



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

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ABSTRACT

In this work, the ground state properties of two dimensional Fermi gas system interacting in a potential consisting 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 ⁴⁰K [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 by including these effects. Additionally, 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

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

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focused on the behaviour of two dimensional Fermi gas system confined in a combination of harmonic potential and a Gaussian one or its 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 an-harmonic 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 non-interacting 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, γ 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 γ 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 γ and y 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., $m_e = 1, \hbar = 1, e = 1$.

2. Theory

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

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

Here, h is the Planck constant, T is the temperature, k is the Boltzmann constant, μ 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

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

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

$$n(r) = \frac{m}{h^2\pi} (\mu - v(r) - V_e(r)). \quad (3)$$

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

$$N = \int_0^{r_0} n(r) 2\pi r dr \quad (4)$$

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

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

and Thomas-Fermi equation can be expressed as

$$\nabla^2 V_e(r) = -\frac{2m}{\hbar^2 \epsilon} (\mu - v(r) - V_e(r)). \quad (6)$$

Here ϵ 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 ($V_e(r_0) = 0$) 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

$$\mu = v(r_0) \quad (7)$$

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

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

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

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

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 for $V_e(r)$ 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 μ , $V_e(r)$ 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],

$$E_k = \int_0^{r_0} \tau(r) 2\pi r dr \quad (11)$$

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

$$E_H = -\frac{1}{2\epsilon} \int_0^{r_0} n(r) V_e(r) 2\pi r dr, \quad (13)$$

Table 1

The comparison of numerical and analytical values for some ground state properties of (μ and n_0) for the cases with different γ and y values.

Non-interacting system					
γ	y	The Chemical Potential (μ)		The Central density (n_0)	
		Analytic results	Numerical results	Analytic results	Numerical results
0.0	–	0.9999	0.9999	0.9999	0.9999
0.1	0.1	1.0050	1,0048	0.9050	0,9048
	0.3	1.0149	1,0149	0.9149	0,9147
	0.5	1.0243	1,0241	0.9243	0,9241
0.5	0.1	1.0247	1,0245	0.5247	0,5245
	0.3	1.0723	1,0722	0.57232	0,5722
	0.5	1.1167	1,1166	0.6167	0,6166
1.0	0.1	1.0488	1,0487	0.0488	0,0487
	0.3	1.1401	1,1400	0.1401	0,1400
	0.5	1.2232	1,2231	0.2232	0,2231

$$E_T = \int_0^{r_0} \tau(r) 2\pi r dr + \int_0^{r_0} n(r) v(r) 2\pi r dr - \frac{\pi}{\epsilon} \int_0^{r_0} n(r) V_c(r) r dr \quad (14)$$

Here, the kinetic energy density can be written as $\tau = \frac{\pi \hbar^2}{2m} n(r)^2$. So the saved results in the numerical procedure can be used for the evaluation of these properties by using a numerical integration method.

3. Results and discussion

In this work, we investigate the effects of confining parameters on the ground-state properties of a two dimensional interacting electron gas in a potential $v(r) = \frac{1}{2} \omega^2 r^2 + \gamma \exp\left(-\frac{r^2}{y}\right)$. The effect of confinement parameters, γ and y on the ground state properties of the system has been discussed in the frame of Thomas-Fermi approximation. The density of electrons, radial distance and number of particles are given in the units of $\left(\frac{m\omega^2\epsilon_0}{\pi}\right)$, $\left(\frac{\epsilon_0}{m}\right)^{1/2}$ and $N = \Omega \cdot \epsilon_0^2 \omega^2$ respectively. All calculations are performed by taking $\Omega = 1$.

In Table 1 we compare the analytical and numerical results for some system properties like the chemical potential (μ) and the central density values of the electrons (n_0) for non-interacting case. Highly precise numerical results reveal the accuracy of the applied procedure. Additionally, we compare numerical results with analytical ones by plotting the variation of the density of non-interacting electrons with radial distance for a special case of $\gamma = 0.5$ and $y = 0.1$ (Fig. 1). As seen from

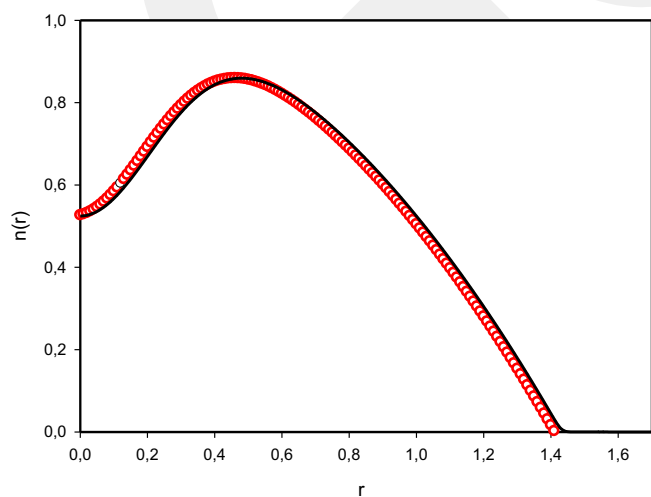


Fig. 1. Variation of the density with radial distance for the case of $\gamma = 0.5$ and $y = 0.1$. The line and the circles correspond to the exact and numerical solutions, respectively, for non-interacting systems.

the figure, the two curves are increasing up to a certain point and then decrease, also the two curves overlap very closely establishing the reliability of the numerical results.

The variation of the confinement potential with radial distance is illustrated in Fig. 2 for low, intermediate and high values of γ separately. The harmonic potential is also shown in Fig. 2(a–c) for comparative purposes. The shape of the trap can be described as almost harmonic which has a very shallow minima at (0, 0.1) coordinates for low γ values. However, it gains new features which can be clearly distinguished from parabolic behaviour for intermediate and high γ values.

In Fig. 3 the density distribution of electrons within the confined radius for different γ and y values are analyzed with the assistance of Fig. 2. Influence of confinement parameters on the density profile can be explained in terms of a) central b) intermediate and c) boundary regions depending on axial parts. The results are also compared with those calculated for the harmonic potential. As can be seen from Fig. 3, the density profiles are very sensitive to γ and y values. For $\gamma = 0.1$, basic attributes of the system show slight changes by the perturbation of the harmonic potential with the exponential term. Electrons are mostly localized at the central part (Fig. 2). An increase in the y value causes a slight decrease in n_0 for all systems. The reduction of the values becomes more noticeable with the inclusion of Coulomb interaction. While a monotonic decrease with radial distance is observed for $y = 0.3$ and $y = 0.5$, the density curve for $y = 0.1$ starts to rise a small amount from its n_0 value then this behaviour subsequently compensated by a smooth decline. This deviation from harmonic behaviour becomes much more striking when the e-e interaction is included in calculations. Generally, it can be concluded that for the low γ value, the effect of confinement parameters is considerable, especially in the central and intermediate parts, however all the curves overlaps with each other and it becomes negligible in the boundary region. On the other hand, it is obvious from Fig. 2(b) and (c) that electrons are more significantly influenced by the shape of the confinement potential. The difference between the density distribution of the systems becomes much more pronounced in all regions for the cases of $\gamma = 0.5$ and 1.0, As γ values increases, more particles will be pushed away from the central region to the other regions which induce a considerable amount of reduction in n_0 values. However, all the electrons are forced back by the potential walls (Fig. 2). So starting from n_0 value, all curves ascent to a certain point in the intermediate region then starts to decrease. The maximum value of the curves shifts outwards to larger radii as y values increases. While a sharp ascent (descent) behaviour observed for $y = 0.1$ value, it becomes smoother for higher values of y . Inclusion of the electron-electron interaction enhances the decrease of the values at the central region. Especially for high values of γ ($y = 0.1$ –0.5) n_0 values converge to 0 for interacting system. Furthermore, Coulomb interactions reduce the sharpness of the curves in the intermediate region.

In order to understand how the parameters, γ and y change the radius of confined system, we focus on the density distributions of the systems (Fig. 3) within the range of $1.4 < r < 1.8$. As expected, Coulomb repulsion causes an increase in r_0 values for all systems. Although r_0 values are independent of y for $\gamma = 0.1$ for both non-interacting and interacting systems, there is an appreciable population of electrons observed in the boundary region for intermediate and high values of γ which causes an increase in the r_0 values.

In Fig. 4 the plots are shown for the chemical potential (μ) (a) and the ratios of kinetic energy (E_K), confining potential energy ($E_{v(r)}$) and Hartree energy (E_H) to total energy E_T (b) for the cases of $\gamma = 0.1, 0.5, 1.0$, separately. The mentioned properties also discussed by considering the effect of e-e interaction. As expected, the chemical potential of interacting system are always higher than those calculated for non-interacting system (Fig. 4(a)). The values also ascent monotonically with y values for all cases. While this increase occurs gradually for $\gamma = 0.1$, it becomes more apparent for $\gamma = 0.5$ and $\gamma = 1.0$ (Fig. 4(a)). In order to understand how γ and y parameters change the qualitative behavior of

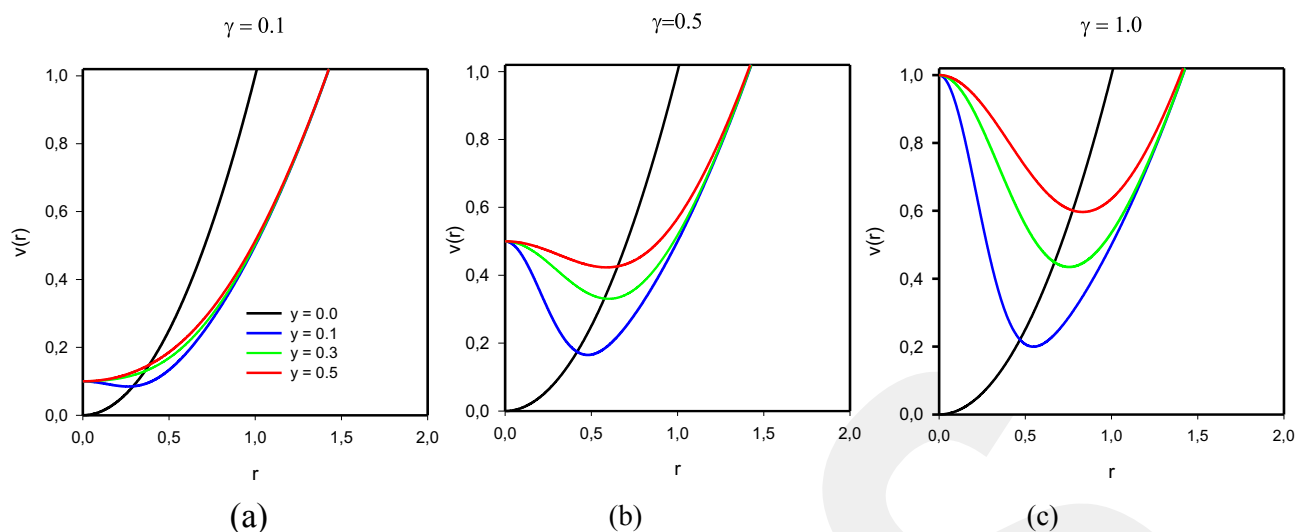


Fig. 2. (a–c) Variation of the confining potential with radial distance. Black, blue, green and red lines correspond to $y = 0.0, 0.1, 0.3, 0.5$, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

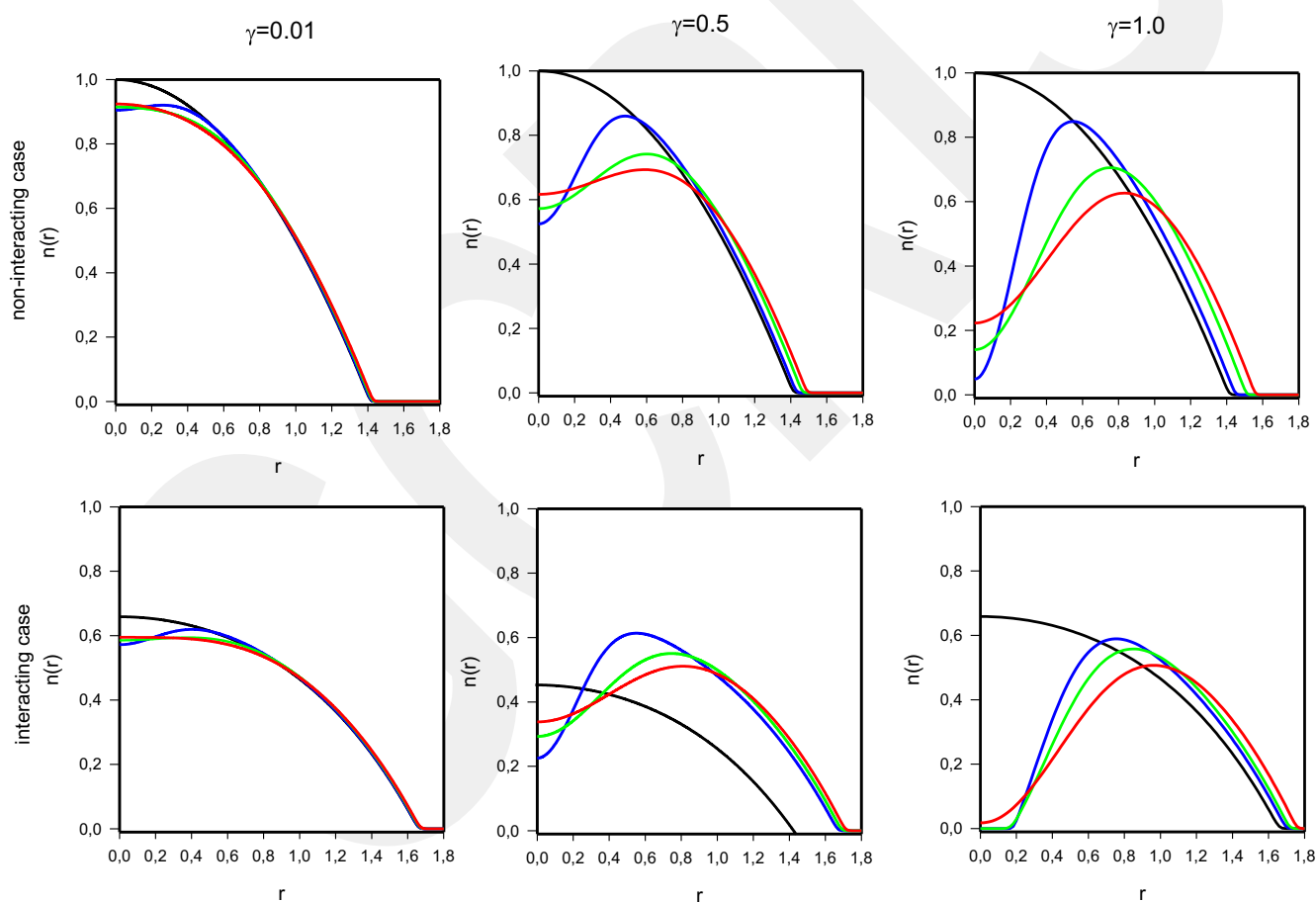


Fig. 3. Variation of the density profiles with radial distance. Black, blue, green and red lines correspond to $y = 0.0, 0.1, 0.3, 0.5$, respectively for both non-interacting and interacting cases. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the energy of the systems, we have performed a detailed analysis by showing the fractional change instead directly relating the energy values with y (Fig. 4(b)). Contrary to the rate of confining potential energy terms to total energy, (E_K/E_T) values decrease with γ . Moreover, the proportion of kinetic energy (E_K) values to (E_T) become smaller with y for both interacting and non-interacting systems and all γ values.

Results also indicate that the contribution of confining potential energy to total energy is always higher than Hartree energy for all y values. While change in the ratios of (E_K/E_T) , $(E_{v(r)}/E_T)$ and (E_H/E_T) per Δy is small for the case of $\gamma = 0.1$, it becomes noticeable as γ increases. One can conclude here that γ and y parameters play really significant role determining the properties stated above.

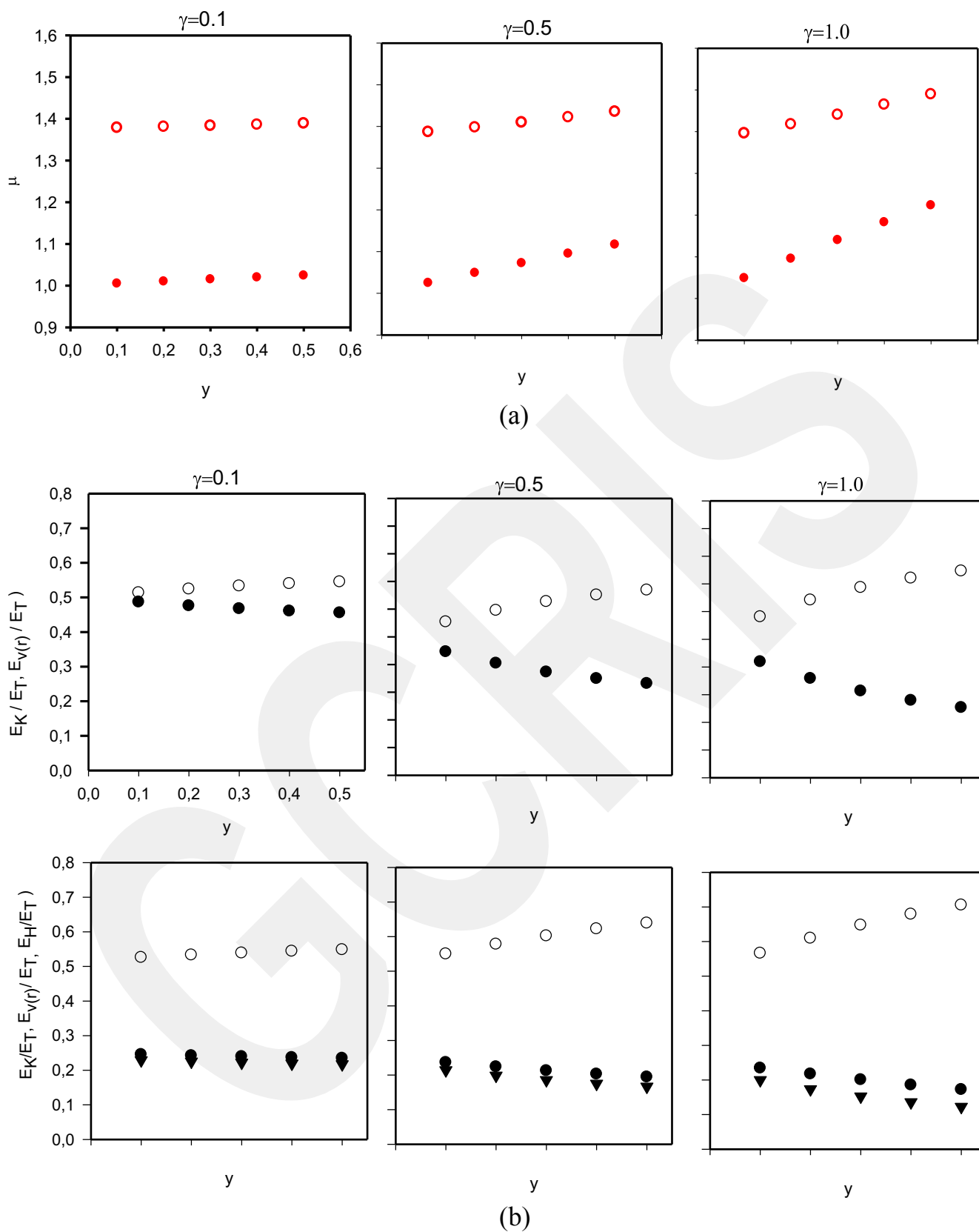


Fig. 4. (a) Variation of the chemical potential (μ) with y for non-interacting (red circles) and interacting cases (white circles) respectively. (b) Variation of the (E_K/E_T) (black circles), (E_H/E_T) (black triangle), $E_{v(r)}/E_T$ (white circles) with y for $\gamma = 0.1, 0.5, 1.0$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4. Conclusion

In this work, we investigate the ground state properties of two dimensional electron gas system confined in a potential of the form $v(r) = \frac{1}{2} \omega^2 r^2 + \gamma \exp(-r^2/\gamma)$ by employing Thomas-Fermi approximation. The results showed that the ground state properties of confined system is strongly modified, especially for intermediate and high γ values. The differences between the system properties due to different γ values become much more striking as γ values increases both for non-interacting and interacting systems. We believe that the results obtained here can be useful for future experimental and theoretical studies on many body effects of ultracold Fermi gases. They also are helpful for designing a planar device [9,38] where electrons within the interface region of hetero-structures are controlled by the diodes in a confining potential modelled here.

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