Kohn-Sham theory of rotating dipolar Fermi gas in two dimensions

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A two-dimensional dipolar Fermi gas in harmonic trap under rotation is studied by solving "ab initio" Kohn-Sham equations. The physical parameters used match those of ultracold gas of fermionic $^{23}Na^{40}K$ molecules, a prototype system of strongly interacting dipolar quantum matter, which has been created very recently. We find that, as the critical rotational frequency is approached and the system collapses into the lowest Landau level, an array of tightly packed quantum vortices develops, in spite of the non-superfluid character of the system. In this state the system looses axial symmetry, and the fermionic cloud boundaries assume an almost perfect square shape. At higher values of the filling factor the vortex lattice disappears, while the system still exhibits square-shaped boundaries. At lower values of the filling factor the fermions become instead localized in a "Wigner cluster" structure.

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Recent developments in the field of ultracold dipolar fermionic and bosonic or fermionic) is the use of rapidly rotating harmonic traps. When the rotational frequency approaches the trap frequency, i.e. just below the limit of centrifugal instability, the single particle energy spectrum becomes highly degenerate and hence the kinetic energy of the Fermi system is much reduced, thus enhancing the role of the interparticle interactions.

A uniform rotation with angular velocity approaching the centrifugal limit is in fact formally equivalent to a magnetic field (in the rotational frame) that re-group single-particle states into discrete, highly degenerate Landau Levels (LL). Such equivalence, which holds in 2D and in the presence of an harmonic trapping potential only, is embodied in the following formal identity $^{13}$ involving the many-body Hamiltonian of the (interacting) system in the rotating reference frame:

$$H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2M} + \frac{M}{2} \omega_i^2 r_i^2 - \Omega \hat{L}_{iz} \right] + V$$

$$= \sum_{i=1}^{N} \left[ \frac{1}{2M} (p_i - M \omega_i e_z \times r_i)^2 + \frac{M}{2} (\omega_i^2 - \Omega^2) r_i^2 \right] + V$$

where $V$ is the interaction energy, $\Omega$ is the rotation frequency and $\hat{L}_{iz}$ is the projection of the angular momentum of the $i$-th particle along the $z$ axis. Here $r_i = x_i e_x + y_i e_y$ is the position vector of the $i$-th particle. When $\Omega = \omega_i$ the non-interacting part reduces to the Landau Hamiltonian of particles with mass $M$ and charge $e$ moving in a constant magnetic field $B = Be_z$, of strength $B = 2M\Omega/e$. The eigenvectors of the non-interacting part span Landau levels with energies $\epsilon_n = h\omega_c (n + 1/2)$, where $\omega_c = 2\Omega$.

We consider in the following a two-dimensional, spin-polarized dipolar fermi gas, characterized by an interaction term in Eq.1 $V = \sum_{i<j} \frac{d}{r_{i,j}^3}$. Here $d$ is the magnetic dipole moment of an atom/molecule and $r_{i,j}$ are coordinates in the 2D $x - y$ plane. Being the dipole moments aligned parallel to the $z$-axis, the (long-range) pair potential is purely repulsive. The range of the dipole-dipole interaction is characterized by the length $r_0 = Md^2/h^2$.

Exotic forms of vortex lattices, e.g. square, stripe-and bubble-"crystal" lattices are expected in rotating...
Bose-Einstein condensates when the critical rotational frequency is approached \[15, 17\]. Rotating dipolar Fermi gases have been proposed \[18, 19\] as suitable candidates to realize Laughlin-like state and more exotic quantum liquids, as well as their crossover behavior to Wigner crystals. At variance with the case of a non-rotating dipolar Fermi gas in a 2D trap, where the crystalline state becomes energetically favored at high densities, in the case of a fast rotating dipolar gas, the situation is reversed \[1\]: rotating dipoles in the Lowest LL (LLL) behave similarly to electrons, where the crystalline phase is stable at low densities. Indeed, it has been shown \[20, 21\] that a rapidly rotating polarized 2D dipolar Fermi gas undergoes a transition to a crystalline state, similar to the two-dimensional Wigner-Seitz electron crystal in a magnetic field, for sufficiently low value of the filling factor, \( \nu < 1/7 \). Here \( \nu = 2\pi l_F^2 n_F \) (where \( n_F \) is the areal density of the fermionic system and \( l = \sqrt{\hbar / M \omega} \) is the magnetic length) gives the fraction of the occupied LLL. At filling factor \( \nu = 1/3 \) the system is instead well described in terms of fractional quantum Hall-like states \[13\].

Density Functional Theory (DFT), which is perhaps the most widely used and successful technique in electronic structure calculations of condensed matter systems, has only recently entered the field of cold gases. The Kohn-Sham (KS) mapping \[22\] of the many-body problem into a non-interacting one makes this approach applicable in practice, often within the so-called Local Density Approximation (LDA) \[22\]. Recently, KS-DFT has been applied to cold atomic Fermi gases in optical lattices \[23\] and to the study of unitary trapped Bose gas \[24\]. DFT approaches have been used recently to describe a Fermi dipolar system in various "single-orbital" approximations (Thomas-Fermi \[9\], Thomas-Fermi-Dirac \[25\], Thomas-Fermi-von Weizsacker \[20, 27\]). In Ref. \[28\] a parameter-dependent DFT-LDA approach was used to study small number of harmonically trapped fermions. A somewhat different density functional formalism, whose applicability is however limited to a small number of particles, and which is based on the self-consistent combination of the weak and the strong coupling limits, has been proposed to study the ground-state properties of strongly correlated dipolar and ionic ultracold bosonic and fermionic gases \[29\].

Here we use the conventional KS approach, based on accurate description for the correlation energy of the dipolar system as provided by Diffusion Monte Carlo calculations \[13\]. Our approach does not require any adjustable parameter, and thus belongs to the family of the "ab initio" methods well known in the electronic structure community. The Kohn-Sham formulation \[22\] of Density Functional Theory \[30\] for an inhomogeneous system of \( N \) interacting particles with mass \( M \) is based on the following energy functional of the density which includes the exact kinetic energy of a fictitious non-interacting system and the interaction energy functional \( E_{HF} \):

\[
E_{KS}[\rho] = -\frac{\hbar^2}{2M} \sum_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d\mathbf{r} + E_{HFC}[\rho] \quad (2)
\]

The \( \{\phi_i(\mathbf{r}), i = 1, N\} \) are single-particle orbitals, forming an orthonormal set, \( \langle \phi_i | \phi_j \rangle = \delta_{ij} \), filled up to the Fermi level. The total density of the system is \( \rho(\mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2 \). \( E_{HFC} \) is the sum of the direct + exchange dipolar interaction term (usually termed "Hartree-Fock" energy, \( E_{HF} \)) and the correlation energy \( (EC) \). The Hartree-Fock energy of a dipolar Fermi gas in 2D has two contributions. The first, for the homogeneous system of surface density \( \rho = N/A \), is:

\[
E_{HF}^{(1)} = \frac{256}{45} N d^2 \sqrt{\pi} \rho^{3/2} \quad (3)
\]

The second term is non-local in nature and is given by \[25, 26\]

\[
E_{HF}^{(2)} = -\pi d^2 \int d\mathbf{r} \rho(\mathbf{r}) \int d\mathbf{r}' \int \frac{dk}{(2\pi)^2} ke^{-i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \rho(\mathbf{r}') \quad (4)
\]

This term vanishes in the uniform limit, while the negative sign crucially lowers the total energy of the system in inhomogeneous configurations. This term has been shown to be essential to stabilize structures such as one-dimensional stripe phases and the Wigner crystal that is expected at high densities \[3\].

In the following we will treat \( E_{HF}^{(1)} \) and \( EC \) within the Local Density Approximation (LDA), i.e.

\[
E_{HF}^{(1)} + EC = \int \left[ \frac{256}{45} d^2 \sqrt{\pi} \rho(\mathbf{r})^{5/2} + \rho(\mathbf{r}) \epsilon_C(\rho(\mathbf{r})) \right] d\mathbf{r} \quad (5)
\]

where \( \epsilon_C(\rho) \) is the correlation energy per particle of the homogeneous system of density \( \rho \), as obtained from the (virtually exact) Diffusion Monte Carlo calculations of Ref. \[13\].

The total energy functional in the co-rotating frame with constant angular velocity \( \Omega \) (where the dipolar system appears at rest) and in the presence of an isotropic harmonic trapping potential of frequency \( \omega_h \), \( U(\mathbf{r}) = \frac{1}{2} M \omega_h^2 (x^2 + y^2) \), is given by:

\[
E[\rho] = E_{KS}[\rho] + \int d\mathbf{r} \rho(\mathbf{r}) U(\mathbf{r}) - \Omega L_z \quad (6)
\]
Here \( \langle L_z \rangle \) is the total angular momentum of the system. Constrained minimization of the above functional leads to the coupled KS eigenvalues equations

\[
\left[ -\frac{\hbar^2}{2M} \nabla^2 + V_{KS} \right] \phi_i(r) = \epsilon_i \phi_i(r) \tag{7}
\]

where

\[
V_{KS}(r) = \epsilon_C(\rho(r)) + \rho(r) \frac{\partial \epsilon_C}{\partial \rho} + \frac{128}{9} d^2 \sqrt{\pi} \rho^{3/2}(r) - \Omega \hat{L}_z - 2\pi d^2 \int dr' \int \frac{dk}{(2\pi)^2} e^{-ik \cdot (r-r')} \rho(r') \tag{8}
\]

and \( L_z = -i\hbar (x\partial / \partial y - y\partial / \partial x) \).

We seek for stationary solutions \( \{ \phi_i(r), i = 1, N \} \) by propagating in imaginary time the time-dependent version\[22\] of the KS equations \(7\). Both the density and the orbitals \( \phi_i \) have been discretized in cartesian coordinates using a spatial grid fine enough to guarantee well converged values of the total energy. The orthogonality between different orbitals has been enforced by a Gram-Schmidt process. The spatial derivatives entering Eq.\(7\) have been calculated with accurate 13-point formulas, while Fast-Fourier techniques have been used to efficiently calculate the non-local term entering the KS potential \( V_{KS} \).

We take in our calculations \( d = 0.8 \) Debye, which is appropriate to \( K_{10}Na_{23} \) molecules in the experimental realization of Ref.[2]. The mass is that of a \( K_{10}Na_{23} \) molecule. The range of the potential is thus \( r_0 = Md^2/\hbar^2 \sim 0.6 \mu m \sim 0.2 a_H, a_H = \sqrt{\hbar/2M\omega_h} \) being the oscillator length. In the ground-state of the non-rotating system, the adimensional interaction strength characterizing the system is \( k_F r_0 \sim 0.9 \) (where \( k_F = \sqrt{\pi \rho_{\text{max}}} \) is the Fermi wavevector of the 2D system at a density equal to the maximum density in the center of the trap), i.e. a relatively weak value which can easily be achieved in experiments. The interparticle distance \( \langle r \rangle \) is larger than the range of the interaction, being \( \langle r \rangle / r_0 \sim 3.6 \). The corresponding dipolar interaction energy \( E_d = d^2 / \langle r \rangle^3 \) approaches 20% of the local Fermi energy \( \hbar^2 k_F^2 / 2M \). In spite of the relatively weak coupling, as a consequence of the rotation, strong correlation effects will show up in the density distribution of the calculated stationary states, as shown in the following. We consider systems with up to \( N = 200 \) fermions.

We show in Fig.1 the evolution of the calculated single particle KS eigenvalues \( \epsilon_i \) for the case \( N = 100 \), as the rotational frequency \( \Omega \) approaches from below the harmonic frequency \( \omega_h \). At \( \Omega = 0.999 \omega_h \) it appears that all the energy levels collapse into a single level, the (highly degenerate) LLL.

It is instructive to follow how the density of the system evolves as \( \Omega \) is increased. This is shown in Fig.2 where the densities of selected configurations corresponding to different values of \( \Omega \) are displayed.

For low values of \( \Omega \) (\( \Omega = 0 \) included) the calculated stationary states have circular symmetry, and the density has the familiar, almost featureless shape of a trapped cold gas cloud. As soon as \( \Omega \) approaches \( \omega_h \), however, a ring of equally spaced deep dimples develop close to the periphery of the cloud, while the systems loses its axi-symmetric shape. Eventually, very close to \( \omega_h \), an array of tightly packed vortices develops, similarly to the
Abrikosov lattice of vortices in rotating superfluids, while the system boundaries acquire a surprising square shape.

The calculated current density in the state with $\Omega/\omega_h = 0.999$ in Fig.2 appears indeed to be circulating around the zero-density minima (black dots in the last panel of Fig.2), as expected for a vortex array. The total angular momentum $\langle L_z \rangle$ shows also the typical behavior associated to the nucleation of quantum vortices, i.e. a sequence of rounded steps (with amplitudes $\sim \hbar$) with increasing rotation frequency $\Omega$, as more vortices are nucleated in the system during the minimization process leading to the stationary state shown in the last panel of Fig.2. The average distance $d_v$ between vortices in the structure shown in Fig.2 is $\sim 20\%$ larger than the one calculated (assuming a triangular vortex lattice of areal density $n_v$) using Feynman’s formula $\frac{\sqrt{3}}{8} \frac{N}{\hbar} = M \Omega/\pi \hbar$.

Quantized vortices in Fermionic cold gases are usually associated to pairing interactions, as in the BCS side of a unitary Fermi gas $\nu$, where they are considered the hallmark of the superfluid character of the system. The presence of vortices in a system with purely repulsive interactions, like the one studied here, has been predicted to occur in fermion systems with purely repulsive interaction such as quantum dots, where the rotation is induced by an external magnetic field (see for instance Ref.33). Indirect evidence of vortices in ultra small fermion droplets ($N = 6$) with aligned dipoles has been provided in Ref.34. However, due to the implicit symmetry constraints in the calculations of Ref.34 multi-vortex structures like the one shown in Fig.2 did not show up in the calculated density profiles.

A striking feature of the $N = 100$ system in the LLL is the lack of axial symmetry represented by the unusual square-shaped boundaries. This seems to be intimately connected with the interactions between fermions: the system shown in Fig.2 under the same conditions but with no interactions between fermions, exhibits density profiles with circular symmetry all the way up to $\omega_h$. Deviations from axi-symmetric configurations in isotropic trapping have been found in fast rotating BEC at overcritical rotation $\nu = 0.999$, as a consequence of the interatomic forces. Stable, non axi-symmetric multi-lobed shapes also characterize the fast rotation of classical liquid droplets $\nu = 0.999$. The configuration shown in the lowest panel of Fig.2 corresponds to a filling factor $\nu \sim 0.77$. By decreasing the number of fermions in the trap we can reach lower values of $\nu$. One example is shown in Fig.2 where $N = 13$. Again, as the centrifugal limit is approached, stationarity configuration with an increasing number of vortices are found: vortices enter the fermion droplet from the low density periphery (a mechanism common to BEC $\nu = 1$ and Helium-4 $\nu = 1$). As $\Omega \sim \omega_h$ (last panel in Fig.2), however, a completely different pattern shows up, resembling a cluster of localized particles (albeit with a partially melted second shell). This configuration is characterized by $\nu \sim 0.18$. We take this as a clear evidence of formation of a "Wigner cluster" structure for sufficiently low values of the filling factor.

Higher values of $\nu$ can be conversely achieved by increasing the fermions number. In this case the vortex lattice disappears, and the smoother structures shown in Fig.3 develop. Here, $\nu = 1.08$ and $\nu = 1.25$, respectively (corresponding to $N = 160$ and $N = 200$ fermions). Note however that the peculiar square-shaped boundaries remain even at higher values of the filling factor.

Although small numbers of cold trapped atoms, like the ones considered here, can nowadays be achieved in experiments, we expect that the surprising phenomenology revealed by our calculations should be present also in larger systems of rotating dipolar fermionic molecules in quasi 2D harmonic traps. Achiev-
ing rotation frequencies $\Omega \sim 0.999 \omega_h$ is a challenging task, but definitely within the reach of current experiments\cite{14}. Due to the relatively high contrast of the vortex array shown in Fig. 2, its observation should be possible by direct imaging of the atomic cloud after expansion (the vortex lattice in quantum dots still awaits experimental detection).

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