CdS/HgS Cylindrical Core/Shell: The simultaneous effect of the hydrostatic pressure and temperature on the diamagnetic susceptibility of hydrogenic donor impurity

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Abstract. One of the most important factors of controlling the properties of the above mentioned systems is hydrostatic pressure and temperature. The effect of the hydrostatic pressure and temperature on diamagnetic susceptibility and binding energy of a center hydrogenic donor impurity has been theoretically investigated in the framework of the effective mass approximation. We describe the quantum confinement by an infinite deep potential. The results for a cylindrical Inhomogeneous quantum dots made out of [CdS (Core) / HgS (Well) / CdS (Shell)] show that (i) when the hydrostatic pressure increase, the diamagnetic susceptibility decreases and the binding energy increases. (ii) The diamagnetic susceptibility increases with the temperature.

1. Introduction

The quantum dots are known by their high quantum efficiency compared to that of quantum wells and wires; however surface states can decrease their optoelectronic performance. Indeed, the surface states trap the charge carriers which decrease their number and consequently reduce the optoelectronic performances. To overcome this problem, it has been thought that the total recovery of a quantum dot by a semiconductor quantum well different from smaller (or larger) forbidden band and of similar mesh parameter can effectively and sustainably suppress the non radiative recombination on the surface of the heart. Among the most remarkable studies, we quote: Hayrapetyan et al [1] studied the Effect of hydrostatic pressure on diamagnetic susceptibility of hydrogenic donor impurity in core/shell/shell spherical quantum dot with Kratzer confining potential. The results show that with the potential minimum point increase, the diamagnetic susceptibility increases until some critical value, after which it decreases. Surajit Saha and coworker [2] have studied Simultaneous influence of hydrostatic pressure and temperature on diamagnetic susceptibility of impurity doped quantum dots under the aegis of noise. Oyoko et al. [3] where studied the effect of a uniaxial stress on the binding
energy of a donor impurity shallow in a GaAs / GaAlAs parallelepiped quantum box using a variational approach and taking into account the position of the ionized donor. Their conclusions are in good agreement with those obtained by Elabsy [4]. The effects of hydrostatic pressure and the magnetic field on optical transitions in InAs / GaAs self-assembled cylindrical quantum dots have also been studied assuming a parabolic potential [5]. This study describes quite well the general aspects reported in experimental measurements [6-8]. Another theoretical model has been developed for a GaAs / GaAlAs quantum wire taking into account the effect of electron-hole correlations [9]. The authors studied variation of the dielectric constant and the size as a function of the pressure. They showed that the impact of these effects on binding energy is considerable. In spherical quantum dots, it has been shown that binding energy increases almost linearly with the hydrostatic pressure and that the slope depends on the radius of the box quantum [10]. The combined effects of pressure and temperature on the energy of donor binding in a double GaAs / Ga\textsubscript{1-x}As quantum well in the presence electric and magnetic fields has been studied using a variational approach [11]. Rahmani et al [12] have studied the magnetic and electric field effect on the binding energy of a shallow donor in Ga\textsubscript{1-x}Al\textsubscript{x}As-GaAs IQD. Their results show that the corrections due to the magnetic and electric field are very important and cannot be neglected or ignored and they show the existence of a critical value which can be used to distinguish the three dimensions confinement from the spherical surface confinement.

In relation to this subject, in order to contribute to the understanding of the effect hydrostatic pressure and temperature on the diamagnetic susceptibility in a cylindrical inhomogeneous quantum dot, we present a complete variational analysis of the problem of a cylindrical quantum dot taking into account the influence of the pressure and the temperature.

2. Theoretical framework

We consider a cylindrical inhomogeneous quantum dot (core/shell) type having inner and outer radii a and b, respectively, and a height H supposed to be longer than b (H >> b) (see figure 1). We assume that the two nested materials used for the core and the shell has a large band gap. CdS/HgS presents a better example: (E\textsubscript{g}(CdS) = 2.5eV and E\textsubscript{g}(HgS) = 0.5eV) [13]

In the context of the effective mass approximation, the Hamiltonian of a donor can be written in the form:

\[ H = \frac{\hbar^2}{2m_e(P,T)} \nabla_e^2 + \frac{e^2}{\varepsilon(P,T)(\mathbf{r}_e - \mathbf{r}_D)} + V_w(r_e) \]  

(1)

Figure 1. schema of a quantum dot of core / shell type with cylindrical geometry with infinite confinement potential.
Where $m_\text{e}^*$ the effective mass of electrons, $e$ is the elementary charge, $\varepsilon$ is the constant static dielectric, $r_x$ and $r_D$ are respectively the positions of the electron and the ionized donor, $V_{w\text{c}}(r_x)$ is the confinement potential, which can be written as the sum of two independent terms:

$$V_{w\text{c}}(r_x) = V_{w\text{c}}^e(\rho_x) + V_{w\text{c}}^\varepsilon(Z_e)$$  \hspace{1cm} (2)

$$\varepsilon(P,T) = \begin{cases}
1.27\exp(-1.67\times10^{-3} P)\exp(9.4\times10^{-5} (T-75.6)) & 0 \leq T \leq 200K \\
13.18\exp(1.73\times10^{-3})\exp(20.4\times10^{-5} (T-300)) & T \geq 200K
\end{cases} \hspace{1cm} (3)$$

$$m_\text{c}^*(P,T) = m_0 \left[1 + 1.71\left(\frac{E_x(P,T)}{E_x(P,T)+E_x(P,T)+\Delta_0}\right)\right]^{-1}$$  \hspace{1cm} (4)

We use the effective Bohr radius $a_B^* = \hbar^2\varepsilon(P,T) / m^*(P,T)\varepsilon^2$ and the effective Rydberg $R_B^* = m^*(P,T)\varepsilon^4 / 2\hbar^2\varepsilon^2(P,T)$ as the units of length and energy. Furthermore, we introduce the dimensionless parameter $\gamma = \frac{\hbar\omega_c}{R}$ and $\omega_c = \frac{eB}{m^*c}$ characterizing the strength of the magnetic field and the effective cyclotron frequency respectively. The Hamiltonian can be expressed in coordinates cylindrical $(\rho,\phi,z)$ as:

$$H = -\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{2}{\sqrt{\rho_0^2 + (z-Z_D)}} + V_1^\varepsilon(\rho_x) + V_2^\varepsilon(Z_e)$$  \hspace{1cm} (5)

Or $\rho_0^2 = \rho_x^2 + \rho_0^2 - 2\rho_x\rho_0\cos(\phi_x - \phi_0)$ is the electron-impurity distance in the xoy plane, $Z_e$ and $Z_D$ are the electron and impurity positions along the oz direction.

In our hypothesis, the confinement potential of the electron in the xoy plane $V_1^\varepsilon(\rho_x)$ and according to the oz direction $V_2^\varepsilon(Z_e)$ write:

$$V_1^\varepsilon(\rho_x) = \begin{cases}
0 & \text{for } a \leq \rho_x \leq b \\
\infty & \text{others}
\end{cases}$$  \hspace{1cm} (6)

$$V_2^\varepsilon(Z_e) = \begin{cases}
0 & \text{for } \left|z_e\right| \leq \frac{H}{2} \\
\infty & \text{others}
\end{cases}$$

Indeed, this approach, of infinite confinement potential, is only valid in heterostructures where the gap of the core material is much greater than the gap corresponding to the shell material. In these Conditions, the maximum probability is located in the shell area. Eq (2) does not admit an analytical solution; we try to solve it by the variational method.

$E_n^\varepsilon$ Energy of the ground state of the donor and the envelope wave function $\psi_D^0$ are solutions of the Schrödinger equation:

$$H\psi_D^0(\rho_e, Z_e, \varphi_e) = E_n^\varepsilon\psi_D^0(\rho_e, Z_e, \varphi_e)$$  \hspace{1cm} (7)

Since the Schrödinger equation cannot be solved exactly, we follow the Hass variational method. We choose the wave function for the impurity ground-state as:

$$\psi_D^0 = N\rho_e(\rho_e)g_e(z_e)\exp(-\alpha\rho_e\rho)_e\exp\beta(z_e - z_D)^2$$  \hspace{1cm} (8)
With $\alpha$ and $\beta$ are variational parameters and $N$ is the normalization constant. The corresponding energy is obtained by minimization with respect to the variational parameters $\alpha$ and $\beta$.

The ground state energy can be obtained by minimizing the average value of $H$ with respect to variational parameters $\alpha$ and $\beta$.

$$E^0_D = \min \left\{ \frac{\langle \psi^0_D | H | \psi^0_D \rangle}{\langle \psi^0_D | \psi^0_D \rangle} \right\}$$  \hspace{1cm} (9)

The binding energy of the donor impurity located at the center of a cylindrical quantum dot is given by:

$$E_b = E^0_e - E^0_D$$  \hspace{1cm} (10)

The Schrodinger equation is solved variational to find the ground state wave function, which has been used in the computation of diamagnetic susceptibility of the hydrogenic donor given as:

$$\chi_{\text{dia}} = -\frac{e^2}{6m_e^*(P,T)c(P,T)c^2} \langle \rho^2_{D} \rangle$$  \hspace{1cm} (11)

Where $c$ is the velocity of light and $\langle \rho^2_{D} \rangle$ is the mean square distance of the electrons from the nucleus. The hydrostatic pressure effect on the diamagnetic susceptibility of a hydrostatic impurity confined in a cylindrical core/shell quantum dot in the presence of a uniform magnetic field is evaluated.

3. Results and Discussion

We compute numerically the donor impurity ground state binding energy in the hollow cylindrical Inhomogeneous quantum dots made out of [CdS/HgS/CdS] under the influence of hydrostatic pressure and temperature. Taking into account the position of the impurity at the center of the shell. The variation of both the hydrostatic pressure and the temperature modify the gap energy and all shell-material parameters.

The physical parameters characterizing the system are given in the table 1:

| Material | $m^*m_0$ | $\varepsilon_0$ | $\varepsilon_0^{\infty}$ | $a^*$ (Å) | $R^*$ (eV) | $E_g$ (eV) |
|----------|----------|-----------------|-----------------|--------|----------|----------|
| CdS      | 0.2      | 9.1             | 5.5             | 5.818  | 3.65     | 2.5      |
| HgS      | 0.036    | 18.2            | 11.36           | 5.851  | 5.0      | 0.5      |

At $P =0$ and $T =300$K, we display in figure 2, the variation of the impurity binding energy as a function of the ratio $a/b$ for different values of the outer radius $b = 1a^*, 2a^*, 4a^*$ and $H=1a^*$. The ratio $a/b$ varies between 0 and 1. We remark that the binding energy increases with ratio $a/b$ increases and decreases with increases of radius $b$ the binding energy approaches the value of $4R^*$ which corresponds to the case of 2D confinement.

In figure 3, we plot the variation of the diamagnetic susceptibility as a function of the ratio $a/b$ for three values of the outer radius ($b = 1a^*, 2a^*, 4a^*$). When the ratio $a/b$ tends to 1, the diamagnetic susceptibility $\chi_{\text{dia}}$ tends to the limit which represents the case of two dimensional. We remark that the diamagnetic susceptibility presents a minimum corresponding to a certain critical value of the ratio $a/b$. From this figure, we can say that the absolute value of the diamagnetic susceptibility $|\chi_{\text{dia}}|$ increases as $b$ increases.
Figure 2. Binding energy as a function of the dot radius $a/b$ for different values of the $b = 1a^*$, $2a^*$, $4a^*$ and $H=1a^*$.

Figure 3. Diamagnetic susceptibility $\chi_{dia}$ as a function of the ratio $a/b$ for different values the radius $b$ ($b=1a^*$, $2a^*$, $4a^*$) and for $H=10a^*$.

We present in the next, the variation of the diamagnetic susceptibility $\chi_{dia}$ as a function of the ratio $a/b$ with the outer radius ($b = 1a^*$) for temperature $T=300K$ and for two values of the hydrostatic pressure ($P=0$ Kbar, $50$ Kbar) (see Figure. 4) and for different values of temperature (see Figure. 5). In all cases, the absolute value of the diamagnetic susceptibility $|\chi_{dia}|$ decreases when the thickness of the shell
decreases in ultimate value, leading to a strengthening of the Colombian term attractive. The behavior in 2D geometry (that is, when a is very close to b) has significant physical properties. Indeed, the structure behaves like a 2D topological configuration. Therefore, the approach variational, taken in the context of the effective mass approximation cannot provide a good description of all the phenomena related to this situation. In the infinite potential case, the electronic wave function confined completely in the shell when the Shell thickness becomes much narrow and cannot penetrate into the barriers. So the probability of the electron to close towards the impurity position becomes very higher. The hydrostatic pressure and temperature increases slightly diamagnetic susceptibility and the influence is more pronounced for the large shell thickness than the small shell thickness.

![Figure 4](image1.png)

**Figure 4.** Diamagnetic susceptibility as a function of the ratio $a/b$ for temperature $T=300K$ of the outer radius ($b = 1a^*$) and for two values of the hydrostatic pressure ($P=0$ Kbar, 50Kbar).

![Figure 5](image2.png)

**Figure 5.** Diamagnetic Susceptibility versus the ratio $a/b$ in absence the hydrostatic pressure of the outer radius ($b = 1a^*$) and for two values of the temperature ($T=300K$, 200K).
4. Conclusion
The binding energy and diamagnetic susceptibility of the donor was studied according to the size of the structure. Our results show that the binding energy of a donor impurity placed in the center of the cylindrical core/ shell, strongly depends on the size of the shell, it increases as the thickness of the shell becomes smaller. The diamagnetic susceptibility in absolute value $|\chi_{\text{dia}}|$ increases with the temperature and decreases with the hydrostatic pressure. On the other hand the effect of temperature and the pressure on the diamagnetic susceptibility is appreciable for large CQD.

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