass and impurity dependent dielectric screening function respectively. \(V_{\text{conf}}(x,y,z)\) is the confining potential of the electron in CQDs which can be expressed by the following form:

\[
V_{\text{conf}}(x,y,z) = \begin{cases} 0 & \text{inside} \\ \infty & \text{outside} \end{cases}
\tag{2}
\]

with \(a = \tan^{-1}(\phi/2)\) and \(\phi\) the apical angle of the cone. In the absence of the impurity centre, we make a change to a new set of variables: \(u = \rho \cos(\phi),\quad v = \rho \sin(\phi),\quad \rho = \sqrt{u^2 + v^2}\) and \(w \in [0,h]\) where \(\rho \in [0,1/a]\). Then, Laplace operator in variables given with these transformations can be written in the form:

\[
\Delta_{\phi\rho w} = \frac{1}{w^2} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2 + 1} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2 \partial^2 \phi^2} \right) + \frac{1}{w^2(\rho^2 + 1)} \frac{\partial}{\partial w} \left( w^2 \frac{\partial}{\partial w} \right), \tag{3}
\]

where \(\rho \in [0,1/a]\).

Owing to the cone symmetry, the following transformations will be used for \(\phi < 90\). In this case, the parameter \(\rho\) will change in the interval. \(0 \leq \rho < 1\). The Equation (3) under the mentioned conditions will reduce to a set of three independent equations associated to each of the new coordinates \(\Psi_\phi(\phi), \Psi_\rho(\rho)\) and \(\Psi_\omega(\omega)\).

\[
\Psi(\phi, \rho, \omega) = \Psi_\phi(\phi)\Psi_\rho(\rho)\Psi_\omega(\omega), \tag{4}
\]
\[
\left\{ \begin{aligned}
\frac{\partial^2 \Psi_{\phi}}{\partial \phi^2} + m^2 \Psi_{\phi} &= 0 \\
\frac{\partial^2 \Psi_\rho}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \Psi_\rho}{\partial \rho} + \left( k_\rho^2 - \frac{m^2}{\rho^2} \right) &= 0 \\
\frac{1}{\omega^2} \frac{\partial^2 \Psi_\omega}{\partial \omega^2} \left( \omega^2 \frac{\partial \Psi_\omega}{\partial \omega} \right) + \left( k^2 - \frac{k_\rho^2}{\omega^2} \right) &= 0
\end{aligned} \right. \quad (5)
\]

It is clear that the solution of the first equation of the system has an exponential form. \( \Psi_{\phi} = C_1 e^{i m \phi} \). The solutions of the second and third equations of the system can be presented via the Bessel function, namely, \( \Psi_\rho = C_2 J_m(k_\rho \rho) \) and \( \Psi_\omega = (C_3/\sqrt{\omega})J_v(k \omega) \). Thus, the solution of the wave equation for the conical quantum dot in Cartesian coordinate system can be rewritten as [16]:

\[
\Psi(x,y,z) = \left( C_c / \sqrt{z} \right) J_v(k z) J_m \left( k_\rho \sqrt{\frac{x^2 + y^2}{z}} \right) e^{i m \phi}, \quad (6)
\]

This wave function is the product of the exponential term and a hydrogenic-like wave function term. The wave function of the correlated electron–impurity can be written as:

\[
\Psi_0(x,y,z) = N \Psi_1(x,y,z) e^{xp(-\alpha r)}, \quad (7)
\]

with \( r = \sqrt{x^2 + y^2 + (z - z_i)^2} \).

\( N \) is the normalization constant and \( \alpha \) is a variational parameter.

2.1. The Effect of Dielectric Screening Function:

The Impurity position-dependent dielectric screening function is given by:

\[
\frac{1}{\varepsilon(r)} = \frac{1}{\varepsilon_0} + \left( 1 - \frac{1}{\varepsilon} \right) e^{-\frac{r}{\beta}}, \quad (8)
\]

where \( \varepsilon_0 \) is the static dielectric constant and \( \beta \) is the screening constant [17,18].

The Hamiltonian when the effect of dielectric screening function is included can be written as:

\[
H = -\frac{\hbar^2}{2m^*} \Delta + V_{\text{conf}}(x,y,z) - \frac{e^2 \varepsilon_0}{r \varepsilon(r)}, \quad (9)
\]

The diamagnetic susceptibility of the hydrogenic donor is given by:

\[
\chi_{\text{dia}} = -\frac{e^2}{6m^* \varepsilon(r) c^2} < r^2 >, \quad (10)
\]

where \( c \) is the velocity of light and \( < r^2 > \) is the mean square distance of an electron from the nucleus [19,20].
3. Results and discussion:

We compute the donor impurity ground state binding energy and diamagnetic susceptibility in the GaAs conical quantum dot, with two fixed values of the apical angle (θ = 30° & 50°) and for an impurity localized at (0, 0, 2h/3). The input parameters for a prototypical GaAs CQD are $\epsilon = 12.35$, $e = 1.6 \times 10^{-19} C$, $c = 3 \times 10^8 m/s$ and $m^* = 0.0665 m_0$ where $m_0$ is the free electron mass.

Figure 1 shows the calculation of the binding energy of the impurity, versus the height of the CQD, with two fixed values of the apical angle (θ = 30° & 50°) and for two different cases with constant dielectric (full line), (dashed line) and with impurity dependent dielectric screening function (dotted line), (dashed-dot line). We see from the figure that the binding energy decreases as the height of CQD increases in all cases. This can be attributed to the weakening of the coupling electron–impurity with the increase of the height. Additionally, the decreasing of the apical angle starts making the electron in a smaller space (the increase of confinement), as a result, it increases the binding energy of impurity, especially for smaller cone. Moreover, it can be observed from the figure that the dielectric screening function affect strongly the impurity binding energy. Indeed, the incorporation of dielectric screening function diminishes the impurity binding energy particularly for a small cone, and this effect enhances as the apical angle of CQD becomes smaller. This behavior is the same as in the case of impurity confined in a quantum well [21] and impurity in a spherical QD [14].
In figure 2, we present the variation of the difference in the binding energy versus the QD height of an impurity confined in a CQD with and without the including the impurity dependent dielectric screening function as a function of the height of the quantum dot for two fixed values of the apical angle ($\theta = 30^\circ$ & $50^\circ$). It is clear from this figure that the dielectric screening function decreases the binding energy especially when the height of the structure becomes smaller, we can explain this behavior by the fact that the Coulomb interaction between the electron and the impurity diminishes due to the gradual weak localization of the electron wave function in the CQD, which leads to a decline of the impurity binding energy [22].

![Figure 2](image_url)

Figure 2. The variation of the difference in the binding energy with excluding and including impurity dependent dielectric screening function as a function of the cone height for two fixed values of the apical angle ($\theta = 30^\circ$ & $50^\circ$).

In figure 3, we depict the results of the magnitude $<r^2>$ of the diamagnetic susceptibility $\chi_{dia}$ as a function of the cone height of an impurity donor confined in a GaAs CQD with constant dielectric (full line), (dashed line) and with impurity dependent dielectric screening function (dotted line), (dashed-dot line) with the same parameters as in the figure 1. It is observed from the figure that for fixed value of the apical angle, the magnitude of the diamagnetic susceptibility with and without dielectric screening increases with increasing the dot size. We can explain this behavior by the reason that when the dimensions of the CQD augment, the wave function of impurity becomes less concentrated around the electron which leads to an increment on the magnitude of the diamagnetic susceptibility. The figure reveals also that for fixed values of the height and the apical angle, the expectation value of $<r^2>$ increases slightly with the inclusion of the dielectric screening function especially for small height. The latter behavior affirms the diminution of impurity binding energy with
the dielectric screening function that observed in figure 1. These results agree well with those obtained for the case in low dimensional semiconducting systems [23].

![Diagram](image)

**Figure 3.** The variation of the magnitude of diamagnetic susceptibility as a function of the cone height with constant dielectric (full line), (dashed line) and with impurity dependent dielectric screening function (dotted line), (dashed-dot line) for an impurity position located at \((0, 0, 2h/3)\).

Figures 4 and 5 present the variation of the diamagnetic susceptibility and the difference between the diamagnetic susceptibility with constant dielectric (full line), (dashed line) and with impurity dependent dielectric screening function (dotted line), (dashed-dot line) respectively as a function of the height of the quantum dot, for two fixed values of the apical angle \((\theta = 30^\circ \& 50^\circ)\) and for an impurity localized at \((0, 0, 2h/3)\). As it can be seen from figure 4, the diamagnetic susceptibility is a decreasing function of the cone height [23,25]. Furthermore, the same figure indicates that there is no appreciable change in the diamagnetic susceptibility for thick dots when the dielectric screening function is introduced. Additionally, it should be noted that the incorporation of the dielectric screening function on the diamagnetic susceptibility is important for smaller CQD (figure 5). These results in the presence of dielectric screening effect are in accordance with the previous investigation carried out by P. Nithiananthi and co-workers [23]. Their study has been focused on the effect of dielectric screening on the diamagnetic susceptibility of a donor in low dimensional semiconducting systems using the variational method within the effective mass approximation.
Figure 4. The diamagnetic susceptibility of an impurity with constant dielectric (full line), (dashed line) and with impurity dependent dielectric screening function (dotted line), (dashed-dot line) as a function of the cone height for two fixed values of the apical angle ($\theta = 30^\circ$ & $50^\circ$) and for an impurity position $(0, 0, 2h/3)$. 
Figure 5. The variation of the difference between the diamagnetic susceptibility with including and excluding the impurity dependent dielectric screening function conversely to figure 1, as a function of the cone height for two fixed values of the apical angle ($\theta = 30^\circ$ & $50^\circ$) for an impurity position $(0,0,2h/3)$.

4. Conclusion

We have investigated the effect of dielectric screening function on the binding energy and the diamagnetic susceptibility of a donor impurity confined in a conical GaAs quantum dot as a function of the geometrical parameters, by utilizing the variational method within the effective-mass approximation. We have shown that the binding energy and the diamagnetic susceptibility are strongly dependent on the size of the dot. Additionally, we have found that the inclusion of the effect of dielectric screening function leads to a diminution of the donor binding energy and the diamagnetic susceptibility. Also, we have shown that the diamagnetic susceptibility decreases drastically for large values of the dimension of the dot. Moreover, the magnitude of the diamagnetic susceptibility increases with inclusion of the effect of dielectric screening function.

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