Journal of Physics: Conference Series **568** (2014) 012020 doi:10.1088/1742-6596/568/1/012020

Density functional theory investigation of two-dimensional dipolar fermions in a harmonic trap

Hande Ustunel[1], Saeed H. Abedinpour[2,3], and B. Tanatar[4]

[1] Department of Physics, Middle East Technical University, 06800, Dumlupinar Blv No: 1, Cankaya, Ankara, Turkey
[2] Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran
[3] School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran 19395-5531, Iran
[4] Department of Physics, Bilkent University, 06800, Bilkent, Ankara, Turkey

E-mail: ustunel@metu.edu.tr

Abstract. We investigate the behavior of polarized dipolar fermions in a two-dimensional harmonic trap in the framework of the density functional theory (DFT) formalism using the local density approximation. We treat only a few particles interacting moderately. Important results were deduced concerning key characteristics of the system such as total energy and particle density. Our results indicate that, at variance with Coulombic systems, the exchange-correlation component was found to provide a large contribution to the total energy for a large range of interaction strengths and particle numbers. In addition, the density profiles of the dipoles are shown to display important features around the origin that is not possible to capture by earlier, simpler treatments of such systems.

1. Introduction

Advances in trapping and cooling polar molecules with large permanent magnetic moments and atoms with electric moments have enabled numerous studies of dipolar quantum gases [1, 2, 3, 4, 5]. An important characteristic of these systems is that the dipole-dipole interaction is long ranged and anisotropic. Similar to the tunability of short-ranged interactions through Feshbach resonances, new techniques have been proposed [6] for controlling the strength and the sign of dipolar interactions. The interaction in three-dimensions is repulsive for dipoles aligned side-by-side and is attractive for dipoles aligned head-to-toe. Because the latter property along with collisional losses may cause instabilities in the system it is suggested that a gas trapped in two-dimensional (2D) geometry will provide a stable system.

Ground-state properties of 2D dipolar fermions have been investigated in a number of works [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. In particular, the ground-state energy, pressure, and compressibility of a uniform gas of 2D fermions have been calculated by Lu and Shlyapnikov [17] up to second order in interaction strength. Recently, Matveeva and Giorgini [18] have performed quantum Monte Carlo (QMC) simulations to obtain the phase diagram of this system over a wide range of coupling constants. Abedinpour et al. [19] developed hypernetted-chain (HNC) approximation to calculate the pair distribution function and static structure factor which agrees very well with the QMC results.

In this work we present a theoretical study of ground-state energy and density profile of a system of 2D polarized dipolar fermions in a harmonic trap potential. Utilizing the parametrized ground-state energy [19] we develop a density-functional formulation within the local-density approximation (LDA). We solve the Kohn-Sham equations iteratively using a simple charge-mixing method using a basis of two-dimensional Hermite functions up to 10 closed shells (i.e. a total of 66 basis functions). In Section 2, we introduce the model and the resulting Kohn-Sham equations followed by a presentation of our results in Section 3. We summarize our conclusions in Section 4.

2. Method

The interaction potential between two dipoles confined to 2D is given by

$$E_{dd} = \frac{C_{dd}}{r^3}\,, \tag{1}$$

where r is the distance between the dipoles which are assumed to align perpendicular to the plane. In the case of an electric dipole with dipole moment d, the interaction strength is given by $C_{dd} = d^2/(4\pi\epsilon_0)$, whereas for a magnetic dipole of magnetic moment μ, it is $C_{dd} = \mu_0\mu^2/(4\pi)$. The many-particle Hamiltonian describing a system of N dipoles in a harmonic trap characterized by an angular frequency ω is

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + \frac{1}{2}\sum_{i=1}^{N}(x_i^2+y_i^2) + \frac{1}{2}\sum_{i\neq j=1}^{N}\frac{g_{dd}}{|\vec{r}_i-\vec{r}_j|^3}\,, \tag{2}$$

where $\vec{r}_i = (x_i, y_i)$ is the position vector of the ith dipole. The Hamiltonian in Eq. (2) is written in harmonic units (h.u.) where lengths are measured in terms of the harmonic length $\ell = \sqrt{\hbar/m\omega}$ and energies in terms of $\hbar\omega$. In this notation, the coupling constant g_{dd} is defined as

$$g_{dd} = \frac{C_{dd}}{\hbar\omega\ell^3}\,. \tag{3}$$

In the LDA treatment of DFT, the total energy is written as a functional of the particle density, $n(\vec{r})$ as

$$E[n] = T_s[n] + E_{trap} + \frac{1}{2}g_{dd}\int d\vec{r}d\vec{r}'\frac{1}{|\vec{r}-\vec{r}'|^3} + \int d\vec{r}n(\vec{r})\epsilon_{XC}(n(\vec{r}))\,, \tag{4}$$

where the first, second and third terms represent the single-particle kinetic energy, the energy associated with the harmonic trap and the classical Hartree energy respectively. The key element of the treatment that determines the accuracy of the energy is the exchange-correlation energy represented by the last term. Here $\varepsilon_{XC}(n(\vec{r}))$ is the exchange-correlation energy (per particle) of a uniform dipole gas with density $n = n(\vec{r})$. Defining the density in terms of auxiliary single-particle orbitals as

$$n(\vec{r}) = \sum_{i}^{N}|\phi_i(\vec{r})|^2\,, \tag{5}$$

and performing a variational minimization of the energy with respect to these orbitals yields the so-called Kohn-Sham equations:

$$\hat{H}\phi_i(\vec{r}) = \left[-\frac{1}{2}\nabla^2 + \hat{V}_{trap} + g_{dd}\int d\vec{r}'\frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|^3} + \hat{V}_{xc}\right]\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r})\,. \tag{6}$$

In Eq. (6), $\hat{V}_{trap} = \frac{1}{2}r^2$ and $\hat{V}_{XC}$ are the external trap and exchange-correlation potentials respectively. $\{\phi_i(\vec{r})\}$ are the Kohn-Sham orbitals and $\{\varepsilon_i\}$ are the corresponding eigenvalues.

Once the system of N nonlinear equations in Eq. (6) are solved simultaneously, the ground state density may be reconstructed from the solutions using Eq. (5).

The exchange-correlation energy $\varepsilon_{XC}(\vec{r})$ used in Eqs. (4) and (6) has been previously derived by two of the authors [19]. In order to overcome the numerical problems caused by the singularity at $r = 0$, we use a regularization scheme to treat the Hartree and exchange potentials together. The regularized interaction is given by

$$v_{\rm reg}(r) = \frac{C_{\rm dd}}{4\pi} \frac{1}{(r^2+\sigma^2)^{3/2}}\,, \tag{7}$$

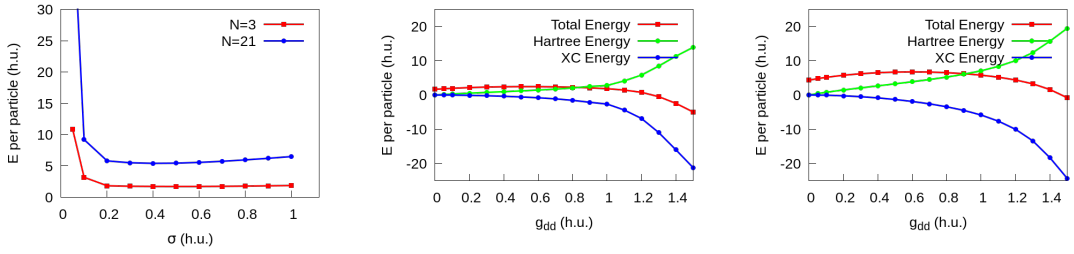
in which σ is a short range cutoff and one recovers the bare interaction in the $\sigma \to 0$ limit. With the introduction of this cutoff, the sum of the Hartree and exchange energy becomes

$$\varepsilon_{\rm HF} = g_{dd}(4\pi n)^{3/2}\frac{32}{45} + \mathcal{O}(\sigma^1)\,, \tag{8}$$

which is regular for small r.

3. Results and Discussion

The results presented in this paper were obtained by means of the self-consistent solution of Eq. (6) varying the two parameters of interest, namely the coupling constant g_{dd} and the particle number N. We present few-particle results, in particular $N = 3$ and $N = 21$ for small to moderate interaction strengths. The effect of varying σ is illustrated in Fig. 1(a) where the total LDA energy per particle is displayed for a fixed g_{dd} value of 1.0 for $N = 3$ and $N = 21$. Good convergence is obtained for both in a rather large range after $\sigma = 0.2$.. All results were obtained for a σ of 0.2ℓ. Fig. 1(b) displays the total LDA energy per particle for a system of 3 particles as a function of g_{dd} while Fig. 1(c) depicts the energy for 21 particles. For $g_{dd} = 0$, the energy for noninteracting, polarized particles in a harmonic trap is recovered. As g_{dd} increases, the energy is initially seen to slowly increase as expected from the repulsive nature of the interaction. However, shortly before $g_{dd} = 1.0$, the energy plunges to negative values and decreases rapidly. This behavior can be explained by considering the Hartree and exchange-correlation energies separately as also presented in Fig. 1. In both cases, the Hartree and exchange-correlation



(a) Energy versus σ (b) $N = 3$ (c) $N = 21$

Figure 1. Total energy per particle as a function of σ (a); total energy (red squares), Hartree energy (green circles) and exchange-correlation energy (blue circles) per particle for $N = 3$ (b) and $N = 21$ (c) as a function of interaction strength, g_{dd}.

energies behave in a similar manner but with opposite signs. In the weak interaction region, the kinetic, trap and Hartree energies keep the total energy positive while as the interaction strength increases, the exchange-correlation energy dominates bringing the total energy down to large, negative values.

The transition in behavior from repulsive to attractive interaction evident from the energies, is also observed in the density profiles. Fig. 2 and Fig. 3 display density profiles for 3 and 21 particles respectively, for a series of selected g_{dd} values.

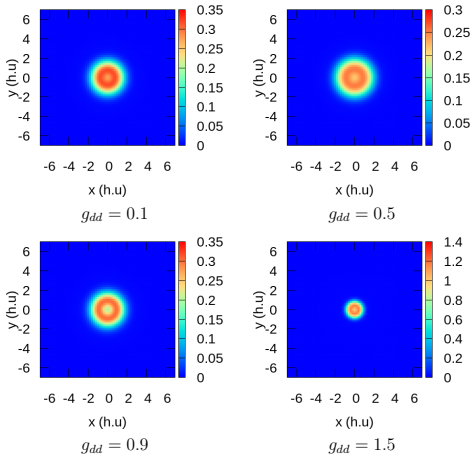


Figure 2. Density profiles for $N = 3$ and g_{dd} values varying between 0 and 1.5.

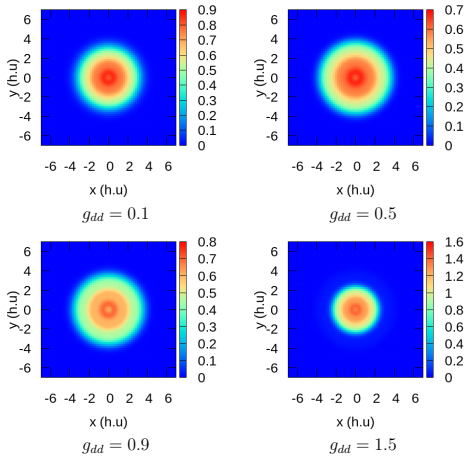


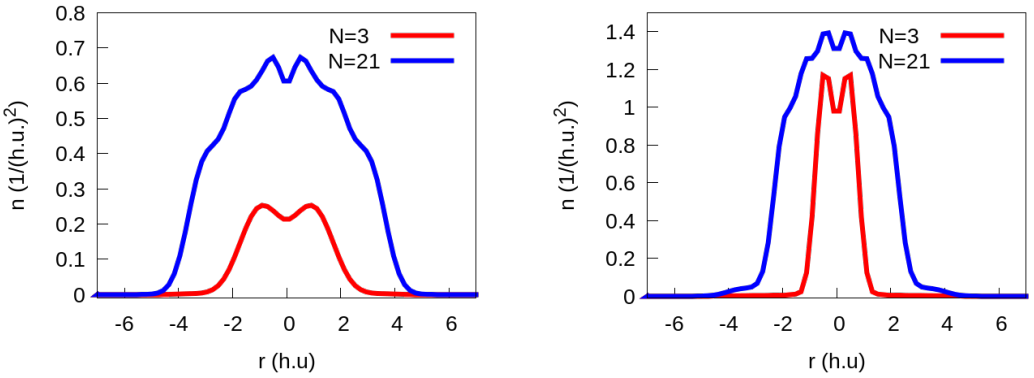
Figure 3. Density profiles for $N = 21$ and g_{dd} values varying between 0 and 1.5.

While the spatial extent of the density is mostly constant in the weak interaction region, a noticeable narrowing is observed once the exchange-correlation term begins to dominate.

In addition to the shift in behavior, the shape of the profiles demands attention. A common feature of all the density profiles obtained in this study is the central crater for $r = 0$ (see Fig. 4). This dip occurs independently of regularization cutoff and interaction strength but its existence depends upon particle number. While some particle numbers a crater as in the present case, others yield a peak. As the density decays away from the origin, well-distinguished terraces are observed as seen in Fig. 4(a) and (b), which are more pronounced for larger particle numbers. These subtle features in the density profile have not been previously identified by using simpler approximations such as variational approaches [20] or the Thomas-Fermi approximation [21, 22].

4. Conclusions

In this short manuscript, an LDA-DFT treatment of dipolar fermions, harmonically confined in two dimensions, was developed. A regularized dipolar interaction has been used to treat the Hartree and exchange-correlation terms in order to avoid singularities. Energies and density profiles for $N = 3$ and 21 particles have been presented for a range of interaction strengths ranging from weak to moderate. In the weak interaction region, the classical part of the energy (kinetic, trap and Hartree) was observed to be the deciding factor for determining the energy values as well as density profiles. For larger interaction strengths, the exchange-correlation term was seen to grow rapidly in the negative direction and dominating the behavior of the system. This result is in contrast to Coulombic systems where exchange and correlation energies are ordinarily a small portion of the total energy. It therefore underlines the importance of the full quantum mechanical treatment of the dipolar problem.



(a) $g_{dd} = 0.5$ (b) $g_{dd} = 1.5$

Figure 4. Cross-section ($y = 0$) of density profiles for $g_{dd} = 0.5$ (a) and $g_{dd} = 1.5$ (b). In each plot, radial density profiles for $N = 3$ and $N = 21$ are displayed.

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