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Role of a uniform magnetic field on the energy spectrum of a single donor in a core/shell spherical quantum dot

by

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Abstract

Using the variational approach within the framework of the effective-mass approximation (EMA), the binding energy of a centred hydrogenic donor impurity in a CdSe/ZnTe core/shell spherical quantum dot (CSSQD) in the presence of an external magnetic field was investigated. In this model, we have taken into account the effect of the radial dependence of the dielectric constant and of the electron effective mass. Our numerical results show a remarkable influence of the nanodot spatial parameters and of the external magnetic field strength on the shallow donor binding energy.

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1 Introduction

As is well-known, the evolution of electronic and optoelectronic devices was always related to the improvement of material properties. Most notably, their optical and electronic properties. Hence the immense need to understand the behavior of charged particles inside materials, particularly in semiconductor nanomaterials, which present the possibility to accurately control both their electronic and optical properties by tuning their size [1, 2, 3] or by the application of an external electric or magnetic field [4, 5, 6] and so on.

The behavior of shallow donors confined in semiconductor quantum dots was extensively investigated and various papers can be found in the literature, such as the study performed by Ribeiro and Latgé [7] concerning the influence of the quantum dot volume and the impurity position on the binding energy. In their investigation, the variational approach was deployed in order to get the binding energy of a shallow donor in a spherical and cubic shaped quantum dot as a function of the nanostructure spatial parameters and the impurity position. The energy spectrum of a hydrogenic donor inside a spherical nanodot was the subject of Ref. [8] that presents a comparative study between the donor binding energy calculated variationally, and by using a perturbation method. To the same end, Li *et al.* [9] have studied the electronic structures and the binding energy of a hydrogenic impurity in a hierarchically self-assembled GaAs/Al_xGa_{1-x}As nanodot. Their paper shows that the binding energy of the acceptor depends more sensitive on the size of the nanodot than that of the donor. The effects of hydrostatic pressure on the energy spectrum of a hydrogenic donor in a GaAs-Ga_{0.7}Al_{0.3}As cylindrical quantum dots was reported in Ref. [10]. It was found that the binding energy increases linearly with pressure in the low pressure regime, while in the high pressure regime the binding energy increases until a maximum value after what it decreases.

In the recent past, more particular attention was awarded to the study of core/shell materials due to their very improved properties. For example in Ref. [11] the energy spectrum of a GaAs/Al_xGa_{1-x}As/AlAs spherical quantum dot, in the presence of impurity, was performed using the fourth-order Runge-Kutta method. So as to perform a comparative study between the binding energy of a shallow donor confined in the center of a CdSe/ZnTe core/shell nanodot and ZnTe/CdSe inverted core/shell quantum dot, Chafai *et al.* [12] deployed a variational study taking into account the radial dependence of the dielectric constant on radius and using a finite confinement potential. It was found that the energy spectrum of nanomaterials is not only affected by nanomaterials size, but also by the localization of charge carriers. On the other hand, the behavior of the binding energy of a shallow donor inside core/shell ZnSe/ZnS submitted to an external magnetic field was the aim of the article of Bhat *et al.* [13]. Their study exhibits a great dependence of the binding energy on the shell thickness and the magnetic field strength. The impact of the core/shell nanodot size, the magnetic field strength and the impurity position on the binding energy was examined by Talbi *et al.* [14]. It was found that in addition to the control of the binding energy by tuning the spatial parameters and the magnetic field strength, the existence of a critical radius which depends on the heteronanodot size and on the material band offset. The impact of an external electric field on the energy spectrum of a hydrogenic donor placed at the center of a CdTe/ZnTe spherical quantum dot is the emphasis of the investigation of Stojanović and Kostić [15]. Deploying the finite difference method Yuan *et al.* [16] studied the nanodot size effect on the energy spectrum

of a donor impurity in GaAs/AlGaAs core/ shell spherical with infinite confinement potential. Then, they have investigated the third-harmonic generation susceptibility for this nanosystem using the compact-density-matrix approach. In Ref. [17] a theoretical study of the energy spectrum, optical absorption coefficients and refractive index of a centered donor confined in a multilayered spherical quantum dot can be found. The authors of this paper have shown that both the electronic and the optical properties of such system can be controlled by turning the strength of the external fields or by tailoring the nanodot size.

In this work, we present a variational study concerning the size control of the shallow donor binding energy in a spherical core/shell nanodot. The impact of the dielectric constant discontinuity at the nanostructure boundaries was also considered. Employing a trial wave function containing three variational parameters the donor binding energy in the presence of an external magnetic field was calculated in the framework of the EMA. the next section is an overview of the applied theory, while section 3 is devoted to the presentation of our numerical results.

2 Model and theory

The nanostructure under study is composed of an on-center donor inside a CdSe/ZnTe core/shell spherical nanodot submerged in a SiO₂ matrix. The global system is the subject of an external magnetic field directed along to the (**OZ**) axis. In Figure 1, a schematic description of our nanoheterostructure is sketched. Where R_C and R_S are, respectively, the inner and outer radii, while $\Delta E_c = U_e$ is the confinement potential of electrons. Within the framework of the (EMA), taking into account the dependence of the electron effective mass on radius and the interaction between the electron and its own image charge due to the dielectric mismatch, the Hamiltonian of our structure reads:

$$H_{D^0} = \left(\mathbf{P} + \frac{e}{c} \mathbf{A} \right) \frac{1}{2m_e^*(r)} \left(\mathbf{P} + \frac{e}{c} \mathbf{A} \right) + U_w(r) + U_{coul}(r) + \Sigma(R_s). \quad (1)$$

The vector potential of the applied magnetic field and the electron momentum are noted, respectively, \mathbf{A} and \mathbf{P} . While the electron mass is assumed to be $m_c^* = 0.13$ ($m_s^* = 0.15$) in core (shell) material. The electron confinement potential, the second term of Eq.(1), is considered to be zero in the core material, while it takes a finite value $U_e = 1.27$ eV [3] when the electron is hosted by the shell material. Otherwise, it becomes infinite. The coulomb interaction and the self-energy are, respectively, given as [18]:

$$U_{coul}(r) = -\frac{e^2}{4\pi \epsilon_0 \tilde{\epsilon} r} - \frac{e^2 (\tilde{\epsilon} - \epsilon_r(\text{SiO}_2))}{4\pi \epsilon_0 \tilde{\epsilon} \epsilon_r(\text{SiO}_2) R_s}, \quad (2)$$

and

$$\Sigma(R_s) = -\frac{e^2}{8\pi \epsilon_0 R_s} \left[\frac{1}{\tilde{\epsilon}} - \frac{1}{\epsilon_r(\text{SiO}_2)} \right] + 0.466 \frac{e^2}{4\pi \epsilon_0 \tilde{\epsilon} R_s} \left[\frac{\tilde{\epsilon} - \epsilon_r(\text{SiO}_2)}{\tilde{\epsilon} + \epsilon_r(\text{SiO}_2)} \right], \quad (3)$$

$\tilde{\varepsilon} = \sqrt{\varepsilon_r(CdSe) \varepsilon_r(ZnTe)} = 10.14$ [19] is the dielectric constant inside the core/shell nanostructure and $\varepsilon_r(SiO_2) = 3.9$ [20] is the dielectric constant of the surrounding medium.

In order to examine the impact of the spatial parameters and the magnetic field strength on the shallow donor binding energy we adopt a variational approach to resolve the Schrodinger equation of our system. In this optic, we have used the following trial wave function:

$$\Psi_{D^0}(r) = \Psi_e(r) e^{-\beta r} e^{-\lambda r^2}, \quad (4)$$

where $\Psi_e(r)$, is the trial wave function of the same system without impurity chosen as:

$$\Psi_e(r) = \begin{cases} N_1 \frac{\sin(\eta_1 r)}{r} e^{-\alpha r^2}, & r \leq R_c \\ N_2 \frac{\sinh(\eta_2 (r-R_s))}{r} e^{-\alpha r^2}, & R_c < r \leq R_s \\ 0, & \text{Otherwise} \end{cases} \quad (5)$$

$\eta_1 = \sqrt{\frac{2m_1^*}{\hbar^2} (E_e - \Sigma(R_s))}$, $\eta_2 = \sqrt{\frac{2m_1^*}{\hbar^2} (U_e + \Sigma(R_s) - E_e)}$. N_i ($i = 1, 2$) and α , β , λ are, respectively, the normalization constants and the variational parameters.

In this context, the energy of an electron under an external magnetic field is given as:

$$E_{D^0} = \min_{\alpha} \left[\frac{\langle \Psi_e(r) | H_e | \Psi_e(r) \rangle}{\langle \Psi_e(r) | \Psi_e(r) \rangle} \right], \quad (6)$$

while the energy of a hydrogenic donor subject to an external magnetic field reads:

$$E_{D^0} = \min_{\beta, \lambda} \left[\frac{\langle \Psi_{D^0}(r) | H_{D^0} | \Psi_{D^0}(r) \rangle}{\langle \Psi_{D^0}(r) | \Psi_{D^0}(r) \rangle} \right]. \quad (7)$$

H_e (H_{D^0}) is the Hamiltonian of the electron (donor) under an external magnetic field.

3 Numerical results

The numerical results presented in this section have performed using $\bar{R}_{D^0} = \frac{\hbar^2}{2\tilde{m}_e^* \bar{a}_{D^0}^2} = 18.478 \text{ meV}$ as unit of energy, $\bar{a}_{D^0} = \frac{\tilde{\varepsilon}_r \hbar^2}{e^2 \tilde{m}_e^*} = 3.842 \text{ nm}$ as unit of length, and the dimensionless magnetic field strength $\gamma = \frac{e \hbar B}{2 \tilde{m}_e^* c \bar{R}_{D^0}}$.

In figure 2, we plot the electron ground state energy as a function of the shell thickness in zero magnetic field ($\gamma = 0$) for various material core sizes: $R_c = 1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$. In this figure, we can observe a great dependence of the electron energy on the nanostructure spatial parameters. In other words, the increase of the shell thickness and the material core size leads to the decrease of the electron ground state energy. It is also

clear that the electron 1s energy is more sensitive to the size of the core material than to the thickness of the shell material which may be explained by the famous quantum confinement effect.

In figure 3, The donor binding energy with zero magnetic field versus the thickness of the shell material for various core radius values: $R_c=1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$ is presented. It is noticeable that the donor binding energy remarkably depends on the nanostructure spatial parameters e.g., when the inner or the outer radius values decrease the binding energy increases which is in good agreement with [21, 22].

In figure 4, we present the electron ground state energy versus the magnetic field strength for a fixed nanostructure size $R_s=2 \bar{a}_{D^0}$ and various material core sizes: $R_c=1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$. This figure shows the possibility to enhance the electron ground state energy, especially in large nanodot, by the application of a uniform magnetic field which might qualified by the existence of a competition between the two coexisting confinement type: the spatial confinement, more pronounced for small nanostructure, and the magnetic confinement more pronounced for large nanostructure.

In figure 5, we draw the donor ground state binding energy as a function of the magnetic field strength for $R_s=2 \bar{a}_{D^0}$ and $R_c=1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$. We can notice from this figure that the effect of the magnetic field is marginalized at the center of the nanodot, on the other hand, his impact on the binding energy is very remarkable near the border of the heteronanodot. That is related to the fact that the presence of an external magnetic field tends to move the charge density toward the center of large nanodot which automatically increases the binding energy. For a small nanostructure and due to the spatial confinement effect, the charge density is compressed around the center of the heterostructure that enhances the binding energy and naturally the effect of the magnetic field is marginalized. As a matter of fact, using the combination effect of an external uniform magnetic field and the core/shell quantum dot size leads to control the donor binding energy. At this spot, we want to draw attention that our results are in good agreement with those obtained in Refs [2, 22].

4 Conclusion

In this investigation, we have studied the combination effect of the spatial confinement and the magnetic field strength on the binding energy behavior of a shallow donor in a CdSe/ZnTe core/shell quantum dot. In order to make our model more realistic, we have taken into account the effect of the dielectric environment and considered a finite confinement potential. Our results provide the possibility to enhance the binding energy via the application of an external magnetic field or the control of the nanodot size. It is also shown that the effect of the magnetic field is more pronounced in regions when the binding energy is low sensitive to the effect of the spatial confinement. In the other case it is marginalized.

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6 Figure captions

Figure 1: On-center donor inside CdSe/ZnTe Spherical heterostructure.

Figure 2: The electron ground state energy as a function of the shell thickness for $\gamma = 0$ and $R_c = 1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$.

Figure 3 The donor binding energy as a function of the shell thickness for $\gamma = 0$ $R_c = 1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$.

Figure 4 The electron ground state energy versus the magnetic field strength for $R_s = 2 \bar{a}_{D^0}$ and $R_c = 1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$.

Figure 5 The donor binding energy versus the magnetic field strength for $R_s = 2 \bar{a}_{D^0}$ and $R_c = 1 \bar{a}_{D^0}$, $1.25 \bar{a}_{D^0}$ and $1.5 \bar{a}_{D^0}$.

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Figure 1









