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Photoionization cross section and Electron binding energy in multilayered spherical quantum dots: Influence of magnetic field and structural dimensions

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Abstract.

Our paper investigates the effects of a magnetic field on the binding energy of a shallow donor impurity placed at the center of a multilayered spher- ical quantum dot. Through the effective mass approximation and finite element method, we computed the electron energy levels in two settings: with and with- out a hydrogenic impurity. Our focus was on understanding the role of geomet- ric parameters-core radius, shell width, and barrier thickness-in shaping these energy levels. This study provides insights into the manipulation of quantum dot properties, which is essential for advancing applications in nanoscale elec- tronics and photonics. These findings are significant for developing innovative applications in fields like nanoelectronics, where precise control over electronic properties is crucial for designing efficient devices.

Keywords: Binding energy, multilayered spherical quantum dots, magnetic field, Finite element method.

1 Introduction

The study of quantum dots (QDs) has garnered significant attention due to their unique optical and electronic properties, which arise from quantum confinement ef- fects. Among the various types of quantum dots, multilayered spherical quantum dots (MSQDs) have emerged as a particularly interesting structure for investigation due to the tunability of their electronic states through structural modifications. MSQDs offer an enhanced level of control over electron confinement by adjusting the core radius, shell width, and barrier thickness, making them suitable for a wide range of applica- tions in fields such as optoelectronics, photonics, and quantum computing.

One of the crucial aspects in studying MSQDs is understanding the behavior of shal- low donor impurities under different external perturbations, such as magnetic fields. Donor impurities, when embedded in quantum dots, can significantly influence the electronic properties, particularly the binding energy and energy levels. The binding energy of impurities is sensitive to various parameters, including the impurity's loca- tion, the size and composition of the quantum dot, and external fields. Previous stud- ies have analyzed impurity binding energies in semiconductor quantum wells and quantum dots, demonstrating how these impurities affect carrier dynamics and optical responses [1], [2]. Research by Zhu, Gu, and Lin highlighted the role of magnetic fields in modifying the electronic states of quantum wells and quantum dots, pointing to the potential for fine-tuning electronic characteristics through applied fields [3].

The theoretical framework for analyzing impurity states in quantum dots has evolved over time. Early studies employed the effective mass approximation (EMA) to model impurity behavior, simplifying the interaction by treating the impurity as a hydrogen- like particle within the quantum dot structure [4], [5]. The EMA is particularly effec- tive in cases where the impurity is shallow, meaning it is weakly bound within the host material. In this study, we use the finite element method (FEM) combined with the EMA, which allows for high-precision modeling of complex geometries, such as MSQDs. The FEM is advantageous in solving the time-independent Schrödinger equation for multilayered structures, as

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it can handle the spatial variations in potential and boundary conditions with greater accuracy compared to traditional methods [6].

The influence of magnetic fields on quantum dot structures has been a subject of re- search due to its potential to control electronic and optical properties. Magnetic fields introduce additional confinement, which alters the energy levels and can enhance or suppress binding energies, depending on the direction and strength of the field. Previ- ous work has shown that magnetic fields can significantly impact the optical absorp- tion and emission spectra of quantum dots, making them tunable for specific applica- tions [7], [8]. Additionally, studies have explored the impact of external fields on the nonlinear optical properties of quantum dots, including phenomena like second har- monic generation and optical rectification, both of which are critical for high-speed optical communication and signal processing [9].

The motivation behind investigating donor impurity binding energy in MSQDs under a magnetic field stems from the potential applications of such structures in nanoelec- tronics and photonics. By understanding and controlling impurity-related effects, MSQDs can be engineered for specific functionalities in optoelectronic devices, such as lasers, photodetectors, and light-emitting diodes (LEDs) [10]. Additionally, quan- tum dot structures with tunable electronic properties are promising candidates for quantum computing applications, where impurity states may act as qubits or help mediate interactions between quantum bits [11]. In the field of sensing, magnetic field-sensitive quantum dots can be integrated into devices for magnetic field detec- tion or as sensors for changes in the local electronic environment, offering possibili- ties in environmental and biomedical applications [12].

Furthermore, the study of impurity binding energies in MSQDs has significant impli- cations for solar energy technologies. Quantum dots with optimized impurity states can enhance the absorption of specific wavelengths of light, contributing to the devel- opment of more efficient solar cells [13]. The tunability provided by magnetic fields and structural modifications enables fine-tuning of the bandgap to match the solar spectrum more closely, improving photon capture efficiency.

In this work, we aim to extend the understanding of shallow donor impurity binding energy within MSQDs subjected to magnetic fields. By calculating energy levels using the effective mass approximation and finite element method, we assess the in- fluence of structural parameters, such as core radius, shell width, and barrier thick- ness, on the electronic behavior of these quantum dots. The insights gained from this study contribute to the design of customizable quantum structures with applications in nano-optoelectronics, quantum computing, and photovoltaic devices. The results are expected to not only add to the fundamental knowledge of impurity effects in MSQDs but also to pave the way for the practical use of these quantum structures in a wide array of high-tech applications.

2 Theoretical model

Figure 1 presents a schematic of a multilayer spherical quantum dot (MSQD), struc- tured with two $GaAs$ quantum dots embedded one inside the other. Each dot is en- cased by layers of $GaAlAs$, creating a finite potential barrier both between the dots and around the outer boundary of the system. The radius of the inner $GaAs$ dot is denoted $R_1 = R_{int}$. The inner barrier width is specified as $W_{b1} = R_2 - R_1$, while the outer barrier width is $W_{b2} = R_4 - R_3$. The well width is defined as $R_w = R_3 - R_2$. Under the effective mass approximation, and taking into account the effects of the magnetic field (B), the Hamiltonian for a donor impurity positioned at the center of the $GaAs/Ga_{1-x}Al_xAs$ MSQD is represented by [14]:

$$H = \frac{1}{*_{(d,b)}}\left(p^{\rightarrow} - \frac{eA^{\rightarrow}}{2m}\right)^2 - \frac{e}{c} \quad N + \frac{\hat{V}(r)}{\varepsilon_{(d,b)}r} \qquad (1)$$

where, Here, e is the elementary charge, $\mathrm{p}^{\rightarrow\rightarrow}$ is the momentum, and $A^{\rightarrow}$ is the magnetic field's vector potential, expressed as: $\vec{A} = \frac{1}{2}(\vec{B} \wedge \vec{r})$, where $B^{\rightarrow\rightarrow}$ applied magnetic field along the z-axis. N denotes the presence $(N = 1)$ and absence $(N = 0)$ of the impuri- ty. In the equation (1), both indices d and b denote the quantum dot $(GaAs)$ and the barrier material $(Ga_{1-x}Al_x As)$. (r) is the confinement potential, which serves to trap the electron inside the structure, is mathematically expressed by:

$$(r) = \begin{cases} 0; & \text{For } GaAs \\ V_{conf}; & \text{For } AlGaAs \end{cases} \qquad (2)$$

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In the equation above, the barrier height V_0, which depends on the aluminum amount x, is specified as follows[15-20]:

$$V_0 = 0.658 \times \Delta E(x) = 0.658(1.155x + 0.37x^2)\ eV \quad (3)$$

$\Delta E(x)$ represents the total energy gap discrepancy between the $GaAs$ QD and the $Ga_{1-x}Al_xAs$ barrier material at the Γ point. $m^*_{(d,b)}$ is the effective mass of electron, it is defined in different regions of the MSQD as [17]:

$$m^*_{(d,b)} = \begin{cases} m^* = 0.067m_0 & \text{for } GaAs \\ m^* = m^* + 0.083xm_0 & \text{for } Ga_{1-x}Al_xAs \end{cases} \quad (4)$$

with m_0 as the free electron mass. The dielectric constant $\varepsilon_{(d,b)}$ is dependent on alu- minum content, it is described for $Ga_{1-x}Al_xAs$ materials as follows [21-22]:

$$\varepsilon(x) = \varepsilon_d - 3.12x \quad (5)$$

The dielectric constant in the dot material ($GaAs$) is given as: $\varepsilon_d = 13.18$.

To obtain the binding energy E_b of the donor hydrogenic impurity, we calculated the difference between the ground state energy of the system without impurity $E_{N=0}$ and the energy of the ground state in the presence of the impurity $E_{N=1}$:

$$E_b = E_{N=0} - E_{N=1} \quad (6)$$

It should be noted that the smallest dot radius of the QD, below which no bound state can be obtained, is given as follows [18]:

$$R_0 = \sqrt{\frac{\pi^2\hbar^2}{8m_d^*V_0} + \frac{\hbar^2}{2m_b^*V_0}\left(\frac{m^*}{m^*_d} - 1\right)}^2 \quad (7)$$

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3 Results and discussion

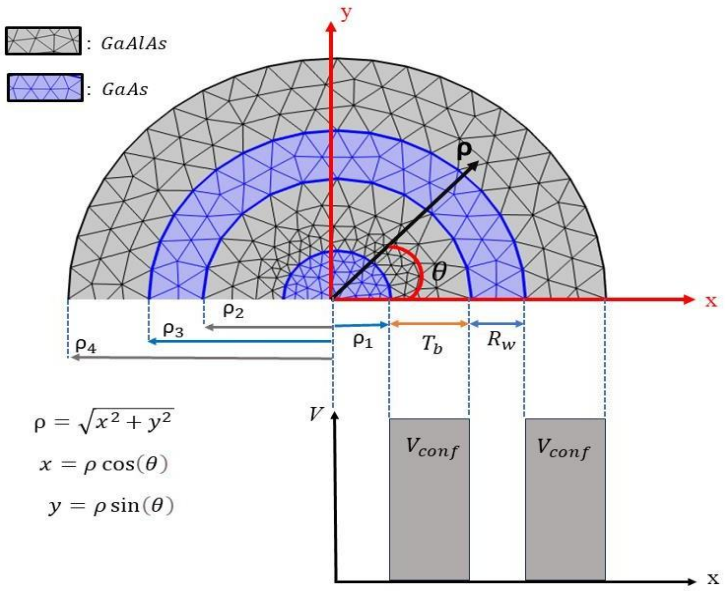

Fig. 1. The multilayer spherical quantum dots and their confinement potential profile in the xy-plane.

This research examines multi-shell quantum dots (MSQDs) depicted in Fig. 1. These MSQDs comprise two concentric $GaAs$ quantum dots enclosed by a $GaAlAs$ barrier material. Figure 1 provides a schematic representation of an MSQD and its potential profile in the xy-plane, with ρ_1 as the core radius, T_b as the barrier width ($\rho_2 - \rho_1$), and Rout as the well width ($\rho_3 - \rho_2$).

In this Fig. 2, we show how the shallow donor impurity binding energy changes with the core radius for various magnetic field strengths. The figure clearly illustrates that for each magnetic field value, the binding energy initially rises sharply as the core radius expands, reaching a peak before decreasing at larger core radii. This observed trend aligns with patterns reported in the literature. As the core radius grows, the con- finement effects diminish, leading to changes in binding energy behavior consistent with established findings. The initial increase followed by a decline demonstrates the impact of core radius on donor binding energy under varying magnetic fields, con- firming similar results documented in previous studies.

The variation of binding energy with core radius in spherical quantum dots (QDs) under different magnetic field strengths reveals crucial insights into their electronic behavior. When a magnetic field is applied, this confinement effect intensifies as the magnetic field strengthens, causing an additional increase in binding energy. For small core radii, even a modest magnetic field can lead to a substantial enhancement in binding energy, as the electron experiences stronger confinement within the QD's limited spatial boundary. In general, for larger core radii in single spherical quantum dots, the impact of the magnetic field is relatively weaker due to diminished confine- ment. Conversely, in multilayered spherical quantum dots with larger core radii, the magnetic field's effect becomes comparatively stronger, owing to the coupling inter- actions between the two GaAs dots.

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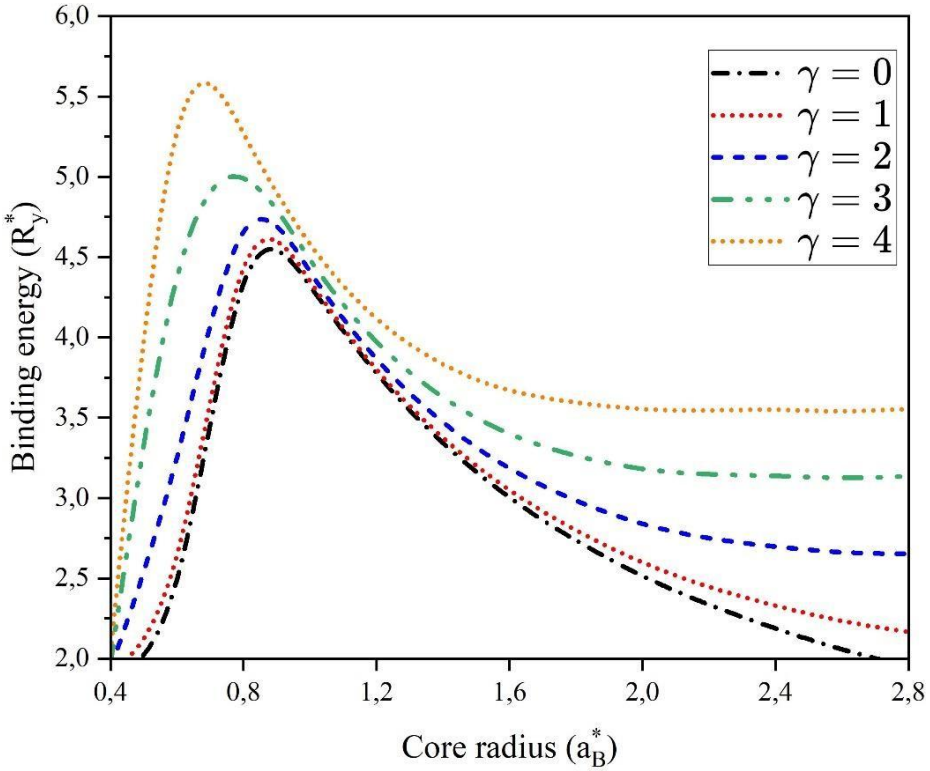

Fig. 2. Variation of binding energy with core radius at different magnetic field strengths.

In Fig. 3, we show how the binding energy of a shallow donor impurity changes with well width under several applied magnetic field strengths. One can see from this fig- ure that without a magnetic field, the binding energy begins from a maximum value and decreases sharply with increasing well width, eventually reaching a minimum and remaining constant with additional increases in width. The obtained outcomes are in agreement with prior research findings. When the structure is exposed to the magnetic field, we observe that the binding energy generally increases. For smaller well widths, this effect is minimal because the confinement effects dominate over the influence of the magnetic field. However, for larger well widths, the impact of the magnetic field becomes more pronounced. A remarkable increase in binding energy was also found for higher well widths and stronger magnetic field values.

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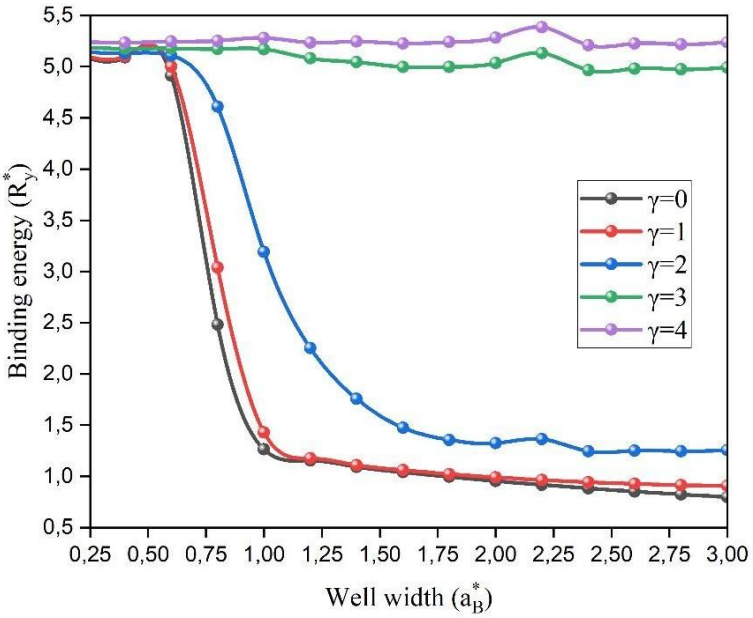

Fig. 3. Variation of binding energy with well width for different values of the magnet- ic field strengths.

In Fig. 4, we examine how the binding energy of a shallow donor impurity varies with changes in the inner barrier width across different applied magnetic field strengths. This analysis shows the influence of both barrier width and magnetic field on impurity binding energy, highlighting how confinement effects are modified by varying these parameters. The binding energy tends to shift distinctly with increasing barrier width, depending on the strength of the magnetic field applied. These varia- tions provide insights into the interplay between magnetic confinement and spatial confinement within the quantum dot structure. The figure illustrates that binding en- ergy shows minimal variation as the barrier width increases. However, for any given barrier width, the binding energy noticeably rises with an increase in the strength of the applied magnetic field.

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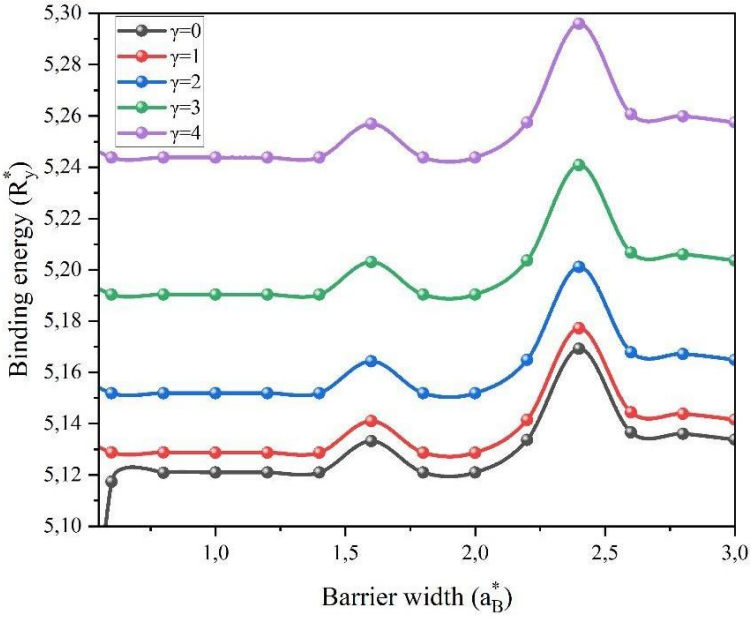

Fig. 4. Variation of binding energy with barrier width for different values of the mag- netic field strengths.

4 Conclusion

In conclusion, our study demonstrates that the binding energy of a shallow donor impurity in multilayered spherical quantum dots (MSQDs) is significantly influenced by both the applied magnetic field and geometric parameters such as the core radius, shell width, and barrier thickness. Through computational modeling using the effec- tive mass approximation and the finite element method, we found that the binding energy exhibits distinct trends based on variations in the inner barrier width and mag- netic field strength. Our analysis reveals that, without a magnetic field, the binding energy decreases as the barrier width expands, stabilizing at a constant level for larger widths. However, when subjected to an applied magnetic field, the binding energy increases notably, particularly at higher field strengths, demonstrating the pronounced effect of magnetic confinement.

Our findings align well with existing literature, underscoring the potential for mag- netic fields to enhance binding energy in quantum dot structures. These results high- light the interplay between magnetic fields and structural confinement, showing that

at smaller barrier widths, the confinement effect dominates, while at larger widths, the magnetic field's influence becomes more pronounced. This tunable behavior provides valuable insights for optimizing MSQD-based devices, particularly in nanoelectron- ics, optoelectronics, and quantum computing applications. By enabling precise control over electronic properties through both structural and magnetic adjustments, MSQDs hold promise for advanced applications in high-speed optical communication, signal processing, quantum computing, and solar energy. This study thus contributes to the fundamental understanding of impurity effects in MSQDs and paves the way for de- signing quantum structures tailored for a range of technological advancements.

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