Journal of Particle Science and Technology 9 (1) (2023) 19-27

Iranian Research Organization for Science and Technology (IROST)

Journal of PARTICLE Science & Technology

JPST
https://jpst.irost.ir

Online ISSN: 2423-4079
Print ISSN: 2423-4087

Theoretical study of quantum and thermal properties of particles' bound state in quantum disks

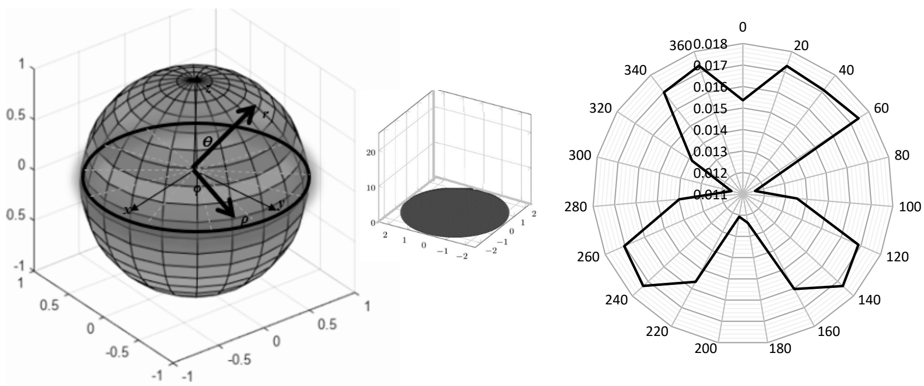
Arezu Jahanshir✉

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

HIGHLIGHTS

- Exciton bound state interaction is described within non-central potential.
- Schrodinger equation is presented based on the Sturmian function.
- Eigenenergy value determined for different strengths of the distortion β_d.
- Distortion potential effect for a fixed quantum disk is calculated at finite temperature.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article type:
Research article

Article history:
Received 19 May 2023
Received in revised form 24 June 2023
Accepted 12 July 2023

Keywords:
Bound state
Distortion potential
Sturmian function
Schrödinger equation

DOI: 10.22104/JPST.2023.6288.1228

ABSTRACT

The present study aims to investigate the thermal properties of low-quantum structures (LQS) with a described non-central potential. Additionally, the study investigates the influence of relativistic parameters such as the constituent mass (effective mass) of particles and the effect of thermal properties. The magnitude of distortion of an LQS due to a non-central potential was found to have a profound effect on the system's quantum and thermal properties, which is crucial to understanding the behavior of practical quantum systems in an LQS. This paper studies the critical concepts in the fundamental optimization of mass and thermal properties of interactions in LQS based on canonical operators. It explores and analytically calculates the radial part of the Schrödinger equation at finite temperatures with two intertwined spaces using the normal ordering method in a combination of the Coulomb potential and the distortion potential. We provide analytical expressions for the ground state energy eigenvalues to define the zeroth approximation with the quantum and thermal effect and properties. Results showed that the energy of a system decreases with an increase in temperature and strength of the distortion.

✉ *Corresponding author: E-mail address:* jahanshir@bzte.ac.ir ; *Tel & Fax:* +9828-33894493

1. Introduction

In recent decades, the field of LQS has proven to be an important foundation of many applications in numerous research areas. Both theoretical and experimental exploration and analysis of their physical, magnetic, and electronic properties have been immensely important, especially concerning thermal effects, and have resulted in various optoelectronic devices, photodetectors, batteries, and sensors, among others. Applications in fields related to energy, bound state mass, and interactions between particles are also possible by exploiting thermal and distorted orientation properties. This issue directly increases the accuracy of theoretical and experimental results in these fields. In recent years, theoretical physicists have become increasingly interested in the study of the relativistic and thermal properties of low-dimensional systems [1,2]. There is a persistent effort to create advanced LQS that feature tunable thermal, electrical, optical, and magnetic properties, as well as a wide range of applications. LQS is a type of nanoscale structure that exhibits quantum mechanical properties due to its small size and unique geometry. LQS is typically composed of semiconducting materials, such as gallium arsenide, and has a thickness of a few nanometers and a diameter of tens or hundreds of nanometers [3,4]. The small size of quantum disks results in the quantization of electronic energy levels, leading to discrete and closely spaced energy levels [5]. This can result in unique optical and electronic properties, such as strong quantum confinement effects, high absorption and emission rates, and the ability to confine and manipulate individual electrons.

LQS have a wide range of potential applications in various fields, such as optoelectronics, nano-photonics, and quantum computing. Researchers are actively studying LQS to better understand their properties and optimize their performance for specific applications. LQS are comparable in size to the charge carrier's de-Broglie wavelength and are classified as either quantum dots, wires, or disks/wells, depending on the number of dimensions that restrict the carrier movement [6]. Among LQS, 2D quantum dots (quantum disks) have been extensively studied due to their myriad applications in fields such as optoelectronics, energy storage, sensors, batteries, and photodetectors [6,7]. Compared to their bulk counterparts, LQS quantum disks' unique properties are attributed to their quantum and thermal effects. The increasing demand for developing advanced LQS devices with quantum and thermal tunable thermal properties has become a continuous endeavor [3-5]. LQS have the potential to open up new research frontiers in low dimensional hi-technology due to their unique properties, which make them promising candidates for next-generation advanced materials.

In LQS, the distortion effect is caused by the distortion potential, which refers to the potential energy arising from deformations in the shape of the disk due to external forces or interactions with other inside particles. The distortion potential refers to a potential energy surface in 2D systems that describes the potential energy of particles or bound states, such as exciton, as a function of the vibrational coordinates [3-5]. The distortion potential arises from the fact that the potential energy of excitons can be affected by changes in their geometry. In particular, it describes how changes in the bond lengths, bond angles, and torsion angles of an exciton affect their potential energy. For example, if an exciton is stretched along its bond, the distortion potential will describe how the potential energy changes as a function of the bond length. Similarly, if an exciton is twisted around its torsion angles, the distortion potential will describe how the potential energy changes as a function of the torsion angle, especially important in strong electron-electron interactions and the presence of a strong magnetic field.

The distortion potential is important in spectroscopy because it affects the frequencies and intensities of the vibrational transitions that a molecule can undergo. By studying the distortion potential of a molecule, researchers can gain insights into its structure, conformational dynamics, and chemical reactivity. These deformations can lead to changes in the electronic structure and the energy levels of the LQS, which can affect its properties and behavior [8,9]. The distortion potential is a key factor in determining the electronic and optical properties of LQS, and it is often used in theoretical models to describe the behavior of these systems. The magnitude and nature of the distortion potential can depend on various factors, including the size and shape of the disk, the composition of the disk material, and the external environment. The study's results are expected to provide guidelines for tuning LQS properties, which will aid the development of practical low-dimensional devices. The remainder of this research is laid out in the following manner: introducing a Sturmian representation in two intertwined spaces and describing the behavior of distortion potentials in LQS, explaining exciton in the distortion Coulombic potential, and presenting the numerical calculation of the mass spectrum and energy eigenvalue of the exciton using quantum and thermal behavior.

2. The behavior of distortion potentials in LQS

Understanding the distortion potential is essential for developing accurate models of LQS and predicting their behavior in different applications. As we know, distortion behavior in a quantum disk can exist even without an external field [9]. Distortion can arise from purely quantum mechanical effects, such as the Coulomb interaction between electrons or electron holes as a disk's bound state system or the disk shape's inherent anisotropy [8]. These effects can cause deformations in the disk shape, which in turn can lead to changes in the electronic structure and energy levels of the disk, affecting its optical and electronic properties. The distortion potential can also arise from the interaction between the quantum disk and its surrounding environment, such as the substrate on which it is grown [9,10]. Therefore, even in the absence of an external field, the distortion potential can still be present and significantly affect an LQS's properties and behavior. An electrically neutral quasi-bound state, known as the exciton, exists within all LQS [7,9].

In this article, the potential interactions of exciting oscillating quantum systems (excitons inside the LQS) with the topology of the 2D semiconductors quantum disk in spherical coordinates are shown in Fig. 1, and the radius of the disk r_0, and boundary conditions through the potential are given by $r < r_0$.

This exotic bound state is comprised of a negatively charged electron and a positively charged hole, which are attracted to each other by the electrostatic Coulomb interaction. Experimentation on LQS led to the discovery of these bound states [10], demonstrated the potential for the existence of multi-exciton states [11], and generated significant interest in their properties, particularly concerning the strength of distortion and the angular position of the distortion. Hence, LQS is described by the combination of the Coulomb potential and the distortion potential ($\hbar = c = 1$) in the polar coordinates (r,φ) as follows (Eq. (1)) [11,12]:

$$V(r,\varphi) = -U(r) + U(r,\varphi) = -\frac{1}{\varepsilon_r r} - \frac{\beta_d Sin(\varphi - \eta)}{2r^2} \qquad (1)$$

where $U(r,\varphi)$ is the potential of the azimuthal distortion that exists due to a hydrogenic impurity that has an electronic

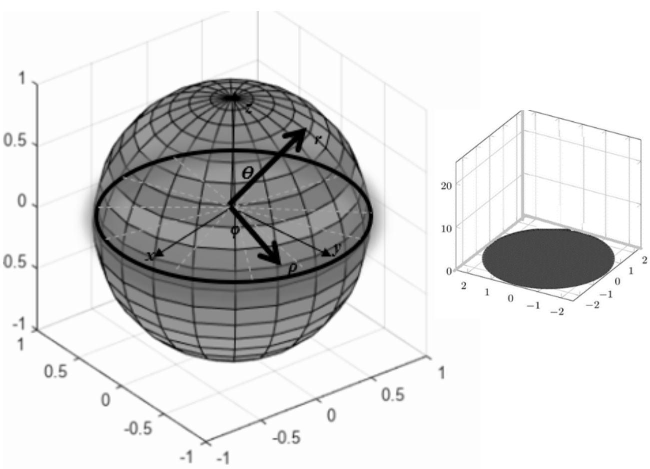


Fig. 1. 2D LQS in spherical coordinate presentation.

structure similar to that of a hydrogen atom with η (the phase of distortion) the angular position of the distortion, β_d is the strength of the distortion and the φ-dependent azimuthal distortion potential. $U(r)$ is the Columbic interaction in the LQS with ε_r the relative static dielectric constant. In this study, we first present the azimuthal distortion effect on quantum disk and its quantum and thermal properties based on exciton bound state. Then, we try to describe the impurity effect using the radial Schrödinger equation of exciton-bound states and define the energy eigenvalue of ground and excited states.

The electronic properties of hydrogenic impurities in semiconductors have been extensively studied, as they can significantly modify the electrical conductivity of the host material. For example, doping silicon with boron, a hydrogenic impurity, can increase the material's electrical conductivity and make it a *p*-type semiconductor [13]. Similarly, doping silicon with phosphorus, which is also a hydrogenic impurity, can increase the electron density in the material and make it an *n*-type semiconductor. Hydrogenic impurities can also be used as quantum bits (qubits) for quantum computing, as the electronic states of the impurity atoms can be manipulated and measured with high precision. For simplicity, the mass spectrum and thermal properties of the LQS are generally studied without external interactions. Furthermore, as mentioned above, the quantum harmonic oscillator, a main unique internal interaction, is an important application and model to describe bound state particles in LQS. Harmonic oscillator eigenvalue problems can be solved analytically when the exact solution of a problem cannot be found; it is advantageous to use approximation methods such as perturbation theory [14]. The perturbation theory approach has been adopted in several approaches to calculate and determine the energy eigenvalues of the ground and excites states of excitons. Theoretically, using a harmonic oscillator method and boundary conditions of the bound state, the quantum and thermal properties of the bound state inside LQS can be solved, providing better experimental results and potential new LQS-based equipment for advanced technologies.

These perturbed harmonic oscillators may be calculated using computational and analytical methods with theoretical contributions. This study used the two intertwined spaces, based on the normal ordering method, which significantly contributes to approximating and developing mathematical techniques for finding the eigenvalues and eigenfunctions of quantum systems with harmonic oscillator main potential and potential in Eq. (1). The normal ordering method is a useful analytical method for solving and approximating the Schrödinger equation in quantum mechanics [14]. It is based on the idea of separating the potential into a nonperturbative and perturbative part, which is then treated separately. The nonperturbative part of the potential can be solved exactly, while the perturbative part can be treated as a perturbation to the nonperturbative part. This method has been successfully applied to study bound systems in various conditions, including the exciton state in this research. Also, in the analysis of the characteristic of the bound states, a transformation from one space to another space is considered to obtain the answer. These intertwined spaces based on the normal ordering method are a useful analytical method for solving and approximating the Schrödinger equation, and it has been successfully applied to study LQS systems [6,14].

The purpose of this research is to use the perturbation and approximate solution method to calculate the zero-energy correction and obtain the generalized energy eigenvalues for exciton with thermal properties. It explores the Schrödinger equation at finite temperatures, applying and implementing the presented transformation and intertwined two-space method for potential parts. We provide analytical expressions for the energy eigenvalues and mass spectrum.

2.1. Transformation and intertwined two spaces method

The article introduces a method for solving the LQS problems based on the Schrödinger equation, which utilizes the Sturmian representation to analyze the exciton properties in the distortion/Coulombic potential. The Sturmian function is a set of eigenfunctions of the Schrödinger equation, which is helpful in addressing specific LQS problems that involve Schrödinger wave functions. Using this approach, the author aims to provide a more effective means of understanding the behavior and properties of LQS.

The Sturmian function

$$\int_0^\infty d^3r\, S_{nl}(r)\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}+\alpha_{nl}U(r)\ -E_{n\ell}\right]S_{nl}(r)=0$$

is the solution of the radial part of the Schrödinger equation [14], where n is the principal quantum number and l is the angular quantum number. These functions, $S_{nl}(r)$, have a notable benefit over Schrödinger functions when used as a basis for expansion since they create a complete set that is not continuous, regardless of the potential between particles. Three key conditions must be satisfied when choosing a different expansion basis of intertwined spaces for the coupled electron-hole state. Firstly, the series must approach convergence at a reasonable rate. Secondly, the continuum and its inherent complexity must be avoided to justify the use of the new series over a usual eigenvector and eigenfunction series. Lastly, the boundary constraints set and restrictions imposed by the new functions must be elementary and uncomplicated. For instance, quantum harmonic oscillator wave functions satisfy the second condition and requirement but at the expense of losing and overburdening the simplicity of their asymptotic behavior of boundary conditions, which makes synthesizing an outgoing spherical symmetric wave difficult. However, we have discovered a set of functions that satisfies the second and third requirements.

Rosner, Quigg, and Gazeau were dealing with the same topic [12]. They drew attention to the fact that the origin of the Sturmian representation and changing the independent coordinate can describe electron-hole bound states problems related to the Schrödinger equation [12]. The mechanism of transforming the independent parameter has long been a useful strategy to solve the Schrödinger equation with different type potentials, like the $V(r,\theta,\varphi) \approx \sum r^{\alpha}$ potential, especially with the bound state interaction. The potential $V(r,\theta,\varphi) \approx \sum r^{\alpha}$ with a variable exponent is a flexible resource that can be utilized to analyze the actions of systems where particles interact with one another, and its usefulness extends to various areas and branches of physics, including condensed matter physics, nanophysics, and semiconductor physics. In this article, the study of coupled electron-hole involves the use of the distortion Coulombic potential because it can define the quantum and thermal properties of LQS. The exciton state issues in LQS can be naturally explained using the origin of the Sturmian representation and the equivalence transformed space for the electron-hole bound state. In cases where solutions for $V(r,\theta,\varphi)$ are not available, a more general equivalence emerges as a change of variable in the total wave function $\Psi(r,\theta,\varphi) = \Re(r)\Theta(\theta)\Phi(\varphi)$ for the large and short distances as follows:

$$\Psi(r,\theta,\varphi)_{r\to\infty} \approx e^{-a(r)}R(r) \approx e^{-r^{1+\sigma}}\Re(r) \tag{2}$$

$$\Psi(r,\theta,\varphi)_{r\to 0} \approx r^{((D-1)/2)}\Re(r) \tag{3}$$

where $r = q^{2\rho}$, $\rho = 1/(1+\sigma)$, and $\sigma \geq 0$, which can be used to map the nonrelativistic Schrödinger equation $\hat{H}\Psi(r,\theta,\varphi) = E_{nl}\Psi(r,\theta,\varphi)$ and its solutions for $V(r,\theta,\varphi) \approx \sum r^{\alpha}$ potential types [13]. For different values of α, the coupled system has to create bound states, with boundary conditions on the wave functions being linked by this transformation. If we focus on long distances limit and use analytical methods, we can typically determine the asymptotic properties and long-term behavior of the wave function as follows:

$$\Psi\big(r\big(q^{\beta}\big),\theta,\varphi\big) \approx e^{-(q)^{2\left(\frac{1}{1+\sigma}\right)}} \tag{4}$$

for $r \to \infty$, where $a(r)$ can be obtained for certain classes of potentials. For large distance potentials, such as Coulomb ($\alpha \leq 0$), $\sigma = 0$.

From the previous references to physics, we have realized that the concept of harmonic oscillators hold significant relevance across various areas of physics, with it being a crucial tool for modeling physical systems. The harmonic oscillator analogy is extensively employed in attempts to solve quantum mechanical problems, as many physical scenarios can be mapped onto a harmonic oscillator with appropriate boundary conditions. This stems from the fact that the harmonic oscillator eigenvalue problem has an analytic solution, allowing more accurate results and better approximation for solutions [14]. We note that Johnson, Quigg and Rosner have studied and analyzed potentials with an adjustable number of power factors of $\sum r^{\alpha}$; they used a variable change to interpret the Sturmian equation and two intertwined spaces in the context of conventional physical Schrödinger equations [12]. We also mention that the electron-hole state with a based-on quantum harmonic oscillator behavior (principal harmonic potential) can be tackled using algebraic methods, such as the normal ordering method. In the following paragraphs, our examination begins with the Schrödinger equation that applies to space with 2-dimensions based on the 3-dimensional Laplacian operator, i.e., we describe the LQS system in spherical coordinates and then calculate equations for $\theta = 0$.

3. Exciton in the distortion Coulombic potential

In this study, theoretically and approximately, the exciton in the LQS solution and eigenvalues answered by the N = 3 dimensional Schrödinger equation in two intertwined spaces based on normal ordering has been described. In the following, we have predicted the mass spectrum in the quantum and thermal conditions using the mechanism of intertwined spaces using the normal ordering method (when all raising operators are to the left of all lowering operators). Our start point is the time-independent Schrödinger equation in 3-dimensional space, which describes the interaction of electron holes with the rest masses m_e, m_h in the potential $V(r,\theta,\varphi)$, that lead us to create the stable bound state and describe properties of the distortion effect based on exciton bound states in LQS. The Schrödinger equation function $\hat{H}\Psi(r,\theta,\varphi) = E_{nl}\Psi(r,\theta,\varphi)$ within potential Eq. (1), and external electric field $V_{ext} = |q|(\boldsymbol{E}\cdot r)$ [14,15] reads as:

$$\int_0^{\infty} d^3r\Re(r)\left(-\frac{1}{2m_e^*}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]-\frac{1}{2m_h^*}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]+\frac{\ell(\ell+1)}{2\mu r^2}+V_c+V_{ext}-E_{n\ell}\right)\Re(r)=0 \tag{5}$$

$$\int_0^{\infty} d^3r\Re(r)(\frac{1}{2\mu}\Delta+\frac{\ell(\ell+1)}{2\mu}+W(U,E_{n\ell}))\Re(r) \tag{6}$$

$$W(U,E_{n\ell}) = -\frac{1}{\varepsilon_r r}-\frac{\beta_d Sin(\varphi-\eta)}{2r^2}+|q|(\boldsymbol{E}\cdot r)-E_{n\ell} \tag{7}$$

where ℓ is the angular momentum quantum number, n is the principal quantum number, and $\frac{1}{m_e^*}+\frac{1}{m_h^*}=\frac{1}{\mu}$ is the reduced mass of the exciton bound state. Using Eq. (6), based on the Laplacian operator effect $\Delta=\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}$, on functions $\Re(r)$ and $\Re(r) \equiv r^{\alpha}\chi(r)$ in 3-dimensional space, one can describe $\Re(r)$ using $\chi(r)$ as a radial weight function (RWF). The RWF is a fundamental concept in quantum mechanics that characterizes the probability density of locating a particle (electron) at a specific distance from another particle (hole) in the bound state (exciton) or electron-nuclei in an atom or molecule's nucleus. RWF is computed as the product of the square of the radial wave function and the square of the radial coordinate and is dependent solely on the radial distance from the constituent particles. This function is essential in determining various properties of bound states in this research. Hence, $\Delta\Re(r) \equiv \Delta(r^{\alpha}\chi(r))$, and we present Eq. (5) as follows:

$$\Re''-\frac{L(L+1)}{r^2}\Re+\frac{W(U,\mathrm{E})}{r^2}\Re=0 \tag{8}$$

where $\Re(r) = r^{\alpha}\chi(r)$, L is a parameter representing a new auxiliary space, i.e., we define the radial Schrödinger equation linked to the 3-dimensional space $L = \ell$. As we introduced in Eq. (4), by changing $r = q^{2\rho}$, $\Re(r) \to \Re(q^{2\rho})$, this means that we can always maps $r = 0$ into $q = 0$ and maps $r = \infty$ into $q = \infty$. Two intertwined spaces are transformed by relations:

$$\frac{d}{dr}=\frac{1}{2\rho}q^{1-2\rho}\frac{d}{dq}$$

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

Hence, the radial Laplacian in a 3-dimensional Riemannian space is:

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

and then by using $\Delta\Re(r) = \Delta(r^{\alpha}\chi(r))$ one can define:

$$\int_0^{\infty} d^3(q^{2\rho})\Phi(q^{2\rho})\left(\frac{d^2}{dq^2}+\frac{1+2\rho}{q}\frac{d}{dq}-\frac{4\ell\rho^2(\ell+1)}{q^2}+4\rho^2q^{4\rho-2}W(q^{2\rho})\right)\Phi(q^{2\rho})=0 \tag{9}$$

where $D = 2 + 2\rho$. After some calculations in the new axillary D-dimensional space $\Phi(q^{2\rho})\rightarrow\aleph(q^{2\rho})=q^{\frac{1-D}{2}}\Phi(q^{2\rho})$ we define:

$$\int_0^\infty d^3(q^{2\rho})\aleph(q^{2\rho})\left(\frac{d^2}{dq^2}+\frac{D-1}{q}\frac{d}{dq}-\frac{4\ell\rho^2(\ell+1)}{q^2}+4\rho^2q^{4\rho-2}W(q^{2\rho})\right)\aleph(q^{2\rho})=0 \quad (10)$$

and then

$$\Phi''-\left[\frac{1-D^2}{2}+(D-1)^2+8\ell\rho^2(\ell+1)\right]\frac{1}{2q^2}\Phi+4\rho^2q^{4\rho-2}W(q^{2\rho})\Phi=0 \quad (11)$$

We generalize this equation within intertwined spaces and determine $L_D=\frac{4\ell\rho+D-3}{2}$ and

$$L_D(L_D+1)=\frac{16\ell\,\rho^2(\ell+1)+(D-2)^2-1}{4} \quad (12)$$

and then one can determine the radial Schrodinger equation in the axillary D-dimensional space ($D = 2L_D - 4\ell\rho + 3$) as follows:

$$\Phi''-\frac{L_D(L_D+1)}{q^2}\Phi+4\rho^2q^{4\rho-2}W(q^{2\rho})\Phi=0 \quad (13)$$

where $\rho > 0$ and $N = 4\ell\rho + D$. Eq. (14) relies on only the parameters D, ρ, and ℓ, which are combined through the parameter L_D. Therefore, it is unnecessary to consider D and ℓ separately, and the number of dimensions is relatively arbitrary. Moving forward, we will treat $L_D = 2\ell\rho + \rho - 0.5$ as a continuous parameter, not restricted to the integral or half-integral values.

4. Exciton mass spectrum in quantum disk

The Radial Schrödinger Eq. (13) in $N = 3$ dimensional axillary space of an electron-hole bound state (exciton) within the distortion-Coulombic potential [16,17] and the external electric field (using the two intertwined space transformation described above) takes the form:

$$\varepsilon_0(E_n)=\int_0^\infty d^3(q^{2\rho})\aleph(q^{2\rho})\left(\frac{\hat{p}_q{}^2}{2}+4\mu\rho^2\hat{q}^{4\rho-2}\left(-\frac{1}{\varepsilon_r\hat{q}^{2\rho}}-\frac{\beta_d Sin(\varphi-\eta)}{2\hat{q}^{4\rho}}+|q|(E\cdot\hat{q}^{2\rho})-E_{n\ell}\right)\right)\aleph(q^{2\rho})=0 \quad (14)$$

As we know, the exciton-bound state wave function becomes an oscillator one. Now, we will analytically calculate the mass spectrum and energy eigenvalue of Eq. (13) using the quantum oscillating properties condition of the bound state with the Hamiltonian $H = H_0 + H_I$, where H_0 is the Hamiltonian of free oscillators and H_I is the Hamiltonian of interactions (or it is directly related to the perturbation of the system). The bound state of the quantum oscillating system can be presented by the normal ordering method in the symplectic space. It is formulating the canonical variables in terms of raising $\hat{a}^+=\frac{\sqrt{2}}{2}\left(\sqrt{m\omega}\hat{q}-\frac{i}{\sqrt{m\omega}}\frac{d}{dq}\right)$ and lowering $\hat{a}=\frac{\sqrt{2}}{2}\left(\sqrt{m\omega}\hat{q}+\frac{i}{\sqrt{m\omega}}\frac{d}{dq}\right)$ operators in the N-dimensional space, i.e., $\hat{q}=\sqrt{2m\omega}(\hat{a}^++\hat{a})$, $\frac{d}{dq}=i\sqrt{\frac{m\omega}{2}}\,(\hat{a}^+-\hat{a})$, where $N = 4\ell\rho + D$, and ω is the quantum oscillator frequency [14]. Substituting the canonical variables $\hat{q},\hat{p}_q=\frac{d}{dq}$ into Eq. (13) and ordering by the creation and annihilation operators, the interaction Hamiltonian is obtained as follows:

$$H=\omega(\hat{a}^+\hat{a})+\frac{N}{2}\omega+\int\left(\frac{dk}{2\pi}\right)^N\breve{W}(k^2)e^{\frac{-k^2}{4\omega}}:e^{ik\hat{q}}:-\frac{\omega^2}{2}\left(:\hat{q}^2:+\frac{N}{2\omega}\right) \quad (15)$$

The normal ordering method in the symplectic space requires that the H_I does not contain the quadratic form of the normal ordering of operators $:\hat{q}^2:$, $\hat{q}^2$, these terms are included in the H_0 (i.e., the distortion potential term in the symplectic space has to be included in the Hamiltonian of free oscillators). Based on this condition, one can determine ω by the relation $\omega^2+\int\left(\frac{dk}{2\pi}\right)^N\left(\frac{k^2}{N}\right)e^{\frac{-k^2}{4\omega}}\breve{W}(k^2)=0$.

The normal product over the canonical operators reads

$$\hat{p}_q^{2u}=\omega^u\frac{\Gamma\left(\frac{N}{2}+u\right)}{\Gamma\left(\frac{N}{2}\right)}+:\hat{p}_q^2:\omega^{u-1}u\frac{\Gamma\left(\frac{N}{2}+u\right)}{\Gamma\left(\frac{N}{2}+1\right)}+:\breve{\beth}:\approx\omega^u\frac{\Gamma\left(\frac{N}{2}+u\right)}{\Gamma\left(\frac{N}{2}\right)}$$

$$\hat{q}^{2u}=\frac{1}{\omega^u}\frac{\Gamma\left(\frac{N}{2}+u\right)}{\Gamma\left(\frac{N}{2}\right)}+:\hat{q}^2:\frac{u}{\omega^{u-1}}\frac{\Gamma\left(\frac{N}{2}+u\right)}{\Gamma\left(\frac{N}{2}+1\right)}+:\beth:\approx\frac{1}{\omega^u}\frac{\Gamma\left(\frac{N}{2}+u\right)}{\Gamma\left(\frac{N}{2}\right)}$$

and then Eq. (14) reads

$$\int_0^\infty d^3(q^{2\rho})\aleph(q^{2\rho})\left(\left(\frac{N}{4}-\beta_d\frac{Sin(\varphi-\eta)}{2}\right)\omega-\frac{4\mu\rho^2}{\varepsilon_r}\hat{q}^{2\rho-2}+4\mu\rho^2|q|(E\cdot\hat{q}^{2\rho})\hat{q}^{4\rho-2}-4\mu\rho^2E_n\hat{q}^{4\rho-2}\right)\aleph(q^{2\rho})=0 \quad (16)$$

We need to ensure that the interaction Hamiltonian has no quadratic terms related to the canonical variables. This condition gives rise to the normal ordering method in the symplectic space condition, which determines the frequency of the oscillator. By following this condition, the distortion potential includes the energy of the ground state or vacuum of the Hamiltonian, and we suppose $:\hat{q}^2:$ (:*:) is the symbol for the Wick ordering or normal ordering in the distortion potential equal zero. Then, we can express the total Hamiltonian in a representation that considers the primary quantum effects on the s ground state of bound particles. For this work, we can simply suppose the spherical coordinate $\Theta \approx 0$ and the external electric field $E \approx 0$ because we are trying to find two intertwined spaces transformation using the normal ordering method in the symplectic space, hence, we use simplified relations. Now using a series of mathematical transformations and applying the main quantum oscillating particles condition, i.e., the bound state exists at the minimum of oscillator frequency and energy eigenvalue. Therefore, $\frac{d\varepsilon_0(E_{n\ell})}{d\rho}=0$ and $\frac{d\varepsilon_0(E_{n\ell})}{d\omega}=0$. Using the first equation, we define parameter ρ as follows:

$$-\frac{1}{\rho}+\frac{1}{2\Gamma\left(\frac{N}{2}\right)}\frac{d}{d\rho}\int_0^\infty x^{\frac{N}{2}-1}e^{-x}dx+\frac{1}{2\Gamma\left(\frac{N}{2}+2\rho-1\right)}\frac{d}{d\rho}\int_0^\infty x^{\frac{N}{2}-2\rho-2}e^{-x}dx-\frac{1}{\Gamma\left(\frac{N}{2}+2\rho-1\right)}\frac{d}{d\rho}\int_0^\infty x^{\frac{N}{2}-\rho-2}e^{-x}dx=0 \quad (17)$$

and using $\frac{d\varepsilon_0(E_{n\ell})}{d\omega}=0$, we determine the quantum oscillator frequency (ω) of the bound state as outlined below:

$$\left[\frac{1}{4\mu\rho^2}\left(\frac{N}{4}-\frac{\beta_d Sin(\varphi-\eta)}{N}\right)\frac{1}{\Gamma\left(\frac{N}{2}+2\rho-1\right)}\int_0^\infty x^{\frac{N}{2}-1}e^{-x}dx\right]\frac{d}{d\omega}\omega^{2\rho}-\left[\frac{1}{4\varepsilon_r}\frac{1}{\Gamma\left(\frac{N}{2}+2\rho-1\right)}\int_0^\infty x^{\frac{N}{2}-\rho-2}e^{-x}dx\right]\frac{d}{d\omega}\omega^{2\rho}=0 \quad (18)$$

and then

$$\omega^{\rho}=\frac{2\mu\rho^2}{\varepsilon_r\left(\frac{N}{4}-\frac{\beta_d Sin(\varphi-\eta)}{N}\right)\Gamma\left(\frac{N}{2}\right)}\int_0^\infty x^{\frac{N}{2}-\rho-2}e^{-x}dx \quad (19)$$

The energy eigenvalue is defined by integrating the two equations $\varepsilon_0(E_{n\ell})=0$ and $\frac{d\varepsilon_0(E_{n\ell})}{d\omega}=0$, so the energy eigenvalue reads

$$E_{n\ell}(\rho,\omega,\mu)=\frac{\omega^{2\rho}}{4\mu\rho^2\Gamma\left(\frac{N}{2}+2\rho-1\right)}\left(\frac{N}{4}-\frac{\beta_d Sin(\varphi-\eta)}{N}\right)\int_0^\infty x^{\frac{N}{2}-1}e^{-x}dx-\frac{\omega^{\rho}}{4\varepsilon_r\Gamma\left(\frac{N}{2}+2\rho-1\right)}\int_0^\infty x^{\frac{N}{2}-\rho-2}e^{-x}dx \quad (20)$$

The thermodynamic properties of quantum and thermal LQS systems can be described and calculated via the partition function [15]. The partition function for n, ℓ states of the quantum oscillator system is $\mathbb{Z}(\lambda,\mu,T)=\sum e^{-\frac{1}{k_bT}E_{n\ell}(\rho,\omega,\mu)}$, where T is the temperature $k_b = 8.617\times10^{-5}$ (eVK^{-1}) is the Boltzmann thermodynamic constant, and $\beta = 1/(k_bT)$. We substitute the energy eigenvalue of LQS systems into the partition function relation and define:

$$\mathbb{Z}(\rho,\mu,T)=exp\left(\beta\frac{1}{2\varepsilon_r{}^2}\frac{\mu\rho^2}{\left(\frac{N}{4}-\frac{\beta_d Sin(\varphi-\eta)}{N}\right)}\frac{\Gamma^2\left(\frac{N}{2}+\rho-1\right)}{\Gamma\left(\frac{N}{2}+2\rho-1\right)\Gamma\left(\frac{N}{2}\right)}\right) \quad (21)$$

Hence, one can determine the mean energy value $U(\rho,\mu,T)=-\frac{d}{d\beta}ln\mathbb{Z}(\rho,\mu,T)$, and the temperature-dependent potential energy can be written as:

$$U(\rho,\mu,T)=k_bTln\left(1+e^{\frac{E_{n\ell}-E_F}{k_bT}}\right) \quad (22)$$

where $E_{n\ell}$ is the energy level of the exciton, and E_F is the Fermi energy of the system.

We used the theoretical parameters appropriate to the semiconductor type of GaAs/AlGaAs for calculating quantum and thermal properties. The effective mass of an electron and a light hole is $m_e^* = 0.067m_e$ and $m_h^* = 0.090m_e$, and $m_e = 0.5$ MeV is the free electron mass. $\varepsilon_r = 12.53\varepsilon_0$ and $\varepsilon_0 = 8.85\times10^{-12}$ F.m^{-1} is the vacuum permittivity. The effective mass of an electron depends on temperature and is defined by

$$m_e^*(T)\cong\frac{m_e}{1+7.51}\left(\frac{2}{E_g}\right),\quad E_g=1.519-\frac{5.4\cdot10^{-4}T^2}{T+204}.$$

Using the spherical-polar coordinate shown in Fig. 1, Fig. 2 presents the distortion potential for a fixed quantum disk with a radius of 50 nm, with some representative values β_d = 0, 0.1, 0.5, 0.7, 1, $\eta = 0$, and temperature T = 100 - 900 K.

The variation of quantum disc radius is given as zero, and the zero-pressure quantum disk radius is constant. As we know, the dependent azimuthal distortion parameters (φ) can affect the physical parameters of exciton-bound states in LQS [18]. This can influence the shape and symmetry of the confinement potential that binds electron-hole carriers in LQS and, consequently, the energy levels and binding energies of the binding states. The dependent azimuthal distortion parameters (φ) can induce distortion of the

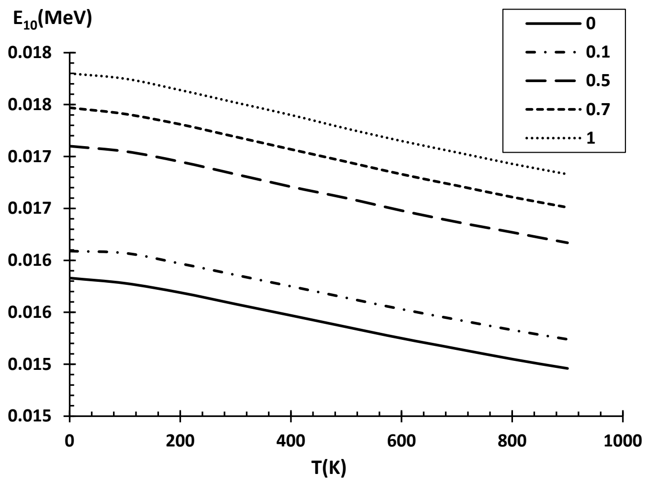


Fig. 2. The ground state energy E_{10} of the exciton for values β_d = 0, 0.1, 0.5, 0.7, 1, $\eta = 0$

confinement potential along certain directions, which can lead to energy level anisotropy and binding state energies. Theoretical calculation of bound state energy eigenvalue and binding energies can also provide information on the effects of distortion, such as photoluminescence spectroscopy . It can be used to measure the emission spectra of bonded states in LQS, providing information about energy levels and binding energies. By analyzing the emission spectra under different orientations, we can study the effect of distortion on energy levels. In general, the effect of distortion on the energy levels of bonding states in LQS depends on the specific properties of the system, such as the structure and the nature of the bonding states, and distortion can be an important factor to consider when designing and optimizing LQS devices based on exciton bound state properties in quantum disks [17,18].

The distortion effect is presented in Fig. 3. As we can see, the dependent azimuthal distortion parameters (φ) at (80°, 300°, and 190°) have extremely lower values than other degrees. Results of the quantum and thermal LQS characteristics were computed using MATLAB R2021a software and are presented in Figs. 2 and 3.

5. Conclusion

This article presents a theoretical approach for determining the energy levels of exciton in the GaAs/AlGaAs quantum disk with a distorted shape, based on transforming N-dimentional coordinate to the D-dimentional coordinate, depending on ρ and ℓ and the external distortion field. The focus was on the generation principles of the ground states and energy levels of the electron-hole bound states in quantum disks. The main cases discussed include the creation of excitons and the distortion effect on eigenenergy and potential energy values when changing the dependent azimuthal distortion parameter. The energy spectrum was determined and calculated for different strengths of the distortion and the dependent distortion potential at finite temperature for a fixed quantum disk with a radius of 50 nm, disk of constant size, taking into account the angular position of the distortion $\eta = 0$, the strength of the distortion β_d, the azimuthal distortion potential φ, and external static electric ($E \approx 0$) field in the consideration of non-central potential, which allows for the possibility of transition rules. The study found that distortion of the quantum disk will be minimal at the angles φ: 80°, 300°, and 190°. The presence of the distortion effect on the exciton bound state leads to extreme changes in eigenenergy value, which may prove useful in certain optoelectronic device design applications.

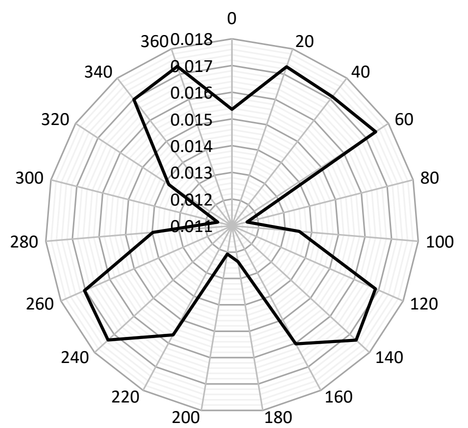


Fig. 3. The potential energy U_0 of exciton in the ground state against the dependent azimuthal distortion parameters (φ) at finite temperature $T = 500$ K.

Overall, the study highlights the importance of considering non-central potential and azimuthal distortion when studying the quantum, thermal, and optical properties of excitons in LQS and quantum disks and provides valuable insights into the behavior of these systems under external fields of varying strengths. In a distorted quantum disk, the thermal conductivity may be affected by various factors, such as the size and shape of the disk, the strength and nature of the distortion, and the temperature. The thermal conductivity of a distorted quantum disk is an important property that can affect its thermal behavior, such as how it dissipates heat or how it responds to environmental changes. The thermal conductivity of a distorted quantum disk can be affected by quantum interactions such as the quanta of lattice vibrations and create a scattering potential for phonons, which can lead to a reduction in the thermal conductivity in LQS. It can also be affected by the presence of impurities or defects in LQS, which can lead to additional scattering that can further reduce the thermal conductivity. Thermal conductivity is important in distorted quantum disks, and we should focus on these topics in future research.

Disclosure statement

No potential conflict of interest was reported by the authors.

References

[1] Shi, B., Qi, P., Jiang, M., Dai, Y., Lin, F., Zhanga, H., & Fang, Z. (2021). Exotic physical properties of 2D materials modulated by moiré superlattices. *Materials Advances*, *2*(17), 5542-5559. https://doi.org/10.1039/D1MA00263E

[2] Manikandan, A., Chen, Y.-Z., Shen, C.-C., Sher, C.-W. Kuo, H.-C., & Chueh, Y.-L. (2019). Critical review on two-dimensional quantum dots (2D QDs): From synthesis toward applications in energy and optoelectronics. *Progress in Quantum Electronics*, *68*, 100226.

https://doi.org/10.1016/j.pquantelec.2019.100226

[3] Singh, K. J., Ahmed, T., Gautam, P., Sadhu, A. S., Lien, D.-H., Chen, S.-C., Chueh, Y.-L. & Kuo, H.-C. (2021). Recent advances in two-dimensional quantum dots and their applications. *Nanomaterials*, *11*(6), 1549. https://doi.org/10.3390/nano11061549

[4] Garshasbia, S., Huangb, S., Valentac, J., & Santamouris, M. (2020). Can quantum dots help to mitigate urban overheating? An experimental and modeling study. *Solar Energy*, *206*, 308-316. https://doi.org/10.1016/j.solener.2020.06.010

[5] Brunetti, M. N., Berman, O. L., Kezerashvili, R. Y. (2019). Optical properties of anisotropic magnetoexcitons in phosphorene. *Physical Review B*, *100*(15), 155433. https://doi.org/10.1103/PhysRevB.100.155433

[6] Jahanshir, A. (2021). Quanto-relativistic background of strong electron-electron interactions in quantum dots under the magnetic field. *Journal of Optoelectronical Nanostructures*, *6*(3), 1-24. https://doi.org/10.30495/JOPN.2021. 28742.1231

[7] Efros, A. L., & Brus, L. E. (2021). Nanocrystal quantum dots: From discovery to modern development. *ACS Nano*, *15*(4), 6192-6210. https://doi.org/10.1021/acsnano.1c01399

[8] Masumoto, Y., & Takagahara, T. (2002). *Semiconductor quantum dots: Physics spectroscopy and applications* (1st ed.). Springer Berlin. https://doi.org/10.1007/978-3-662-05001-9

[9] Ghosh, D., Sarkar, K., Devi, P., Kim, K.-H., & Kumar, P. (2021). Current and future perspectives of carbon and graphene quantum dots: From synthesis to strategy for building optoelectronic and energy devices. *Renewable and Sustainable Energy Reviews*, *135*, 110391. https://doi.org/10.1016/j.rser.2020.110391

[10] Talwar, S. L., Lumb, S., & Prasad, V. (2022). Optical properties of hydrogenic impurity in a distorted quantum disk. *The European Physical Journal Plus*, *137*, 175. https://doi.org/10.1140/epjp/s13360-022-02393-4

[11] a. Gambhir, M., & Prasad, V. (2021). Dependence of nonlinear optical properties on electrostatic interaction in an excitonic parabolic quantum dot in a static magnetic field. *Journal of Modern Optics*, *68*(10), 542-554. https://doi.org/10.1080/09500340.2021.1927228

b. Chouef, S., Mommadi, O., Boussetta, R., Belamkadem, L., Hbibi, M., El Moussaouy, A., Vinasco, J. A., Duque, C. A., El Hadi, M., & Falyouni, F. (2022). Impact of applied temperature and hydrostatic pressure on the off-center donor spectrum in spherical quantum dot. *Solid State Phenomena, 335*, 31-41. https://doi.org/10.4028/p-6h7el8

[12] Johnson, B. R., (1980). On a connection between radial Schrodinger equations for different power-law potentials. *Journal of Mathematical Physics*, *21*, 2640-2647. https://doi.org/10.1063/1.524378

[13] De Guzman, J. A. T., Markevich, V. P., Coutinho, J., Abrosimov, N. V., Halsall, M. P., & Peaker, A. R. (2022). Electronic properties and sructure of boron–hydrogen complexes in crystalline silicon. *Solar RRL, 6*(5), 2100459. https://doi.org/10.1002/solr.202100459

[14] Dineykhan, M., Efimov, G. V., Ganbold, G., & Nedelko, S. N. (1995). *Oscillator representation in quantum physics* (1st ed.). Springer Berlin. https://doi.org/10.1007/978-3-540-49186-6

[15] Avery, J. S. (1989). *Spherical harmonics: Applications in quantum theory* (2nd ed.). Springer.

[16] Lumb, S., Talwar, S. L., & Prasad, V. (2022). Hydrogenic impurity in a distorted quantum disk: Effects of hydrostatic pressure and temperature on the optical properties. *The European Physical Journal Plus*, *137*, 672. https://doi.org/10.1140/epjp/s13360-022-02882-6

[17] Gerlach, B., Wüsthoff, J., Dzero, M. O., & Smondyrev, M. A. (1998). Exciton binding energy in a quantum well, *Physical Review B*, *58*(16), 10568-10577. https://doi.org/10.1103/PhysRevB.58.10568

[18] Vurgaftman, I., Meyer, J. R., Ram-Mohan, L. R. (2001). Band parameters for III–V compound semiconductors and their alloys. *Journal of Applied Physics*, *89*(11), 5815-5875. https://doi.org/10.1063/1.1368156

Additional information

Correspondence and requests for materials should be addressed to A. Jahanshir.

HOW TO CITE THIS ARTICLE

Jahanshir, A. (2023). Theoretical study of quantum and thermal properties of particles' bound state in quantum disks. *J. Part. Sci. Technol. 9(1) 19-27.*

DOI: 10.22104/JPST.2023.6288.1228
URL: https://jpst.irost.ir/article_1288.html