

Comparison of Exciton Mass from Symplectic Space and Artificial Neural Network Methods in Nanostructures

Arezu Jahanshir 

Department of Physics and Engineering Sciences, Buein Zahra Technical University, Iran

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Corresponding

Authors:

Arezu Jahanshir

Email:

jahanshir@bzte.ac.ir

ABSTRACT

Recent advances in artificial neural network methods and modeling have opened new pathways for understanding and predicting the exotic bound state properties in semiconductor nanostructures. In this theoretical and modeling work, we propose a combined artificial neural network-based framework for calculating and investigating bound state effects in confined semiconductor nanocrystals, with emphasis on calculating the exciton effective mass, binding energy, and wavefunction. The model is based on quantum field theory and a nonrelativistic Hamiltonian, enabling the prediction of bound state properties. Unlike conventional perturbative methods, the proposed approach captures confinement effects and multi-exciton interactions in regular semiconductor nanostructures. The study further identifies confinement potential by correlating it with specific physical effects. The obtained theoretical and artificial neural network-based framework provides a true and computationally efficient approach for calculating exciton bound state properties in semiconductor $GaAs/Al_{0.3}Ga_{0.7}As$ quantum dot. The developed methodology offers reliable numerical and computational tools for investigating confined excitonic systems and may be extended to other low-dimensional semiconductor nanostructures, designing a new generation of optoelectronic, biomedical diagnostics, genomic, and medical analysis tools, and bio-imaging semiconductor nanocrystals technologies, and two-dimensional nanomaterials.

KEYWORDS: Neural network; Schrödinger equation; Exciton; Bound state; Nano-semiconductor

1. Introduction

Semiconductor nanostructures (SNs) play a progressively important role in modern optoelectronics, photonics, spintronics, and advanced technologies in genomics and biosensing. Nanoscale structures or devices such as transistors, integrated circuits, modern CPUs, GPUs, memory chips, phones, AI hardware, and biological DNA sensors depend on the specific electronic and optical properties of semiconductors to detect optoelectrical or biological interactions with high sensitivity and precision [1,2]. The physical phenomena in semiconductor

nanostructure systems are excitons (electron–hole pair bound state in the material) and exciton–electron–hole interactions. Excitonic effects in SNs are strongly influenced by electrostatic interactions, relativistic effects such as spin interactions, fine-structure splitting, quantum confinement, surface defects, and charge dynamics. These features modify the exciton energy, lifetime, and optical properties in the presence or absence of an external electromagnetic field. Therefore, excitonic effects in SNs are crucial for many optoelectrical and bioanalytical devices. The interaction between excitons, electrons, holes, and SNs' material properties is important for the design and optimization of next-generation SNs-based biosensors and genomic analytical systems. For example, in bio and genomic sensors, DNA biomolecules fix to the surface of SNs. Under these conditions, DNA biomolecules can shift the local electromagnetic field, as a result modifying the absorption or emission rate and properties, thus enabling bio and genomic detection [3-5]. For this reason, the subject of this theoretical research requires a review of SN concepts, which we will briefly review. Usual classification of SNs in this article includes semiconductor nanocrystals (SNCs) and quantum dots (QDs), which have different formation in dimensions (directions). SNCs are a general term for any crystal in which only one dimension is in the range of 1 – 100 nm. SNs can be rods (anisotropic shape, not confined in three directions) or quantum wells (quantum confinement in one dimension with two free directions). Examples of SNs include rods, wells, and various material compositions such as *CdSe/CdS*, *CsPbBr₃*, *ZnO*, *Fe₃O₄*. SNs may be spherical, ellipsoidal, strongly ellipsoidal, rod, plate, etc. QDs are a specific category of SNs in which all three dimensions are in the range of less than 10 nm, where electrons and holes are confined in all three directions, such as *CdSe* spherical 4 nm dots, *InP*, *PbSe*, and *PbS* [6,7]. These electron–hole bound states may be referred to as artificial atoms (excitons) and produce quantized energy levels (discrete energy levels). In recent years, with the advancement of high technologies, the importance of exciton bound state characteristics in semiconductor nanostructures is undeniable. Quantum properties of excitons in semiconductor nanostructures have industrialized the cadmium free QD light-emitting diode displays, green/red emitters, developed Perovskite QDs in ultra-high color purity, next generation of single-photon sources, low-threshold lasers, light-emitting semiconductor diode [8-10], infrared photodetectors, high-sensitivity infrared sensors, thermoelectric, tunable mid-infrared lasers [11], and established quantum communication, entangled photon generation at two main optical communication bands used in fiber optics with wavelengths (1310/1550 nm) [12], complementary metal-oxide-semiconductor fabrication technology (compatible quantum bits) [13], nonvolatile memory [14], photonics, infrared optoelectronics, quantum logic devices, topological quantum materials [15], mid-infrared detection, spin–orbit devices [16, 17], exciton–polariton devices [18, 19], etc. Sectors of common and modern high technologies that utilize SNs are included in Table .1.

Table 1: Technologies that use SN systems

Biomedical diagnostics	- Analysis microarrays
	- Lab-on-a-chip devices
	- Point-of-care medical tests
	- Disease detection platforms
Genomic and medical diagnostics	- DNA sequencing chips
	- Nano-biosensors
	- Fluorescence detection systems
	- Microfluidic diagnostic platforms
Transistors and integrated circuits	- Modern CPUs, GPUs, memory chips
	- Especially FinFET and GAAFET transistors
	- Used in computers, phones, and AI hardware
Sensors	- Gas sensors
	- Chemical sensors
	- Biosensors for DNA, proteins, glucose
	- Nanowires, QDs, or thin-film semiconductors
Optoelectronics	- LEDs
	- Laser diodes
	- Photodetectors
	- Solar cells
	- Display technologies
Quantum technologies	- Quantum dots
	- Single-electron devices
	- Qubits in some platforms
	- Quantum computing and quantum sensing
Nanoelectronics	- Extremely small circuit elements
	- Low-power and high-speed devices
	- Computing and communication systems

The theoretical and analytical study of SNCs with different corrections are an important subject in optoelectronic devices and modern high technology research. The importance of SNCs and QDs in modern and high technologies has motivated interest in studying exciton bound states interactions in SNC systems, which play a main role in controlling exciton bound state behavior. Hence, the theoretical investigation using artificial neural network (ANN) methods in SNCs and QDs has contributed to describing properties of excitons in quantum electronics and optoelectronics. SNs, as an important part of theoretical and experimental research in modern technology, help us analyze, model, and optimize complex SN systems that are difficult to describe with traditional methods[2-,24]. ANN methods can be used in SN research for predicting physical behaviors, optimizing SN material properties, calculating energy eigenvalues and spin interactions, analyzing experimental data, and accelerating design processes; hence, ANN-based approaches are a valuable part of high-tech nanoelectronics, optoelectronics, and quantum device research. One can use an ANN method for calculating the

mass-energy spectra of the exciton bound state in SNCs [23,24]. Hence, the physical appearance and properties of an exciton, as the electron-hole bound state within the confinement potential, are investigated and defined. The confinement potential determines the exciton mass spectrum, and the properties and modification effects in the effective mass of the electron and hole, which do not match the rest mass of each particle. The different effects in SNCs and QDs is also associated with a greater emission band compared to non-nano-dimensional semiconductors. The group of excitonic interactions (exciton-exciton, biexciton-exciton, and biexciton-biexciton) in SNCs and QDs can be described collectively as multi-exciton correlations [25,26]. Quantum correlations presents innovative nonlinear optical effects and result in intertwined conditions forming new quantum states and phenomena [27,28]. These effects directly depend on important SNCs' structural factors, including the dimensions (size), profile, composition of SNCs, and shape. For example, the structural factors of ellipsoidal and spherical SNCs differ significantly from each other and from those of strongly ellipsoidal SNCs. Absorption peaks of ellipsoidal SNCs are expanded a bit compared with spherical QDs, and exhibit clearer peak splitting and stronger shifts in strongly ellipsoidal SNs due to confinement differing along different axes [29-31]. Redshift or blueshift (depending on the long or short axis confinement) shows dependence on particle orientation in differently shaped SNs. Photoluminescence in ellipsoidal SNCs may remain relatively sharp, while strongly ellipsoidal SNs often become more polarization-dependent and exhibit larger Stokes shifts. Ellipsoidal SNs show moderate polarization anisotropy, whereas strongly ellipsoidal SNs show much stronger linearly polarized absorption and emission along the long axis. The more important SN's property depends on the exciton fine structure. Ellipsoidal SNs exhibit some splitting of exciton states due to broken symmetry, whereas strongly ellipsoidal SNs show larger splitting and stronger mixing of states. These effects are experimentally observable as changes in low-temperature spectra, exciton state lifetimes, temperature dependence of emission, direction-dependent conductivity, electroabsorption, nonlinear optical behavior, and others. This study provides guiding principles for modifying the properties of SN-based electrical devices through nano-quantum physics and optoelectronics. It highlights the simplicity and efficiency of applying ANN modeling to account for different effects and corrections. Therefore, we focus on exciton bound states in SNCs and QDs. Then, using an ANN algorithm framework, we attempt to calculate the bound state effects and highlight their importance in nano quantum physics and optoelectronics [27-32]. The determination of the exciton energy spectrum through Salpeter, Dirac, or modified Schrödinger equations represents a fundamental problem in the study of SNs. Because analytical solutions to these equations are very difficult, computational strategies are typically required. In this work, we introduce a novel method that integrates quantum field theory (QFT), combined with ANN algorithms, to calculate the energy eigenvalues and wavefunction. Numerical results are presented for the vacuum and excited states in the Coulombic potential, and these outcomes are compared with other theoretical methods.

The comparison shows that, in addition to computational accuracy and speed, the ANN-based method provides accurate mass estimation and can be extended to multi-exciton systems, which can be utilized in SNs. The article is organized as follows: 1) determination of the exciton bound state properties based on QFT, 2) transformation of intertwined spaces in quantum mechanics (QM) and QFT, and 3) explanation of the exciton energy spectrum, which could model the exciton spectrum.

2. Theoretical formulation of the Sturmian function in SNs

Excitons can be created in certain SNs under specific photoelectric and electromagnetic field conditions. We study an exciton as an electrostatic electron-hole bound state in SNs (Fig.1).

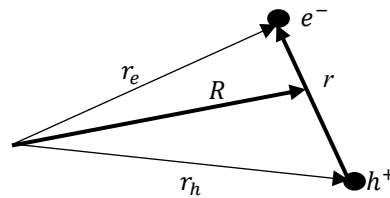


Fig.1: The relative motion of the two-particle bound state in SNs.

Now, applying a Jacobian coordinate transformation to the electron-hole bound state, we consider the effective masses. m_e^* , m_h^* of the carrier electron and hole in SNs, along with the reduced effective mass μ^* in SNs. We determine

$$r_e = \frac{m_h^*}{M} r + R, \quad r_h = \frac{m_e^*}{M} r + R, \quad M = m_e^* + m_h^*, \quad \mu^* = \frac{m_e^* m_h^*}{m_e^* + m_h^*}$$

where r is the relative motion vector, and R is the center of mass vector. The effective mass of particles in SNs is a concept from solid state physics that describes how a particle behaves within the crystal lattice of a material or under the external electromagnetic field, and is different from the free electron mass $m_e = 0.511 \text{ MeV}$. The total Hamiltonian of the exciton contains the relative H_r and the centers of mass H_R Hamiltonians in spherical coordinates [33]

$$H\Psi(r, R) = (H_R + H_r)\Psi(r, R) \rightarrow H = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2\mu^*}\Delta_r + V(r) \quad (1)$$

where $\Delta_r = \frac{d^2}{dr^2} + \frac{n-1}{r} \frac{d}{dr} - \frac{\ell(\ell+n-2)}{r^2}$, $\Delta_R = \frac{d^2}{dR^2} + \frac{n-1}{R} \frac{d}{dR} - \frac{\ell(\ell+n-2)}{R^2}$ are the radial Laplacian operators

defined in the 3-dimensional space $n = 3$, and ℓ is the main orbital angular momentum quantum number.

Hence, the total radial Schrödinger equation (SE) of relative motion, including the spin interactions

Hamiltonian H_s and the interaction potential $V(r)$, is defined as

$$\left[-\frac{\hbar^2}{2m_e^*} \left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right] - \frac{\hbar^2}{2m_h^*} \left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right] + V(r) + H_s - E_l(\mu^*) \right] \Psi(r, l) = 0 \quad (2)$$

To define an ANN-based algorithm using the Sturmian function (SF) transformation [33-35], we first describe an exciton bound state in SNs as a harmonic quantum oscillator system, and then apply equation (2) to this system in the form

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right] + V(r) + H_s - E_l(\mu^*)\right)\Psi(r, l) = 0 \quad (3)$$

Now we represent equation (3) based on the SF transformation and the second quantization method in QM for solving the radial SE of an exciton bound state in the SNs system. Applying SF in equation (3) is one of the main techniques in QM and QFT that leads us to solve the SE and define specific properties of SNs [34, 35]. The SF transformation is a valuable mathematical tool and technique that can transform the second-order linear differential equation of the SE for studying various aspects of excitons in SN systems. Moreover, the SF transformation method can explain exciton bound state properties in different areas of solid-state physics and chemistry. This tool helps us define several features of SN systems (wavefunctions, binding energy, effective mass, and quantum-optical characteristics). In this research, we present the SF transformation to study the electron-hole bound state with the reduced effective mass μ^* in SNs and represent the radial SE without spin interaction using the SF transformation wavefunction $S(r, l)$ as follows [33]

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right] + V(r) - E_0(\mu^*)\right)S(r, l) = 0 \quad (4)$$

Or

$$\left(-\frac{\hbar^2}{2\mu^*}\hat{p}_r^2 + V(r) - E_0(\mu^*)\right)S(r, l) = 0 \quad (5)$$

We consider that the wavefunction of a bound state is of the Gaussian type. Based on the Gaussian wavefunction, QFT, and QM principles, we choose a new variable $r = q^{2\xi}$ for the SF wavefunction in the intertwined space (auxiliary space) $\Psi(r, l) \rightarrow S(r, l) = q^{2\xi}\varphi(q)$, where $S(r, l) \approx e^{-a(r)} \approx e^{-r^\xi}$. ξ is a variational parameter to be determined. The first and second derivatives of the transformed space r to the auxiliary space q read [36-40]

$$r = q^{2\xi} \rightarrow \frac{d}{dr} = \frac{dq}{dr} \frac{d}{dq} = \frac{1}{2\xi} q^{1-2\xi} \frac{d}{dq},$$

$$\frac{d^2}{dr^2} = \left(\frac{dq}{dr} \frac{d}{dr}\right) \left(\frac{dq}{dr} \frac{d}{dr}\right) = \frac{1}{4\xi^2} q^{2-4\xi} \left[\frac{d^2}{dq^2} + \frac{1-2\xi}{q} \frac{d}{dq}\right]$$

Thus, the radial Laplacian operator in the transformed intertwined space $r = q^{2\xi}$ represent as

$$\Delta_r = \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \rightarrow \Delta_q = \frac{d^2}{dq^2} + \frac{\beta-1}{q} \frac{d}{dq}$$

Where $\beta = 4\xi\ell + 2\xi + 2$ is the dimension of the auxiliary space under the intertwined new coordinate $r = q^{2\xi}$. Therefore, the SF has a notable advantage as a basis for expansion over equation (4) when explaining the

equation with a different basis of intertwined space for an exciton bound state. To solve the modified radial SE, we know that the harmonic quantum oscillator wavefunction must satisfy the SF-transformed condition over intertwined spaces. Hence, the modified radial SE reads

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{q^{2-4\xi}}{4\xi^2}\hat{p}_q^2\left(\frac{d^2}{dq^2}+\frac{\beta-1}{q}\frac{d}{dq}\right)\right]+V(q)-E_l(\mu^*)\right)\varphi(q,l)=0 \quad (6)$$

or

$$\left(-\frac{\hbar^2}{2\mu^*}\hat{p}_q^2+V(q)-E_l(\mu^*)\right)\varphi(q,l)=0 \quad (7)$$

and can be used with numerous types of potential models, such as the Coulomb potential $V_C(r) = -\frac{e^2}{4\pi\epsilon_r\epsilon_0}\frac{1}{r} = -\frac{\alpha}{\epsilon_r r}$, Yukawa-type or screened Coulomb potential $V_Y(r) = \frac{e^2}{4\pi\epsilon_r\epsilon_0}\frac{e^{-\alpha r}}{r}$, harmonic confinement potential $V_H(r) = \frac{1}{2}m_e^*\omega^2 r^2$, and Rytova–Keldysh potential $V_{RK}(r) = -\frac{e^2}{8r_0\epsilon_r\epsilon_0}\left(S_0\left(\frac{r}{r_0}\right)-Y_0\left(\frac{r}{r_0}\right)\right)$ in SNs [41–43]. Where e is the elementary charge, ϵ_0 is the vacuum permittivity, ϵ_r is the relative permittivity of SNs, r_0 is the screening length, S_0 is the Struve function, Y_0 is the Bessel function of the second kind, r is the relative distance between electron and hole in the exciton bound state, α is the inverse screening parameter, ω is the angular frequency of harmonic oscillation. To solve the modified radial SE under the ANN method, the exciton state in SNs is described using equation (7) by the Wick ordering technique (WOT) in the standard formalism for the harmonic oscillator with the Hamiltonian $H = \frac{1}{2m}(\hat{P}^2 + m^2\omega^2\hat{Q}^2)$. The commutation relation of canonical operators is $[\hat{Q}, \hat{P}] = i\hbar\delta_{ij} = i\hbar\beta$, where $\hat{Q}, \hat{P} = \frac{\hbar}{i}\frac{\partial}{\partial q}$. For simplicity, we consider dimensionless operators. $\hat{Q}^2 = \frac{\hbar}{m\omega}\hat{q}^2$, $\hat{P}^2 = m\omega\hbar\hat{p}^2$ and substitute them into H . Then, one can obtain the dimensionless (or normalized) form of Hamiltonian: $H = \frac{m\omega\hbar}{2m}\hat{p}^2 + \frac{m\omega^2\hbar}{2m\omega}\hat{q}^2 = \frac{1}{2}\hbar\omega(\hat{p}^2 + \hat{q}^2)$. We choose the quantum harmonic oscillator because it has simple energy levels and simple Gaussian-type wavefunctions. WOT is a second quantization method based on creation $\hat{a}^\dagger$ and annihilation $\hat{a}$ operators in QM. WOT helps us to solve the SE and define properties of mass, energy, spin interactions, etc., of bound states. Now, we begin with a rapid analysis of $\hat{a}^\dagger$ and $\hat{a}$ operators in QM. Creation and annihilation operators act on a Hilbert space and satisfy the relations $[\hat{a}, \hat{a}^\dagger] = \delta_{ij} = \beta$ and $\hat{a}|0\rangle = 0$, where $|0\rangle$ is the vacuum state. This commutation relation is fundamental in the context of QM and QFT. Thus, $\hat{a}^\dagger$ and $\hat{a}$ operators are connected to dimensionless coordinate and momentum operators $\hat{p}, \hat{q}$ in natural units $\hbar = c = m = 1$, and take the form $\hat{a}^\dagger = \frac{(m\omega\hat{Q} - \frac{\partial}{\partial\hat{Q}})}{\sqrt{2m\omega}} = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p})$, $\hat{a} = \frac{(m\omega\hat{Q} + \frac{\partial}{\partial\hat{Q}})}{\sqrt{2m\omega}} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p})$, where $\hat{Q} = \frac{(\hat{a} + \hat{a}^\dagger)}{\sqrt{2m\omega}}$ and $\hat{P} = i\frac{\sqrt{m\omega}(\hat{a}^\dagger - \hat{a})}{\sqrt{2}}$. WOT over the canonical operators gives us a new presentation of canonical operators based on the vacuum state frequency of the exciton bound state system ω , and the dimension of the auxiliary space β under the intertwined new space $r = q^{2\xi}$. Therefore,

we define even orders of canonical operators $\hat{q} = \frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)$ and $\hat{p} = i\sqrt{\frac{\omega}{2}}(\hat{a}^\dagger - \hat{a})$, using $[\hat{a}, \hat{a}^\dagger] = \beta$ as follows [36-38]

$$\begin{aligned}\hat{q}^2 &= \left[\frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)\right]\left[\frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)\right] = \frac{1}{\omega} \frac{\Gamma(\frac{\beta+1}{2})}{\Gamma(\frac{\beta}{2})} : \hat{q}^2 = \frac{\beta}{2\omega} : \hat{q}^2 :, \\ \hat{q}^4 &= \left(\left[\frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)\right]\left[\frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)\right]\right)\left(\left[\frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)\right]\left[\frac{1}{\sqrt{2\omega}}(\hat{a} + \hat{a}^\dagger)\right]\right) = \frac{\beta(\beta+2)}{4\omega^2} + \\ &\frac{\beta+2}{\omega} : \hat{q}^2 : + : \hat{q}^4 : = \frac{1}{\omega^2} \frac{\Gamma(\frac{\beta+2}{2})}{\Gamma(\frac{\beta}{2})} + \frac{2}{\omega} \frac{\Gamma(\frac{\beta+2}{2})}{\Gamma(\frac{\beta}{2})} : \hat{q}^2 : + : \hat{q}^4 :, \\ &\vdots \\ \hat{q}^{2\tau} &= \frac{1}{\omega^\tau} \frac{\Gamma(\frac{\beta+2\tau}{2})}{\Gamma(\frac{\beta}{2})} + \frac{\tau}{\omega^{\tau-1}} \frac{\Gamma(\frac{\beta+2\tau}{2})}{\Gamma(\frac{\beta}{2})} : \hat{q}^2 : + : \hat{q}^{2\tau} :, \tau = 1, 2, 3, \dots\end{aligned}\quad (8)$$

and

$$\hat{p}_q^2 = \left[i\sqrt{\frac{\omega}{2}}(\hat{a}^\dagger - \hat{a})\right]\left[i\sqrt{\frac{\omega}{2}}(\hat{a}^\dagger - \hat{a})\right] = \frac{\beta\omega}{2} : \hat{p}^2 : = \omega \frac{\Gamma(\frac{\beta+1}{2})}{\Gamma(\frac{\beta}{2})} : \hat{p}^2 : \quad (9)$$

where $: \cdot :$ represents the WOT symbol. We consider that in the new intertwined space $r = q^{2\xi}$ the interaction Hamiltonian doesn't contain $: \hat{q}^2 :$ and $\hat{q}^2$ terms (these terms are postulated to be contained within the free oscillator part). This condition is a main principle of the symplectic intertwined spaces method (SISM) (the oscillator representation method in QM and QFT), and yields the equation for the frequency ω . Therefore, the normalized Hamiltonian based on WOT (the normal ordering form of creation and annihilation operators) in the natural units $\hbar = c = m = 1$ reads $H = \frac{1}{2}\omega(\hat{p}^2 + \hat{q}^2) = \omega(\hat{a}^\dagger \hat{a}) + \frac{\beta\omega}{2} = H_0 + \epsilon_0$, where H_0 is the free oscillator Hamiltonian and ϵ_0 is the energy of the vacuum state of the Hamiltonian. Thus, we can define the ground state ($n = 0$) wavefunction $|0\rangle = \left(\frac{\omega}{\pi}\right)^{\beta/4} e^{-\frac{\omega}{2}\hat{q}^2}$ with the conditions $\hat{a}|0\rangle = 0$, $\langle 0|0\rangle = \int_{-\infty}^{+\infty} \left(\frac{\omega}{\pi}\right)^{\beta/2} e^{-\omega\hat{q}^2} dq = 1$ and for all excited states n take the form $\langle n|m\rangle = \delta_{nm}n!$, $H_0|0\rangle = n\omega|0\rangle$, $H_n|n\rangle = \omega\left(n + \frac{\beta}{2}\right)|n\rangle$, $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle$ and for all the orthonormality conditions of radial excited states in the R^β space with $\ell = 0$, the allowed radial quantum number n_r can take infinitely many

values in principle $n_r = 0, 1, 2, \dots$, each different n_r labels a different radial excitation with the same $\ell = 0$ and read as $|n_r\rangle = \left(\frac{\Gamma(\beta/2)}{4^{n_r} n_r! \Gamma(\beta/2 + n_r)}\right)^{1/2} (\hat{a}^\dagger)^{n_r} |0\rangle$, where $\langle n_r | m_r \rangle = \delta_{n_r m_r}$ and $H_0 |n_r\rangle = 2n_r \omega |n_r\rangle$.

3. Solving the Schrödinger equation

In QM and QFT, SISM is based on the transformation $r = q^{2\xi}$, use auxiliary position $\hat{q}$ and momentum $\hat{p}_q$ variables in a $\beta = 4\xi\ell + 2\xi + 2$ dimensional space to analyze and calculate the mass-energy spectrum of few-body bound state systems. As a powerful mathematical tool, SISM provides a deeper understanding of system dynamics. This technique is beneficial for solving the SE for exciton bound states and for calculating their properties and characteristics in SNs. Hence, the total Hamiltonian in the natural units $\hbar = c = 1$ with the specific interaction potential takes the form [33, 36, 37]

$$H\Psi = E\Psi \rightarrow \left[\frac{\hat{p}_r^2}{2m} + V_{conf}(r) + V(r)\right]\Psi = E\Psi \quad (10)$$

Under SISM and WOT methods, as described in the previous section, the total Hamiltonian based on equations (6) and (7) defines

$$H = H_0 + \epsilon_0 + H_I = \omega(\hat{a}^\dagger \hat{a}) + \frac{\beta}{2}\omega + \int \left(\frac{dk}{2\pi}\right)^\beta \check{V}(k^2) e^{\frac{-k^2}{4\omega}} : e^{ik\hat{q}} : - \frac{\omega^2}{2} \left(:\hat{q}^2: + \frac{\beta}{2\omega}\right) \quad (11)$$

Where $V(q) \int \left(\frac{dk}{2\pi}\right)^\beta \check{V}(k^2) e^{ikq}$ is the interaction potential, $H_0 = \omega(\hat{a}^\dagger \hat{a})$ is the

Hamiltonian of the free oscillator, $\epsilon_0 = \frac{\beta\omega}{4} + \int \left(\frac{dk}{2\pi}\right)^\beta \check{V}(k^2) e^{\frac{-k^2}{4\omega}}$ is the vacuum energy

(ground state energy), and $H_I = \int \left(\frac{dk}{2\pi}\right)^\beta \check{V}(k^2) e^{\frac{-k^2}{4\omega}} : e^{ik\hat{q}} :$ is the interaction Hamiltonian.

Also, based on the SISM condition, one can determine the equation for the frequency state

$$\omega^2 + \int \left(\frac{dk}{2\pi}\right)^\beta \left(\frac{k^2}{\beta}\right) e^{\frac{-k^2}{4\omega}} \check{V}(k^2) = 0. \text{ Now, as presented, canonical variables } \hat{p}_r^2 = \frac{q^{2-4\xi}}{4\xi^2} \hat{p}_q^2$$

and $r = q^{2\xi}$ operators in equation (7), the SE in SISM within Coulomb interaction potential, and SISM conditions about interaction Hamiltonian for electron-hole bound state, one can define equation (11) in the form

$$\epsilon_0 \varphi(q, l) = \left(\frac{1}{2\mu^*} \left[\frac{q^{2-4\xi}}{4\xi^2} \hat{p}_q^2 \right] + V_{conf}(r) + V(q) - E_l(\mu^*) \right) \varphi(q, l) = 0 \quad (12)$$

Thus under $\hat{q}^{2\tau} = \frac{1}{\omega^\tau} \frac{\Gamma(\frac{\beta}{2} + \tau)}{\Gamma(\frac{\beta}{2})}$ and $\hat{p}_q^2 = \frac{\beta\omega}{2}$ the SE reads

$$\epsilon_0 \varphi(q, l) = \left(\frac{\beta\omega}{4} + 4\mu^* \xi^2 q^{4\xi-2} [V(q^{2\xi}) + V_{conf}(q^{2\xi}) - E_l(\mu^*)] \right) \varphi(q, l) = 0 \quad (13)$$

Thus, the vacuum energy of a bound state in the SISM under WOT is realized by the following equation

$$\epsilon_0 = \frac{\beta\omega}{4} + 4\mu^* \xi^2 q^{4\xi-2} [V(q^{2\xi}) + V_{conf}(q^{2\xi}) - E_l(\mu^*)] \quad (14)$$

Hence, applying the SISM condition, one can represent two conditions $\frac{d\epsilon_0}{d\omega} = 0$ and $\frac{d\epsilon_0}{d\xi} = 0$ to define the ground state energy eigenvalue ϵ_0 and the variational parameter ξ . As we know, bound states form in confined states at the lowest ϵ_0 and ω states. Thus, by decreasing SN dimensions and profile shape, the electron-hole pairs become closer, leading to stronger Coulombic coupling and exciton bound states. Furthermore, applying an external electromagnetic field to SNs can increase the coupling constant strength, making spin interactions an important term in the total Hamiltonian. Hence, the total Hamiltonian, which describes all interaction potentials, is defined as $H = \epsilon_0 + H_{SS} + H_{LS} + H_T$ [43]. Thus, the ground state energy of an exciton bound state within the Coulombic interaction $V_C(r) = -\frac{e^2}{4\pi\epsilon_r\epsilon_0 r} = -\frac{\alpha}{\epsilon_r r}$ and confined potential, $V_{conf}(r) = +V_{conf}^e(r) + V_{conf}^h(r)$ under SISM-WOT with the variational parameter ξ , defined as follows

$$\epsilon_0 = \frac{\hat{p}_q^2}{2} + 4\mu^* \xi^2 q^{4\xi-2} \left[-\frac{\alpha}{\epsilon_r q^{2\xi}} + V_{conf} - E_l(\mu^*) \right] \quad (15)$$

The variational parameter ξ is determined using the condition $\frac{d\epsilon_0}{d\xi} = 0$, and for Coulomb interaction is $\xi =$

1, therefore equation (13) under transformation of $\hat{q}^2 = \frac{\beta}{2\omega}$, and $\hat{p}_q^2 = \frac{\beta\omega}{2}$, gets the form [36,37]

$$\epsilon_0 = \frac{\beta\omega}{4} - 4\frac{\alpha}{\epsilon_r} \mu^* + 2\mu^* \frac{\beta}{\omega} V_{conf} - 2\mu^* \frac{\beta}{\omega} E_l(\mu^*) = 0 \quad (16)$$

Hence, the theoretical method and then ANN formalism using the transformation from SE to radial equation is presented in the following manner $\Psi(r, \theta, \phi) = R(r)Y(\theta, \phi) \rightarrow \Psi(r, \theta, \phi) = ru(r)Y(\theta, \phi)$ where the reduced radial wavefunction is $u(r) = rR(r)$, by eliminating the first-order derivative term and transforms equation

(10), $\frac{-1}{2\mu} \frac{d^2 u(r)}{dr^2} + \left[\frac{\ell(\ell+1)}{2\mu r^2} + V_{conf}(r) + V(r) \right] u(r) = Eu(r)$, and in the ANN approximates the reduced radial wavefunction by $u(r_i, l) = r e^{(yr)^a} \sum_{i=1}^n u_i f(r, v_i, w_i)$, where $\sum_{i=1}^n u_i f(r, v_i, w_i)$ is the neural-network output and v_i, w_i denote all trainable parameters (weights, biases, decay parameters, reduced mass, and energy eigenvalue).

4. Schrödinger equation within artificial neural networks

A numerical method in nanophysics using the radial SE and fundamental single-layer ANN algorithms founded on ANN is proposed for calculating properties of excitons, exciton-polaritons, and other exotic bound states in SN systems [44-46]. The ANN implementation consists of a fully connected feed-forward neural network with one input neuron representing the radial coordinate r , one hidden layer containing $d = 15$ neurons, and one output neuron corresponding to the reduced radial wavefunction. The network parameters include input weights, output weights, and neuron biases. The hidden neurons employ the Softplus activation function, while its first and second derivatives are evaluated analytically during optimization. In this article, the standard MATLAB functions are represented. However, we used the open-source GNU Octave 13.3.0 software instead of MATLAB to avoid copyright and licensing restrictions. The ANN parameters are optimized using the MATLAB `fminsearch` algorithm with a maximum of 3500 iterations, 7000 function evaluations, convergence tolerances of $TolX = 10^{-6}$ and $TolFun = 10^{-8}$. The computational domain is $r \in [10^{-3}, 5]$, discretized into 120 collocation points. To this end, the boundary conditions of the exciton bound state wavefunction in the limits $r \rightarrow 0$ and $r \rightarrow \infty$ are taken into account, and ANN algorithms are employed to normalize and optimize the first and second-order derivatives of the SE to compute the wavefunction, mass-energy spectrum, and spin interactions. For the initial configuration of the ANN, we start from equation (3) and the activation functions of the ANN algorithm that have a high level of agreement between the analytical and numerical solutions. We will compare the results in R^3 spherical coordinates (r, θ, φ) under the ANN algorithm and in R^3 spaces under SISM and WOT for the exciton bound state system in the Coulomb potential with α coupling constant in SNs. Now, we proceed with the numerical solution of equation (3) using the extended ANN algorithms of Kosmas-Lagaris [47] under the feedback control function $F_N(r, \vec{u}, \vec{v}, \vec{w})$, where $\vec{u}, \vec{v}, \vec{w}$ are parameter vectors, and one can determine them through the minimization process of equation (3) with the ANN algorithm to avoid the trivial solution $S(r, \ell) = 0$ everywhere in the domain of r . This is done within the approximation for solving first- and second-order differential equations. For this purpose, we need to obtain an initial value for the eigenvalue $E_l(\mu^*)$. If we use another type of interaction potential, unlike the Coulomb potential of the hydrogen atom model, the eigenvalue is not easily determined. Therefore, we need to use an initial approximate Gaussian wave function for initialization and optimization in subsequent neurons, which is incorporated at the beginning

of the algorithm, to approximate its value. Thus, we consider the behavior of the reduced wavefunction of an exciton bound state within the Coulomb potential on the ANN in the form $S(r, \ell) = S_0(r, \ell, n)e^{-\mu^* ar}$ in the natural units $\hbar = c = 1$, with the normalization condition $\int r^2 |S(r, \ell)|^2 dr = 1$. Simplify equation (3), using $u(r, l) = r S(r, l)$ and under $\int |u(r, \ell)|^2 dr = 1$, the normalization condition; we consider this normalization in order to avoid $u(r, l) = 0$. Hence, the reduced radial SE takes the following form [47-49]

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + 2\mu^* \left[-\frac{\alpha}{\varepsilon_r r} + V_{conf} - E_l(\mu^*)\right]\right) u(r, l) = 0 \quad (17)$$

Using equation (16), we define the energy eigenvalue. Now, we explain that the main structure of the network dimensions is defined by a length a from the origin to the point where the wavefunction vanishes, and it is divided into smaller networks of size $i = 1, 2, \dots, n$. To obtain the bound state wavefunction and mass-energy spectrum, it is necessary to know the energy eigenvalue $E_l(\mu^*)$ to satisfy SE's equation (15) with high accuracy at every point in the network based on the ANN method; we choose

$$u(r, l) = re^{-a} F_N(r, \vec{v}, \vec{w}, \vec{u})$$

The reason we used and parameterized $u(r, l)$ with the neural network function $F_N(r, \vec{v}, \vec{w}, \vec{u})$ include in considering the conditions $u(r, l) = 0$ and $u(r, l) \rightarrow 0$ if $r \rightarrow \infty$. Thus, to achieve high accuracy at every point in the network, we use the residual function $\mathbb{R}(r_i)$ and error function (loss function) $\mathbb{E}(r_i)$, due to measures of how far the network output is from the target data, and the differential-equation mismatch (what we try to minimize) [47, 50]. Hence, the sum of squares of the minimum residual function and the error function across the entire networks of size $i = 1, 2, \dots, n$ are considered and expressed by equations

$$\sum_{i=1}^n \left[\left(-\frac{d^2}{dr_i^2} + \frac{\ell(\ell+1)}{r_i^2} + 2\mu^* \left[-\frac{\alpha}{\varepsilon_r r_i} + V_{conf} - E_l(\mu^*) \right] \right) u(r_i, l) \right]^2 \quad (18)$$

$$\mathbb{E}(r_i, l) = \sum_{i=1}^n [\mathbb{R}(r_i, l)]^2 \quad (19)$$

Thus, the residual function is the local differential-equation mismatch, and the error function is a global quantity made from residuals and is the square of that residual function. It refers to a function that returns the differences between observed and simulated values in a model (in other words, the error between predicted and actual values), helping assess model accuracy. Residual plots are key to understanding how well the regression model based on ANN works. The ANN algorithm parametrizes the reduced wavefunction using the feedback function $F_N(r, \vec{u}_i, \vec{v}_i, \vec{w}_i) = \sum_{i=1}^n u_i f(r, v_i, w_i)$ in the form of activation functions of the algorithm $f(r, v_i, w_i)$ of ANN, can be rewritten as

$$u(r_i, l) = re^{-ar - \beta r^2} \sum_{i=1}^n u_i f(r, v_i, w_i) \quad (20)$$

where n is the number of required neurons in the hidden layer of the network, specified in the feedback function, and activation functions are represented as $f(r, v_i, w_i) = f(rv_i + w_i)$. Activation functions enable the final processing of ANN vectors' effects and the approximation of non-linear and complex relationships in the hidden

layer for all characteristic vectors and parameters of the system at any moment. Ultimately, the input, hidden, and output layers of the network yield calculations that satisfy the problem's boundary conditions. In neural networks, especially in this research, we describe parameters $\vec{v}_i, \vec{w}_i, \vec{u}_i$ as parameter vectors because vectors allow representing multiple parameters simultaneously; each component of a vector corresponds to a specific weight, bias, or feature. Parameter vectors in the notation context of ANN refer to a vector of weights and contain the trainable parameters of the ANN, with the component $\vec{u}_i = \sum_{i=1}^n u_i, \vec{v}_i = \sum_{i=1}^n v_i$ and $\vec{w}_i = \sum_{i=1}^n w_i$. Components u_i, v_i, w_i of $\vec{u}_i, \vec{v}_i, \vec{w}_i$ vectors correspond to a specific weight that the network learns during the training process, and each $\vec{v}_i, \vec{w}_i, \vec{u}_i$ vectors for a given neuron indexed as i is a vector in a R^n real space: $(u_i, v_i, w_i) \in R^n$, where n is the number of hidden neurons and represents the number of neurons in the hidden layer of the ANN. Therefore, the parameter vector $\vec{v}_i = \sum_{i=1}^n v_i$ represents the weighted scale for the variable r before entering the i -th hidden neuron unit. These show the sensitivity of the i -th neuron to changes in r . The parameter vector $\vec{w}_i = \sum_{i=1}^n w_i$ is trainable and determines the shift of the activation threshold of each network neuron with its dimensional variations on the wave function. A complete ANN algorithm is used for variational searching, where the structure of the feedback function $F_N(r, \vec{u}_i, \vec{v}_i, \vec{w}_i,)$ defines the generation of radial wavefunctions, the calculation of the mass-energy spectrum, and spin interaction corrections. To solve the radial SE, an initial variational ANN is considered and defined by the application functions of the algorithms under two ANN activation functions

$$\text{Softplus: } f(x) = \ln(1 + e^x)$$

$$\text{Sigmoid: } f(x) = (1 + e^{-x})^{-1}$$

Softplus is employed as the hidden-layer activation function, whereas its derivative, the Sigmoid function, is used in the analytical evaluation of the first and second derivatives of the trial wavefunction. Activation functions are necessary in solving the first- and second-order derivatives of SE to show a positive, smooth, and stable physical nature to the output function $F_N(r, \vec{u}_i, \vec{v}_i, \vec{w}_i,)$ of ANN. The results of their effect are substituted into $u(r, l)$. The output function serves as an approximator, which is placed within the optimization cycle of ANN parameters to obtain the physical nature of the original wavefunction measures and minimizes the residual function $\mathbb{R}(r, l)$ in SE. In our code, the residual is calculated in the Loss function section, and the hidden neurons employ the Softplus activation function, rather than the ReLU. The Softplus function enables the analytical evaluation of the first and second derivatives required by the kinetic-energy operator in the SE. It is applied directly within the neural-network representation of the reduced wavefunction, ensuring a differentiable trial solution throughout the optimization process. Therefore, in any case, based on ANN modeling, we can use the ReLU activation function $f(x) = \max(0, x)$ in a deep learning ANN method in the SE. This activation function shows specific outputs with conditions: *i*) returns the input unchanged for positive values: if $x > 0$, then $f(x) = x$, *ii*) returns the input to zero when it is negative or zero: if $x \leq 0$, then $f(x) = 0$. We include it to define a non-negative value for the exciton bound state mass spectrum. Activation functions Softplus and Sigmoid are necessary in solving the radial SE to determine a positive and stable physical nature to the output function $F_N(r, \vec{u}_i, \vec{v}_i, \vec{w}_i,)$ of ANN. The results of their effect are substituted into $u(r, l)$. The output function

acts as an approximator, which is placed within the optimization cycle of ANN parameters to obtain the physical nature of the original function in such a way that the wavefunction measures and minimizes the residual $\mathbb{R}(r, l)$ in SE. Therefore, the applied ANN algorithm in this research is proposed to approximate the radial Schrödinger wavefunction and mass-energy spectrum of the exciton bound state in $GaAs/Al_xGa_{1-x}As$, SNs. Hence, composition-dependent value for effective electron and hole in $GaAs/Al_xGa_{1-x}As$ approximately are used as follows [51-53]

$$m_e^*(x) \approx (0.067 + 0.083x)m_e$$

$$m_{hh}^*(x) \approx (0.34 + 0.13x)m_e$$

$$m_{lh}^*(x) \approx (0.087 + 0.02x)m_e$$

Thus, typical effective masses for electron and hole in $GaAs/Al_xGa_{1-x}As$ are considered in Table 2.

Table 2: The effective masses for electron and hole in $GaAs/Al_xGa_{1-x}As$

x	m_e^*/m_e	m_{hh}^*/m_e	m_{lh}^*/m_e
0.0	0.067	0.340	0.087
0.1	0.075	0.353	0.089
0.2	0.084	0.366	0.091
0.3	0.092	0.375	0.093
0.4	0.100	0.392	0.095
0.5	0.109	0.405	0.097

As we know, the light hole effective mass depends on the crystal direction and changes with V_{conf} . It can be strongly affected by heavy hole/light hole mixing in SNs, and we should consider confinement direction mass or in-plane direction mass. In this research, we choose the confinement potential that depends on x . In NSs, shifting x changes $E_g(x)$, and creates the barrier potential. The common approximation band gap for electrons $E_g(x)$ of $GaAs/Al_xGa_{1-x}As$ in eV unit is

$$E_g(x) \approx 1.424 + 1.247x$$

and the band gap difference is

$$\Delta E_g(x) \approx E_g(x) - E_g(0)$$

Now, we define a parameter ϑ as an offset ratio that describes the split between the conduction and valence bands at the interface between two SNs, for $GaAs/Al_xGa_{1-x}As$, it is taken to be around 0.6 to 0.7. Hence, the jump in the conduction ΔE_c and valence ΔE_v band edges between two materials in $GaAs/Al_xGa_{1-x}As$ are defined in the form

$$\Delta E_c = \vartheta \Delta E_g$$

$$\Delta E_v = (1 - \vartheta) \Delta E_g$$

Hence, the structural and material properties of SNs, such as nanostructure size, well width, barrier width, composition fraction, defect density, surface roughness, layer thickness, etc., are used as important features in the ANN modeling algorithm. The physical model and the material parameters employed in the ANN calculations.

The reduced mass is evaluated from $\mu = \frac{m_e^* m_{hh}^*}{m_e^* + m_{hh}^*}$.

The interaction potential consists of the screened Coulomb attraction together with a weak confinement contribution, $V(r) = -\frac{\alpha}{\epsilon_r r} + V_{\text{conf}}(r)$,

and the radial SE in the ANN calculations is solved for the ground state $\ell = 0$ subject to the physical boundary conditions $u(0) = 0$ and $u(r) \rightarrow 0$ as $r \rightarrow \infty$, together with wavefunction normalization $\int_0^\infty |u(r, l)|^2 dr = 1$. Therefore, in this research, the ANN algorithm on the exciton with heavy hole properties in GaAs SNs under the Aluminum matrix is applied

$$\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}: \text{GaAs}/\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$$

and physical properties are considered as follows

$$m_e = 0.511 \text{ MeV}$$

$$m_{hh}^* = 0.375 m_e$$

$$m_{lh}^* = 0.093 m_e$$

$$m_e^* = 0.092 m_e$$

$$\epsilon_r = 12.9$$

$$\vartheta = 0.65$$

$$V_{\text{conf}}^e = \Delta E_c \approx 0.243 \text{ eV}$$

$$V_{\text{conf}}^{hh} = V_{\text{conf}}^{lh} = \Delta E_v \approx 0.131 \text{ eV}$$

proposed with the aim of approximating the radial SE wavefunction and mass-energy spectrum. The results of the exciton mass calculations of the ground state in $\text{GaAs}/\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$, using theoretical SE and ANNs with $n = 100$ neurons are defined. The results of the mass spectrum, energy eigenvalue, and electron-hole reduced mass of the exciton bound state in the ground state solving SE with the theoretical SISM-WOT method and ANN algorithm in $\text{GaAs}/\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$, are presented in Table 3.

Table 3: Mass M , interaction potential E_{col} , energy eigenvalue E , and the reduced mass μ of heavy and light excitons bound state in $\text{GaAs}/\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$, in units of MeV .

Heavy exciton	ANN	Theo. (SISM-WOT)
M	0.2386	0.2386
E_{col}	-6.04327	-6.04327
E	5.6732	5.6732
μ	0.03774	0.03775
Light exciton	ANN	Theo. (SISM-WOT)
M	0.09453	0.09454
E_{col}	-3.78328	-3.78328
E	3.41328	3.41328
μ	0.02357	0.02363

To evaluate the numerical stability of the ANN model, the calculations were repeated using different numbers of hidden neurons ($n = 5, 10, 15, 20, 30$, and 100). The exciton mass obtained for the largest network ($n = 100$) was taken as the reference value. For each network size, the absolute error and relative error were calculated according to $\Delta M = |M(n) - M_{\text{ref}}|$, and $\delta = \frac{|M(n) - M_{\text{ref}}|}{M_{\text{ref}}}$. The results show that the predicted exciton mass becomes essentially independent of the number of hidden neurons,

for light exciton:

$$M = 0.0945349955 \pm 5.921 \cdot 10^{-9} \text{ MeV } (\text{mean} \pm \text{std})$$

for heavy exciton:

$$M = 0.2386369942 \pm 1.360 \cdot 10^{-9} \text{ MeV } (\text{mean} \pm \text{std})$$

indicating that the ANN solution has converged with respect to the network size, and a hidden layer containing n neurons was adopted throughout the present work. And the ground state radial and reduced wavefunctions have been plotted in Fig. 2 based on ANN, and Fig. 3 was constructed using the theoretical SISM-WOT method. The comparison in Table 1 shows that, in addition to accuracy and speed of calculations, the ANN-based method provides mass estimation with good accuracy in addition to its high estimation accuracy [54], and can be extended to a multi-exciton system, which can be used in SNs.

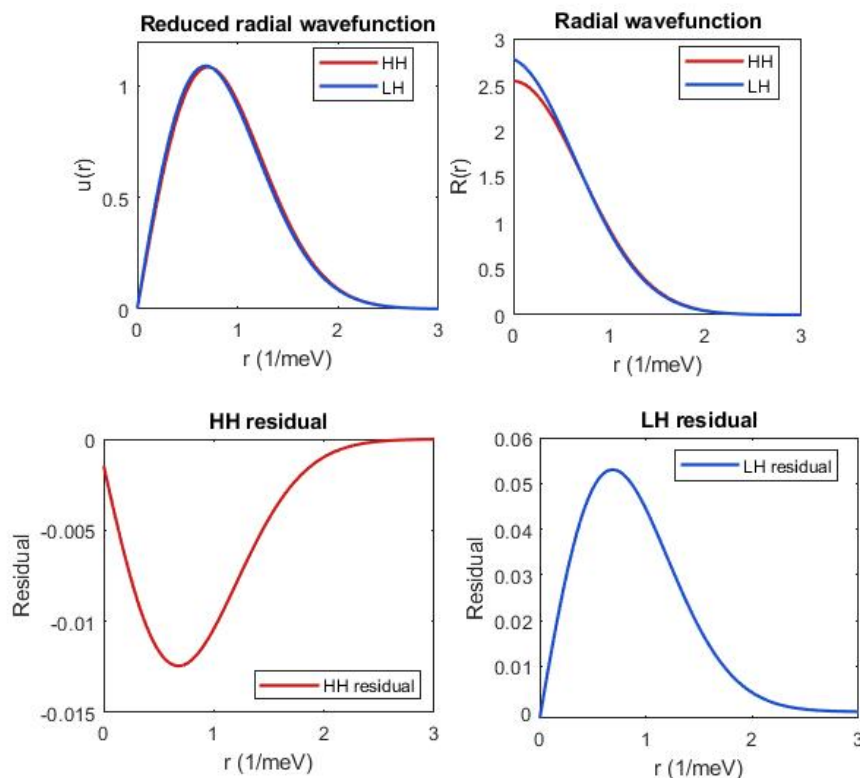


Fig. 2. The radial, reduced and residual wavefunctions of the exciton in $GaAs/Al_{0.3}Ga_{0.7}As$, using the ANN algorithm.

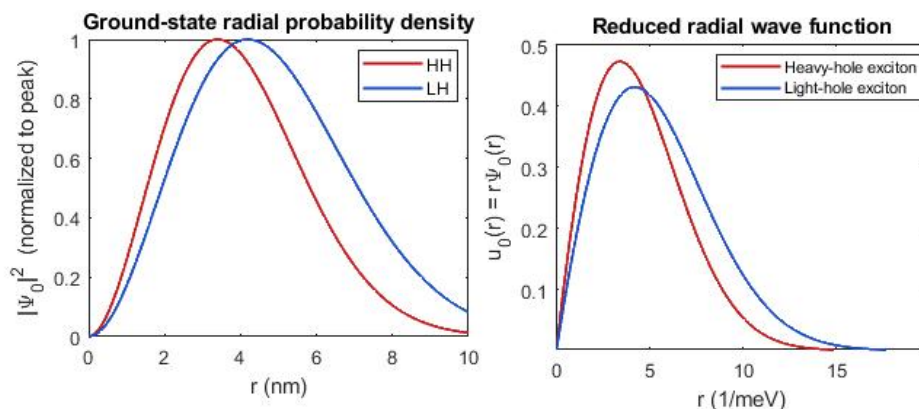


Fig. 3. The radial and reduced wavefunctions of the exciton in $GaAs/Al_{0.3}Ga_{0.7}As$, using the theoretical SISM-WOT method.

5. Conclusion

The electron-hole bound state (an exciton system) in SNs as a quantum system in nano-physical science is described by radial SE of first- and second-order differential equations. These differential equations are usually very hard to solve analytically; however, the common radial SE must be solved numerically based on advanced integration techniques. In this theoretical-numerical research, we present an ANN algorithm technique to solve the radial SE equation and a theoretical-analytical method based on SISM-WOT. The radial SE results of these methods with the corresponding energy eigenvalue and mass spectrum are compared to estimate the performance of our work and calculations. Therefore, theoretical and ANN methods in the spherical $GaAs/Al_{0.3}Ga_{0.7}As$ are presented. The radial SE for the exciton has motivating optoelectrical properties due to interaction near the electron-hole confinement in SNs. In SNs, n -body clusters of n -exciton bound states, such as biexcitons, etc., have different properties from the single exciton. Hence, the transition energy of an exciton cluster can be explained using the ANN method. As we know, the exciton cluster optical spectrum is conventionally connected to the energy eigenvalues of the electron-hole bound state, which allows full energy levels of n -body electron-hole system in $GaAs/Al_{0.3}Ga_{0.7}As$, SNc. In Coulombic interaction near the confinement potential of the electron-hole system, particles can interact with other photons, excitons, and phonons in SNs. The presented research, applying SISM-WOT and ANN methods, directly affects the calculation of spin-orbit interactions, quantum mechanical properties, and the optical and optoelectrical characteristics that enable the modification of properties in SNs; and a convergence study with respect to the hidden-layer size confirmed that the predicted exciton mass is insensitive to further increases in the number of hidden neurons, demonstrating the numerical robustness of the proposed ANN model. Some of research categories that can be defined and explained using based on presented SISM-WOT and ANN methods included in these subcategories as they have consequences in quantum information processing, fundamental studies of solid state and semiconductor physics, nanoelectronics technologies and devices: *i*) Quantum-mechanical related properties are directly described the wavefunction behavior, confinement, band structure, energy eigenvalue, bandgap energies, wavefunction distribution, tunneling probability, carrier effective mass, localization length, spin-dependent properties, transmission coefficient, and etc. *ii*) Optoelectrical and optoelectronic properties relate to light-SNs interaction, absorption coefficient, emission wavelength, responsivity, photoluminescence intensity, electroluminescence efficiency,

photoconductivity, carrier mobility, and etc. *iii*) Transport and electronic properties of SNs are used in devices to define conductivity, resistivity, mobility-lifetime product, carrier concentration, current–voltage characteristics, thermionic emission and etc. *iv*) Thermal and stability properties are useful to define thermal conductivity, specific heat, thermal stability, phonon scattering rate, electron–phonon coupling, temperature dependence of bandgap, temperature dependence of mobility, and etc. *v*) Spin and magnetic properties for advanced NSs such as spin polarization, spin relaxation time, spin lifetime, magneto-optical response, Zeeman splitting, magnetic anisotropy, spin Hall effect, Rashba splitting, and etc.

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Data availability

All data reported in this article were obtained from the analytical equations discussed within the article and are available on request by contacting the corresponding author of the study.

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Conflict of Interest

The authors affirm that they have no competing monetary interests that could influence the work reported in this paper.

References

- [1] J. Ameixa, L. Sala, J. Kocišek, I. Bald, Radiation and DNA Origami Nanotechnology: Probing Structural Integrity at the Nanoscale, *ChemPhysChem* 26 (2025) e202400863. <https://doi.org/10.1002/cphc.202400863>.
- [2] Z. Han, A.X. Guo, T. Luo, T. Cai, C.A. Mirkin, Biomaterialization of semiconductor quantum dots using DNA-functionalized protein nanoreactors, *Sci. Adv.* 11 (2025) eadv6906. <https://doi.org/10.1126/sciadv.adv6906>.
- [3] Y. Shang, N. ul Ain, J.A. Kimbro, A. Jamil, J.J. Waggoner, S.M. Hecht, S. Chen, Enzyme-free, femtomolar detection of dengue virus RNA via hierarchical quantum dot signal amplification and toehold-mediated strand displacement, *Microchem. J.* (2026) 118498. <https://doi.org/10.1016/j.microc.2026.118498>.
- [4] H. Ishiwata, J. Song, Y. Shigeno, K. Nishimura, N. Yanai, Molecular quantum nanosensors functioning in living cells, *Sci. Adv.* 12 (2026) eab5422. <https://doi.org/10.1126/sciadv.aeb5422>.
- [5] Y.D. Cho, S.H. Park, J.H. Huh, A. Gopinath, S. Lee, DNA as grabbers and steerers of quantum emitters, *Nanophotonics* 12 (2023) 399–412. <https://doi.org/10.1515/nanoph-2022-0602>.
- [6] J. Lim, M. Park, W.K. Bae, D. Lee, S. Lee, C. Lee, K. Char, Highly efficient cadmium-free quantum dot light-emitting diodes enabled by the direct formation of excitons within InP@ZnSeS quantum dots, *ACS Nano* 7 (2013) 9019–9026. <https://doi.org/10.1021/nn403594j>.
- [7] G. Singh, Recent advances on cadmium free quantum dots-liquid crystal nanocomposites, *Appl. Mater. Today* 21 (2020) 100840. <https://doi.org/10.1016/j.apmt.2020.100840>.
- [8] J. Yurek, Z. Luo, The Next Chapter for Quantum Dot Displays, *Inf. Display* 42 (2026) 13–13. <https://doi.org/10.1002/msid.70038>.
- [9] V.K. Agrahari, P.K. Aich, A. Yadav, B. Pal, S. Sadhu, D.S. Pandey, Quest of Ideal Precursors for RT Synthesis of Luminescent CsPbBr₃ Perovskite QDs for LED Phosphor Applications, *Chem. Eur. J.* (2026) e70954. <https://doi.org/10.1002/chem.70954>.
- [10] Y. Liu, D. Chen, Z. Zhang, W. Li, J. Fan, Emerging low-dimensional perovskite photoferroelectrics: From crystallographic microstructure to applications, *Nano Energy* 136 (2025) 110774. <https://doi.org/10.1016/j.nanoen.2025.110774>.

- [11] Y. Fang, Y. Shen, E. Wang, Y. Wen, G. Li, W. Li, X. Guo, et al., High-power, 2.6–10.6 μm tunable mid-infrared laser with refined Sellmeier equations using an end-mirror dielectric-coating-free ZGP OPO, *Opt. Laser Technol.* 201 (2026) 115364. <https://doi.org/10.1016/j.optlastec.2026.115364>.
- [12] A.S. Raevskii, Y.V. Raevskaja, A.Y. Sedakov, Calculation of a single-mode fiber optic attenuator, in: *Optical Technologies for Telecommunications 2024*, Proc. SPIE 13738 (2025) 185–194.
- [13] Y. Wan, W. He, J. Jaussi, L. Liao, D.Z. Pan, J.E. Bowers, H. Rong, Integrating silicon photonics with complementary metal–oxide–semiconductor technologies, *Nat. Rev. Electr. Eng.* 3 (2026) 15–31. <https://doi.org/10.1038/s44287-025-00223-0>
- [14] J. Shi, Z. Liu, J. Wei, A. Azam, C.H. Lin, Y. Liu, S. Li, Revolutionizing nonvolatile memory: advances and future prospects of 2D floating-gate technology, *ACS Nano* 19 (2025) 21905–21926. <https://doi.org/10.1021/acsnano.5c02740>
- [15] A. Nasir, A. Arshad, H. Chen, T. Zhang, T. Raza, T. Yang, S. Yun, et al., Advances in topological quantum materials for energy conversion, *J. Mater. Chem. A* 13 (2025) 26936–26966. <https://doi.org/10.1039/D6TA00807K>
- [16] M. Li, M. Wang, X. Xu, K. Meng, B. He, G. Yu, Y. Jiang, et al., A flexible field-free spin-orbit torque driven programmable spin logic device, *Adv. Funct. Mater.* 36 (2026) 2424086. <https://doi.org/10.1002/adfm.202424086>
- [17] J.D. Gerber, E. Ersoy, M. Masseroni, M. Niese, M. Laumer, A.O. Denisov, A. Knothe, et al., Tunable spin–orbit splitting in bilayer graphene/WSe2 quantum devices, *Nano Lett.* 25 (2025) 12480–12486. <https://doi.org/10.1021/acs.nanolett.5c02309>
- [18] X. Xie, Q. Li, C. Liu, Y. Liu, C. Lee, K. Sun, H. Deng, 2D material exciton-polariton transport on 2D photonic crystals, *Sci. Adv.* 11 (2025) eads0231. <https://doi.org/10.1126/sciadv.ads0231>
- [19] L. Huang, F. Jin, F. Shen, M. Hu, R. Su, Advances in exciton-polaritons with bound states in the continuum, *Laser Photonics Rev.* (2026) e03270. <https://doi.org/10.1002/lpor.202503270>
- [20] S.K. Dubey, H. Islahi, R. Singh, Solutions to the Schrödinger equation using deep neural networks for integrated photonics, *J. Opt. Commun.* 46 (2025) 969–976. <https://doi.org/10.1515/joc-2024-0193>
- [21] W.E. Azogor, T.I. Uza, N.O. Edodi, Analytical solutions of Klein–Gordon equation for a central inverse square potential using Nikiforov–Uvarov method, *Glob. J. Pure Appl. Sci.* 31 (2025) 397–412. <https://doi.org/10.4314/gjpas.v31i2.25>
- [22] M. Jaouane, et al., Optical properties of an exciton in core/shell/shell spherical quantum dot under an electric field, *J. Phys. Chem. Solids.* 208 2 (2025) 12:113169. <https://doi.org/10.1016/j.jpcs.2025.113169>
- [23] Hayrapetyan, Binding and recombination energies of quasi-one-dimensional excitonic complexes in ellipsoidal quantum dot, *Foundations* 2 (2022) 219–227. <https://doi.org/10.3390/foundations2010015>.
- [24] H.H. Xie, L.G. Jiao, A. Liu, Y.K. Ho, High-precision calculation of relativistic corrections for hydrogen-like atoms with screened Coulomb potentials, *Int. J. Quantum Chem.* 121 (2021) e26653. <https://doi.org/10.1002/qua.26653>
- [25] K.G. Dvovyan, D.H. Kazaryan, E.M. Kazaryan, Direct interband light absorption in a strongly oblated ellipsoidal quantum dot, *Nanoscale Res. Lett.* 4 (2009) 106–112. <https://doi.org/10.1007/s11671-008-9209-2>.
- [26] D.B. Hayrapetyan, Direct interband light absorption in a strongly prolated ellipsoidal quantum dot, *J. Contemp. Phys.* 42 (2007) 292–297. <https://doi.org/10.3103/S1068337207060175>.
- [27] D.A. Baghdasaryan, D.B. Hayrapetyan, E.M. Kazaryan, Optical properties of narrow-band prolate ellipsoidal quantum layers ensemble, *J. Nanophotonics* 10 (2016) 033508. <https://doi.org/10.1117/1.JNP.10.033508>.
- [28] Y.Y. Bleyan, et al., Non-linear optical properties of biexciton in ellipsoidal quantum dot, *Nanomaterials* 12 (2022) 1412. <https://doi.org/10.3390/nano12091412>.
- [29] V. Kumar, S. Bhardwaj, R.M. Singh, F. Chand, Optical properties and effect of magnetic field on energy spectra of a GaAs spherical quantum dot, *Eur. Phys. J. Plus* 138 (2023) 191. <https://doi.org/10.1140/epjp/s13360-023-03810-y>.
- [30] Z.H. Zhang, J.H. Yuan, Electronic and nonlinear optical properties in Al_xGa_{1–x}As/GaAs Gaussian confinement quantum dot under applied electric field, *Physica E* 147 (2023) 115594. <https://doi.org/10.1016/j.physe.2022.115594>.
- [31] A. Jahanshir, E. Omugbe, Relativistic mass of spherical layered quantum dots within harmonic potential, in: *Proc. 2nd National Conference on Technological Advances in Applied Physics*, Graduate University of Advanced Technology, Iran, 2023.
- [32] C. Chang, X. Li, X. Wang, C. Zhang, Nonlinear optical properties in GaAs/Ga_{0.7}Al_{0.3}As spherical quantum dots with Like–Deng–Fan–Eckart potential, *Phys. Lett. A* 467 (2023) 128732. <https://doi.org/10.1016/j.physleta.2023.128732>.
- [33] M.E. Peskin, *An Introduction to Quantum Field Theory*, CRC Press, Boca Raton, 2018.
- [34] M.J. Ambrosio, et al., Mathematical properties of generalized Sturmian functions, *J. Phys. A Math. Theor.* 45 (2011) 015201. <https://doi.org/10.1088/1751-8113/45/1/015201>.

- [35] G. Gasaneo, et al., Three-body Coulomb problems with generalized Sturmian functions, *Adv. Quantum Chem.* 67 (2013) 153–216. <https://doi.org/10.1016/B978-0-12-411544-6.00007-8>.
- [36] M. Dineykan, G. Efimov, G. Ganbold, S. Nedelko, *Oscillator Representation in Quantum Physics*, Springer, Berlin, 2008.
- [37] A. Jahanshir, Quanto-relativistic background of strong electron–electron interactions in quantum dots under magnetic field, *J. Optoelectron. Nanostruct.* 6 (2021) 1–24. <https://doi.org/10.30495/JOPN.2021.28742.1231>.
- [38] E. Hiyama, Y. Kino, M. Kamimura, Gaussian expansion method for few-body systems, *Prog. Part. Nucl. Phys.* 51 (2003) 223–307. [https://doi.org/10.1016/S0146-6410\(03\)90015-9](https://doi.org/10.1016/S0146-6410(03)90015-9).
- [39] M.A. de Gosson, *Symplectic Geometry and Quantum Mechanics*, Springer, Basel, 2006.
- [40] M. Bojowald, Canonical description of quantum dynamics, *J. Phys. A Math. Theor.* 55 (2022) 504006. <https://doi.org/10.1088/1751-8121/acafb0>.
- [41] M.I. Eides, H. Grotch, V.A. Shelyuto, Theory of light hydrogenlike atoms, *Phys. Rep.* 342 (2001) 63–261. [https://doi.org/10.1016/S0370-1573\(00\)00077-6](https://doi.org/10.1016/S0370-1573(00)00077-6).
- [42] H. Yukawa, On the interaction of elementary particles, *Proc. Phys.-Math. Soc. Jpn.* 17 (1935) 48–57.
- [43] M. Dineykan, R. Nazmitdinov, Ground state spin oscillations of a two-electron quantum dot in a magnetic field, *J. Phys. Condens. Matter* 11 (1999) L83–L88. <https://doi.org/10.1088/0953-8984/11/11/002>.
- [44] Y. Zhang, B. Jiang, H. Guo, Schrodinger Net: A universal neural network solver for the Schrodinger equation, *J. Chem. Theory Comput.* 21 (2025) 670–677. <https://doi.org/10.48550/arXiv.2408.04497>
- [45] I.A. Moloshnikov, A.G. Sboev, A.A. Kutukov, R.B. Rybka, M.S. Kuvakin, O.O. Fedorov, S.V. Zavertyaev, Analysis of neural network methods for obtaining soliton solutions of the nonlinear Schrödinger equation, *Chaos Solitons Fractals* 192 (2025) 115943. <https://doi.org/10.1016/j.chaos.2024.115943>
- [46] L. Serkin, T.L. Belyaeva, Physics-informed neural networks for higher-order nonlinear Schrödinger equations: Soliton dynamics in external potentials, *Mathematics* 13 (2025) 1882. <https://doi.org/10.1016/j.jjleo.2023.170739>
- [47] T.S. Kosmas, I.E. Lagaris, On the muon–nucleus integrals entering the neutrinoless $\mu^- \rightarrow e^-$ conversion rates, *J. Phys. G Nucl. Part. Phys.* 28 (2002) 2907–2925. <https://doi.org/10.1088/0954-3899/28/12/302>
- [48] I.G. Tsoulos, O.T. Kosmas, V.N. Stavrou, Dirac Solver: A tool for solving the Dirac equation, *Comput. Phys. Commun.* 236 (2019) 237–243. <https://doi.org/10.1016/j.cpc.2018.10.010>
- [49] F. Salvat, J.M. Fernández-Varea, RADIAL: A Fortran subroutine package for the solution of the radial Schrödinger and Dirac wave equations, *Comput. Phys. Commun.* 240 (2019) 165–177. <https://doi.org/10.1016/j.cpc.2019.02.011>
- [50] S. Manzhos, T. Carrington, An improved neural network method for solving the Schrödinger equation, *Can. J. Chem.* 87 (2009) 864–871. <https://doi.org/10.1139/V09-025>
- [51] J.S. Blakemore, Semiconducting and other major properties of gallium arsenide, *J. Appl. Phys.* 53 (1982) R123–R181. <https://doi.org/10.1063/1.331665>
- [52] H. Uchida, C.J. Curtis, P.V. Kamat, K.M. Jones, A.J. Nozik, Optical properties of gallium arsenide nanocrystals, *J. Phys. Chem.* 96 (1992) 1156–1160. <https://doi.org/10.1021/j100182a026>
- [53] A. Jahanshir, Combination of Artificial Neural Networks and Polarization Loop in Calculating Hadronic Mass Spectrum, in: *Proc. 7th National Conference on computational physics*, Shahid Beheshti University, Iran, 2025.
- [54] Y.I. Diakite, S.D. Traore, Y. Malozovsky, B. Khamala, L. Franklin, D. Bagayoko, Accurate electronic, transport, and bulk properties of gallium arsenide (GaAs), *arXiv:1601.05300* (2016). <https://doi.org/10.48550/arXiv.1601.05300>