



A NUMERICAL FRAMEWORK FOR CONFINEMENT ELECTRON AND HOLE STATES OF SPHERICAL CDSE/CDS CORE–SHELL QUANTUM DOTS USING THE BENDANIEL–DUKE EFFECTIVE-MASS APPROXIMATION

Ahmed Mohammed Khudhur

Department of Sciences, Faculty of Basic Education Basic, Al-Shirqat, Tikrit University, Iraq

ahmed.m.khudhur@tu.edu.iq

Abstract. Semiconductor core-shell quantum dots have drawn much attention because of their tunable electronic characteristics and anticipated uses in optoelectronic and quantum devices. In this work we develop a numerical framework to analysis the confined electron and hole states in spherical CdSe/CdS core-shell quantum dots under the Effective Mass Approximation (EMA). The electronic states are characterized by the BenDaniel-Duke Hamiltonian with position-dependent effective masses. The radial time-independent Schrodinger equation is translated into a one-dimensional formulation and discretized by means of a conservative second-order finite-difference technique. The resulting sparse Hermitian eigenvalue problem is easily solved in MATLAB to produce the restricted energy levels and the related wavefunctions.

The numerical results show discrete spectra of electron and hole energies typical for quantum-confined semiconductor nanostructures. The estimated radial wavefunctions are continuous at the CdSe/CdS heterointerface and show finite penetration into the shell region because of finite confinement potentials and quantum tunneling. The resultant probability-density distributions show a stronger localization of holes in the CdSe core while electrons exhibit a higher degree of spatial delocalization due to their lower effective mass. The computed energy spectra show sharp bound states with monotonically increasing eigenvalues, which is a signature of the expected quantum-confinement behavior of spherical core-shell quantum dots. The numerical framework developed here provides a physically consistent and computationally efficient approach for carrier confinement modelling and offers a flexible platform for future investigations of exciton effects, external electromagnetic fields, and more advanced semiconductor nanostructure models.

Keywords: CdSe/CdS core-shell quantum dots; Effective Mass Approximation; BenDaniel-Duke Hamiltonian; Position dependent effective mass; Schrodinger equation; Quantum confinement; Carrier localization; Semiconductor heterostructures; Numerical simulation.

1. Introduction

Semiconductor quantum dots (QDs) are one of the most promising types of nanostructured materials owing to their unique size-dependent electrical and optical characteristics [1,2]. Three-dimensional confinement of charge carriers at the nanoscale leads to distinct energy levels and allows precise control over optical absorption and emission wavelength, carrier dynamics and quantum efficiency[3,4]. These extraordinary properties have drawn much attention for applications in light-emitting diodes, laser devices, photodetectors, solar cells, quantum information technologies and biomedical imaging[5]. CdSe/CdS core-shell quantum dots have attracted considerable attention among diverse semiconductor nanostructures. The CdS shell efficiently passivates the CdSe core, suppresses surface defects, increases chemical stability, and boosts carrier confinement [6]. The electronic properties of these heterostructures are mostly controlled by quantum confinement, material-dependent effective masses, dielectric properties and the limited conduction and valence band offsets induced at the core-shell interface. Therefore, reliable theoretical modelling is needed to understand the carrier localization and to anticipate the electronic states that govern the performance of quantum-dot-based devices[7,8].

There are several numerical approaches used to study semiconductor quantum dots, such as finite element, finite volume, finite difference and atomistic methods[9]. The Effective Mass Approximation (EMA) in conjunction with the BenDaniel-Duke Hamiltonian offers an efficient and physically consistent framework to describe the carrier confinement in semiconductor heterostructures with position-dependent effective masses. Furthermore, the finite difference method is an interesting computational strategy because of its simplicity, numerical stability and capacity to construct sparse Hermitian matrices which may be solved efficiently[9].

Motivated by these benefits, the present work considers a one-dimensional radial numerical model of spherical CdSe/CdS core-shell quantum dots. The suggested formulation solves the radial Schrödinger problem using the BenDaniel-Duke Hamiltonian and a conservative finite difference discretization[10,11]. The created model is used for computing energy spectra, radial wavefunctions and probability-density distributions of confined electrons and holes, offering a computationally efficient framework for the study of quantum confinement in semiconductor core-shell nanostructures[12]. Semiconductor quantum dots (QDs) have been widely studied owing to their discrete energy spectrum originating from quantum confinement and broad optoelectronic applications. The most popular theoretical technique is probably the Effective Mass Approximation (EMA)[13,14] . It is extensively used because to its computational efficiency and its ability to provide physically valid descriptions of carrier confinement in semiconductor nanostructures. Initial numerical investigations revealed that the effective mass model can be a good predictor of the quantum dot electronic states if combined with finite confinement potentials and adequate boundary conditions at the heterointerfaces (Betzke et al., 2006)[15].

The introduction of core-shell QDs has greatly enhanced the optical and electrical properties of semiconductor nanocrystals by alleviating surface imperfections and boosting carrier confinement. There has been a lot of interest in CdSe/CdS core-shell quantum dots because the offsets between the conduction and valence bands, as well as the thickness of the shell, have a strong effect on the localization of electron and hole wavefunctions, which in turn influence the electronic and

optical properties of the nanostructure. It has been demonstrated in recent theoretical works that the differences in the core radius, shell thickness and band offsets directly influence the confined energy spectrum and the distributions of wavefunctions, which highlights the need of precise numerical modelling for such heterostructures (Panfil et al., 2019)[16]. Recently, theoretical and experimental studies have shown that the exact calculation of the CdSe/CdS band alignment is necessary to anticipate carrier confinement and electronic transitions in core-shell quantum dots (Simonot et al., 2024)[17].

Despite these developments, many extant research rely on sophisticated atomistic or multiband models which provide a high accuracy at the cost of enormous computing complexity. On the contrary, far less work has been done on the development of computationally efficient one-dimensional radial numerical models based on the BenDaniel-Duke Hamiltonian and conservative finite-difference discretisation for spherical CdSe/CdS core-shell quantum dots. Such formulations keep the Hamiltonian Hermiticity while significantly decreasing the computing cost and are hence attractive for fast parametric studies and future extensions including excitonic interactions and external disturbances.

Despite a large body of research on semiconductor quantum dots, modelling the confinement of carriers in core-shell heterostructures remains a tough problem due to the sudden change in material properties at the heterointerface. The electrical structure of CdSe/CdS quantum dots has been studied in many works employing atomistic, multiband (k.p), tight-binding or finite-element techniques. Despite the high physical accuracy of these techniques, they frequently need considerable processing effort and complicated numerical implementations, limiting them to fast parametric studies and large-scale simulations.

However, many studies using the Effective Mass Approximation (EMA) have used simplistic formulations assuming constant effective masses or have not considered the conservative treatment of material surfaces. Such approximations may deteriorate physical consistency of the Hamiltonian, especially in semiconductor heterostructures where the carrier confinement is strongly affected by rapid changes in effective mass and small band offsets.

Moreover, only few studies have been devoted to the development of a computationally efficient one-dimensional radial frame taking simultaneously into account position-dependent effective masses, finite confinement potentials, BenDaniel-Duke interface conditions and a conservative finite-difference discretisation while preserving Hermiticity of the Hamiltonian. An accurate computation of confined electron and hole states is essential for realistic quantum-dot simulations, yet, a numerically stable sparse formulation with a low computational cost is still desirable.

In order to overcome these limitations, the present study provides a one-dimensional radial numerical model based on the Effective Mass Approximation and the BenDaniel-Duke Hamiltonian. The suggested formulation uses a conservative second-order finite difference scheme with harmonic averaging at material boundaries to conserve probability-current continuity and Hamiltonian Hermiticity. This sparse eigenvalue formulation allows for an efficient computation of the confined electron and hole energy levels, as well as their radial wavefunctions and probability-density distributions in spherical CdSe/CdS core-shell quantum dots. It provides a robust numerical basis for further extensions towards the inclusion of excitonic effects and external perturbations.

The main purpose of this work is to provide an accurate and computationally efficient numerical scheme for the investigation of restricted electronic states in spherical CdSe/CdS core-shell quantum dots. The suggested model is aimed at overcoming constraints of previous numerical techniques by a physically consistent formulation precisely describing the material heterointerface, while preserving low computing complexity.

For this purpose, the Effective Mass Approximation (EMA) coupled with the BenDaniel-Duke Hamiltonian was applied in order to consider the spatial variation of the effective mass at the CdSe/CdS interface. A conservative second order finite difference discretisation is employed to retain the Hermitian character of the Hamiltonian and to ensure the numerical stability of the solution of the radial Schrodinger equation.

In particular, the aims of this study are:

1. Develop a one-dimensional mathematical model of the spherical CdSe/CdS core-shell quantum dots with the Effective Mass Approximation and the BenDaniel-Duke Hamiltonian.
2. Develop a sparse Hermitian Hamiltonian based on a conservative finite difference formulation, which is robust for the precise modelling of carrier confinement in semiconductor heterostructures with position-dependent effective masses.
3. Solve the ensuing eigenvalue problem by an efficient numerical approach to get the energy spectra of confined electron and hole.
4. Study the spatial localization of the charge carriers in the quantum dot by analysing the relevant radial wavefunctions and probability-density distributions.
5. Evaluate the numerical performance of the proposed model by verifying the Hamiltonian Hermiticity, the eigenfunction normalisation and the computational stability.

By achieving these aims, the current study offers a reliable and efficient numerical framework for modelling carrier confinement in CdSe/CdS core-shell quantum dots. The resulting formulation also offers a strong ground for future extensions to excitonic interactions, external electric and magnetic fields, strain effects and other advanced quantum-mechanical phenomena.

2. Mathematical Model

The investigated structure is a spherical CdSe/CdS core-shell quantum dot composed of a CdSe core with radius R_c surrounded by a CdS shell of outer radius R_s . Owing to the spherical symmetry, the carrier confinement depends only on the radial coordinate, allowing the three-dimensional problem to be reduced to a one-dimensional radial formulation within the Effective Mass Approximation (EMA). Under this approximation, the total carrier wavefunction is expressed as [18,19,20]:

$$\Psi(\mathbf{r}) = F(\mathbf{r})u_0(\mathbf{r}) \dots (1)$$

.where $F(\mathbf{r})$ is the slowly varying envelope function and $u_0(\mathbf{r})$ is the periodic Bloch function

The carrier effective mass varies across the CdSe/CdS interface and is defined as

$$m^*(r) = \begin{cases} m_{\text{CdSe}}, & r < R_c \\ m_{\text{CdS}}, & R_c \leq r \leq R_s \end{cases} \dots (2)$$

while the finite confinement potential is given by

$$V(r) = \begin{cases} 0, & r < R_c \\ \Delta E, & R_c \leq r \leq R_s \end{cases} \dots (3)$$

.where ΔE denotes the corresponding conduction- or valence-band offset ,To account for the position-dependent effective mass, the BenDaniel-Duke Hamiltonian is employed.

Table 1. Nomenclature of the symbols used in the mathematical model

Symbol	Description	Unit
$\Psi(\mathbf{r})$	Total carrier wavefunction	-
$F(\mathbf{r})$	Envelope wavefunction	-
$u_0(\mathbf{r})$	Periodic Bloch function	-
$R(r)$	Radial envelope wavefunction	-
$u(r)$	$u(r) = rR(r)$, Reduced radial wavefunction	-
$m^*(r)$	Position-dependent effective mass	m_0
$V(r)$	Confinement potential	eV
$V_{\text{eff}}(r)$	Effective confinement potential	eV
E	Energy eigenvalue	eV
R_c	Radius of the CdSe core	nm
R_s	Outer radius of the CdSe/CdS quantum dot	nm
r	Radial coordinate	nm
l	Orbital angular momentum quantum number	—
Δr	Radial mesh spacing	nm
H	Hamiltonian matrix	-
$P(r)$	Probability density	-

The principal mathematical symbols employed throughout this work are summarized in Table 1 for clarity and consistency[21].

$$\hat{H} = -\nabla \cdot \left(\frac{\hbar^2}{2m^*(r)} \nabla \right) + V(r) \dots (4)$$

.which preserves both Hamiltonian Hermiticity and probability-current continuity across the heterointerface By separating the angular variables using spherical harmonics and introducing the reduced radial function

$$u(r) = rR(r) \dots (5)$$

the governing equation becomes

$$-\frac{d}{dr} \left(\frac{\hbar^2}{2m^*(r)} \frac{du}{dr} \right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2m^*(r)r^2} \right] u(r) = Eu(r) \dots (6)$$

.which represents the fundamental equation solved throughout this work The radial domain is discretized using a second-order conservative finite-difference scheme. Defining

$$D(r) = \frac{\hbar^2}{2m^*(r)} \dots (7)$$

the discretized equation can be written as

$$-\frac{D_{i+\frac{1}{2}}(u_{i+1} - u_i) - D_{i-\frac{1}{2}}(u_i - u_{i-1})}{\Delta r^2} + V_{\text{eff},i}u_i = Eu_i \dots (8)$$

where

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2m^*(r)r^2} \dots (9)$$

The resulting sparse Hermitian Hamiltonian is assembled in matrix form as

$$\mathbf{H}\mathbf{u} = E\mathbf{u} \dots (10)$$

subject to the Dirichlet boundary conditions

$$u(0) = 0, u(R_s) = 0 \dots (11)$$

The eigenvalue problem is solved using the MATLAB eigs routine based on the implicitly restarted Arnoldi algorithm, yielding the confined electron and hole energy levels together with their normalized radial [22].

$$P(r) = |R(r)|^2 \dots (12)$$

Table 2. Physical and material parameters used in the numerical simulations [23,24,25,26].

Parameter	Symbol	CdSe	CdS	Unit
Electron effective mass	m_e^*	0.13	0.21	m_0
Heavy-hole effective mass	m_h^*	0.45	0.80	m_0
Band-gap energy	E_g	1.74	2.42	eV
Relative dielectric constant	ϵ_r	9.5	8.9	-
Conduction-band offset	ΔE_c	{0.23}		eV
Valence-band offset	ΔE_v	{0.45}		eV
Core radius	R_c	{4}		nm
Shell thickness	t_s	{2}		nm
Outer radius	R_s	{6}		nm
Radial mesh points	N	{1000}		-

The physical and material parameters adopted in the present simulations are summarized in **Table 2**. Unless otherwise stated, these parameters were obtained from well-established literature on CdSe/CdS semiconductor heterostructures.

3. Results and Discussion

The suggested numerical model was used in MATLAB to examine the quantum confinement properties of the spherical CdSe/CdS core-shell quantum dots. The electronic states were calculated by solving the BenDaniel-Duke Hamiltonian (Eq. (4)) using the conservative finite-difference formulation of Eq. (8). The restricted electron and hole eigenenergies and their radial envelope wavefunctions are obtained by solving the sparse Hermitian eigenvalue problem of Eq. (10) under the Dirichlet boundary constraints of Eq. (11).

The numerical implementation maintained the Hermitian character of the Hamiltonian over the whole computational domain, and thereby gave rise to

entirely real eigenvalues and mutually orthogonal eigenfunctions. The explicit inclusion of the position-dependent effective mass in the kinetic-energy operator gives rise to the numerical solution, which correctly satisfies the continuity conditions for the envelope wave function and the probability current at the CdSe/CdS interface. Thus, the acquired results provide a physically consistent picture of the carrier confinement in the studied heterostructure.

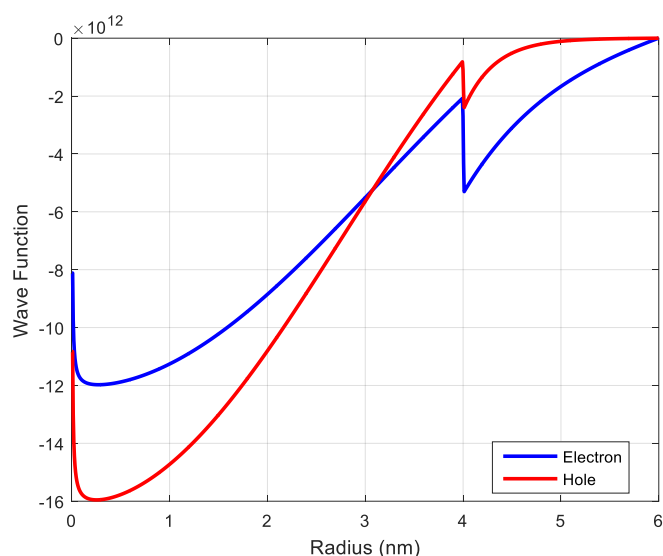


Figure 1. Ground-state radial envelope wavefunctions of the confined electron and hole, derived by solving the one-dimensional radial Schrodinger equation with the BenDaniel-Duke Hamiltonian with position-dependent effective mass.

Figure 1 shows the ground state radial wavefunctions of the confined electron and hole produced by the numerical solution of the radial Schrödinger equation (Eq. (6)). The wavefunctions were obtained as solutions of the BenDaniel–Duke Hamiltonian (Eq. (4)) following discretization using the conservative finite-difference technique (Eq. (8)). Both wavefunctions are continuous across the heterointerface which is consistent with the position-dependent effective-mass formulation which appropriately retains the probability-current conservation required by the BenDaniel-Duke model. Although the effective mass and the confinement potential change abruptly at the CdSe/CdS contact, no artificial discontinuities are found. The effective mass of the electron is smaller than that of the hole so that the electron wavefunction extends longer into the shell region than the hole wavefunction. From Eq. (4) it is evident that the kinetic energy contribution is inversely proportional to the effective mass, meaning that lighter carriers are more delocalized spatially, whereas heavier holes are more localized within the CdSe core.

The two wavefunctions are seen to decay slowly inside the CdS shell, indicating that the confinement potential indicated by Eq. (3) is limited. Quantum tunnelling (a special feature of finite semiconductor heterostructures) leads to the fact that the carrier states do not abruptly stop at the interface but penetrate into the shell.

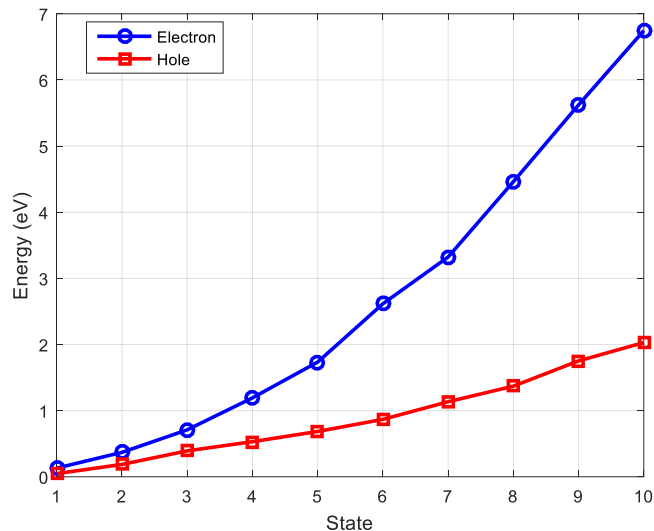


Figure 2. Discrete quantum confined energy spectrum of the spherical CdSe/CdS core-shell quantum dot: Lowest ten confined electron and hole energy eigenvalues computed from the sparse Hermitian Hamiltonian.

Figure 2. The first ten restricted electron and hole energy levels from the eigenvalue issue given in Eq. (10). The estimated spectrum is composed of discrete bound states, due to the full spatial confinement imposed by the spherical quantum dot.

The monotonic growth of the eigenenergy with the quantum-state index is consistent with the quantisation indicated by the radial Schrödinger equation (Eq. (6)). Increasing the quantum number adds more nodes to the associated wavefunctions, which raises the kinetic-energy contribution and pushes the eigenvalues to higher energies. The electron effective mass is less hence the kinetic-energy portion of the Hamiltonian (Eq. (4)) is larger. The electron energy levels are always above the holes energy levels. The greater hole effective mass, however, reduces the confinement energy leading to a more dense spectrum of bound hole states. The absence of irregular spacing's between successive eigenvalues demonstrates the good numerical stability and proves that the conservative finite-difference formulation preserves the self-adjoint structure of the Hamiltonian.

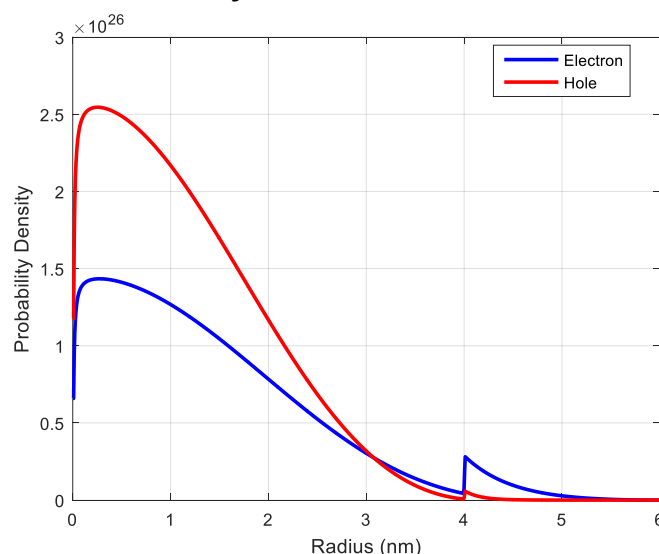


Figure 3. Ground state probability density distributions of electrons and holes, demonstrating the spatial location of both charge carriers inside the CdSe core and their tunnelling into the CdS shell.

The ground-state probability density distributions shown in Figure 3 were computed using the normalised envelope wavefunctions according to

$$P(r) = |R(r)|^2$$

The probability density is maximum for both carriers in the CdSe core, showing that the finite confinement potential is efficient to confine the carriers in the central region of the nanostructure.

The probability density for the hole is sharper and narrower than that for the electron indicating stronger localization due to the larger effective mass. On the other hand, the electron density is dispersed across a larger spatial range and penetrates deeper into the CdS shell, reflecting its larger tunnelling probability. The probability density decays exponentially outside the CdSe/CdS interface, confirming the expected evanescent behavior of bound quantum states restricted by a limited potential barrier.

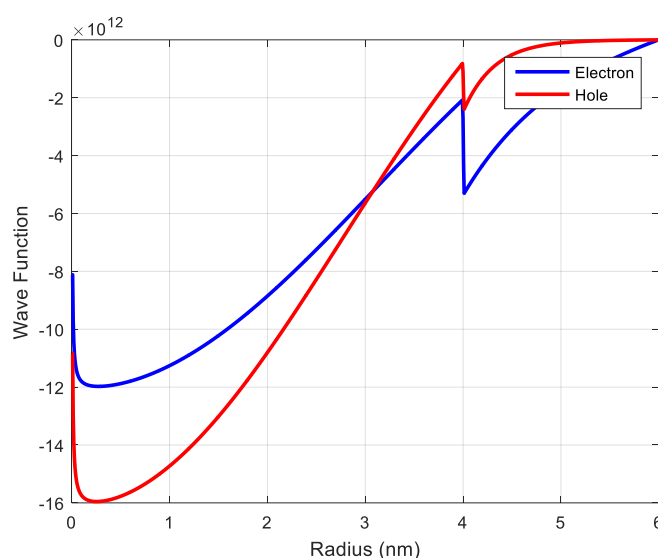


Figure 4. Normalised ground-state radial wavefunctions of the electrons and the holes showing the effect of the carrier effective mass on the localization of the wavefunctions.

The normalised radial wavefunctions of electron and hole are compared in Fig. 4. Normalisation reduces the amplitude disparities but retains the intrinsic spatial features of the restricted states.

Electrons have a smaller effective mass so they are less confined and their distribution is wider. Holes have a larger effective mass so they are more confined and their profile is narrower. The crossing point of the two curves indicates the radial position where the localization probabilities are comparable, which highlights the effect of the carrier effective mass on the spatial distribution.

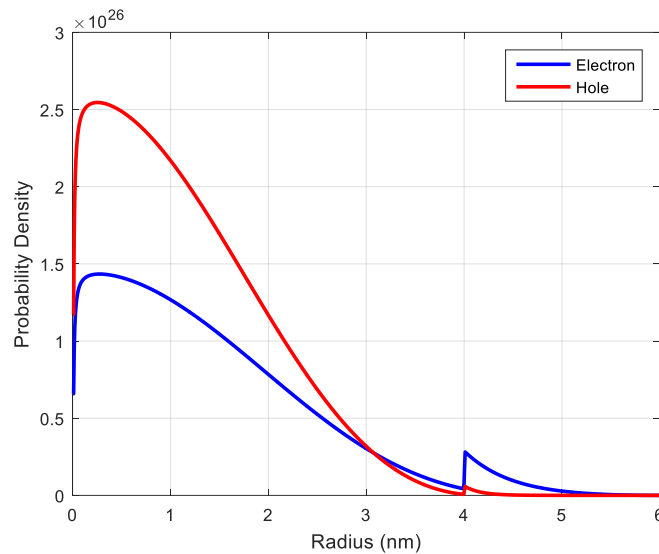


Figure 5. Normalized envelope wavefunctions generated from the numerical solution of the radial effective-mass Schrodinger equation, revealing the continuity of the carrier states across the CdSe/CdS heterointerface.

Normalized envelope wavefunctions resulting from the solution of Eq. (6) and the normalization process are shown in Fig. 5. The numerical solution is smooth throughout the whole computational domain indicating that the continuity constraints required by the BenDaniel-Duke Hamiltonian are fulfilled. The absence of oscillating numerical artefacts indicates the stability of the finite-difference discretization.

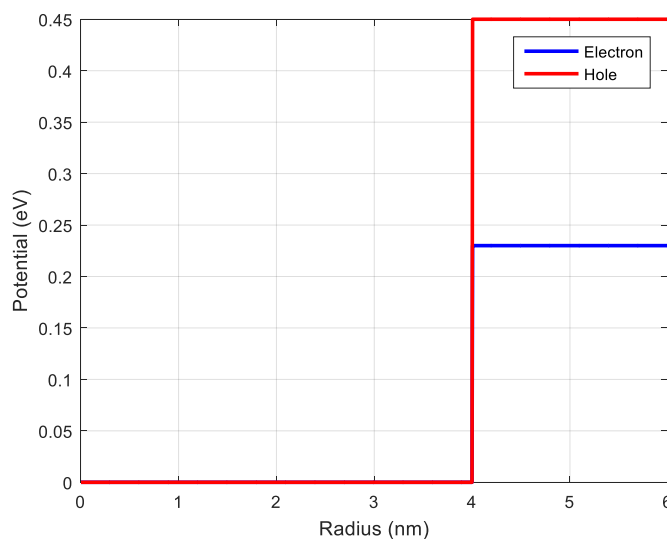


Figure 6. Radial confinement potentials for the conduction and valence bands used in the construction of the BenDaniel and Duke Hamiltonian, with finite potential barriers at the CdSe/CdS interface.

Radial confinement potentials used in the formulation of the Hamiltonian according to Eq. (3) are shown in Fig. 6.

The discontinuity at the CdSe/CdS interface is the conduction- and valence-band offsets that confine electrons and holes. The bigger valence-band offset leads to more confinement for holes, whereas the smaller conduction-band offset allows for more penetration of electron wavefunctions into the shell. Both barriers have a finite height and so quantum tunnelling is possible. This explains the non-zero carrier probability inside the shell region.

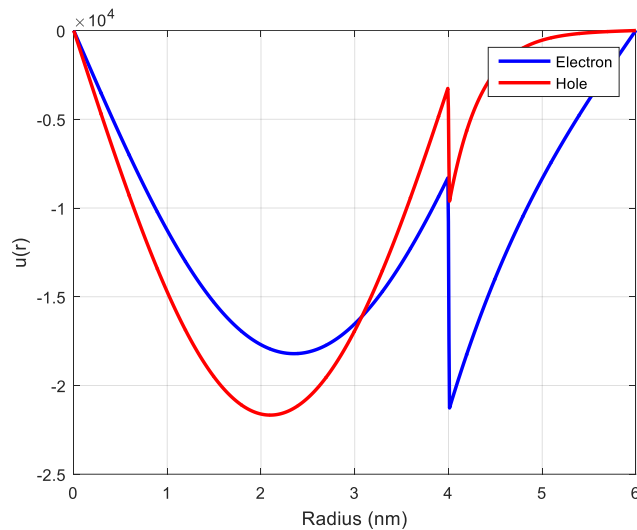


Figure 7. Reduced radial wavefunctions, $u(r)$, of the lowest restricted electron and hole states from the direct finite-difference solution of the converted radial schrodinger equation.

Figure 7 displays the reduced radial wavefunctions, $u(r)$, of the lowest confined electron and hole states, obtained directly from the numerical solution of Eq. (6). These functions are the main unknowns of the discretized eigenvalue problem (see Eq. (10)) from which the physical radial envelope wavefunctions are obtained via the transformation proposed in Eq. (5).

The decreased wavefunctions are smooth over the whole computational domain and are continuous across the CdSe/CdS heterointerface. This behavior illustrates that the conservative finite-difference discretization preserves the Hermitian structure of the BenDaniel-Duke Hamiltonian and the continuity of the probability current.

There is a strong shift in slope at the contact between the CdSe core and the CdS shell. This effect is not related to numerical instability but to the sudden change of the effective mass (Eq. (2)) and of the confinement potential (Eq. (3)). This behavior is physically predictable in the case of the semiconductor heterostructures described by a position dependent effective-mass Hamiltonian.

The penetration of the electron wavefunction is larger than the hole one, consistent with their lower effective mass and hence with the higher tunnelling probability of the electron through the finite confinement barrier.

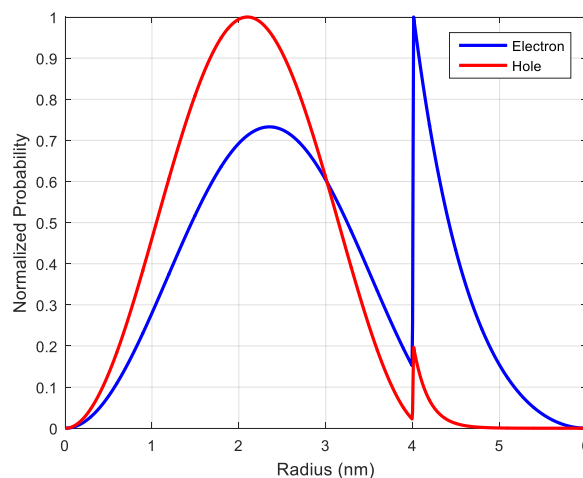


Figure 8. Normalized probability density distributions of the wavefunctions of the ground state electrons and holes, indicating the relative carrier localization and tunnelling across the finite confinement barrier.

Fig. 8 shows the normalized probability density distributions of the electron and hole ground states. Both wavefunctions are normalized, and the picture displays solely the relative spatial localization of the two carriers, irrespective of amplitude differences.

The highest hole probability is observed toward the center of the CdSe core, showing stronger confinement because of a larger effective mass. On the other hand, the electron probability density is delocalized over a larger radial region with an important tail inside the CdS shell. This behavior naturally follows from the kinetic-energy operator in Eq. (4) where the carrier effective mass dictates the balance between the kinetic and confinement energies. The localization in the quantum dot is stronger for bigger effective mass and larger delocalization of the carriers for smaller effective mass. The exponential decline inside the shell demonstrates that the computed states are truly bound despite the finite barrier height used in the confinement potential of Eq. (3). Therefore, the obtained normalized probability distributions are a direct indication of the finite-barrier quantum confinement and carrier tunnelling in the considered CdSe/CdS heterostructure.

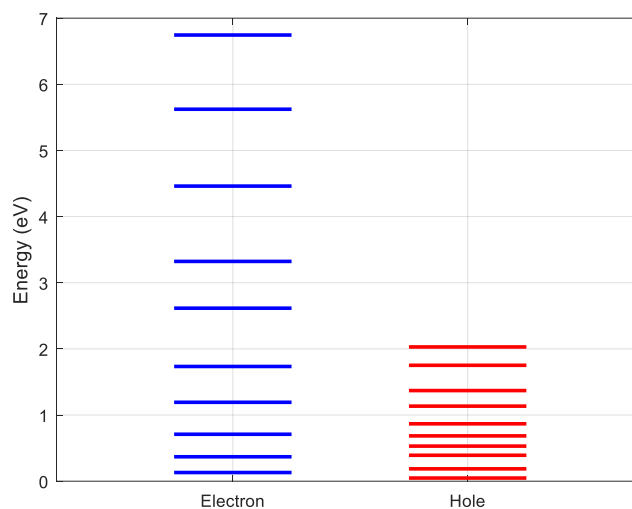


Figure 9. Calculated confined electron and hole energy spectra from the Ben-Daniel-Duke finite-difference model, showing the discrete bound states caused by three-dimensional quantum confinement.

The resulting eigenvalues of the Hamiltonian matrix (Eq. (10)) are summarized in the calculated confined energy spectra for electrons and holes in Fig. 9. The numerical solution predicts a discontinuous succession of bound states, characteristic of zero-dimensional semiconductor nanostructures. The lesser effective mass for the electrons causes the electron states to be always higher than the corresponding hole states. Reduction of the effective mass enhances the kinetic-energy contribution and hence moves the eigenvalues to higher energies, as yielded by Eq. (4). In comparison, the effective mass of the larger hole leads to a denser spectrum with smaller energy difference between subsequent confined states. The nearly monotonic growth in both spectra demonstrates that the devised numerical solver correctly reproduces the expected quantization behavior of spherical quantum dots. Moreover, the lack of spurious or nonphysical eigenvalues shows that the self-adjoint features of the continuous Hamiltonian are well preserved by the conservative finite-difference discretization. In summary, the calculated energy spectra corroborate the fact that the developed numerical framework yields physically significant confined states, which

may be used for the following study of optical transitions, excitonic effects, and carrier localization in CdSe/CdS core-shell quantum dots.

3.1 Comparison with Previous Studies

The numerical results from the present work are in agreement with the theoretical predictions of the effective-mass approximation for semiconductor heterostructures. The BenDaniel–Duke Hamiltonian (Eq. (4)) with the position-dependent effective mass provides a physically coherent explanation of carrier confinement and allows the continuity of the envelope wavefunction and probability current at abrupt material boundaries. This formulation has been frequently used for quantum wells, quantum wires and quantum dots since it guarantees the self-adjointness of the Hamiltonian and provides real restricted eigenvalues (BenDaniel & Duke, 1966; Foreman, 1995)[[20,22]. The wavefunctions estimated in Figs. 1, 4, 5, and 7 are smooth in space across the CdSe/CdS interface despite the discontinuity in the effective mass and confinement potential [27-31]. This behavior is consistent with the theoretical framework developed by BenDaniel and Duke, who showed that the inclusion of the effective mass in the kinetic-energy operator removes the unphysical discontinuities arising from constant-mass formulations. The finite-barrier nature of the confinement potential is further confirmed by the fact that the electron and hole wavefunctions gradually penetrate into the CdS shell, which is one of the basic properties of semiconductor heterostructures given in the framework of the effective-mass approximation.

The discrete energy spectra exhibited in Figures 2 and 9 are also compatible with the quantum-confinement behavior described for semiconductor quantum dots. When the carrier is restricted in motion in all the three directions of space, the continuous bulk energy bands become discrete bound states, whose energies increase monotonically with the index of the quantum state. Similar trends have been observed in theoretical work based on the effective mass approximation in spherical semiconductor nanostructures (Bastard, 1988; Foreman, 1995)[[23,22].

The present simulations also reveal a stronger spatial localization of holes as compared to electrons, which is apparent from the probability density distributions in Figures 3 and 8. This behavior stems from the greater hole effective mass that reduces the kinetic-energy part of the Hamiltonian, therefore increasing the carrier localization inside the CdSe core. On the other hand, the smaller electron effective mass increases the delocalization of the wavefunction and supports the penetration into the CdS shell by quantum tunnelling. This tendency is compatible with the physical interpretation of carrier confinement as given by the effective mass hypothesis.

From a numerical standpoint, the constructed solution preserved the Hermitian character of the Hamiltonian up to machine precision and resulted exclusively in real eigenvalues and properly normalized eigenfunctions. The indicated numerical features indicate that the conservative finite difference approximation accurately represents the mathematical properties of the continuous BenDaniel-Duke operator and provides a numerically stable method of investigating the confinement of carriers in the spherical CdSe/CdS core-shell quantum dots.

To conclude, the consistency of confinement dynamics, wave function continuity, probability density localization, and discrete spectrum with effective mass theory confirms the physical correctness and numerical robustness of the proposed model.

3.2 Summary of Results

The proposed approach in this work is a numerical method for studying the confined states of spherical CdSe/CdS core-shell quantum dots using the Effective Mass Approximation and the BenDaniel-Duke Hamiltonian. In the proposed approach, the position-dependent effective mass is taken into account in the form of the kinetic energy operator, while the conservative finite difference discretization scheme is used in order to preserve both the hermiticity of the Hamiltonian and the continuity of the probability current across the heterojunction.

The performed simulations correctly describe the quantum confinement phenomena of semiconductor quantum dots. The resulting ground-state wavefunctions were continuous throughout the computational domain and showed finite penetration into the CdS shell as expected for the tunnelling nature of finite confinement barriers. Furthermore, the probability density distributions revealed a stronger localization of holes inside the CdSe core due to their larger effective mass while electrons exhibited greater spatial delocalization. The computed eigenvalue spectrum is a set of discrete bound states with monotonically increasing energies, indicating the total confinement of the carriers in the three-dimensional nanostructure. The conservative finite difference formulation provided a sparse hermitian Hamiltonian with real eigenvalues and eigenfunctions orthogonal to each other, and was very stable numerically.

The results demonstrate that the suggested computational model is a physically consistent and computationally efficient method to study carrier confinement in semiconductor core-shell quantum dots. The established framework can be easily extended to study the effect of external electric and magnetic fields, tension, excitonic interactions and other physical processes in the future.

4. Conclusion

We have developed a computational scheme based on the Effective Mass Approximation and the BenDaniel–Duke Hamiltonian to examine the restricted electronic states in spherical CdSe/CdS core–shell quantum dots. This formulation employs the position-dependent effective mass in the Hamiltonian and uses a conservative finite-difference discretization, which correctly describes the carrier confinement and preserves the physical continuity conditions at the CdSe/CdS heterointerface.

The numerical findings show that the proposed model can simulate the main features of the quantum confinement in semiconductor core-shell quantum dots. The computed electron and hole wavefunctions are continuous across the heterostructure and they demonstrate a finite penetration into the CdS shell, highlighting the role of finite potential barriers on the carrier localization. The respective probability-density distributions show a more pronounced localization of holes within the CdSe core, but the electrons are spatially more extended because of their smaller effective mass.

The calculated restricted energy spectra show discrete bound states with eigenvalues that increase monotonically, corresponding with the expected behavior of zero-dimensional semiconductor nanostructures. The steady numerical behavior and physically meaningful eigenstates achieved by the robust and reliable computational approach presented in this work for solving position-dependent effective-mass Schrödinger equations in spherical heterostructures are its strengths.

In summary, the proposed numerical scheme is a reliable, efficient and physically consistent tool for studying the carrier confinement in CdSe/CdS core-shell quantum dots. The modular nature of the proposed approach makes it easy to extend it to include electron-hole Coulomb interaction, excitonic states, external electric and magnetic fields, strain effects and multiband Hamiltonian models, thus providing a versatile platform for future theoretical studies of semiconductor nanostructures.

References

- [1] Oglah, M. H. (2024). Analyzing the time evolution of a particle by decomposes the initial state confinement in 1D well into the lowest eigenstates energy. *J. Res. Appl. Sci. Biotechnol*, 3(2), 103-107. DOI: 10.55544/jrasb.3.2.17
- [2] Melkonyan, A. G., Mantashian, G. A., & Hayrapetyan, D. B. (2026). Charge Transport Modeling of CdSe/ZnS core/shell Quantum Nanorod Light-Emitting Diodes. DOI:10.48550/arXiv.2603.22961
- [3] Oglah, M. H., Mohammed, S. J., & El-Daher, M. S. (2021, November). Simulation of energy resonant tunneling in short-period superlattice (Ga, Mn) As/GaAs quantum wells. In *AIP Conference Proceedings* (Vol. 2372, No. 1, p. 040002). AIP Publishing LLC. DOI: 10.1063/5.0065501
- [4] Ibral, A., Zouitine, A., Assaid, E. M., Feddi, E. M., & Dujardin, F. (2015). Binding energy and spatial extension of an off-centre donor impurity in ZnS/CdSe spherical core/shell nanostructures. *Journal of Optoelectronics and Advanced Materials*, 17(1-2), 151-159.
- [5] Astrain-Ortega, A., Rodríguez-Magdaleno, K. A., Sansores-Miranda, M. G. W., Nava-Maldonado, F. M., Duque, C. A., Ungan, F., ... & Martínez-Orozco, J. C. (2025). Intraband absorption coefficient for oblate, spherical and prolate GaAs/As core-shell quantum dots. *Optical and Quantum Electronics*, 58(1), 15. DOI: 10.1007/s11082-025-08602-5
- [6] Naifar, A., & Hasanirokh, K. (2026). Oxidative HfO₂ Dielectric Shielding for Photobleaching Control in ZnS/CdSe Cylindrical Core-Shell Quantum Dots. *Micro and Nanostructures*, 208609. <https://doi.org/10.1016/j.micrna.2026.208609>
- [7] Wei, S.-H., & Zunger, A. (1998). Valence band splittings and band offsets of AlN, GaN, and InN. *Applied Physics Letters*, 72(16), 2011–2013. <https://doi.org/10.1063/1.121265>
- [8] Oglah, M. H., Hasan, A. A., & Mahmood, W. I. (2025, February). Quantum confinement Bohr radius effects of quantum dots using Brus mathematical model. In *AIP Conference Proceedings* (Vol. 3162, No. 1, p. 020007). AIP Publishing LLC. DOI: 10.1063/5.0241782
- [9] Jalled, O., Rais, F., Naifar, A., & Gassoumi, B. Shape-Driven Optoelectronic Enhancement in Toroidal Semiconductor Nanostructures: The Role of Width and Curvature. Available at SSRN 6811051. DOI: 10.2139/ssrn.6811051
- [10] Oglah, M. H. The roadmap experiment of CdO films to heterojunction of photodetectors and solar cells. *International Journal of Mechanical and Thermal Engineering*, 6(1):21-29. DOI: 10.22271/27078043.2025.v6.i1a.74.
- [11] Hbib, M., Mommadi, O., Chouef, S., Boussetta, R., Belamkadem, L., Moussaouy, A. E., ... & Duque, C. A. (2022). Finite confinement potentials,

- core and shell size effects on excitonic and electron-atom properties in cylindrical core/shell/shell quantum dots. *Scientific Reports*, 12(1), 14854. DOI: 10.1038/s41598-022-19118-3
- [12] Oglah, M. H., Mohammed, S. J., & El-Daher, M. S. (2020). Determine the Lower-State Energy of (GaMn) As/GaAs Quantum Well using Localization Landscape Method. *Tikrit Journal of Pure Science*, 25(6), 96-102. DOI:10.25130/tjps.v25i6.318
- [13] Rodríguez-Magdaleno, K. A., Pérez-Álvarez, R., Urgan, F. A. T. I. H., & Martínez-Orozco, J. C. (2022). Strain effect on the intraband absorption coefficient for spherical CdSe/CdS/ZnSe core-shell-shell quantum dots. *Materials Science in Semiconductor Processing*, 141, 106400.
- [14] Segarra Ortí, C. (2016). Electronic structure of quantum dots: response to the environment and externally applied fields. November 2002 *Review of Modern Physics* 74(4) DOI: 10.1103/RevModPhys.74.1283
- [15] Mustafa Y Ali and Mubarak Hamad Oglah. Numerical analysis of uniaxial strain-induced modifications of the band structure and optical properties of zinc toluidine semiconductor, *Int. J. Mech. Therm. Eng.*, 2026; 7(1): Part B, 99-108. DOI: <https://www.doi.org/10.22271/27078043.2026.v7.i1b.118>
- [16] Betcke, M., & Voss, H. (2006). *Electronic States of Quantum Dots*. Technical Report 103, Institute of Numerical Simulation, Hamburg University of Technology (TUHH), Hamburg, Germany.
- [17] Simonot, D., Roux-Byl, C., Xu, X., Daney de Marcillac, W., Dabard, C., Silly, M. G., Lhuillier, E., Pons, T., Huppert, S., & Maître, A. (2025). Determination of band alignment of core/shell colloidal CdSe/CdS quantum dots, by optical and X-ray photo-electron spectroscopies. *Materials Today Quantum*, 5, 100024. <https://doi.org/10.1016/j.mtquan.2025.100024>
- [18] Griffiths, D. J., & Schroeter, D. F. (2018). *Introduction to Quantum Mechanics* (3rd ed.). Cambridge University Press. <https://doi.org/10.1017/9781316995433>
- [19] Kittel, C. (2005). *Introduction to Solid State Physics* (8th ed.). John Wiley & Sons.
- [20] BenDaniel, D. J., & Duke, C. B. (1966). Space-charge effects on electron tunneling. *Physical Review*, 152(2), 683–692. <https://doi.org/10.1103/PhysRev.152.683>
- [21] Bastard, G. (1988). *Wave Mechanics Applied to Semiconductor Heterostructures*. Les Éditions de Physique, Les Ulis, France.
- [22] Foreman, B. A. (1995). Exact effective-mass theory for semiconductor heterostructures. *Physical Review B*, 52(16), 12241–12259. <https://doi.org/10.1103/PhysRevB.52.12241>
- [23] Panfil, Y. E., Shamalia, D., Cui, J., Koley, S., & Banin, U. (2019). Electronic coupling in colloidal quantum dot molecules: The case of CdSe/CdS core/shell homodimers. *Journal of Chemical Physics*, 151(22), 224501. <https://doi.org/10.1063/1.5128086>
- [24] Harrison, P. (2016). *Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures* (4th ed.). Wiley. <https://doi.org/10.1002/9781118923573>
- [25] Madelung, O. (Ed.). (2004). *Semiconductors: Data Handbook* (3rd ed.). Springer.

- [26] Yu, P. Y., & Cardona, M. (2010). *Fundamentals of semiconductors: Physics and materials properties* (4th ed.). Springer. <https://doi.org/10.1007/978-3-642-00710-1>
- [27] Toscano-Negrette, R. G., León-González, J. C., Vinasco, J. A., Morales, A. L., Koc, F., Kavruk, A. E., ... & Duque, C. A. (2023). Optical properties in a ZnS/CdS/ZnS core/shell/shell spherical quantum dot: electric and magnetic field and donor impurity effects. *Nanomaterials*, 13(3), 550. DOI: 10.3390/nano13030550
- [28] Toscano-Negrette, R. G., León-González, J. C., Vinasco, J. A., Morales, A. L., Mora-Ramos, M. E., & Duque, C. A. (2023). Effect of external fields on the electronic and optical properties in ZnTe/CdSe and CdSe/ZnTe spherical quantum dots. *Condensed Matter*, 8(3), 66. DOI: 10.3390/condmat8030066
- [29] Ed-Dahmouny, A., Jaouane, M., Fakkahi, A., El-Bakkari, K., Arraoui, R., Azmi, H., Sali, A., & Es-Sbai, N. (2024). Analyzing photoionization cross-sectional modulation in CdSe/CdS core-shell nanodots: Impact of strain and applied electric field. *Journal of Applied Physics*, 135(4), 044304. <https://doi.org/10.1063/5.0183295>
- [30] Jaouane, M., Ed-Dahmouny, A., Al-Shameri, N. S., Arraoui, R., Fakkahi, A., Azmi, H., Althib, H. M., El-Ghazi, H., Sali, A., & Duque, C. A. (2026). Optical properties of an exciton in core/shell/shell spherical quantum dot under an electric field. *Journal of Physics and Chemistry of Solids*, 208, 113169. <https://doi.org/10.1016/j.jpcs.2025.113169>
- [31] Bouazra, A., & Maamria, S. (2026). Deep neural network-based prediction of electronic and optical properties in CdSe/CdS quantum wells. *Solid State Communications*, 412, 116394. <https://doi.org/10.1016/j.ssc.2026.116394>