Contents lists available at ScienceDirect

## **Chemical Physics**

journal homepage: www.elsevier.com/locate/chemphys

# The ground state properties of two dimensional Fermi gas system confined in a potential composed of harmonic and a Gaussian terms



CHEMICAL

### Berna Gülveren<sup>a,\*</sup>, Mehmet Şahin<sup>b</sup>, Ülfet Atav<sup>a</sup>

<sup>a</sup> Selçuk University, Faculty of Science, Physics Dept., Campus 42130, Konya, Turkey

<sup>b</sup> Abdullah Gul University, Material Science and Nanotechnology Eng., Sumer Campus, Kocasinan, 38080 Kayseri, Turkey

ARTICLE INFO	A B S T R A C T
Keywords: Fermi gas Thomas-Fermi approximation Gaussian potential Harmonic potential	In this work, the ground state properties of two dimensional Fermi gas system interacting in a potential con- sisting of harmonic and Gaussian terms are investigated in the frame of Thomas-Fermi approximation. The depth and the curvature of the potential are changed by varying confinement parameters and the influence of the constraining conditions on the system properties like the density profile, the kinetic and the potential energy of the fermionic system is analyzed comprehensively. The deviations of the results due to the Gaussian potential are also determined by comparing the results with those obtained for pure harmonic potential. Calculations are also performed analytically for non-interacting case for comparative purposes. The results show that the confinement parameters play crucial role on the ground state properties of confined system.

#### 1. Introduction

Since the remarkable experiments beginning with the observation of Bose-Einstein condensation [1–2] and soon after followed by the realization of the degenerate Fermi gas of <sup>40</sup>K [3], there have been great interest to investigate the characteristics of both confined Fermi and Bose systems at low temperatures.

Fermions can be experimentally trapped in a two dimensional (2D) space by optical lattice [4,5] and the physics of these systems is very significant for many aspects. For example, constraining a Fermi gas in the boundary conditions of 2D space reveals some exiting many body effects as compared to three dimensional counterparts [6]. Some photoemission-type experiments on atomic two dimensional Fermi gas [4,5] has shown some remarkable changes attributed to stronger pairing fluctuations due to the reduction of dimensions. Watanabe et al. [6] investigated the physical properties like local density of states of a two dimensional Fermi gas can be formed within the interface region of hetero-structures and establish a basis for future device applications [7–9].

The shape of a trap influences the behaviour of the confined gas, noticeably. In the past, the physical properties such as density and momentum distribution of two dimensional gas trapped in a perfect harmonic potential have been investigated extensively by many authors [10–15]. However, recent developments in laboratory techniques have

\* Corresponding author. *E-mail address:* berna@selcuk.edu.tr (B. Gülveren).

https://doi.org/10.1016/j.chemphys.2018.09.035 Received 7 July 2018; Accepted 24 September 2018 Available online 27 September 2018 0301-0104/ © 2018 Elsevier B.V. All rights reserved. allowed experimentalist to form a confinement in various shapes which provide an opportunity to analyze some unusual effects due to the change in the spatial constraining [16–22]. For example, Hueck et al. [16] have carried out an experiment trapping two dimensional Fermi gas in a box potential and observe the Pauli blocking in the momentum space for attractive interacting Fermi systems. They also perform measurements on the density distribution of Fermi gas as a function of the chemical potential for non-interacting case and show the accuracy of their results by comparing with the corresponding statistical physics equations. Koinov [18] has investigated the collective excitations of fermion and boson mixture within the Hubbard model in a sufficiently deep periodic optical lattice potential obtained by standing waves of laser light. By superimposing a laser beam on to a harmonically confined condensate, some experimental groups have successfully observed some unusual effects which are not encountered in a pure harmonic trap [19]. In that case, the confining potential has been approximated by the combination of harmonic and Gaussian terms [19-22]. Many theoretical studies have reported predictions of various interesting physical properties of Bose systems [23-25] for such type of confinement or its reduced forms (quartic plus quadratic) obtained by weak laser beam approximation. For example, Aftalion and Mason [24] have performed calculations on the density profile of rotating Bose-Einstein condensates trapped in a potential composed of harmonic and Gaussian terms. The variation of density profile with radial distance also discussed for different potential constants. A few studies have been



focused on the behaviour of two dimensional Fermi gas system confined in a combination of harmonic potential and a Gaussian one or it's reduced form. Howe et al. [26] studied on the fascinating properties of rotating polarized Fermi systems trapped by an an-harmonic potential consisting of harmonic and quartic terms. Ögren and Heiselberg [27] calculated the level densities and shell oscillations and other system properties of ultra-cold dilute gas of fermionic atoms confined by anharmonic quartic trap potentials by Hartre-Fock approximation.

The strength of interaction between the fermions is also an influencing factor determining the physical properties of confined systems [17,27–28]. For example, Hagymási et al. [28] examine how electron interactions modify the momentum distribution of heavy fermions in an extended periodic Anderson model by comparing the system with noninteracting case. We have also previously discussed the crucial role of electron interaction strength and confining potential type on the physical properties of Fermi system for different potentials in the frame of Thomas-Fermi approximation [8,14–15,29–33].

Recent experiments on trapped atomic gases [19-22] have stimulated us to perform a detailed analysis on the ground state behavior (such as the density distribution, the chemical potential, kinetic and potential energy) of two dimensional electron gas confined in a potential consisting of harmonic and Gaussian terms by using Thomas-Fermi method. The potential have been taken in the form of  $v(r) = \frac{1}{2} \omega^2 r^2 + \gamma \exp(-r^2/y)$  (where,  $\gamma$  and y are characteristic potential parameters) and the ground state properties of a fermionic system have been investigated by altering the y parameters from 0.1 to 0.5 for low, intermediate and high values of  $\gamma = 0.1$ , 0.5, 1.0. An iterative numerical procedure is applied to solve Thomas-Fermi equation for interacting electron gas. Here, we are particularly focused on the influence of the characteristic potential parameters  $\gamma$  and y on the ground state properties of both non-interacting and interacting fermionic systems. The deviations of the results due to the Gaussian potential and hence  $\gamma$  and v terms are also discussed by comparing the results with those calculated for pure harmonic potential. Throughout the work, all calculations are performed in atomic units, i.e.,  $m_e = 1$ , h = 1, e = 1.

#### 2. Theory

For an electron gas confined in a two dimensional space, the density of a system can be expressed as [33]

$$n(r) = \frac{1}{h^2} \int_0^\infty \frac{4\pi p \, dp}{b^{-1} e^{((p^2/2m) + V_\ell(r) + v(r))/kT} + 1}$$
(1)

Here, h is the Planck constant, T is the temperature, k is the Boltzmann constant,  $\mu$  is the chemical potential,  $V_e(r)$  is the electron-electron (e-e) interaction potential, v(r) is the confining potential,  $b = e^{\mu/kT}$  is the fugacity function respectively. Eq. (1) can be written in terms of Fermi-Dirac integrals  $f_1(b')$  [33–35] as

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

where,  $b' = e^{(\mu - v(r) - V_e(r))/kT}$ . In the limit of low temperatures (T ~ 0 K), the reduced form of the Eq. (1) can be obtained by using Sommerfeld's lemma [35]

$$\mathbf{n}(r) = \frac{m}{\hbar^2 \pi} (\mu - \upsilon(r) - V_e(r)). \tag{3}$$

The total number of electrons confined in a two dimensional space can be clearly written in terms of density of electrons as

$$N = \int_{0}^{r_0} n(r) 2 \pi r \, dr \tag{4}$$

To determine the ground state properties of the interacting confined system, Eq. (3) can be related with Poisson equation

$$\nabla^2 V_e(r) = -\frac{2\pi}{\varepsilon} n(r) \tag{5}$$

and Thomas-Fermi equation can be expressed as

$$\nabla^2 V_e(r) = -\frac{2m}{\hbar^2 \varepsilon} (\mu - \upsilon(r) - V_e(r)).$$
(6)

Here  $\varepsilon$  is the dielectric constant of the material and  $\nabla^2 = (1/r)(\partial/\partial r)r(\partial/\partial r)$ . It is obvious that the density of electrons should vanish at the boundaries due to the confinement. So it can be taken as zero at the radius of the confined space  $r_0(n(r_0) = 0)$ . We also assume that electron-electron interaction is zero at this point ( $V_e(r_0) = 0$ ) to make the system as electrically neutral [29–30,37].

The ground state properties of non-interacting (ideal) system ( $V_e(\mathbf{r}_0) = 0$ ) can be directly obtained by relating the boundary conditions with Eq. (3) and determining the positive root of f (r) function for  $r_0$  value for a constant number of particles

$$\mu = v(r_0) \tag{7}$$

$$f(\mathbf{r}_0) = \mathbf{N} - \int_0^{r_0} n(r) 2 \,\pi r \, dr = 0 \tag{8}$$

respectively. For a system confined with  $v(r) = \frac{1}{2} \omega^2 r^2 + \gamma \exp(-r^2/y)$  (where,  $\gamma$  and y are confinement parameters.), the chemical potential and the radius of confinement can be obtained from the equations written below

$$\mu = \frac{1}{2} \omega^2 r_0^2 + \gamma \exp(-r_0^2/y), \tag{9}$$

$$f(r) = \frac{1}{4}\omega^4 r_0^4 + \gamma \exp(-r_0^2/y)[y + r_0^2] - N - \gamma y = 0$$
(10)

According to our knowledge there is no analytical solution of Thomas-Fermi equation for an interacting electron system confined in a potential  $v(r) = \frac{1}{2} \omega^2 r^2 + \gamma \exp(-r^2/y)$ . So the solution will be realized by solving Eqs. (4) and (6) with the iterative numerical method summarized with some general steps;

- (i) Start with an initial guess for the chemical potential: In this stage, an arbitrary value for the chemical potential is determined. To avoid the waste of time, the values can be chosen from analytically known results in the literature [37].
- (ii) Obtain a solution forV<sub>e</sub>(r)by substituting the chemical potential μ in to Eq. (6).
- (iii) Determine a new chemical potential value by inserting the solution for  $V_e(r)$  into Eq. (4).
- (iv) Evaluation of the results: A tolerance value which stops the iteration is determined and the chemical potentials are updated until the difference of old and new generated values is smaller than the prescribed tolerance value.
- (v) Save the calculated values for  $\mu$ ,  $V_e(r)$  and n(r).

The same procedure can be used to evaluate the ground state properties of the non-interacting case by taking $V_e(r) = 0$ . The accuracy of the results can be checked by comparing them with the analytical results obtained by using Eqs. (3), (9) and (10) for non-interacting case. And also by taking  $\gamma = 0$ , we compare our results with those given for harmonically confined  $(v(r) = \frac{1}{2}m\omega^2 r^2)$  interacting system [37]. Within the *T*-F approach, the other system properties such as the kinetic, energy  $(E_K)$ , the confining potential energy  $(E_{v(r)})$  and Hartree energy  $(E_H)$  and in turn the total energy  $(E_T)$  can be calculated via density values [30,36],

$$E_{\rm k} = \int_0^{r_0} \tau({\bf r}) 2 \,\pi {\bf r} \,\mathrm{d}{\bf r} \tag{11}$$

$$E_{\nu(r)} = \int_0^{r_0} n(r)\nu(r) 2\,\pi r\,dr$$
(12)

$$E_{H} = -\frac{1}{2\varepsilon} \int_{0}^{r_{0}} n(r) V_{e}(r) 2\pi r \, dr, \qquad (13)$$

Download English Version:

# https://daneshyari.com/en/article/10998097

Download Persian Version:

https://daneshyari.com/article/10998097

Daneshyari.com