Thomas-Fermi Approach to the Ground State of a Morse-Confined Quantum Dot with Interacting Electrons

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Abstract

In this study, a quantum dot (QD) system with many interacting electrons confined in a Morse potential is analyzed. The ground state properties, including electron density, chemical potential, kinetic energy, and Hartree energy, are examined using the Thomas-Fermi (TF) model. The novelty of this study lies in employing the Morse potential to explore the effects of confinement on quantum dots, which has not been extensively studied compared to harmonic or quartic potentials. Using the Thomas-Fermi (TF) model, the electron density for the two-dimensional electron gas interacting with the Morse potential at low temperatures is derived and solved numerically. The results demonstrate that the depth and curvature of the Morse potential significantly alter the electron interactions and overall system properties. These findings provide insights into the tunability of QD properties for potential applications in optoelectronics and nanotechnology.

Key words: Quantum Dot, Interacting Electrons, Morse Potential, Electron Density, Ground State Properties, Confinement Potential, Thomas-Fermi

Introduction

Quantum dots (QDs) are low-dimensional semiconductor nanoparticles that confine electrons in three spatial dimensions. Their size-dependent optical and electronic properties, driven by quantum confinement effects, make them highly versatile for various applications [1-5]. Quantum confinement is a phenomenon in quantum mechanics where the dimensions of a system are reduced to a scale small enough to restrict the motion of charge carriers, such as electrons or holes, to a region smaller than their wavelength. This confinement affects the system's electronic density of states, causes energy levels to split, and leads to significant changes in the system's electronic and optical properties, enabling QDs to be treated as artificial atoms. QDs have discrete quantized energy levels rather than a continuous range of energy

levels, as seen in bulk materials. Additionally, their band gaps can be controlled by adjusting their size.

The size-dependent optical, electronic, and structural properties of QDs make them highly attractive for applications (Figure 1) in photovoltaics [6-10], biological imaging [11-13], biomedical applications [14-18], and semiconductor lasers [19]. The expanding scope of QD applications now includes healthcare facilities [20,21], pathology laboratories, artificial intelligence (AI) [22], and quantum computing [23,24]. Different types of QDs are used based on their application areas and physical properties [25-31].

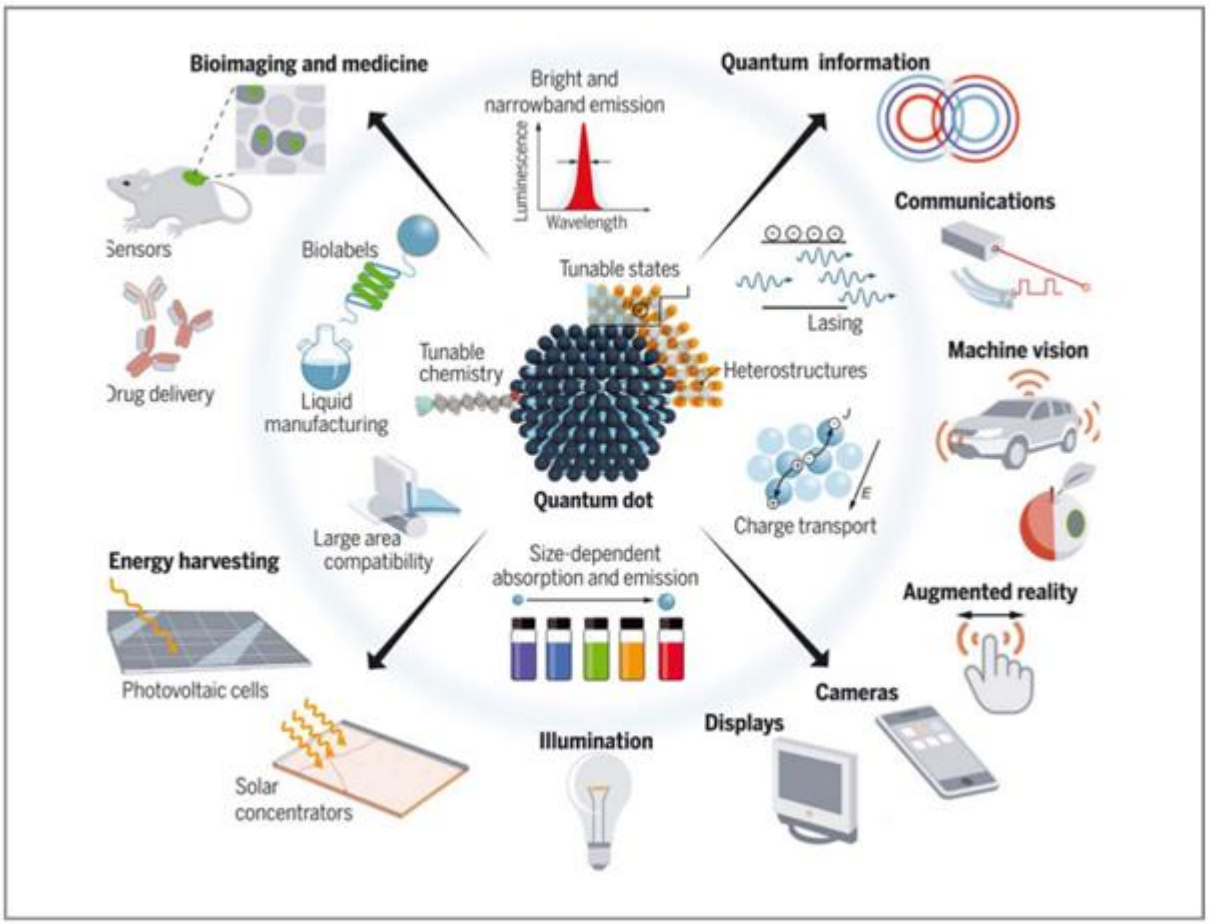

Figure 1. Applications of QDs [25].

QDs can be produced using various methods such as lithography [32-35], epitaxial growth [36,37], and colloidal synthesis [38,39]. The number of confined electrons varies depending on the QD size. As a result, studying their physical properties with classical methods becomes

increasingly difficult. The Thomas-Fermi (TF) model is a statistical method that directly relates the particle density of atoms and molecules to the electrostatic potential [40-44]. Despite its simplicity, it has been highly successful in predicting the key properties of multiparticle systems. The method and its modified versions have been applied to atoms, ions, nanocrystals, and nanostructures [45].

The shape of the confinement potential significantly influences the physical properties of QDs [46]. This is particularly evident in anisotropic confinement potentials, which allow tuning of electronic properties. While harmonic and quartic potentials have been extensively studied [47], the Morse potential provides a unique framework due to its flexibility in modeling anharmonic systems Non-parabolic confinement effects in two-dimensional quantum dots further highlight the advantages of Morse over harmonic models. Unlike harmonic potentials, the Morse potential excels by capturing anharmonic effects with decreasing energy level spacings at higher levels, offering a realistic model for electron-phonon interactions and optical properties in quantum dots (QDs). Its adjustable parameters allow flexible modeling of shallow and steep confinements, enabling simulation of diverse shapes and phenomena like tunneling that harmonic models overlook. By incorporating finite depth and dissociation, it accurately represents bond breaking and electron escape in high-energy scenarios, crucial for nanostructure deformation studies. The Morse potential better fits experimental spectroscopic data, enhancing predictions for energy spectra under magnetic fields and improving absorption/emission calculations in QDs. In nanostructures, it outperforms harmonic assumptions by modeling binding energies, thermodynamic behaviors, and surface modifications under electric fields, though its complexity arises from additional parameters.

However, studies investigating the ground state properties of QDs confined in Morse potentials remain scarce.

In literature surveys, there are far fewer articles compared to harmonic or parabolic potentials; the existing ones generally focus on optical properties, exciton states, or bound state energies, and comprehensive research directly targeting ground state properties remains limited [48,49]. Theoretical studies on optical properties with different confinement potentials underscore the need for Morse-based models. Direct studies on electronic and optical properties under Morse confinement confirm its novelty. Thermodynamic properties under Morse potential further illustrate these effects.

This study, therefore, addresses the identified research gap by employing the Thomas-Fermi (TF) model to systematically investigate the ground-state properties of a quantum dot (QD) confined by a Morse potential. A key component of our investigation is a comparative analysis with non-interacting systems, which serves to isolate and clarify the specific effects of electron-electron interactions. Furthermore, we elucidate how varying the strength of the confinement potential influences critical properties, including the electron density distribution and the total ground-state energy. For consistency and simplicity in our calculations, all presented results utilize atomic units, where $m_e = \hbar = e = 1$.

Theoretical Approach

The ground state properties of an interacting electron gas confined in a Morse potential were investigated using the TF model. The electron density in the two-dimensional system was expressed as [50-53]:

$$n(r) = \frac{1}{h^2} \int_0^\infty \frac{4\pi p dp}{c^{-1} e^{((p^2/2m)+V_0(r)+v(r))/kT}+1} \tag{2.1}$$

Here, h is the Planck constant, $c = e^{\frac{\mu}{kT}}$ is fugacity function, μ is the chemical potential, p is momentum, k is the Boltzmann constant, T is the temperature, $V_0(r)$ is Coulomb potential, $v(r)$ is the confining potential. Eq. (2.1) can be rewritten as follows using $f_n(y')$ Fermi-Dirac integrals [54-56]

$$n(r) = \frac{mkT}{\hbar^2\pi} f_1(y') = \frac{mkT}{\hbar^2\pi} ln(1+y') \tag{2.2}$$

where, $y' = e^{(\mu - v(r) - V_0(r))/kT}$. At low temperatures ($T \sim 0\ K$), Eq. (2.2) for the confined system is reduced to the following form by the Sommerfeld model [57,58]:

$$n(r) = \frac{m}{\hbar^2\pi}\big(\mu - v(r) - V_0(r)\big) \tag{2.3}$$

For the system confined in a two-dimensional space, the total number of electrons can be clearly written in terms of density of electrons as

$$N = \int_O^{r_o} n(r) 2\pi r dr \tag{2.4}$$

To determine the ground state properties of the interacting confined system, equation (2.3) can be formulated in relation to the Poisson equation,

$$\nabla^2 V_0(r) = -\frac{2\pi}{\varepsilon} n(r) \tag{2.5}$$

and the TF equation can be obtained for the electrons interacting in a two-dimensional quantum dot system as:

$$\nabla^2 \mathrm{V}(r) = -\frac{2m}{\hbar^2 \varepsilon} (\mu - v(r) - V_0(r)) \tag{2.6}$$

where $\nabla^2 = (1 / r)\ (\partial / \partial r)\ r\ (\partial / \partial r)$ and ε are the dielectric constant of the material. It is evident that due to the confinement the electron density will approach zero at the boundaries. Therefore, it can be taken as zero at the radius r_0 of the confined region ($n(r_0) = 0$). Furthermore, the electron-electron interaction potential will be assumed to be zero at this point ($\mathrm{V}_0(r_0) = 0$).

The ground state properties of a non-interacting system, boundary conditions are connected to equation (2.3), and for a constant number of particles, they can be directly determined using the positive root of the (r) function.

$$\mu = v(r_0) \tag{2.7}$$

$$f(r_0) = N - \int_O^{r_o} n(r) 2\pi r dr = 0 \tag{2.8}$$

In the framework of the TF approach, the total energy (E_T) can be expressed in terms of density values;

$$E_T = \int_O^{r_o} \tau(r) 2\pi r dr + \int_0^{r_o} n(r) v(r) 2\pi r dr + \frac{1}{2\varepsilon} \int_0^{r_o} n(r) V_0(r) 2\pi r dr \tag{2.9}$$

Here, the kinetic energy density can be written as $\tau(r) = \frac{\pi\hbar^2}{2m} n(r)^2$. Here, the first term is the kinetic energy (E_K), the second term is the confining potential energy ($E_U(r)$), and the third term is the Hartree energy (E_H) [59,60]. Reviews on kinetic energy density functionals for non-homogeneous systems provide deeper insights into TF approximations [61,62].

Results and Discussions

Using the TF model, QD structures containing N electrons confined to $v(r) = V_0(1 - e^{-br})^2$ in Morse potential were investigated. By taking $V_0 = 5, b = 0.5$; $V_0 = 7, b = 0.5$ and $V_0 = 7$, $b = 1.0$, the effect of the confinement potential on the electrical properties of the system (such as electron density $n(r)$, μ chemical potential, total energy E_T) was investigated for three different potentials. In all calculations, atomic units (such as m_e=1, $\hbar = 1$,…) were used. Electron density $(m\omega^2\varepsilon_0)/\pi$, radial distance $(\varepsilon_0 m)^{\frac{1}{2}}$ and number of total particles are given as $N = \Omega\varepsilon_0^2\,\omega^2$. All calculations are performed for the case of $(\Omega = 0.05)$.

In figure 2, the variation of the confinement potential $(v(r) = V_0(1 - e^{-br})^2)$ depending on the potential coefficients V_0 and b is examined for three different cases. At $V_0 = 5$, $b = 0.5$, the potential is more diffuse. When the coefficient of b is increased by keeping V_0 constant ($V_0 =$, $b = 0.5$ and $b = 1.0$), the confinement shape narrows to push the particles towards the center. Here, if the coefficient of b is kept constant and V_0 is enlarged further ($V_0 = 5$ and $V_0 = 7, b = 1.0$), the effect of the confinement potential to gather the particles towards the center increases further, and it becomes more effective in determining the electrical properties of the confined electron gas.

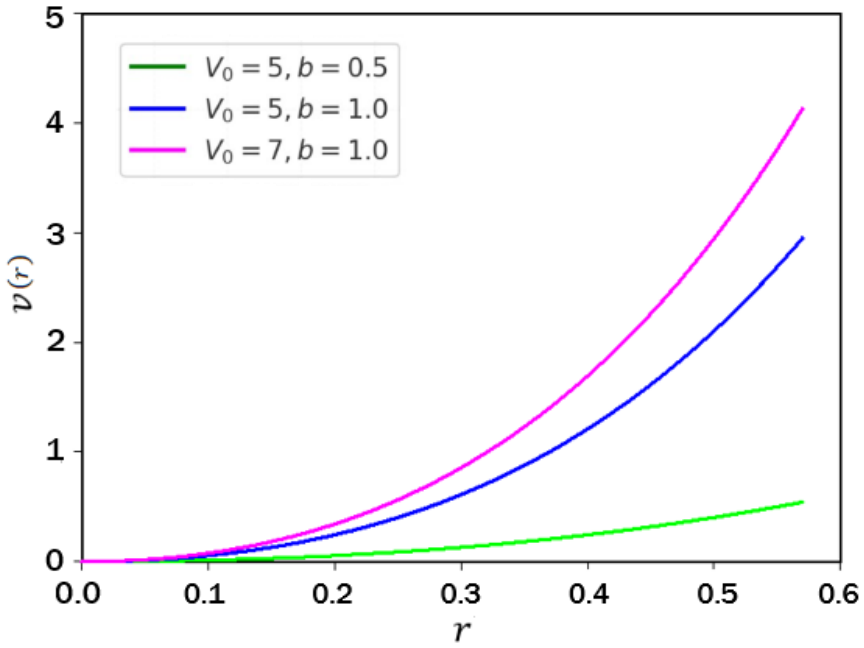

Figure 2. The variation of the confining potential as a function of radial distance for three different cases.

In figure 3, the numerical and analytical results obtained when the potential coefficients are taken as $V_0 = 5, b = 0.5$ for the system where particle interaction is ignored ($V_e = 0$) are compared.

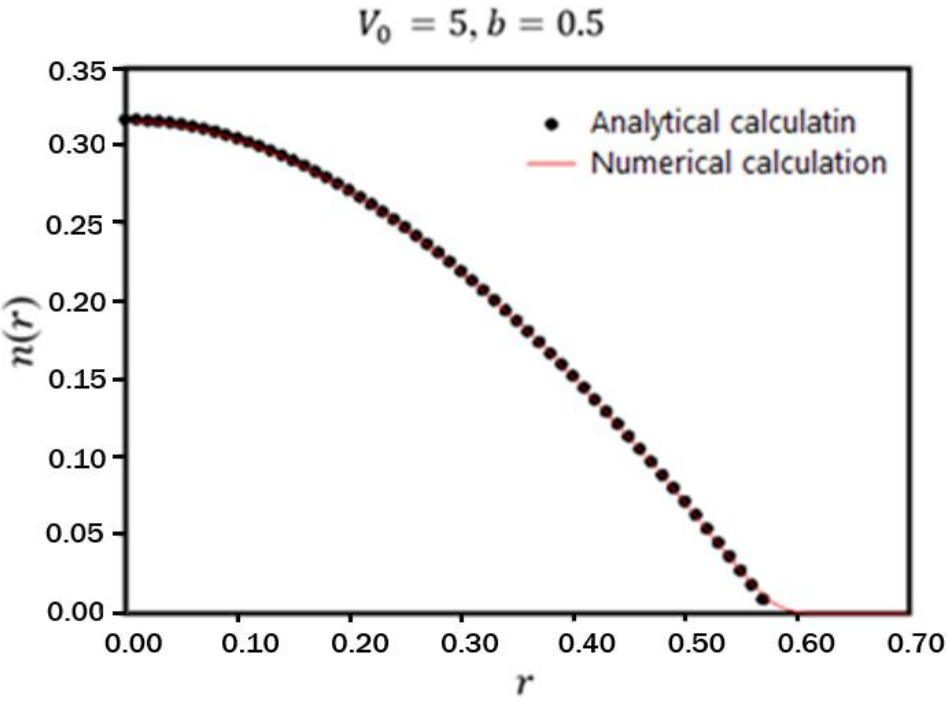

Figure 3. The variation of electron density with dot radius for $V_0 = 5, b = 0.5$.

The line shows numerical results, and dots show analytical results. According to this, it can be concluded that the numerical and analytical results are compatible, and the applied numerical procedure is quite effective in determining the physical properties of the electron gas confined in the dot structure.

In figure 4 and 5, the effect of the confinement parameters (V_0 and b) on the Coulomb interaction of the electron gas and the determination of the physical parameters such as density ($n(r)$) and dot radius were investigated in detail. As can be easily seen from figure 3, for all confinement parameters (a-c), the center electron density ($n(0)$) of the interacting (dotted line) systems is lower than that of the non-interacting (solid line) system. However, for all cases (a-c) electron densities decrease with radial distance. Accordingly, as the central electron density

decreases, the radial distance increases so that the total number of particles remains constant. As expected, the dot radius of the interacting system is larger than the dot radius of the non-interacting system, as the Coulomb interaction propagates the electrons within the confined system.

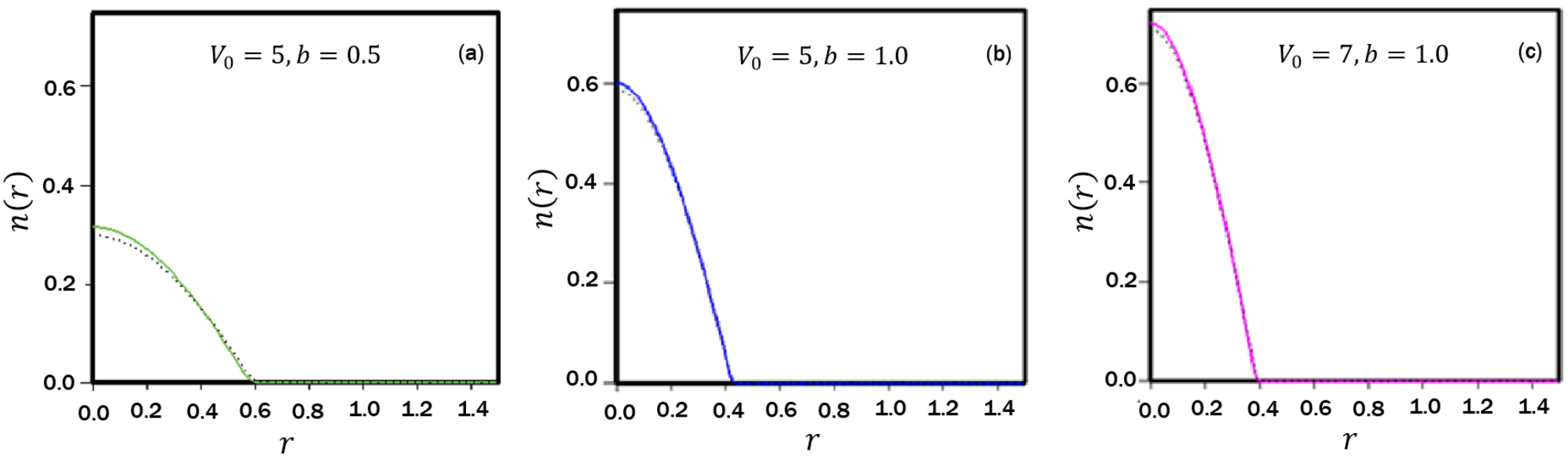

Figure 4. Determination of the effect of interaction on density for electrons at different confinement potentials ($\Omega = 0.05$). The line is given for the case where the interaction is ignored, and the dotted line is for the case where the Coulomb interaction is considered.

In figure 3a and 3b, when the b coefficient is increased ($V_0 = 5$, $b = 0.5$ and $b = 1$) by keeping the V_0 value constant, the central electron densities of the interacting and non-interacting systems increase, and the dot radius decreases. However, as in figure 3b and 3c, if the value of V_0 is increased, and the number of b coefficients is kept constant ($V_0 = 5$, $V_0 = 7$, $b = 1$), the center electron density increases even more and the dot radius decreases in parallel. Increasing the confinement coefficients reduces the difference between the distributions of interacting and non-interacting systems within the dot. For the case $V_0 = 7$, $b = 1.0$, the difference between the dot radii of the interacting and non-interacting systems and their distribution in the potential is quite small compared to the other two cases. Nonetheless, the center density gets its highest value (and therefore the lowest value of the dot radius) in the case of $V_0 = 7$, $b = 1.0$ for both the interacting and non-interacting systems (Figure 4 a,b).

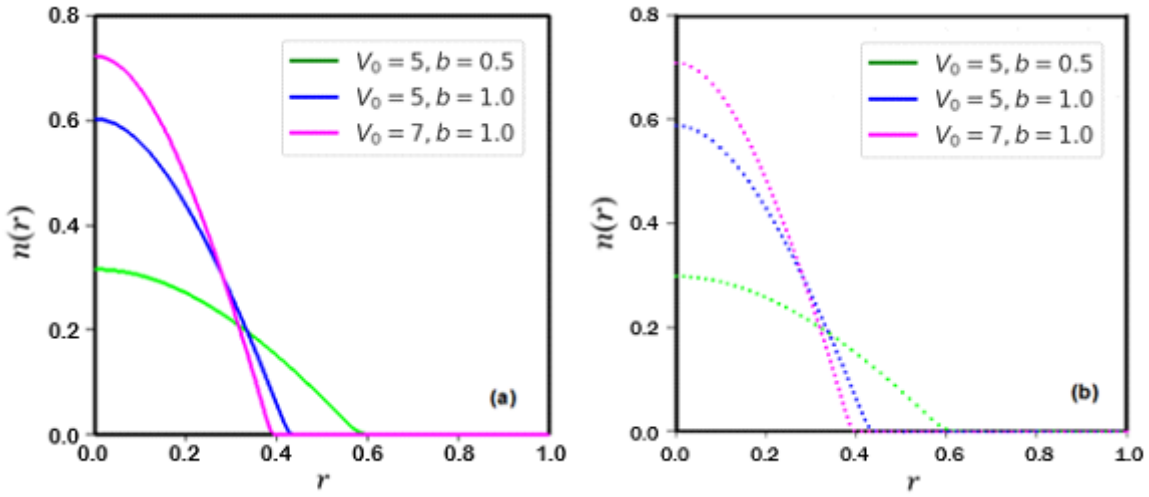

Figure 5. Determination of the effects of confinement parameters (a) non-interacting (b) interacting systems on electron distribution ($\Omega = 0.05$). The line is given for the case where the interaction is ignored, and the dotted line is for the Coulomb interaction.

Change in chemical potential (μ), kinetic energy (E_K), Hartree energy (E_H), confinement potential energy $E_{v(r)}$, and total energy (E_T) values of interacting and non-interacting systems depending on different limitation parameters ($\Omega = 0.05$) is calculated with equation (2.9) and is given in table 1. From the calculations, it can be said that as the confinement potential strength increases, μ, E_K, $E_{U(r)}$, E_T values increase for both cases. However, for a constant confinement potential, it can be seen that the, $E_{U(r)}$ and E_T of the interacting system are larger compared to

that of the non-interacting system. The interaction significantly changes the value of μ. However, due to the Coulomb interaction, the Hartree energy contributes E_H to the total energy. When all cases are compared, the total energy is highest for the interacting system at $V_0 = 7, b = 1.0$.

Table 1. Change in chemical, kinetic, Hartree, confinement and total energies of systems depending on different confinement parameters ($\Omega = 0.05$).

V_0	b	Chemical Potential μ	Kinetic Energy E_K	Hartree Energy E_H	Confinement Pot. Energy $E_{U(r)}$	Total Energy E_T
Non-Interacting System						
5	0.5	0.3157	0.0050	0.0000	0.0056	0.0107
	1.0	0.6018	0.0095	0.0000	0.0110	0.0205
7	1.0	0.7221	0.0114	0.0000	0.0131	0.0246
Interacting System						
5	0.5	0,3373	0,0047	0,0013	0,0059	0,0120
	1.0	0,6302	0,0092	0,0017	0,0110	0,0220
7	1.0	0.7520	0.0111	0.0018	0.0131	0.0260

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