Dipolar fermions in a two-dimensional lattice at non-zero temperature

Anne-Louise Gadsbølle\textsuperscript{1,2} and G. M. Bruun\textsuperscript{2}

\textsuperscript{1}Lundbeck Foundation Theoretical Center for Quantum System Research
\textsuperscript{2}Department of Physics and Astronomy, University of Aarhus, Ny Munkegade, DK-8000 Aarhus C, Denmark

We examine density ordered and superfluid phases of fermionic dipoles in a two-dimensional square lattice at non-zero temperature. The critical temperature of the density ordered phases is determined and is shown to be proportional to the coupling strength for strong coupling. We calculate the superfluid fraction and demonstrate that the Berezinskii-Kosterlitz-Thouless transition temperature of the superfluid phase is proportional to the hopping matrix element in the strong coupling limit. We finally analyze the effects of an external harmonic trapping potential.

INTRODUCTION

An increasing number of experimental groups are trapping and cooling atoms or molecules with a permanent magnetic or electric dipole moment. Bose-Einstein condensates of \textsuperscript{52}Cr atoms \textsuperscript{[1,2]} and of \textsuperscript{164}Dy atoms \textsuperscript{[3]} with large magnetic dipole moments have been realized. Fermionic gases of \textsuperscript{40}K\textsuperscript{87}Rb \textsuperscript{[4]} and \textsuperscript{23}Na\textsuperscript{6}Li \textsuperscript{[5]} molecules with an electric dipole moment have been created, and the first steps toward the formation of fermionic \textsuperscript{23}Na\textsuperscript{40}K molecules have been reported \textsuperscript{[6]}. Also, experimental progress toward realizing dipolar molecules in an optical lattice have recently been presented \textsuperscript{[7]}. The anisotropy of the dipole interaction results in many intriguing effects. In a two-dimensional (2D) lattice, the existence of density ordered phases with a complicated unit cell \textsuperscript{[8]}, liquid crystal phases \textsuperscript{[9]}, and a supersolid phase \textsuperscript{[10]} have been predicted when the dipole moments are perpendicular to the lattice plane. Tilting the dipoles toward the lattice plane leads to density order with different symmetry, superfluidity and bond-solid order at zero temperature \textsuperscript{[11,13]}. When a trapping potential is present, these phases were shown to coexist, forming ring and island structures \textsuperscript{[12]}. In this paper, we examine fermionic dipoles in a 2D square lattice including the presence of a harmonic trapping potential. Focus is on the effects of a non-zero temperature and the melting of density ordered and superfluid phases. We determine the critical temperature for the density ordered phases and find that it is proportional to the interaction strength in the strong coupling regime. For the superfluid phase, we calculate the superfluid fraction and the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature, which is proportional to the hopping matrix element in the strong coupling limit. We analyze the effects of an external trapping potential showing that for experimentally realistic systems, the ordered phases exist in the center of the trap with melting temperatures close to that which can be obtained from a local density approximation.

MODEL

We consider fermionic dipoles of mass $m$ and dipole moment $\mathbf{d}$ moving in a 2D square lattice with lattice constant $a$. The dipole moment is aligned by an external field to form an angle $\theta_P$ with respect to the $z$ axis which is perpendicular to the lattice plane and an angle $\phi_P$ with respect to a lattice vector chosen as the $x$ axis. The Hamiltonian is $\hat{H} = \hat{H}_{\text{kin}} + \hat{V}$ where

$$\hat{H}_{\text{kin}} = -t \sum_{\langle ij \rangle} \left( \hat{c}_i^\dagger \hat{c}_j + \text{h.c.} \right) + \sum_i \left( \frac{1}{2} m \omega^2 r_i^2 - \mu \right) \hat{n}_i$$

and

$$\hat{V} = \frac{1}{2} \sum_{i \neq j} V_D(\mathbf{r}_{ij}) \hat{n}_i \hat{n}_j$$

where $\mathbf{r}_i$ denotes the position of lattice site $i$ and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\hat{c}_i$ is the annihilation operator that removes a dipole at site $i$, and $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ is the number operator. The chemical potential is $\mu$ and $t$ is the hopping matrix element between nearest neighbors $\langle ij \rangle$. We include the effects of a harmonic potential with trapping frequency $\omega$ exactly in our analysis. The interaction between two

![FIG. 1: (color on-line) Dipoles move in a 2D square lattice with lattice constant $a$. They are aligned forming an angle $\theta_P$ with the $z$ axis perpendicular to the lattice plane, and the azimuthal angle $\phi_P$ with the $x$ axis which is parallel to a lattice vector.](https://example.com/fig1.png)
dipoles separated by \( \mathbf{r} \) is given by

\[
V_D(\mathbf{r}) = \frac{D^2}{r^3} \left( 1 - 3 \cos^2 \theta_{\mathbf{r}} \right)
= \frac{D^2}{r^3} \left[ 1 - 3 \cos^2(\phi_\mathbf{r} - \phi) \sin^2 \theta_\mathbf{r} \right]
\tag{3}
\]

with \( D^2 = d^2/4\pi\epsilon_0 \) for electric dipoles and \( \theta_{\mathbf{r}} \) the angle between the dipole and \( \mathbf{r} = r \cos(\phi, \phi, 0) \), see Fig. 1. We define \( g = D^2/a^3 \) as a measure of the interaction strength.

The anisotropy of the dipolar interaction (3) with attractive and repulsive regions gives rise to both density ordered and superfluid phases [8, 11, 12]. We capture the existence of these competing phases using mean-field theory including the Hartree terms and the pairing terms, which we expect to be reasonably accurate due to the long range nature of the interaction. The mean-field Hamiltonian is diagonalized by solving the Bogoliubov-de Gennes equations [12]

\[
\sum_j \left( L_{ij} - \Delta_{ij} \right) \begin{pmatrix} u_{ij}^\dagger \varepsilon_j \end{pmatrix} = E_n \begin{pmatrix} u_{ij}^\dagger \varepsilon_j \end{pmatrix},
\tag{4}
\]

where \( \Delta_{ij} = V_D(\mathbf{r}_{ij})/\hat{\mathbf{c}}_i \hat{\mathbf{c}}_j \)

\[
L_{ij} = -t\delta_{ij} + \sum_k V_D(\mathbf{r}_{ik})/\langle n_k \rangle + \frac{m}{2} \omega^2 r_i^2 - \mu \delta_{ij},
\tag{5}
\]

Here \( \delta_{ij} \) and \( \delta_{(ij)} \) are the Kronecker delta functions connecting on-site and nearest neighbor sites, respectively. Self-consistency is obtained iteratively through the usual relations

\[
\langle \hat{n}_i \rangle = \sum_{\mathbf{r}_k \neq 0} \left[ (1 - f_{\mathbf{r}_k})|u_{\mathbf{r}_k}|^2 + f_{\mathbf{r}_k}|u_{\mathbf{r}_k}^*|^2 \right]
\]

and

\[
\langle \hat{c}_i \hat{c}_j \rangle = \sum_{\mathbf{r}_k \neq 0} \left[ u_{\mathbf{r}_k}^* u_{\mathbf{r}_k} (1 - f_{\mathbf{r}_k}) + u_{\mathbf{r}_k} u_{\mathbf{r}_k}^* f_{\mathbf{r}_k} \right],
\]

with \( f_{\mathbf{r}_k} = \exp(E_{\mathbf{r}_k}/T) + 1 \)^{-1} the Fermi function for the temperature \( T \). We use units where \( k_B = h = 1 \). To analyze the melting of the superfluid phase, we shall use the framework of BKT theory.

**STRIPE MELTING AT HALF FILLING**

We first analyze the case of no trapping potential and half filling, \( N/N_k = 1/2 \), with \( N_k \) the number of lattice sites and \( N = \sum_i \langle \hat{n}_i \rangle \) the total number of particles. When the dipoles are perpendicular to the lattice, it follows from the perfect nesting of the Fermi surface that a phase with checkerboard density order persists down to \( g/t \to 0 \) for \( T = 0 \) [8]. In the limit of strong interaction \( g/t \gg 1 \) where the kinetic energy can be neglected and the problem becomes classical, it was shown that the checkerboard phase is replaced by a striped phase when the dipoles are tilted at a sufficiently large angle \( \theta_p \) [12]. We now examine the melting of these density ordered phases at a non-zero temperature. The melting is in the Ising universality class due to the discreteness of the lattice, and we therefore expect mean-field theory to yield a qualitatively correct value for the transition temperature.

For the case of stripes along the \( x \) direction, we express the density as \( \langle \hat{n}_i \rangle = 1/2 [1 + M(-1)^x] \) with \( M \) the order parameter. The corresponding mean-field Hamiltonian can be written as \( H = \sum_{\mathbf{r}_k > 0} c_{\mathbf{r}_k}^\dagger c_{\mathbf{r}_k} + E_1k |\gamma_{\mathbf{r}_k}|^2 + E_2k |\gamma_{\mathbf{r}_k}|^2 \) with the single particle energies

\[
E_1k = \xi_k + \sqrt{(2t \cos k_y a)^2 + [V_D(0, \pi/a) M/2]^2}
\tag{6}
\]

where \( \xi_k = -2t \cos k_x a - \mu + V_D(0, 0)/2 \). We have defined the Fourier transform \( V_D(\mathbf{k}) = \sum \exp(-i\mathbf{k} \cdot \mathbf{r}_i) V_D(\mathbf{r}_i) \). The energy \( E_2k \) is given by (3) with a minus-sign in front of the square root. The self-consistency equation reads

\[
1 = \frac{1}{N_L} \sum_{\mathbf{k} \neq 0} \frac{V_D(0, \pi/a)|f_{\mathbf{r}_k} - f_{\mathbf{r}_k}^*|}{(2t \cos k_y a)^2 + [V_D(0, \pi/a) M/2]^2},
\tag{7}
\]

where the sum is over half the first Brillouin zone with \( k \neq 0 \). In the limit of strong interaction \( g/t \gg 1 \), Eq. (7) yields

\[
T_c^{st} = -\frac{1}{4} \frac{V_D(0, \pi/a)}{\gamma_k(0, \pi/a)}.
\tag{8}
\]

When the dipoles are aligned in the lattice plane with \( (\theta_p, \phi_p) = (\pi/2, 0) \), Eq. (5) gives \( T_c^{st} \approx 1.27g \). A similar analysis for the checkerboard phase yields \( T_c^{cb} = -V_D(\pi/a, \pi/a)/4 \) in the strong coupling limit, which gives \( T_c^{cb} \approx 0.66g \) for \( \theta_p = 0 \) [8].

Figure 2 shows the critical temperature as a function of the interaction strength for the checkerboard phase with \( \theta_p = 0 \) and for the striped phase with \( (\theta_p, \phi_p) = (\pi/2, 0) \). The \( \phi \)'s and \( x \)'s are numerical results for the stripe and checkerboard phases respectively, obtained from solving (4), and the lines the analytical results for the strong coupling limit discussed above. Finite size effects of the system are eliminated by neglecting the high temperature tail of the order parameter. For example, for the lower right inset in Fig. 2 the elimination of the high temperature tail gives the critical temperature \( T_c^{cb}/t = 0.4 \). We see that the numerical results agree well with the strong coupling results for \( g/t \gg 1 \) whereas the critical temperature becomes exponentially suppressed in the weak coupling limit. Note that the critical temperature of the striped phase is almost twice that of the checkerboard phase, which makes it easier to observe experimentally. The upper left inset shows how the striped order parameter \( M \) decreases with \( T \) for \( (\theta_p, \phi_p) = (\pi/2, 0) \) and \( g/t = 3.3 \), and the lower right inset shows the checkerboard order parameter \( M \) as a function of \( T \) for \( \theta_p = 0 \) and \( g/t = 1 \).

Figure 3 shows the critical temperature of the striped and the checkerboard phase as a function of \( (\theta_p, \phi_p) \) in the strong coupling regime. It is obtained from
For smaller filling fractions, the system can be in a superfluid state with \( p \)-wave symmetry for large enough \( \theta_p \) \cite{as}. This leads to a competition between density and superfluid order in analogy with dipoles moving in a 2D plane without a lattice \cite{as2,as3}. As an example, we now consider the melting of the superfluid and the striped phase for the filling fraction \( N/N_L = 1/3 \) and \( (\theta_p, \phi_p) = (\pi/2, 0) \). For these parameters, mean-field theory predicts the system to be superfluid for \( g/t \leq 1.15 \) and to exhibit stripe order for \( g/t > 1.15 \) at \( T = 0 \) \cite{as2}.

For the 2D system considered here, the melting of the superfluid phase is of the BKT type with a transition temperature determined by the phase stiffness of the order parameter \cite{as4,as5}. The phase stiffness \( J_x \) associated with a phase twist of the superfluid order parameter in the \( x \) direction is determined from the energy cost

\[
F_\Theta - F_0 \simeq \frac{J_x}{2} \sum_i \delta \Theta^2.
\]

Here, \( F_\Theta \) is the free energy when the phase of the order parameter varies by \( \delta \Theta \) between neighboring sites in the \( x \) direction and \( F_0 \) is the free energy when there is no phase twist \cite{as6}. Associated with the phase twist, we define the superfluid fraction \( \rho_{s,x} \) by writing

\[
F_\Theta - F_0 = \frac{N}{2} \rho_{s,x} m^* v_s^2 = \frac{N}{4} t \rho_{s,x} \delta \Theta^2,
\]

where \( v_s = \delta \Theta/2m^*a \) is the superfluid velocity of the Cooper pairs with mass \( 2m^* \). The effective mass for the dispersion \(-2t(\cos k_x a + \cos k_y a)\) is \( m^* = 1/2ta^2 \). Note that the superfluid fraction is dimensionless. Similar expressions hold for the phase stiffness \( J_y \) and the superfluid fraction \( \rho_{s,y} \) for the \( y \) direction.

A linear phase twist along the \( x \) direction is equivalent to acting on the Hamiltonian with the unitary gauge transformation

\[
\hat{H}_\Theta = e^{-i\delta \Theta \sum_i \hat{\xi}_i/a} \hat{H} e^{i\delta \Theta \sum_i \hat{\xi}_i/a}.
\]
where $x_l$ is the $x$-coordinate of particle $l$ \[19\]. We have $\delta \Theta = 2\delta \theta$ since the superfluid order parameter involves two particles so that the gauge transformation gives $\Delta_{ij} \to \Delta_{ij} \exp[i(x_l + x_j)\delta \theta/a]$. The gauge transformation only affects $\hat{H}_{\text{fin}}$ by introducing a phase factor $t_{c}^{\dagger}c_{i+e_x} \to t_{c}^{\dagger}e^{\pm i\delta \theta}c_{i+e_x}$ on the hopping terms connecting neighboring sites in the $x$ direction. Here, $e_x$ denotes one lattice step in the $x$ direction. Since we only need the energy cost to lowest order in the phase twist to determine $J$ from Eq. \[9\], it is sufficient to use perturbation theory in $\delta \theta$. Expanding to second order in $\delta \theta$, we obtain $\hat{H}_{\theta} \equiv \hat{H} + \hat{J} + \hat{T}$ with

$$
\hat{J} = -i\delta \theta \sum_i \left( c_i^\dagger c_{i+e_x} - c_i^\dagger c_{i-e_x} \right)
$$

$$
\hat{T} = \frac{t}{2\delta \theta^2} \sum_i \left( c_i^\dagger c_{i+e_x} + c_i^\dagger c_{i-e_x} \right).
$$

(12)

Since the unitary transformation conserves particle number, we can take $F_{\theta} - F_0 = \Omega_{\theta} - \Omega_0$ where $\Omega = F - \mu N$ with $N$ the total number of particles \[20\]. The linked cluster expansion gives \[21\]

$$
\Omega_{\theta} - \Omega_0 = \langle \hat{T} \rangle - \frac{\beta}{2} \langle J^2 \rangle
$$

(13)

where $\langle \ldots \rangle$ denotes the thermal average with respect to the untwisted Hamiltonian and we have used that there is no current in the untwisted case, i.e. $\langle \hat{J} \rangle = 0$. Mean-field theory gives after some lengthy but straightforward algebra

$$
\langle \hat{T} \rangle = \frac{t}{2\delta \theta^2} \sum_{\eta,i} (u_{\eta}^{\dagger}u_{\eta}^{\dagger}e_x + u_{\eta}^{\dagger}u_{\eta}e_x) f_{\eta}
$$

(14)

and

$$
\langle J^2 \rangle = -t^2\delta \theta^2 \sum_{ij} \sum_{\eta \alpha} \sum_{k,l} \kappa \left[ u_{\eta}^{\dagger}u_{\alpha}^{\dagger}u_{\alpha}^{\dagger}u_{\eta}^{\dagger}e_x + u_{\eta}^{\dagger}u_{\eta}e_x \right] \left( u_{\eta}^{\dagger}u_{\alpha}^{\dagger}u_{\alpha}^{\dagger}u_{\eta}^{\dagger}e_x + u_{\eta}^{\dagger}u_{\eta}e_x \right) f_{\eta}(1 - f_{\alpha}).
$$

(15)

The sums in Eqs. \[14\]-\[15\] are taken over positive as well as negative energies, and we have made use of the duality $(u_{\eta}, v_{\eta}, E_{\eta}) \leftrightarrow (v_{\eta}^{\dagger}, u_{\eta}^{\dagger}, -E_{\eta})$ of the Bogoliubov-de Gennes equations.

When there is no trap, the Bogoliubov-de Gennes equations are straightforward to solve and Eqs. \[10\], \[14\], and \[15\] yield

$$
\rho_{s,x} = \frac{1}{N} \sum_k \left[ n_k \cos k_x a - \frac{2t}{T} E_k (1 - f_k) \sin^2 k_x a \right].
$$

(16)

Here $E_k$ are the BCS quasiparticle energies for the $p$-wave paired state, and $n_k = u_{k}^{\dagger}u_{k} + v_{k}^{\dagger}v_{k}(1 - f_k)$. In the continuum limit $a \to 0$ keeping the density $N/N_x a^2$ constant, this reduces to the usual expression $\rho_{s,x} = 1 + (3m^*)^{-1}(2\pi)^{-3} \int d^3k \partial E_k f_k k^2$ for a single component superfluid \[22\].

From the phase stiffness, we can extract the transition temperature as $T_{\text{BKT}} = \pi J/2$ \[16\] \[17\] where we have taken the average $J = (J_x + J_y)/2$ to account for the anisotropy of the $p$-wave pairing. Equations \[9\]-\[10\] give $J = N\rho_s t/2NL$ with $\rho_s = (\rho_{s,x} + \rho_{s,y})/2$, and we finally obtain

$$
T_{\text{BKT}} = \frac{\pi N}{4NL} \rho_s t = \frac{\pi}{8} \frac{n_s}{m^*}
$$

(17)

with the superfluid density defined as $n_s = N\rho_s/N_L a^2$.

In Fig.\[4\] we plot $T_{\text{BKT}}$ as a function of the coupling strength obtained from Eq. \[17\]. For comparison, we plot the mean-field superfluid transition temperature $T^*$. We also plot the critical temperature $T^{*}\text{c}$ for the stripe phase which is the ground state for $g/t > 1.15$. For weak coupli-
is interesting that both critical temperatures, $T_{\text{BKT}} \sim t$ and $T_{c}^{\text{st}} \sim g$, can be much higher than that of the antiferromagnetic phase for atoms in a 3D lattice, which scales as $T_N \sim t^2/U$ in the strong coupling limit with $U \gg t$ on the on-site interaction [24, 25].

In Fig. 5 we plot the superfluid fraction and the nearest neighbor order parameter as a function of $T$ for various coupling strengths. As usual for a 2D system, the superfluid fraction is discontinuous at the critical temperature. Contrary to a translationally invariant system, the superfluid fraction is less than 1, even for $T = 0$ [20]. In the inset, we plot the superfluid fraction and the nearest neighbor pairing as a function of $T$ for various coupling strengths.

![FIG. 5: (color on-line) The superfluid fraction $\bar{\rho}_s$ and the nearest neighbor pairing $|\langle \hat{c}_{i+e_y} \hat{c}_i \rangle|$ as a function of $T$ for various coupling strengths. $|\langle \hat{c}_{i+e_y} \hat{c}_i \rangle|$: Pink ×’s for $g/t = 0.7$, pink △’s for $g/t = 0.8$, and pink ▲’s for $g/t = 1.5$. △’s: Blue V’s for $g/t = 0.7$, blue ○’s for $g/t = 0.8$, and blue ○’s for $g/t = 1.5$. The numerical calculations are performed on a $27 \times 27$ lattice with one third filling. Inset: The nearest neighbor pairing $|\langle \hat{c}_{i+e_y} \hat{c}_i \rangle|$ (green ○’s) and the superfluid fractions $\rho_{s,x}$ (pink ×’s) and $\rho_{s,y}$ (red △’s) as a function of $g$ for $T = 0$.](image)

TRAPPED SYSTEM

The harmonic trapping potential is always present in atomic gas experiments. For $T = 0$, this leads to the coexistence of superfluid and density ordered phases forming ring and island structures [12]. We now investigate these effects at a non-zero temperature.

Figure 6 (top) shows the density and the checkerboard order parameter as a function of temperature for the dipoles aligned perpendicularly to the lattice plane with $(\theta_P, \phi_P) = (0, 0)$. We have chosen $\bar{\omega} = \omega a \sqrt{m/t} = 0.24$, $g/t = 1$, and $\mu/t = 4.23$ for the numerical calculations, giving $N = 207 - 210$ dipoles trapped and an average filling fraction close to 1/2 in the center of trap. For these parameters, there is a large region in the center of the trap with checkerboard density order for $T = 0$. With increasing temperature, the radius of the checkerboard phase in the center shrinks and it melts completely for $T/t \gtrsim 0.4$. In Fig. 6 (bottom), we compare the central value of the density order parameter with that of an untrapped system at half-filling performed on a $30 \times 30$ lattice with the same interaction strength. We see that the critical temperature of the trapped system is close to that of an untrapped system. This shows that the system essentially behaves according to the local density approximation.

In Fig. 7 (top), we plot the density and the stripe or-
Numerical calculations leading to an increased density with increasing temperature is so small. The pairing increases slightly to mean-field theory to be small since the critical temperature is superfluid for $T/t = 0$ and there is no stripe order. As expected, the pairing decreases with increasing $T$ and it disappears for $T/t \approx 0.11$. The critical temperature is calculated using mean-field theory. We expect corrections to mean-field theory to be small since the critical temperature is so small. The pairing increases slightly with increasing $T$ at low temperature. This is because we for simplicity keep the chemical potential fixed in the numerical calculations leading to an increased density with increasing $T$. A number conserving calculation would yield a monotonically decreasing pairing with increasing $T$.

These results illustrate that even in the presence of a trap, one can observe the superfluid and density ordered phases predicted for the infinite lattice systems, provided the system is large enough. In particular, the transition temperature is determined by the parameters in the center of the trap, and the results for a system with no trap can be used.

**CONCLUSION**

In conclusion, we examined the density ordered and superfluid phases of fermionic dipoles in a square 2D lattice. We determined the critical temperature of the density ordered phases and demonstrated that it is proportional to the interaction strength for strong coupling. We calculated the superfluid fraction and showed that the critical temperature of the superfluid phase is proportional to the hopping matrix element for strong coupling. Finally, we analyzed the effects of the harmonic trapping potential showing that for systems of a realistic size, the density ordered and superfluid phases exist with critical temperatures close to those obtained from a local density.
approximation.

A.-L. G. is grateful to N. Nygaard for valuable discussions concerning the superfluid density and to S. Gammelmark for Fig. 1.

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