

Theoretical Study of Spin-Orbit Interaction in CdSe/CdS core-shell elliptical quantum dots Subjected to External Magnetic Fields

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ABSTRACT

This work presents a complete numerical study of confined electron states in CdSe/CdS core-shell elliptical quantum dots, within the single-band effective mass approximation and BenDaniel–Duke Hamiltonian. The position-dependent effective mass is used for a correct description of carrier transport through the CdSe/CdS heterointerface and the two-dimensional Schrodinger equation under finite confinement conditions is discretized and solved by the finite difference method. The developed numerical framework is applied to study the influence of the quantum dot geometry on its electronic properties. In particular, the influences of core size, shell thickness, and aspect ratio on the confined energy levels and electron wavefunctions are studied systematically. Contour plots, 3D surface visualizations, and 1D cross-sectional profiles of the spatial distribution of the ground and excited states are used to demonstrate the localization behavior of the confined electron. In addition, a mesh convergence study is conducted to confirm the numerical accuracy and stability of the proposed method. The effect of the geometric deformation on quantum confinement is examined by comparing elliptical and circular quantum dots. The results show that the increase of core size reduces the confinement strength and hence the confined electron energy levels. The effects of the changes in shell thickness and aspect ratio are also reflected in the energy spectrum and spatial localization of the electron wavefunctions. The results show that the electronic structure depends strongly on the quantum dot geometry. The proposed computational framework provides an accurate and computationally efficient tool for analysis and design of semiconductor core-shell quantum dots and can be readily extended to consider more advanced nanostructures involving external electric and magnetic fields, spin-related effects and excitonic interactions.

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1. Introduction

Semiconductor quantum dots (QDs) have attracted considerable interest in the last few decades because of their unique size-dependent electronic and optical properties that originate from quantum confinement. When the size of a semiconductor nanostructure is comparable to the Bohr radius of the exciton, the continuous energy bands split into discrete energy levels. This leads to the emergence of atom-like properties, which are not present in bulk materials[1,2]. These remarkable properties have made quantum dots increasingly important in many applications such as light-emitting diodes, semiconductor lasers, photodetectors, solar cells, biological imaging, quantum information technologies, and nanoscale optoelectronic devices[3,4].

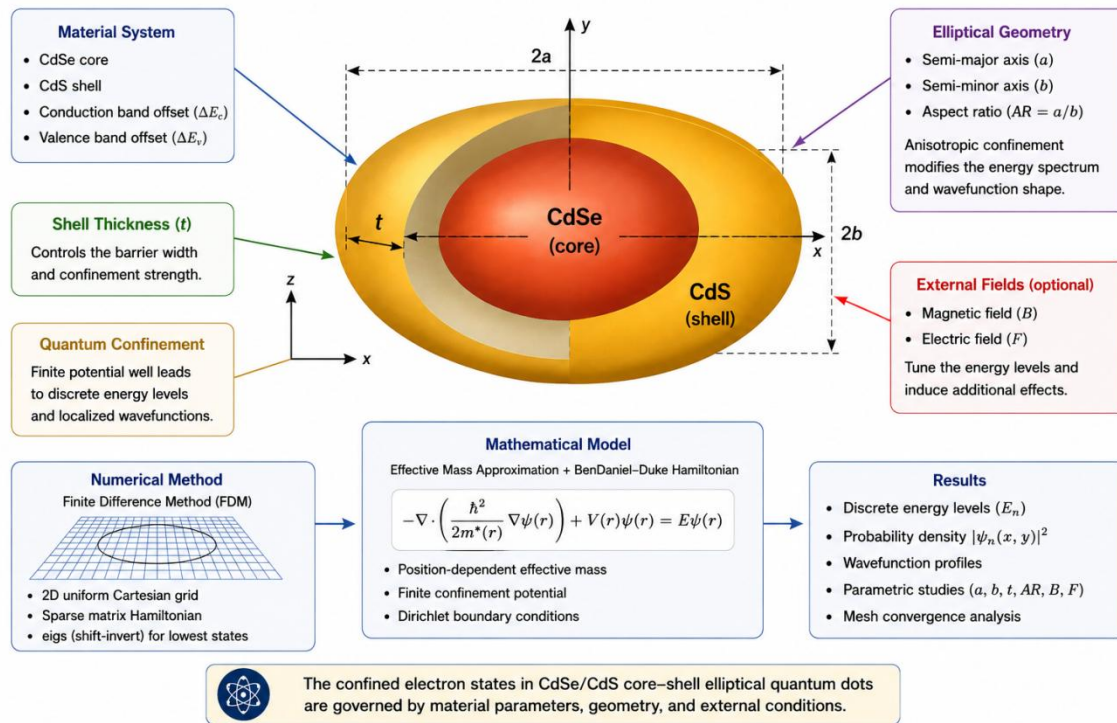
Core-shell quantum dots (CSQDs) are one of the most promising candidates among various semiconductor nanostructures, due to their improved carrier confinement,

enhanced structural stability and reduced surface recombination as compared to single material quantum dots. The core-shell heterostructures offer an additional degree of freedom to engineer the confinement potential and to tailor the electronic states by combining two semiconductor materials with different electronic band structures. In particular, CdSe/CdS core-shell quantum dots have been extensively studied due to their favorable band alignment, high optical efficiency, relatively low density of surface defects and excellent chemical stability. All these characteristics give them potential to become good building materials for fast and efficient optoelectronics and photonics applications[5].

The electronic properties of semiconductor quantum dots depend not only on the material used but also on its geometrical form[6]. Quantum confinement effect and energy levels directly depend on the core size, shell thickness, and

symmetry of the nanostructure. Spherical quantum dots have been widely studied due to their mathematical simplicity, however, many experimentally fabricated nanostructures exhibit deviations from perfect spherical symmetry[7]. In particular, elliptical quantum dots produce anisotropic

confinement, giving rise to unique electronic properties that cannot be mimicked in circular or spherical geometries. So it becomes very important to comprehend the significance of geometrical anisotropy in the design of semiconductor nanostructures.



Graphical abstract: Schematic of the conceptual CdSe/CdS core-shell elliptical quantum dot studied in this work. The diagram shows the geometrical parameters controlling the nanostructure, semi-major axis ((a)), semi-minor axis ((b)), shell thickness ((t)) and aspect ratio ((AR=a/b)). Material composition and finite confinement potential are also shown. It also gives a summary of the mathematical model in terms of the effective mass approximation and the BenDaniel-Duke Hamiltonian, and the finite difference method used to calculate the confined electron states. Then the electronic properties are discussed in terms of the energy spectrum, the electron probability density, the distributions of wavefunctions and the effects of the geometrical parameters and external fields.

Proper treatment of the spatial variation of the material properties across heterointerfaces is needed in the theoretical modeling of semiconductor heterostructures. The standard constant-mass Schrodinger equation cannot be used to describe the carrier confinement in core-shell systems where the electron effective mass is different from one material to another[8]. The single-band Effective Mass Approximation (EMA) with the BenDaniel-Duke Hamiltonian gives a physically consistent description of the position-dependent effective mass, while keeping the Hamiltonian Hermitian and the probability current continuous at the material interfaces. It strikes an effective balance between computational efficiency and physical realism and has been one of the main theoretical approaches used for the study of confined electronic states in semiconductors.

The numerical solution of the Schrodinger equation obtained must be done using efficient discretization methods for any geometry and material inhomogeneity. Among the available numerical approaches, the Finite Difference Method (FDM) provides a simple and computationally efficient framework

for solving two-dimensional eigenvalue problems, when the position-dependent material parameters and the finite confinement potentials are included. Moreover, the FDM technique enables convergence analysis and offers the possibility of parametric analysis depending on structural parameters without complicating computational effort considerably [9]. In view of these considerations, the present study aims at developing a comprehensive numerical model to study the electronic states of CdSe/CdS core-shell elliptical quantum dots. The model is a combination of Effective Mass Approximation, BenDaniel–Duke Hamiltonian and Finite Difference Method to solve the two dimensional Schrödinger equation with finite confinement conditions. Specifically, the modifications in the core parameters, the shell thickness, and aspect ratio and how they affect the energy and wave function of the confined electrons are discussed. In addition to the evaluation of the electronic energy spectrum, the work also reports detailed analyses of the spatial probability density, wavefunction localization, numerical convergence and the influence of geometrical deformation by comparison

with the corresponding circular quantum dot. The proposed computational scheme may serve as a sound theoretical background for analyzing the issue of quantum confinement in semiconductor core-shell nanostructures, and can form the basis for future research into other effects such as influence of external electric and magnetic fields, spin effects, etc.

The theoretical approach has been widely applied to the analysis of semiconductor quantum dot electronic properties in particular due to its difficulty to experimentally characterize the quantum dots. The Effective Mass Approximation (EMA) together with the BenDaniel–Duke Hamiltonian is one of the most used theoretical approaches for the study of carrier confinement in semiconductor heterostructures with position dependent effective mass[10].

A pioneering contribution to this field was made by BenDaniel and Duke (1966) who formulated the boundary conditions for envelope functions at semiconductor heterojunctions. The continuity of wavefunction and probability current was assured by their definition. This formed the theoretical foundation for dealing with mass-discontinuity issues in semiconductors. Even today, in the field of quantum wells and wires, the same boundary conditions have remained the standard [11]. Based on this, Bastard (1988) showed that the Effective Mass Approximation gives an efficient and physically consistent description of the confined electronic states in semiconductor heterostructures with a relatively low computational complexity. His work established the envelope-function formalism as a main theoretical tool for the analysis of quantum-confined systems and remains a corner stone reference for the modelling of semiconductor nanostructures[8].

Harrison (2016) then gave a thorough theoretical treatment of quantum wells, quantum wires and quantum dots using the effective-mass approach. The study discussed the finite confinement potentials, position dependent effective mass and numerical solution techniques applicable to the semiconductor heterostructures of arbitrary geometries. It also stressed the importance of the correct boundary conditions as well as the numerical discretization to obtain physically meaningful confined states[12].

Tan et al. (2011) presented a numerical study of the calculation of confined electron states in CdTe/CdS core-shell quantum dots using the finite difference method combined with the BenDaniel–Duke Hamiltonian. Their study demonstrated that the finite difference approach reproduces the correct behaviour of the lowest confined energy levels and the corresponding wave functions, while retaining the effects of finite confinement and the effective-mass discontinuity. However, the analysis was limited to spherically symmetric quantum dots and one dimensional radial modeling[13]. More recently, Tyrrell and Smith (2011) studied the electronic and excitonic properties of the type-II core-shell quantum dots CdTe/CdSe and CdSe/CdTe within the framework of the effective-mass theory. By comparing single-band and multiband formulations, they have demonstrated that more sophisticated band models give a better description of higher excited states and optical transitions. However, their work was mainly concerned with the exciton properties of spherical nanocrystals, but not with

geometrical anisotropy of the confined electron states[14, 15].

Recent theoretical works have continued to use the Effective Mass Approximation and BenDaniel–Duke boundary conditions to study semiconductor core-shell nanostructures with finite confinement potentials. These studies have demonstrated that the electronic structure and optical response of semiconductor quantum dots are strongly influenced by material composition, band offsets and structural dimensions. Despite these advances, the majority of the numerical studies are still limited to spherical or radially symmetric geometries, while little attention has been paid to two-dimensional elliptical core-shell quantum dots with position-dependent effective mass directly solved by the finite difference method[16].

Despite the multiple theoretical and numerical studies of the semiconductor quantum dots, many important research challenges are to be solved. Most of the present studies have been mainly focused on spherical or circular quantum dots due to the geometrical symmetry which facilitates the mathematical formulation and numerical implementation. As a result, the study of elliptical core-shell quantum dots has been relatively limited, although geometrical anisotropy can play a significant role in modifying the electronic confinement properties and the localization of the wavefunction. Furthermore, many previous studies have used simplified theoretical models based on constant effective mass or infinite confinement potentials. These assumptions have greatly reduced the computational complexity, but do not capture the actual scenario of the semiconductor heterostructures in practice, where the effective mass is discontinuous across the interfaces of the materials, and the confinement potential is finite. Hence, such simplified models might not fully incorporate the effect of the heterointerface properties on the confined electronic states.

Another limitation found in the literature is that a lot of studies are mainly focused on the calculation of a limited number of energy eigenvalues without a thorough analysis on the corresponding wavefunctions, probability-density distributions, geometrical deformation effects, numerical convergence and comparative evaluation with reference geometries. Thus, the combined effect of the core dimensions, shell thickness and aspect ratio on the electronic properties of CdSe/CdS core-shell elliptical quantum dots has not yet been systematically investigated within a unified computational framework.

In the present work, such limitations are overcome by developing a two dimensional numerical model based on the Effective Mass Approximation and BenDaniel–Duke Hamiltonian with position dependent effective mass. The proposed model uses the Finite Difference Method to solve the Schrödinger equation in finite confinement conditions and presents a detailed analysis of the confined electron states. Apart from the energy spectrum, such aspects of quantum confinement as probability-density distributions, wavefunction localization, the effect of geometrical parameters and the mesh convergence are analyzed by comparison of the elliptical and the circular quantum dots. The current analysis provides a complete picture of quantum confinement in the CdSe/CdS core-shell structures and serves

as a basis for further investigations considering external perturbations and more complicated physical effects.

The goal of this research is to construct an efficient numerical model of confined electron states in CdSe/CdS core-shell elliptical quantum dots. The approach used in this study is based on the use of the Effective Mass Approximation (EMA), the BenDaniel-Duke Hamiltonian and the Finite Difference Method (FDM) to solve the Schrödinger equation with the position-dependent effective mass and finite confinement potential in two dimensions. This approach is applied to construct a two-dimensional model to obtain numerically the energy eigenvalues and normalized wavefunctions for the quantum system under consideration.

The constructed model allows one to investigate the distribution of electrons in the considered quantum dot by calculating probability-density contour maps, three-dimensional wavefunction distributions and one-dimensional wavefunction cross-sections. The main attention is paid to the effect of core size, shell thickness and the aspect ratio of the quantum dot on the electronic energy spectrum and wavefunction properties, which gives the insight into the influence of the geometrical structure on quantum confinement. The mesh convergence analysis is carried out to ensure the numerical reliability of the used approach. The electronic properties of elliptical and circular quantum dots are compared to evaluate the effect of geometrical anisotropy, which further proves the capability of the proposed method. The resulting computational framework provides a solid basis for further investigations on the effects of external electric and magnetic fields, spin-dependent interactions, excitonic effects and more sophisticated semiconductor nanostructures and thus represents a valuable tool for the design and optimization of next generation nanoelectronic and optoelectronic devices.

2. Mathematical Model

The physical system considered in this work is a two-dimensional CdSe/CdS core-shell elliptical quantum dot. The electronic motion is assumed to be confined within the $x - y$ plane, while the confinement along the growth direction is sufficiently strong that the problem can be treated as effectively two-dimensional[8,11,12,13].

The boundary of the elliptical core is defined by

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} \leq 1 \dots (1)$$

where a and b denote the semi-major and semi-minor axes, respectively. The geometrical deformation of the quantum dot is characterized by the aspect ratio

$$AR = \frac{a}{b} \dots (2)$$

Since the present work focuses on the electronic states close to the conduction-band minimum, the envelope-function

approximation together with the single-band effective mass approximation is adopted [17].

Within this framework, the total electron wavefunction is expressed as

$$\Psi(\mathbf{r}) = F(\mathbf{r})u_c(\mathbf{r}) \dots (3)$$

where $u_c(\mathbf{r})$ is the periodic Bloch function and $F(\mathbf{r})$ is the slowly varying envelope function

The effective mass approximation has been extensively employed for semiconductor heterostructures

because it provides an accurate description of confined electronic states while maintaining a relatively simple mathematical formulation (Bastard, 1988; Harrison, 2016)[8,9].

Unlike homogeneous semiconductors, the effective mass varies across the CdSe/CdS heterointerface. Consequently, the conventional kinetic-energy operator

$$-\frac{\hbar^2}{2m^*}\nabla^2$$

cannot be used because it no longer guarantees a Hermitian Hamiltonian.

To preserve Hermiticity and ensure current conservation across the material interface, the kinetic-energy operator is replaced by the BenDaniel-Duke operator, yielding the Hamiltonian

$$H = -\frac{\hbar^2}{2}\nabla \cdot \left(\frac{1}{m^*(x,y)}\nabla \right) + V(x,y) \dots (4)$$

Equation (4) has become the standard Hamiltonian for semiconductor heterostructures with position dependent effective mass and is widely used for quantum wells, quantum wires, and quantum dots.

The electron effective mass is assumed to be piecewise constant:

$$m^*(x,y) = \begin{cases} m_{\text{CdSe}}, & \frac{x^2}{a^2} + \frac{y^2}{b^2} \leq 1, \\ m_{\text{CdS}}, & \frac{x^2}{a^2} + \frac{y^2}{b^2} > 1. \end{cases} \dots (5)$$

This representation accurately models the abrupt heterointerface between the CdSe core and the CdS shell.

The conduction-band confinement is represented by a finite potential barrier

$$V(x,y) = \begin{cases} 0, & \frac{x^2}{a^2} + \frac{y^2}{b^2} \leq 1 \\ V_0, & \frac{x^2}{a^2} + \frac{y^2}{b^2} > 1 \end{cases} \dots (6)$$

where V_0 corresponds to the conduction-band offset between CdSe and CdS.

Substituting Eqs. (5) and (6) into Eq. (4) yields the governing equation

$$-\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m^*(x,y)} \nabla \psi \right) + V(x,y) \psi = E \psi \dots (7)$$

Equation (7) constitutes the fundamental eigenvalue problem solved throughout this work.

At the CdSe/CdS interface, the envelope function satisfies the BenDaniel-Duke boundary conditions. First, the wavefunction remains continuous.

$$\psi_1 = \psi_2 \dots (8)$$

while conservation of the probability current requires:

$$\frac{1}{m_1} \frac{\partial \psi_1}{\partial n} = \frac{1}{m_2} \frac{\partial \psi_2}{\partial n} \dots (9)$$

These interface conditions naturally arise from Eq. (4) and guarantee both Hermiticity and current continuity across the heterojunction.

To eliminate the influence of the computational boundary, the numerical domain is selected sufficiently, larger than the quantum dot dimensions, and homogeneous Dirichlet boundary conditions are imposed.

$$\psi = 0 \dots (10)$$

Finally, the confined electronic states are obtained by solving

$$H \psi_n = E_n \psi_n \dots (11)$$

where E_n denotes the n -th energy eigenvalue and ψ_n is the corresponding normalized envelope wavefunction.

The calculated eigenpairs are subsequently used to generate the energy spectrum, probability-density distributions, contour maps, three-dimensional wavefunction surfaces, and all parametric analyses presented in this study [18,19].

For numerical implementation, the BenDaniel-Duke Hamiltonian given in Eq. (4) is expanded explicitly in Cartesian coordinates. This transformation provides the differential form required for the finite difference discretization while preserving the Hermitian nature of the Hamiltonian.

Starting from Eq. (4)

$$H = -\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m^*(x,y)} \nabla \right) + V(x,y) \dots (12)$$

the divergence operator is written in Cartesian coordinates as

$$\nabla \cdot \left(\frac{1}{m^*} \nabla \psi \right) = \frac{\partial}{\partial x} \left(\frac{1}{m^*} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{m^*} \frac{\partial \psi}{\partial y} \right) \dots (13)$$

Applying the product rule to each derivative yields

$$\frac{\partial}{\partial x} \left(\frac{1}{m^*} \frac{\partial \psi}{\partial x} \right) = \frac{1}{m^*} \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial}{\partial x} \left(\frac{1}{m^*} \right) \frac{\partial \psi}{\partial x} \dots (14)$$

and

$$\frac{\partial}{\partial y} \left(\frac{1}{m^*} \frac{\partial \psi}{\partial y} \right) = \frac{1}{m^*} \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial}{\partial y} \left(\frac{1}{m^*} \right) \frac{\partial \psi}{\partial y} \dots (15)$$

Substituting Eqs. (14) and (15) into Eq. (13), the governing Schrödinger equation can be written explicitly as

$$-\frac{\hbar^2}{2} \left[\frac{1}{m^*} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + \frac{\partial}{\partial x} \left(\frac{1}{m^*} \right) \frac{\partial \psi}{\partial x} + \frac{\partial}{\partial y} \left(\frac{1}{m^*} \right) \frac{\partial \psi}{\partial y} \right] + V \psi = E \psi \dots (16)$$

Equation (16) is the complete Cartesian representation of the BenDaniel-Duke Hamiltonian for a position dependent effective mass. The first two terms correspond to the conventional kinetic-energy operator, whereas the additional first-order derivative terms originate from the spatial variation of the effective mass across the CdSe/CdS heterointerface [20]. These correction terms are essential for maintaining Hermiticity and ensuring the continuity of the probability current. For homogeneous materials, where the effective mass is spatially constant.

$$\frac{\partial m^*}{\partial x} = \frac{\partial m^*}{\partial y} = 0 \dots (17)$$

Eq. (16) reduces to the conventional effective-mass Schrödinger equation

$$-\frac{\hbar^2}{2m^*} \nabla^2 \psi + V \psi = E \psi \dots (18)$$

Therefore, Eq. (16) represents the generalized form applicable to semiconductor heterostructures with abrupt material interfaces and serves as the starting point for the finite difference discretization developed in the next section. The obtained eigenvalues E_n represent the quantized electron energy levels, whereas the corresponding normalized eigenfunctions $\psi_n(x,y)$ describe the spatial probability distribution of the confined electron inside the elliptical quantum dot. All subsequent numerical analyses (such as the energy spectrum, probability-density distributions, contour maps, 3D wavefunction visualizations, mesh-convergence analysis, and the investigation of geometrical effects) were based upon these quantities linked to changes in core radius, shell thickness and aspect ratio.

3. Results and Discussion

The electronic properties of semiconductor quantum dots are governed by the interplay of geometrical confinement, material composition and quantum mechanical boundary conditions. In this paper we calculate the electronic states of a CdSe/CdS core-shell elliptical quantum dot by solving the two-dimensional BenDaniel–Duke Schrödinger equation in the effective mass approximation (EMA). The Hamiltonian was discretized using the Finite Difference Method (FDM) on a uniform Cartesian mesh, which enabled the inclusion of both the position-dependent effective mass and the finite conduction-band confinement potential. The resulting

eigenvalue problem gives the quantised electron energy spectrum and the corresponding wavefunctions, which are employed as a basis for studying the influence of structural geometry on carrier confinement. The elliptical shape, instead of the idealized circular quantum dot, results in anisotropic confinement, which leads to electrons moving differently along the major and minor axes. Thus, the spatial distribution of the wavefunction and the quantized energy spectrum are very sensitive to the aspect ratio of the quantum dot. The physical meaning of each numerical result is discussed in the next section and the observed trends are connected to the underlying quantum mechanical formulation.

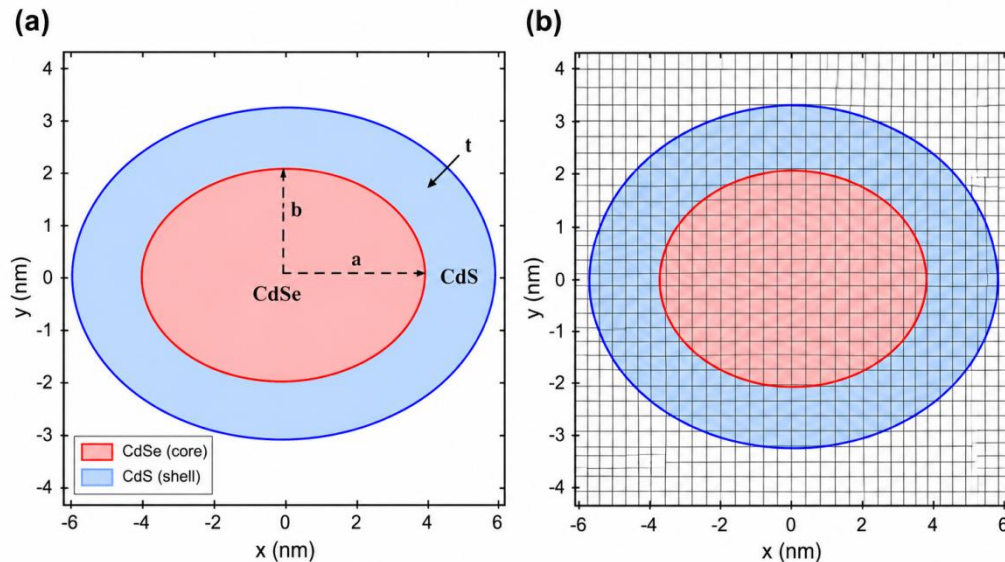


Figure 1. (a) Schematic representation of the CdSe/CdS core-shell elliptical quantum dot, showing the CdSe core, CdS shell, semi-major axis a , semi-minor axis b , shell thickness t , and computational domain. (b) Finite-difference mesh used to discretize the computational domain for solving the two-dimensional BenDaniel–Duke Schrödinger equation.

Figure 1 shows the geometrical configuration used in the whole investigation. The model comprises an elliptic CdSe core and a uniformly thick CdS shell, with the confinement geometry characterized by the semi-major axis (a), semi-minor axis (b) and shell thickness (t). This setup allows a realistic representation of experimentally fabricated core-shell nanostructures and at the same time allows a systematic investigation of geometrical anisotropy. From the theoretical point of view, the elliptical geometry changes the spatial boundary conditions appearing in the 2D Schrödinger equation. Unlike a circular quantum dot which possesses a rotationally symmetric confinement potential, the elliptical structure has different confinement lengths along two principal directions. The kinetic-energy operator in the BenDaniel–Duke Hamiltonian involves spatial derivatives of the electron wavefunction. Because the kinetic energy operator is a differential operator, the boundary conditions on the wavefunction are not automatically satisfied[21].

$$-\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m^*(x, y)} \nabla \psi \right)$$

The different geometrical sizes naturally induce anisotropic wavefunction localization. Consequently the confinement energy is not only dependent on the size of the quantum dot, but also on the aspect ratio, which becomes an additional design parameter to tune the electronic properties.

The numerical implementation starts with the discretization of the computational domain as shown in Figure 1. A uniform Cartesian finite-difference mesh is used for both the quantum dot and the surrounding shell. The use of a structured mesh leads to a significant simplification of the discretization of the BenDaniel–Duke operator, while preserving the second-order accuracy in the spatial domain. The finite difference approximation converts the continuous differential equation into a sparse algebraic eigenvalue problem, greatly increasing computational efficiency without loss of physical accuracy. A second important point is that the mesh goes beyond the boundaries of the heterostructure so that the numerical boundary conditions do not artificially influence the confined

electronic states. The uniform grid spacing also ensures that the truncation errors in both spatial directions are the same, hence the anisotropy that is observed can only be attributed to the elliptical geometry and not the numerical discretization. This is a commonly used approach to semiconductor quantum dot simulations as it guarantees stable convergence and respects the continuity conditions at the material interfaces.

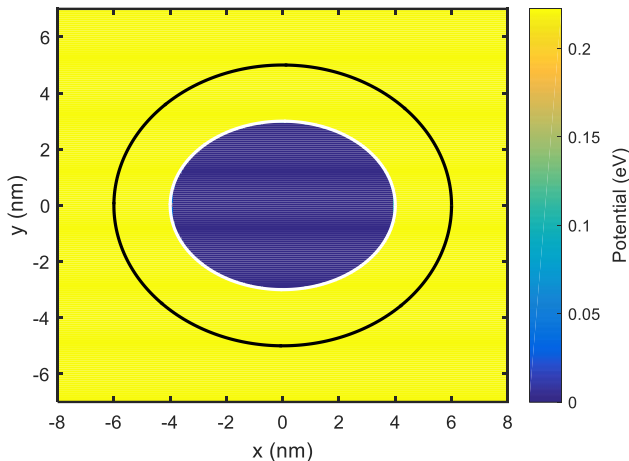


Figure 2. Two-dimensional contour map of the conduction band confinement potential. The electron is confined in the CdSe core ($V=0$) and experiences a finite potential barrier (V_0) in the surrounding CdS shell which corresponds to the conduction-band offset of the heterostructure.

The confinement potential used in the present work is shown in Figure 2. Here the CdSe core is taken as zero reference potential and the surrounding CdS shell provides a finite conduction band barrier corresponding to the conduction band offset between the two semiconductor materials[22]. The finite potential profile is one of the main advantages of the present model compared to simpler infinite-potential approximations. In practice, the finite potential barrier allows the electron wavefunctions to partially penetrate into the CdS shell, so that the electrons are not perfectly confined in the CdSe core[23,24]. The penetration obeys the quantum mechanical continuity conditions at the heterointerface and leads to an evanescent wave behaviour inside the shell. The resulting leakage reduces the effective confinement strength and thus modifies both the eigenenergies and probability density distributions. Mathematically, the confinement potential enters the Hamiltonian directly through the potential-energy term, $H = -\frac{\hbar^2}{2m^*}\nabla^2\psi + V\psi$ and any change in the potential profile directly changes the eigenstates calculated. Thus, the finite barrier presented in Fig. 2 causes the localization of the electron and the tunnelling probability through the interface CdSe/CdS.

The spatial variation of the effective electron mass is shown in Figure 3, where the heterostructure composition considered in the numerical model is reflected in the sharp transition between the CdSe core and the CdS shell. In the present work the position-dependent effective mass is explicitly incorporated in the BenDaniel-Duke Hamiltonian,

rather than assuming a constant effective mass throughout the computational domain. This approach yields a much more realistic description of the carrier dynamics as the effective mass appears directly in the kinetic-energy operator[14].

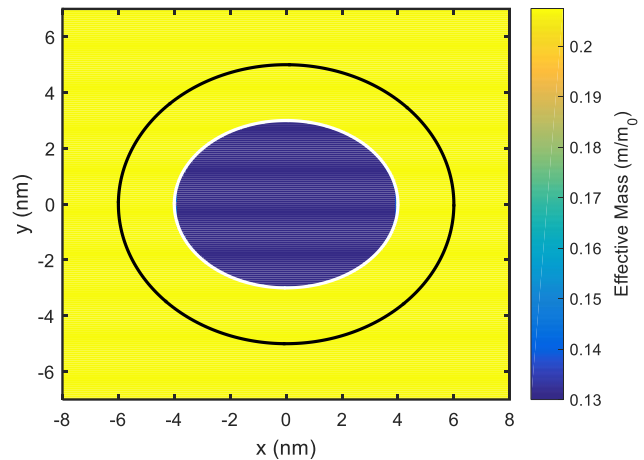


Figure 3. Spatial distribution of the position-dependent effective mass of the electrons used in the BenDaniel-Duke Hamiltonian. The heterointerface between CdSe and CdS is represented by the abrupt change and is included via the position-dependent effective mass formulation.

Electrons physically have higher mobility in regions of lower effective mass. Regions of higher effective mass slow down the carrier motion by increasing inertial response. This is because CdSe has a lower electron effective mass than CdS that favors the localization of the electron wavefunction within the core, while its penetration into the shell is progressively attenuated. This behaviour follows naturally from the solution of the Schrodinger equation and does not require additional fitting parameters.

Furthermore, the discontinuity in the effective mass results in the BenDaniel-Duke interface condition that must be satisfied in order to ensure the continuity of the probability current density through the heterojunction. Fulfillment of this condition is vital for preserving the Hermitian form of the Hamiltonian and providing the physical meaning of the eigenvalues. Therefore, the effective mass profile in Fig. 3 is a fundamental element of the structure, which defines the properties of the electronic confinement in the CdSe/CdS core-shell elliptical quantum dot.

The distributions of the electron probability densities shown in Figs. 4-6 represent a direct illustration of the quantum nature of the confinement of carriers in the studied heterostructure. The probability density equals the square of the absolute value of the normalized wave function ($|\psi(r)|^2$). As a result, the probabilities of finding the confined electron in the different points inside the heterostructure were calculated and plotted in Figs. 4-6. They were obtained from the solutions of the two-dimensional BenDaniel-Duke Hamiltonian and therefore can be considered a physical interpretation of the quantized solutions of the Schrödinger equation.

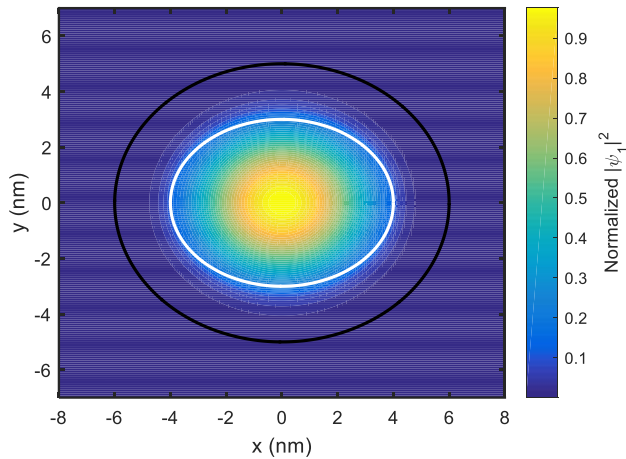


Figure 4. Probability density of ground-state electrons $|\psi(\mathbf{r})|^2$ of the core-shell elliptical quantum dot CdSe/CdS. The quantum confinement results in an extremely localized probability density distribution within the quantum dot.

Fig. 4 illustrates the probability density normalized to unit area for the ground state of the exciton. The probability distribution function features a pronounced maximum in close proximity to the geometric center of the CdSe core, gradually fading off near the heterointerface and slightly extending into the outer layer of the CdS shell. Such an energy level distribution is characteristic of the first excited state in quantum confined structures and is explained by the electron's inclination towards the lowest energy state. From the mathematical point of view, the ground state wavefunction is the one corresponding to the lowest eigenvalue of the Hamiltonian, and thus minimizing the total energy functional under the normalization condition. Thus, there are no internal nodes in the confinement region since the existence of nodes would increase the curvature of the wavefunction and, according to the kinetic-energy operator $-\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m^*(x,y)} \nabla \psi \right)$ would have to increase the kinetic energy. The absence of nodal structures is thus a direct consequence of the variational principle of the quantum mechanical ground state.

The observed confinement within the CdSe core further confirms that the finite conduction-band offset provides a sufficient potential depth to support strongly localized bound states. However, the probability density does not drop sharply to zero at the CdSe/CdS interface. Instead one observes a gradual attenuation in the shell region due to the finite potential barrier. This exponential infiltration is connected to quantum mechanical tunnelling and is a major difference between finite and infinite confinement models. Such a penetration is physically expected, since the electron has a finite probability to exist within classically forbidden regions whenever the confining potential is finite.

The spatial distribution of the first excited state probability density plotted in Fig.5 is quite different from that of the ground state. Instead of a single central maximum the probability density is divided into two symmetric lobes

separated by a nodal region through the center of the quantum dot. This nodal pattern is a direct consequence of the orthogonality condition between different eigenfunctions of the Hamiltonian.

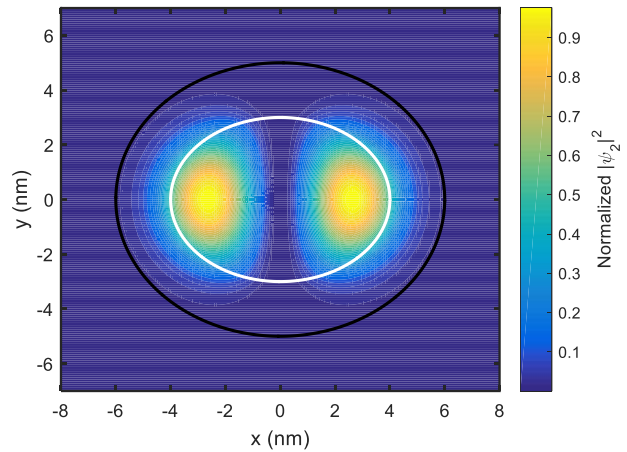


Figure 5. Probability density distribution of the first excited electron state $|\psi(\mathbf{r})|^2$. The spatial symmetry and nodal structure of the first excited confined state in the elliptical quantum dot have been determined.

Quantum mechanically the first excited state has an additional quantum number compared to the ground state leading to a sign change of the wavefunction across the nodal plane. The probability density is positive (proportional to $|\psi(\mathbf{r})|^2$ anyway) but the underlying wavefunction has sign changes across the node, hence the double-lobed distribution we observe. This behavior is perfectly consistent with analytical properties of excited-state solutions of confined quantum systems. The appearance of the nodal region in turn explains the larger energy of the first excited state with respect to the ground state. Adding a node increases the spatial curvature of the wavefunction, and this increases the expectation value of the kinetic-energy operator. This means the corresponding eigenvalue goes to higher energy. Such a relation between the nodal structure and the ordering of the energies is one of the basic principles governing the eigenstates of quantum-confined systems and is well reproduced by the present numerical model.

Another point worth mentioning is the symmetry of the probability distribution. Although the quantum dot has an elliptical geometry, rather than perfect rotational symmetry, the first excited-state wavefunction retains reflection symmetry about the principal coordinate axes. This implies that the adopted computational model correctly preserves the geometrical symmetry of the confinement potential and at the same time anisotropic confinement effects can naturally arise from the numerical solution.

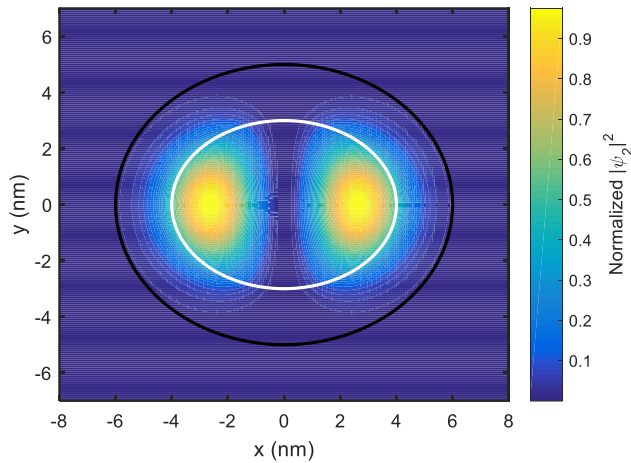


Figure 6. Three-dimensional surface representation of the ground state electron probability density. The surface plot shows the localization of the electron wavefunction in the quantum-confined region.

Figure 6 displays a complementary representation of the ground-state wavefunction as a three-dimensional surface for the probability density. The surface plot is a better representation of the amplitude variation across the confinement region, than the contour representation shown above. The central peak is the most probable localization. The gradual decrease towards the boundaries shows the decreasing of the electron confinement when approaching to the potential barrier.

The smooth shape of the probability surface also demonstrates the numerical stability of the finite difference solution. No artificial oscillations or discontinuities appear near the material interface, which demonstrates that the discretized BenDaniel-Duke Hamiltonian preserves both wavefunction continuity and probability current conservation across the CdSe/CdS heterojunction. These properties are important to obtain physically meaningful eigenstates in semiconductor heterostructures with position-dependent effective masses[25].

From a device perspective, the strong localization observed in Figures 5-7 has important implications in optoelectronic applications. Confinement of carriers is stronger, optical transition is more efficient, and overlap of carriers with the holes that are confined is also more when electron wave functions are highly localized. Due to these characteristics, these quantum dots become effective for emitting quantum light, and are therefore suitable for photodetectors and optoelectronic devices. Furthermore, the accurate prediction of both the ground and excited-state wavefunctions provides a sound basis for further studies of excitonic interactions, optical absorption, and external-field perturbations.

The dependence of the confined electronic states on the geometrical parameters of the CdSe/CdS core-shell elliptical quantum dot is shown in Figs. 7-10. The eigenvalues obtained from the BenDaniel-Duke Hamiltonian correspond to the quantized electronic energy levels. The kinetic and potential energy terms in the Schrödinger equation change when the confinement geometry is changed. Therefore, the electronic spectrum is directly affected by the variations of

the core dimensions, the shell thickness and the geometrical anisotropy, through the changes in the spatial confinement experienced by the electron.

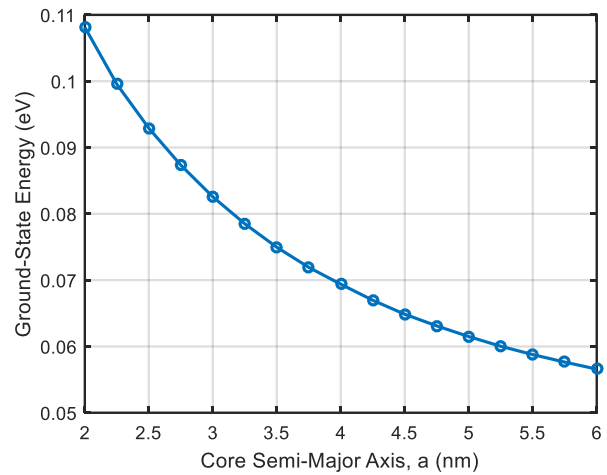


Figure 7. Lowest confined electron energy levels as a function of the core semi-major axis. By increasing the core size, the quantum confinement becomes weaker, and the energy levels become lower.

The dependence of the ground state energy on the semi-major axis of the CdSe core is shown in Fig. 7. It is found that the ground-state energy decreases monotonically as the semi-major axis increases from 2 to 6 nm. This behaviour is in complete agreement with the fundamental principles of quantum confinement and expresses the inverse dependence of the confinement strength on the characteristic size of the nano-structure[26].

Mathematically, making the semi-major axis larger leads to a greater effective area over which the electron wavefunction can spread out, reducing its curvature in space. The kinetic-energy part of the Hamiltonian is proportional to the Laplacian of the wavefunction. So reducing the curvature reduces the expectation value of the kinetic-energy operator. Therefore, the total eigenenergy shifts to lower values. This is consistent with the well-known scaling law of quantum confinement, where the confinement energy decreases approximately with the increase of confinement dimensions. Also a physical interpretation can be obtained by taking into account the electron de Broglie wavelength. The size of the quantum dot is reduced to be comparable to the electron wave length. Strong confinement confines the electron to strongly localized states, the kinetic energy of which is increased by the uncertainty principle. Increasing the semi-major axis relaxes this spatial confinement and allows to wavefunction to extend over a larger volume. The reduction in localization reduces the uncertainty in the electron momentum and hence the confinement energy. The nonlinearity of the curve also implies that the strongest confinement is achieved for the smallest quantum dots, while the sensitivity is gradually reduced as the structure size approaches the weak-confinement regime.

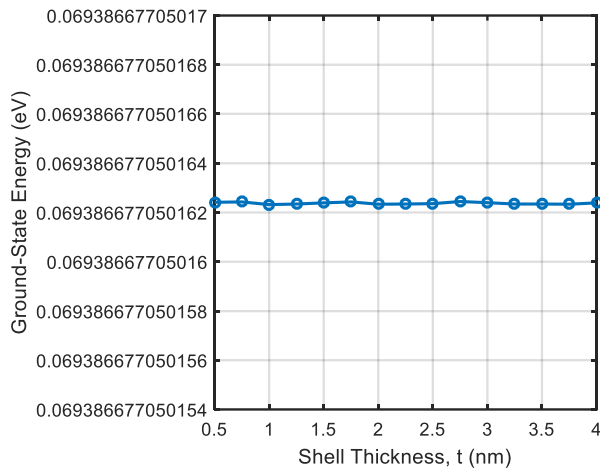


Figure 8. Dependence of the confined electron energy spectrum on the thickness of the CdS shell. The results show how the shell thickness changes the confinement potential and influences the electronic states.

The effect of the thickness of CdS shell is shown in Fig. 8, where the change of the ground-state energy with the increase of the thickness of shell is depicted. In contrast to the pronounced dependence found for the core dimensions, the calculated energy is almost constant over the whole range of investigated thickness, showing only very small numerical variations.

This behaviour has a significant physical meaning. The finite conduction band offset mainly confines the electron in the CdSe core leading to a strong localization of the wavefunction in this region. If the shell thickness is larger than the characteristic penetration depth of the evanescent wavefunction in the CdS barrier, increasing the shell thickness further does not alter the electron confinement. In other words, the electron "does not feel" the additional shell material because the probability density has decayed to negligible values before reaching the external shell boundary. The mathematical explanation is simply from the exponential decay of the wavefunction within finite potential barriers, $\psi(x) \propto e^{-\kappa x}$ where the decay constant (κ) depends on the barrier height and effective mass in the CdS shell. The penetration depth is much smaller than the shell thicknesses studied, so that the overlap of the confined electron wave function with the boundary of the outer shell becomes marginal. Thus, the Hamiltonian matrix is almost invariant, which explains the almost invariant eigenenergy found numerically.

This result is interesting in particular because it indicates that in the range of parameters explored, the shell is mainly a protective barrier and not an active confinement parameter. Such a behaviour has also been reported in theoretical studies of finite core-shell heterostructures, where thick enough shells decouple the confined electronic states from the external environment without significantly changing the ground-state energy. The current simulations thus show that increasing the shell beyond a certain point does not add much to the electronic confinement, although it may improve

optical stability and prevent surface recombination in real devices.

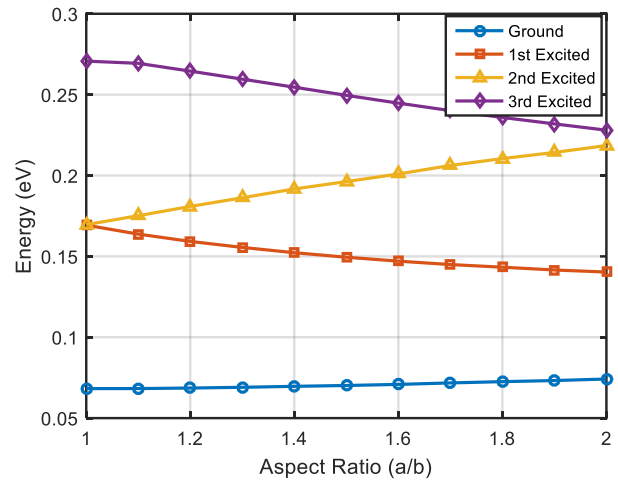


Figure 9. Evolution of the confined electron energy levels as a function of the aspect ratio of the elliptical quantum dot. The geometrical deformation changes the anisotropic confinement, which produces systematic shifts of the quantized energy spectrum.

The role of geometrical anisotropy is much more pronounced in Fig. 9 where the first four energy levels of confined electrons are presented as a function of aspect ratio (a/b). With increasing aspect ratio, the confinement symmetry is gradually broken, and the electronic spectrum is systematically shifted. The response, however, varies from eigenstate to eigenstate, indicating that each quantum state interacts differently with the anisotropic confinement potential. The ground state energy increases slightly with increasing aspect ratio, while the first excited state decreases monotonically. In contrast, the second excited state is increased and the third excited state shows a gradual decrease. The contrary behaviour arises as a result of geometrical deformation causing different variations in nodal structures of each eigenfunction. In particular, states whose probability densities are preferentially oriented along the elongated axis will be less confined and consequently have reduced energy, while states confined along the compressed axis have increased confinement and, thus, higher energies. This is a typical indicator of anisotropic quantum confinement effect. Degeneracy (or near-degeneracy) of excited states in circular quantum dots can be attributed to the presence of rotational symmetry. Geometrical deformation causes breakdown of the rotational symmetry and redistribution of confinement energy among various quantum states. This change in energy, therefore, is brought about by geometrical lifting of the degeneracy due to the presence of the elliptic geometry.

In addition, the gradual and smooth variation of energy levels in all cases indicates that the geometrical deformation causes gradual and smooth variation of the confinement potential without any numerical instability. This further supports the physical validity and the stability of the Hamiltonian.

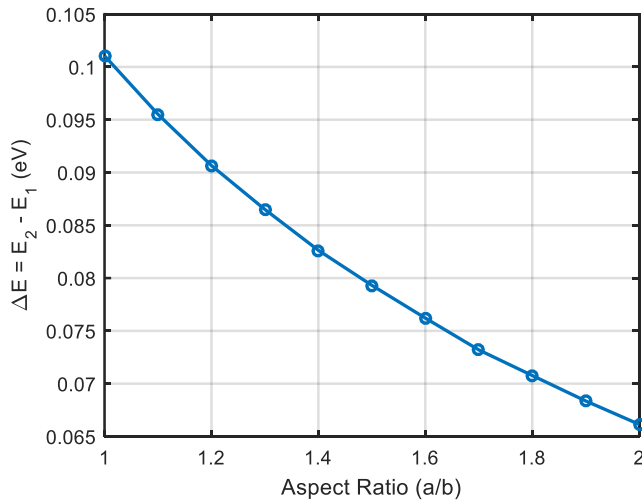


Figure 10. Energy spacing between the first excited and ground states (E_2-E_1) vs. aspect ratio. The variation of the energy gap mirrors the effect of geometrical anisotropy on electronic confinement.

The change of the energy spacing between the ground and first excited states is summarized in Fig. 10. The results show that the energy gap decreases gradually with increasing aspect ratio. This means that the elliptical deformation leads to compression of the low energy electronic spectrum.

Such behaviour can be explained by the fact that increasing the aspect ratio decreases the confinement strength mainly along one of the principal directions while a stronger confinement is maintained along the orthogonal axis. The effect of the reduction of the confinement in the elongated direction is more pronounced for the excited states than for the ground state, as the wavefunctions of the excited states extend over larger spatial regions, and are more subject to the boundary geometry. Hence, the energy spacing between consecutive eigenstates decreases as the anisotropy increases. From a practical point of view, this is an important result because the energy spacing sets a number of optical properties, such as the intersubband transition energies, absorption spectra, spontaneous emission wavelengths, and carrier relaxation dynamics. Therefore, the aspect ratio provides an efficient geometrical route to engineer the electronic spectrum of CdSe/CdS QDs without changing their material composition. This ability provides great flexibility for the design of nanoscale optoelectronic devices with desired transition energies and tailored optical responses.

The one-dimensional cross sections of the normalized wavefunction of the ground state, are shown in figure 11. The probability density is calculated along both the major (x) and minor (y) axes of the elliptical quantum dot. Unlike the previously shown two-dimensional probability maps, these cross-sectional profiles provide a quantitative description of the strength of the confinement along each principal direction and clearly reveal the anisotropic nature of the electronic localization. The calculated profiles show a strong maximum at the centre of the quantum dot where the electron

localization probability is maximal. Moving away from the centre the probability density decreases continuously until it becomes negligible outside the confinement region. This behavior is the hallmark of a bound quantum state and confirms that the calculated wavefunction satisfies the localization requirements imposed by the finite confinement potential.

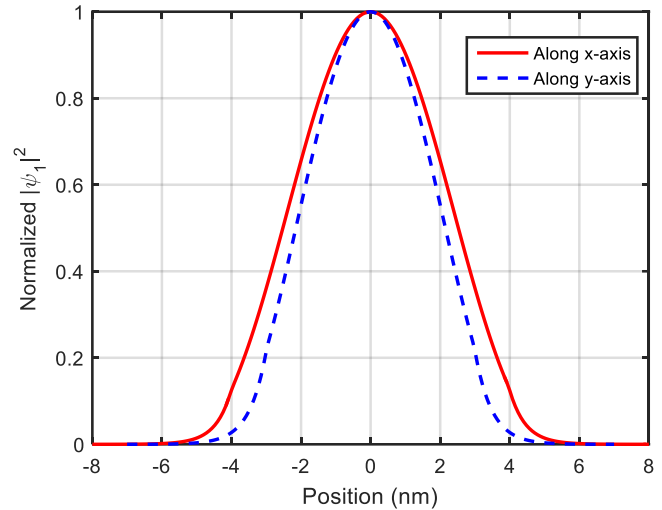


Figure 11. One-dimensional cross sections of the normalized ground state wavefunction along the principal axes (x) and (y). The profiles show the anisotropic spatial confinement caused by the elliptical geometry.

There is a noticeable difference between the two spatial directions. The distribution of probabilities is more elongated in the x-direction which is related to the semi-major axis of the ellipse, while it decays faster in the y-direction due to shorter confinement length. This effect is a result of the ellipsoid geometry. Along the major axis of the confinement potential, which extends over a larger distance, the electron wavefunction is weaker confined and is thus more spread out in space. On the other hand, the smaller dimension along the minor axis means a stronger confinement and the wavefunction has to shrink faster. This anisotropy in localization is a result of the kinetic-energy operator in the BenDaniel-Duke Hamiltonian. The wavefunction acquires a spatial distribution such that the total energy is minimized subject to the imposed boundary conditions. Thus, the spatial width of the ground state wavefunction becomes proportional to the available length of confinement in each direction. The present results thus provide clear evidence that the electronic properties of elliptical quantum dots cannot be described using isotropic confinement models even in the case of the same material composition [27]. From the optical point of view, the anisotropic wavefunction presented in Figure 11 is expected to affect some important physical quantities such as transition dipole moments, polarization-dependent optical absorption, oscillator strength and spontaneous emission characteristics. Thus the geometrical deformation provides an extra degree of freedom for engineering the optical response of semiconductor quantum dots beyond the traditional choice of materials.

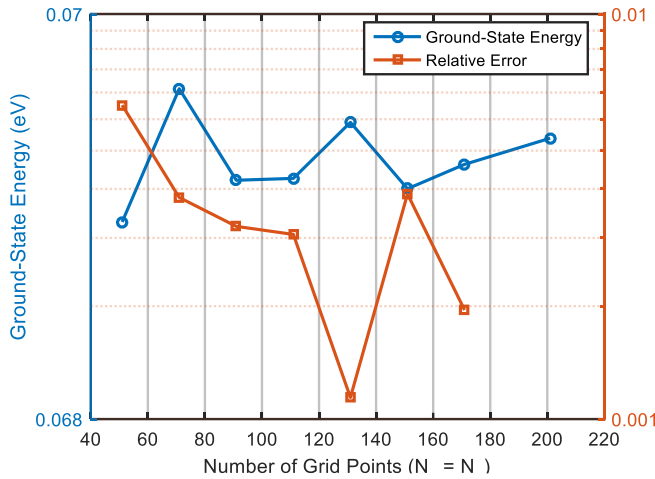


Figure 12. Mesh convergence analysis showing the dependence of the calculated ground-state energy on the finite-difference mesh density. The convergence behavior confirms the numerical stability and accuracy of the discretization scheme used.

The numerical stability of the proposed computational framework is studied in Fig. 12, which shows the mesh convergence analysis of the ground-state energy as a function of the finite-difference grid density. With the increase of the number of grid points, the calculated ground-state energy converges to a nearly constant value and the relative numerical error is reduced substantially. This behaviour suggests that the finite-difference discretization adopted converges to the continuous solution of the Schrödinger equation.

The convergence behaviour has an important mathematical significance. The continuous second order spatial derivatives are replaced by algebraic expressions in the finite difference approximation, with a truncation error proportional to the square of the mesh spacing. Hence, a finer computational grid reduces the discretization error and the numerical Hamiltonian can better approximate the continuous BenDaniel–Duke operator. As shown in Figure 12, the calculated eigenvalue gradually stabilizes, which indicates that the mesh density chosen is adequate to describe the essential physics of the confined electron without introducing significant numerical artifacts.

At intermediate mesh densities small variations are observed but these are extremely small compared to the overall energy scale and diminish with finer mesh. Such behaviour is expected for sparse eigenvalue problems with position-dependent material parameters and is not an indication of numerical instability. Instead, the concurrent decrease of the relative error confirms that the numerical solution is approaching grid independence, i.e., the reported electronic energies are mainly determined by the physical model rather than the discretization scheme.

The convergence analysis also explains how the BenDaniel–Duke interface conditions are implemented. In the heterointerface CdSe/CdS, the abrupt change of effective mass makes the maintenance of the probability-current continuity a must for the physically meaningful eigenvalues. The smooth convergence seen in Figure 12 is thus an indirect

confirmation that the interface treatment and the Hamiltonian assembly have been correctly implemented.

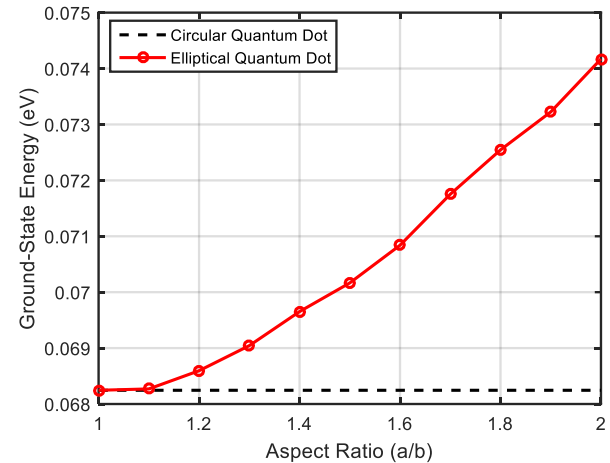


Figure 13. Comparison of confined electron energy levels in elliptical and circular CdSe/CdS quantum dots. The results show the effect of geometrical deformation on the electronic confinement properties and the energy spectrum.

Finally, in Fig. 13 we show the ground-state energies of elliptical and circular CdSe/CdS quantum dots for the range of aspect ratios studied here. The elliptical geometry naturally tends to the circular case for the aspect ratio equal to 1 and both structures show almost the same confinement energies. However, as the aspect ratio increases, the electronic energy of the elliptical quantum dot increases progressively, whereas the circular quantum dot retains almost a constant energy because of its rotational symmetry and unchanged confinement dimensions. The result clearly shows that the geometrical deformation itself is an independent mechanism of confinement. Increasing the aspect ratio makes the confinement potential asymmetric in one direction which changes the relative kinetic and potential energies of the Schrödinger equation. While the available confinement region may still be comparable, the unequal spatial dimensions alter the electron probability distribution and change the curvature of the wavefunction, resulting in measurable shifts in the eigenenergy [28].

Another important effect due to the ellipse-like distortion is the rotational symmetry. In case of circular confinement, isotropy is achieved, which means that equal restoring force is exerted on the electrons in all in-plane directions. However, in case of elliptical dots, anisotropy is introduced due to the variation in the strength of confinement along different directions. This anisotropic behaviour cannot be reproduced using simplified circular models and thus highlights the necessity of considering realistic geometrical configurations for predicting the electronic properties of semiconductor nanostructures.

As can be seen from the data presented in Fig. 13, once more, the geometrical engineering represents an effective tool for the manipulation of the electronic structure without changing the material constituents or the heterostructures boundaries. Such structural optimization is especially appealing for practical device fabrication as the aspect ratio can be often

controlled in experiments during crystal growth with the same semiconductor materials. Therefore, elliptical quantum dots are more versatile than conventional circular structures in tuning energy levels, optical transition energies, polarization characteristics and carrier localization as per desired device requirements. The overall results reported in Figures 11-13 validate the physical validity and the numerical robustness of the proposed computational framework. The anisotropic wavefunction distributions reproduce correctly the effect of elliptical confinement. The convergence analysis confirms the stability and accuracy of the finite-difference implementation. The comparison with circular quantum dots shows that the geometrical deformation is an efficient way to tailor the electronic properties of CdSe/CdS core-shell nanostructures [29]. Taken together, these results demonstrate that the two-dimensional BenDaniel-Duke effective-mass model developed in this work offers a reliable and physically consistent platform to explore the quantum confinement effects in semiconductor heterostructures and to assist future designs of advanced optoelectronic devices based on quantum dots.

4. Conclusions

A two-dimensional numerical model has been developed for the study of confined electron states in CdSe/CdS core-shell elliptical quantum dots using the single-band Effective Mass Approximation, BenDaniel-Duke Hamiltonian and Finite Difference Method. The adopted formulation considers the position dependent effective mass and the finite conduction band confinement potential, thus allowing a physically consistent description of the electronic states in the heterostructure.

The mathematical model successfully described the energy levels of the electrons, wave functions and their probability distribution. From the findings it is clear that the geometry of the quantum dots significantly affects their electronic properties. The core dimensions are increased, thus decreasing the quantum confinement and the confined energy levels, while variations in shell thickness and aspect ratio modify the confinement profile and hence the spatial localization of the electron wavefunction.

The calculated probability-density distributions show that the ground-state electron is mostly localized inside the CdSe core, whereas the excited states are more spatially extended and exhibit nodal structures. Moreover, the comparison of elliptic and circular quantum dots shows that the geometrical anisotropy plays an important role in the energy spectrum and the wavefunction distribution, confirming the aspect ratio as an effective design parameter for the electronic properties of semiconductor nanostructures. The mesh convergence analysis shows that the finite difference discretization used in this work can provide stable numerical results with refinement of the computational grid, and thus supporting the applicability of the proposed numerical approach for modeling of semiconductor core-shell quantum dots.

In conclusion, the proposed computational framework provides an efficient basis for the analysis of confined electron states in semiconductor heterostructures, and can be

extended to include additional physical phenomena such as external electric and magnetic fields, spin-related interactions, strain effects and excitonic corrections, thus providing a versatile platform for the design and optimization of future nanoelectronic and optoelectronic devices.

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