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Effect of a Finite Number of Electrons on the Physical Properties of Two Dimensional Parabolic Quantum Dot

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Abstract

The effect of number of particles on the physical properties of a two dimensional parabolic quantum dot system is investigated numerically at finite temperature. The Thomas-Fermi equation is solved self consistently with Poisson equation. The changes induced by electron-electron interaction are also analyzed. It is shown that the numerical procedure that is applied to solve the problem is very efficient at all temperatures.

1. Introduction

In recent years, advances in nanotechnology allow manufacturing quantum dot structures in which a finite number of electrons are confined in a finite area by applying various voltages. Especially, their optical and magnetic properties are well-investigated [1–4]. Quantum dots are commonly fabricated by various techniques such as etching or modulation of electric field [5, 6]. Several interesting effects such as electron-electron interaction, quantum confinement on the determination of physical properties of quantum dot structure have been studied both experimentally and theoretically [7–14]. The number of confined electrons also has strong effect on the determination of electronic structure of such systems. When the number of confined electrons is large enough, it is appropriate to treat the system in statistical sense.

Thomas-Fermi method is a semi-classical method to describe the electrostatic potential and the electron distribution of the system. In this model, electrons are considered to form an ideal gas obeying Fermi-Dirac statistics. The method, since first proposed by Fermi [15] and Dirac [16] has been applied to many areas, particularly in atomic systems, condensed matter and molecular systems [17–22]. It has also some applications in nano-structures [23–32]

We have previously discussed the physical properties like chemical potential, electron density of two dimensional parabolic quantum dot at T=0 K and finite temperature [31, 32]. In this work, we will also consider the effect of a finite number of particles on the determination these properties at finite temperature. In section II, we solve numerically the Thomas-Fermi equation in conjuction with Poisson equation for the system at finite temperature. In section III, we present the reliability of the numerical procedure by comparing our results with analytical limits given for T=0 K in the literature and expand our discussion for non-interacting system. We discuss the effect of number of electrons on determination of the physical properties both for non-interacting and interacting systems.

2. Theory

The number density of electrons described the Fermi-Dirac statistics in n-dimensional space is given as [33],

$$n\,(r) = \int_0^\infty \frac{2j\,\left(\frac{C_j}{\hbar^j}\right) p^{j-1} dp}{e^{\left(\frac{p^2}{2m^*}+V(r)-\mu\right)/\,kT}+1} \quad , \tag{1}$$

where, $C_j R^j$is the volume of a j dimensional sphere of radius R and $C_j = \frac{\pi^{j\,/2}}{\Gamma(\frac{j}{2}+1)}$, m^* is the effective mass of electrons, μ is the chemical potential, k is the Boltzmann constant. For a system composed of interacting many electrons confined in a two dimensional quantum dot Eq. (1) can be written as,

$$n_e(r) = \frac{m^* kT}{\hbar^2 \pi} \int \frac{dx}{e^{x-\eta}+1} \quad . \tag{2}$$

Here, $x = \frac{p^2}{2m^* kT}$, $\eta = \frac{\mu - \upsilon\,(r) - V_e(r)}{kT}$, $\upsilon(r)$ is the confining potential and $V_e(r)$ is the electrostatic potential. Using the Fermi integration [34],

$$f_l(z) = \quad \frac{1}{\Gamma(l)} \int \frac{x^{l-1} dx}{z^{-1} e^x + 1} \quad , \tag{3}$$

Eq. (2) may be expressed as,

$$n_e(r) = \quad \frac{m^* kT}{\hbar^2 \pi} F_0(\eta)\,. \tag{4}$$

Case $l = 0$ has the simple solution $F_0(\eta) = ln\,(\,1 + e^\eta\,)$ so Eq. (4) becomes,

$$n_e(r) = \frac{m^* kT}{\hbar^2 \pi} ln\,(\,1 + e^\eta\,)\,, \tag{5}$$

and

$$N = \int_0^{r_0} 2\pi\, r n_e(r)\, dr = \frac{2\,m^* kT}{\hbar^2 \pi} \int_0^{r_0} r ln\,(\,1 + e^\eta\,) dr \tag{6}$$

where, r_0 is the radius of the dot. Then two dimensional Poisson equation leads to the Thomas-Fermi equation

$$\nabla^2 V_e \quad = \quad -\frac{2\,\pi}{\varepsilon} \frac{m^* kT}{\hbar^2 \pi} ln\,(\,1 + e^\eta\,), \tag{7}$$

where ε is the dielectric constant of the material. Eq.(7) reduces to

$$\nabla^2 V_e \quad = \quad -\frac{2\,\pi}{\varepsilon} \frac{m^* kT}{\hbar^2 \pi} \eta, \tag{8}$$

for $T \approx 0K$. It is really hard to solve Eq. (7) analytically for $T \neq 0K$, when the confining potential is of the parabolic form (i.e., $\upsilon\,(r) = \frac{1}{2}\, m^* \omega^2\, r^2$, where ω is the strength parameter of the potential). Therefore, we apply the numerical methods by which convergence to a self consistent solution is achieved. We keep N= const. and take the dot radius as the point at which the density vanishes. Eq.(6) is used to determine the chemical potential of the system. We first determine V_e by using Eq. (7) starting form the initial guess for chemical potential. Then, we update chemical potential in Eq. (6) by using temporarily determined V_e. This procedure is repeated until the difference between the chemical potentials is smaller than a predetermined tolerance value. We repeat our steps for T=0 K and compare our results in Figure 1 with the ones that is given analytically for electron density in Ref. [23] as a check on accuracy of our solution.

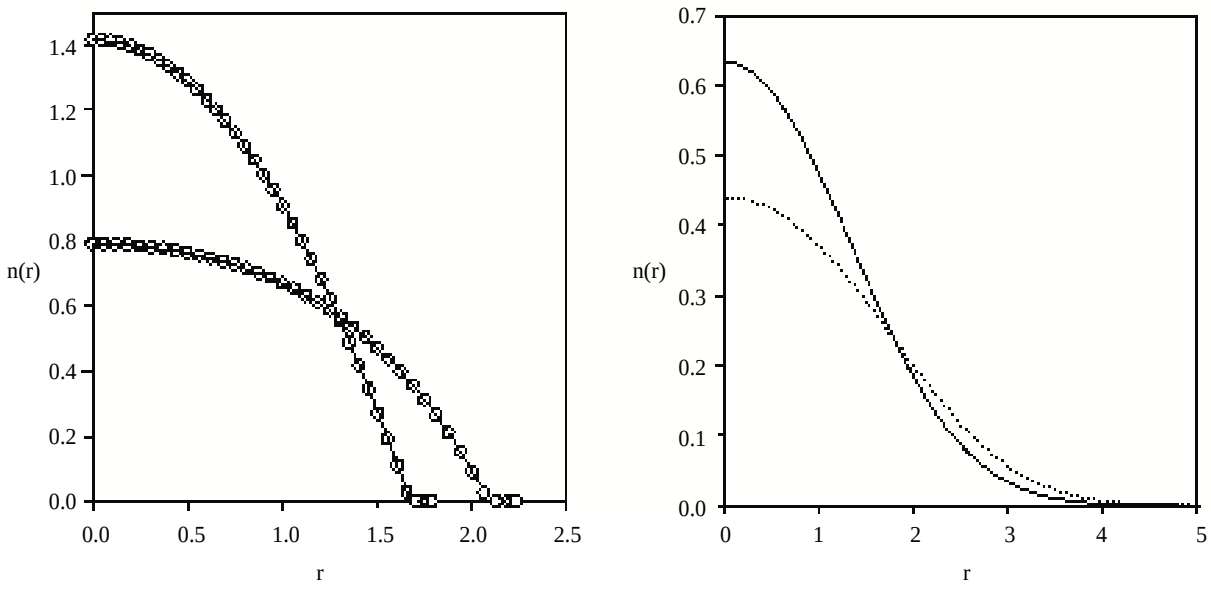


Figure 1. (a)The variation of electron density in the radial direction for $\Omega = 2$ and $\frac{T}{T_F} = 0.01$. Circles correspond to analytical results and solid lines show the analytical results for non-interacting and interacting cases. (b)The variation of electron density with respect to dot radius r for $\Omega = 2$ and $\frac{T}{T_F} = 1.0$. Dotted line and solid lines correspond to interacting and non-interacting cases respectively.

3. Results and Discussion

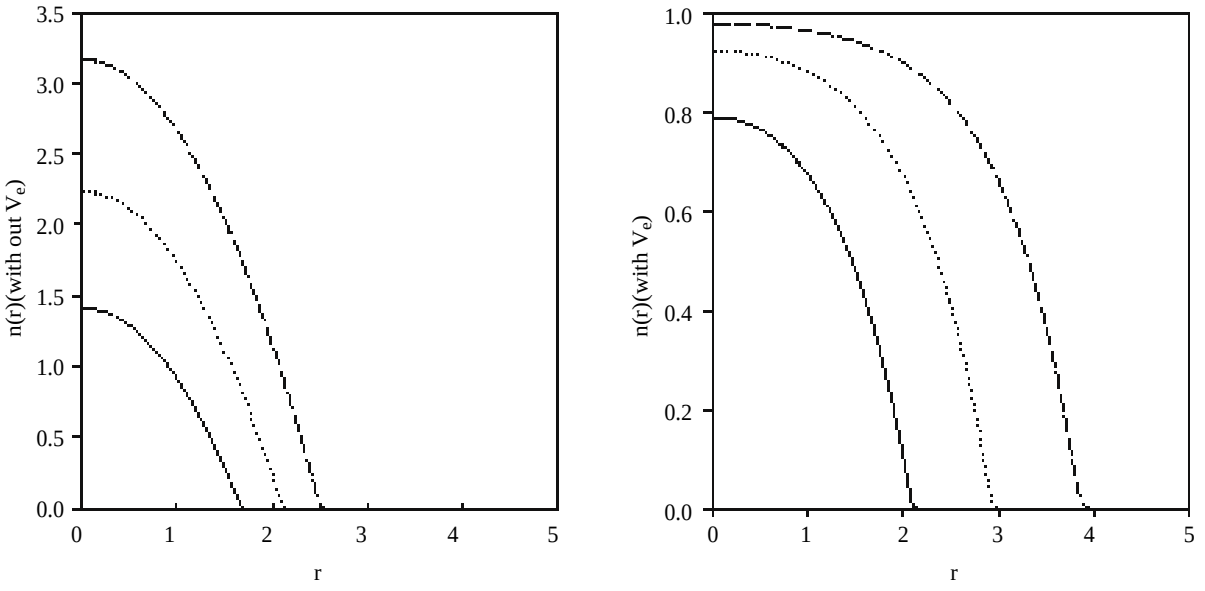
In this paper, all the chemical potentials and temperatures are given in terms of the Fermi energy and Fermi temperature of a dot containing N non-interacting electrons. Also density has been measured in units of $\frac{m^*\omega^2\varepsilon}{\pi}$, r in units of $\left(\frac{\varepsilon}{m^*}\right)^{1/2}$and we give the number of particles in terms of a parameter Ω, defined as $\Omega = \left(\frac{N}{\varepsilon^2\omega^2}\right)$.

In Figure 1, the variation of the electron density with the radial distance is shown for very low (a) and high (b) temperatures for both interacting and non-interacting system. In Figure 1(a) we compare our numerical results for very low temperatures with exact solution for zero temperature [23], where the circles and lines represent the numerical results and analytical results, respectively. The results obtained by the numerical method is found very close to exact values for T=0 K. Increasing the temperature results in spreading of electrons in the dot. The results for high temperatures are presented in Figure 1(b), the curves represent the expected behavior for both interacting and non-interacting systems.

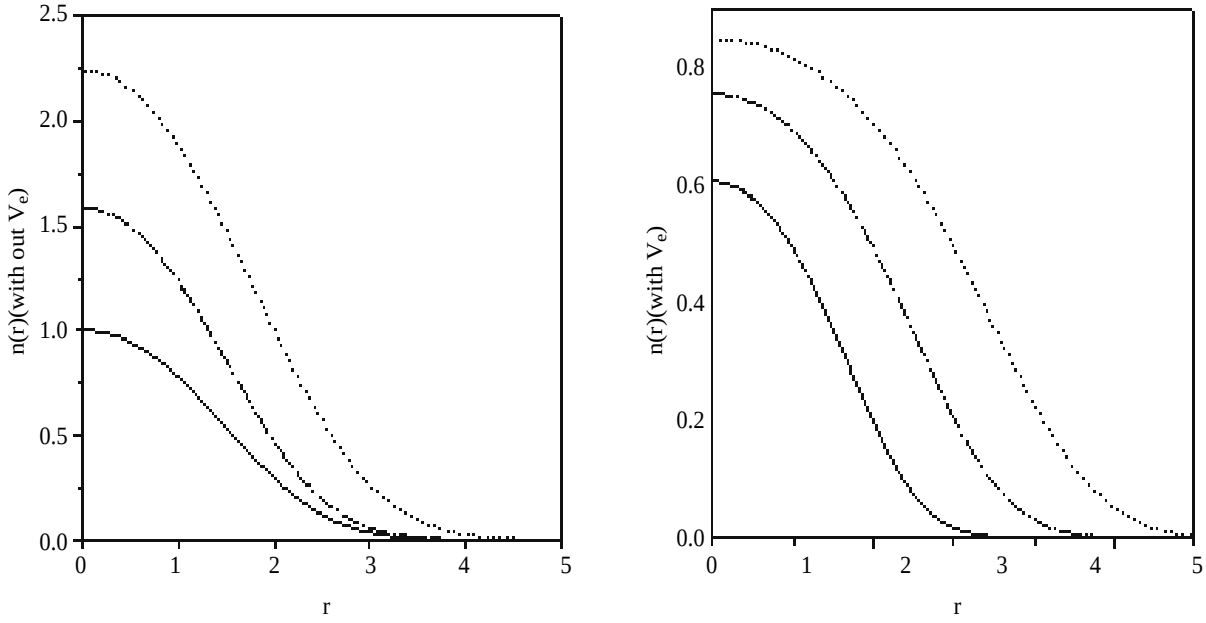
In Figure 2, we analyze the effect of number of particles on density profile at low ($T/T_F = 0.01$) and intermediate temperatures ($T/T_F = 0.5$) for interacting and non-interacting systems. At low temperatures, the central density is proportional to $\sqrt{N}$ of non-interacting system, whereas the central density of interacting system increases monotonically for interacting system and converges to 1 (in our units) as $N \to \infty$. As temperature increases, electrons of the interacting system will be affected not only by the repulsion of electrons but also by thermal effects. From the figure, one can say that the effect of electron-electron interactions is more pronounced at lower temperatures and higher number of particles.

In Figure 3, we investigate the dependence of chemical potential to the number of particles both for non-interacting and interacting systems at three different temperatures ($T/T_F = 0.01$, $T/T_F = 0.5$, $T/T_F = 1.0$). The chemical potentials of the systems are increasing with the increasing number of particles. The temperature has a more significant effect on the chemical potentials of both systems containing small number of particles as compared with high number of particles. If we compare the chemical potentials of both systems, the effect of temperature is more apparent for large non-interacting system with a high number of particles.

The results that are obtained in this report might be used to calculate the other properties like total energy and differential capacitance. We hope that such calculations are particularly useful in model quantum



(a) $\frac{T}{T_F} = 0.01$



(b) $\frac{T}{T_F} = 0.5$

Figure 2. Density profiles of the systems containing different number of (Ω = 2, 5, 10) non-interacting and interacting electrons with radial distance at (a) $\frac{T}{T_F} = 0.01$(b) $\frac{T}{T_F} = 0.5$.

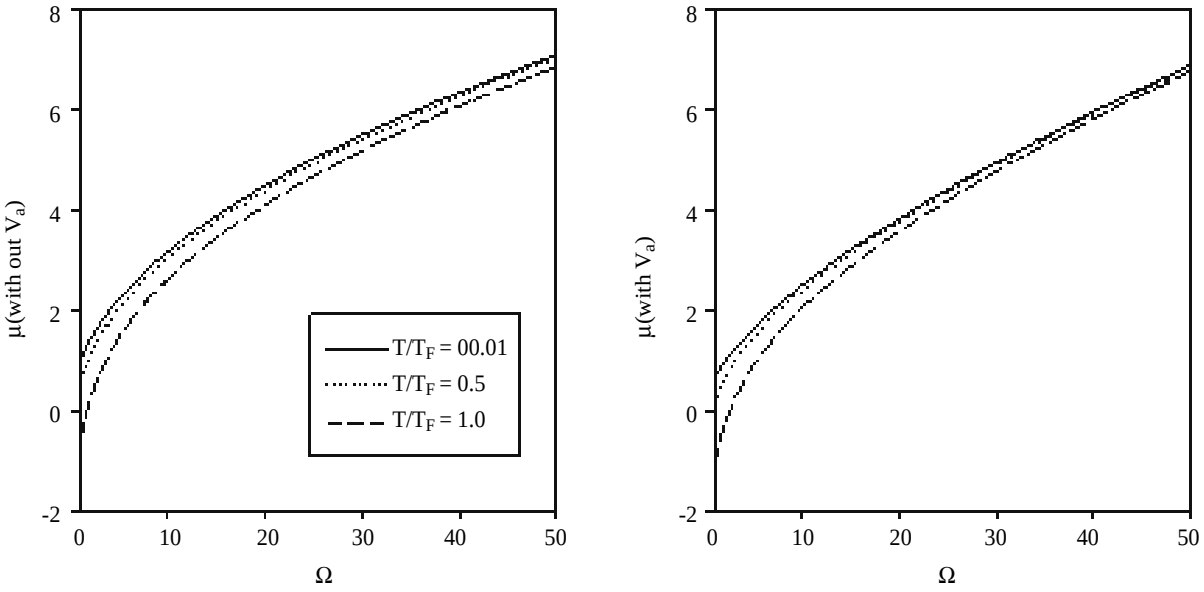


Figure 3. The curves of chemical potential versus Ω for non-interacting and interacting number of electrons at $\frac{T}{T_F} = 0.01, 0.5, 1.0$.

dot systems where one might plan experiments controlling the number of particles.

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