Quantum phases of a two-dimensional dipolar Fermi gas

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We examine the superfluid and collapse instabilities of a quasi two-dimensional gas of dipolar fermions aligned by an orientable external field. It is shown that the interplay between the anisotropy of the dipole-dipole interaction, the geometry of the system, and the p-wave symmetry of the superfluid order parameter means that the effective interaction for pairing can be made very large without the system collapsing. This leads to a broad region in the phase diagram where the system forms a stable superfluid. Analyzing the superfluid transition at finite temperatures, we calculate the Berezinskii–Kosterlitz–Thouless temperature as a function of the dipole angle.

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Trapped ultracold gases are increasingly being used to simulate solid-state systems, where clear experimental signatures of theoretical predictions are often lacking [1]. A limitation of these gases is that the interactions are typically s-wave [2] whereas order parameters in solid state systems exhibit richer p- and d-wave symmetries. Recent progress in the production of trapped, cold dipolar gases [3, 4, 5] promises to change this since the dipole-dipole interaction is long-range and anisotropic. Importantly, the interaction in fermionic heteronuclear Feshbach molecules can be large, with electric dipole moments on the order of a Debye [5, 6, 7]. This opens the door to experimentally reaching the superfluid phase. One complicating feature is that the gases tend to become unstable when interactions are sufficiently strong and attractive.

In this letter, we propose confining a gas of fermionic dipoles of mass $m$ in the 2D plane by a harmonic trapping potential $V_z(z) = m \omega_z^2 z^2/2$. For $\hbar \omega_z \gg \epsilon_F$ where $\epsilon_F = k_F^2/2m$ is the Fermi energy, determined by the 2D density $n_{2D} = k_F^2/4\pi$, the system is effectively 2D. The dipoles are aligned by an external field $E$ (see Fig. 1), subtending an angle $\Theta$ with respect to the $x$-$y$ plane. The interaction between two dipole moments $\mathbf{d}$ separated by $r$ is given by $V(\mathbf{r}) = D^2(1 - 3 \cos^2 \theta_{rd})/r^3$. Here, $D^2 = \epsilon_d^2/4\pi \epsilon_0$ for electric dipoles and $\theta_{rd}$ is the angle between $\mathbf{r}$ and $\mathbf{d}$. The strength of the interaction is parametrized by the dimensionless ratio $g = 2D^2 k_F^2/(3\epsilon_F)$. Since we consider identical fermions at low temperatures $T$, additional short range interactions are suppressed. We show that in this configuration, the effective interaction for pairing has p-wave symmetry and can be made large without the system collapsing. This makes the 2D system of dipoles a promising candidate to study quantum phase transitions and pairing with unconventional symmetry.

A key point is that the effective dipole-dipole interaction in the $x$-$y$ plane can be tuned by changing the angle $\Theta$. This gives rise to several interesting effects. For $\Theta = \pi/2$, the interaction is repulsive and isotropic in the $x$-$y$ plane and the dipoles are predicted to undergo a quantum phase transition to a crystalline phase for $g \simeq 27$ at $T = 0$ [8]. As $\Theta$ is decreased, the interaction becomes anisotropic in the $x$-$y$ plane and for $\Theta < \arccos(1/\sqrt{3})$, an attractive sliver appears along the $x$ axis as illustrated in Fig. 1. This gives rise to two competing phenomena: superfluidity and collapse [4]. The resulting phase diagram is shown in Fig. 2 and is the main focus of this letter.

We first examine the critical angle $\Theta_c$ below which the attractive part of the interaction overcomes the Fermi pressure and the gas is unstable towards collapse. The instability is identified with a negative value of the inverse compressibility $\kappa^{-1} = n_{2D}^2 \partial^2 E/\partial n_{2D}^2$. We analyze the stability of the dipolar Fermi gas using the normal phase
anisotropy of the interaction, by writing the superfluid and stable for Θ attractive interaction overcomes the Fermi pressure and the gas collapses. The system is superfluid and stable for Θ critical angle Θ for weak coupling, there is a contribution to the energy arising from the con- 2D limit ℏ = ℏ/2m, all dipoles reside in the superfluid and normal regions are separated by a quantum phase transition. For comparison, we also plot as dashed lines the phase diagram calculated with no Fermi surface deformation effects (α = 1).

energy density \( \mathcal{E}_n = \mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{dir}} + \mathcal{E}_{\text{ex}} \) with

\[
\mathcal{E}_{\text{kin}} = \frac{1}{(2\pi)^2} \int d^2k \frac{k^2}{2m} f_k = \frac{\pi n_D^2}{2} \frac{1}{\alpha^2 + \alpha^2}, \tag{1}
\]

the kinetic energy density. We allow for the possibility that the Fermi surface can deform due to the anisotropy of the interaction, by writing the \( T = 0 \) Fermi distribution function as \( f_k = \Theta(k_F^2 - k^2) / (\alpha^2 + k^2) \). The direct and exchange energies are \( r \equiv r_1 - r_2 \)

\[
\mathcal{E}_{\text{dir}} = -\frac{1}{2L^2} \int d^3r_1 d^3r_2 n(r_1, r_2)V(r)n(r_2, r_1) \tag{2}
\]

and

\[
\mathcal{E}_{\text{ex}} = -\frac{1}{2L^2} \int d^3r_1 d^3r_2 n(r_1, r_2)V(r)n(r_2, r_1) \tag{3}
\]

with \( n(r_1, r_2) \equiv \langle \tilde{\psi}^\dagger(r_1) \tilde{\psi}(r_2) \rangle \), \( \tilde{\psi} \) the dipolar field operator, and \( L^2 \) the size of the gas. In the superfluid phase, there is a contribution to the energy arising from the condensation energy \( \mathcal{E}_c \propto \Delta_0^2 / \epsilon_F \) which is small for \( \Delta_0 \ll \epsilon_F \). We ignore this contribution in the following.

In the 2D limit \( \hbar \omega_z \gg \epsilon_F \), all dipoles reside in the lowest harmonic oscillator level \( \Phi(z) \) in the z-direction. We then have \( n(r_1, r_2) = \Phi(z_1)\Phi(z_2)n_{2D}(\rho) \) with

\[
n_{2D}(\rho) = \int \frac{d^2k}{(2\pi)^2} f_k e^{i\mathbf{k} \cdot \mathbf{r}} = \frac{k_F}{2\pi F(\rho)} J_1 [k_F \tilde{r}(\rho)]. \tag{4}
\]

Here, \( J_1(x) \) is the Bessel function of first order, \( \rho = (x, y) \), and \( \tilde{r}(\rho) = \sqrt{x^2 + \alpha^2 y^2} \). Evaluating the integrals in \[2\] and \[3\], we find

\[
\mathcal{E}_{\text{dir}} + \mathcal{E}_{\text{ex}} = -\frac{8n_D^2}{3\pi m^2} g I(\alpha, \Theta) \tag{5}
\]

where

\[
I(\alpha, \Theta) = \int_0^{\infty} dv \int_0^{2\pi} d\phi (1 - 3 \cos^2 \Theta \cos^2 \phi) \left\{ \frac{4J_1^2(t)}{t^2} - 1 \right\} \tag{6}
\]

is a dimensionless function of the Fermi surface deformation parameter \( \alpha \) and the dipole angle \( \Theta \), and \( t \equiv v \sqrt{\alpha^2 \sin^2 \phi + \cos^2 \phi / \alpha^2} \). Equations \[1\], \[5\], and \[6\] give the energy as a function of \( g, \Theta, \phi, \alpha \). For a given coupling strength \( g \) and angle \( \Theta, \phi, \alpha \) is found by minimizing \( \mathcal{E} \). In general, this has to be done numerically. However, for small Fermi surface deformation \( \alpha \approx 1 \) we can expand \[6\] in the small parameter \( t - v \).

The resulting \( \phi \) integrals are straightforward and using \( \int_0^{\infty} dv [4J_1^2(t)/v^2 - 1] v^{-2} \approx -0.9 \) we obtain

\[
\alpha^4 \approx \frac{1 + 1.06g(1 - \frac{2}{3} \cos^2 \Theta)}{1 + 1.06g(1 - \frac{4}{3} \cos^2 \Theta)}. \tag{7}
\]

Note that \( \alpha < 1 \) as expected.

Since \( \mathcal{E} \propto n_D^2 \), it is now straightforward to evaluate the compressibility \( \kappa(\alpha, \Theta) \). The resulting region of the collapse instability is shown in Fig. 2. There is a large region where the system is stable even though the interaction is strong \( (g > 1) \) and partly attractive \( (\Theta < \arcsin(1/\sqrt{3}) \). This is most easily understood by ignoring the Fermi surface deformation \( (\alpha = 1) \), which yields \( \Theta_c \rightarrow \arcsin 1/\sqrt{3} \) for \( g \rightarrow \infty \). In this limit, the interaction energy dominates and the gas collapses when the dipole-dipole interaction is attractive in more than half the \( x \)-\( y \) plane, i.e. for \( \Theta < \arcsin 1/\sqrt{3} \). Fermi surface deformation effects are significant however; in Fig. 3 we show how \( \alpha(g, \Theta) \) deviates substantially from 1 along the critical line \( \Theta_c(g) \) for collapse.

The stability of the 2D system for a strong, attractive interaction makes it a promising candidate to observe superfluid pairing with unconventional symmetry. To investigate this, we solve the effective 2D BCS gap equation at \( T = 0 \), derived from the usual 3D BCS pairing Hamiltonian using \( \psi(\mathbf{r}) = \tilde{\psi}(\mathbf{r}) \Phi(z) \). This ansatz results in a 2D gap equation in terms of an effective interaction \( \psi(\mathbf{r}) = \int d\mathbf{z} \Phi(\mathbf{z})V(\mathbf{r}) \), where \( \Phi(\mathbf{z}) = \exp[-z^2/2\ell_z^2]/\pi^{1/4} \ell_z^{1/2} \) with \( \ell_z = \sqrt{2m\omega_z} \) is the lowest harmonic oscillator wavefunction for the reduced mass \( m/2 \). Using the rescaled momentum \( \mathbf{k} = (\tilde{k}_x, \tilde{k}_y) = (\alpha k_x, k_y/\alpha) \) to describe pairing about the deformed Fermi surface, the 2D gap equation becomes

\[
\Delta_k = -\frac{\int d^2k'}{(2\pi)^2} \tilde{V}_{2D}(\mathbf{k}, \mathbf{k}') \frac{\Delta_k}{2E_k} \tag{8}
\]
with $E_k = (\xi_k^2 + \Delta_k^2)^{1/2}$, $\xi_k = \tilde{k}^2 / 2m - \mu$, and $\mu$ the chemical potential. $V_{2D}(k, k')$ is the Fourier transform

$$V_{2D}(k, k') = \int d^2 \rho \sin(k \cdot \rho) V_{2D}(\rho) \sin(k' \cdot \rho). \quad (9)$$

of $V_{2D}(\rho)$, expressed in terms of the scaled momenta $\tilde{k}, \tilde{k}'$; i.e. $V_{2D}(\tilde{k}, \tilde{k}') = V_{2D}(k, k')$. Note that only sin components contribute to the Fourier series since the order parameter is antisymmetric. The Pauli exclusion principle therefore cancels the short range $r^{-3}$ divergence in the dipole-dipole interaction, making the Fourier transform (9) finite even in the 2D limit.

Using the expansions $\Delta_k = \sum_{n=1}^{\infty} \Delta_n (\tilde{k}) \cos[(2n - 1)\phi]$ and $\tilde{V}_{2D}(\tilde{k}, \tilde{k}') = \sum_{nn'} \tilde{V}_{nn'}(\tilde{k}, \tilde{k}') \cos(2n - 1)\phi \cos(2n' - 1)\phi'$ in (8), where $\phi$ is the angle between $\tilde{k}$ and the $x$ axis, we find numerically that $V_{nn} \gg V_{nn'}$ for $n' \neq n$ and all angles $0 \leq \Theta \leq \pi/2$. This shows that to a very good approximation the gap is $p$-wave, $\Delta_k = \Delta_0 \cos \phi$, and we can replace $\tilde{V}_{2D}(\tilde{k}, \tilde{k}')$ with $V_{11}(\tilde{k}, \tilde{k}') \cos \phi \cos \phi'$. Using this in (8), it reduces to

$$1 = -\frac{4\pi g_s / m}{m} \int d^2 \tilde{k}' \frac{g_s(\tilde{k}, \tilde{k}') \cos^2 \phi'}{2E_{k'}} \quad (10)$$

where $4\pi g_s / m \equiv V_{11}$.

The dimensionless effective pairing interaction $g_s$ corresponds to the dipole-dipole interaction averaged over the deformed Fermi surface, weighted by the $p$-wave symmetry of the order parameter. After a straightforward but lengthy calculation, we find

$$g_s(k, k') = gM(k, k')I_s[\Theta, \alpha(g, \Theta)] \quad (11)$$

Here, $I_s$ and $M$ are dimensionless functions given by

$$I_s = \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{(1 + \cos 2\phi)(1 - 3\cos^2 \phi \cos^2 \phi')}{(\alpha^2 \cos^2 \phi + \sin^2 \phi / \alpha^2)^{3/2}} \quad (12)$$

and $M(k, k') = \frac{k'^2}{2\pi} \int [(1 + x)E(x) + (x - 1)K(x)] \frac{d\phi}{2\pi} \cos(2k'\phi)$ for $k < k'$ and $k'\ell_z < 1$; for $k' < k$ one simply swaps $k$ and $k'$. $\ell(z) = E(2) = 1.5, 2, 3$ for collapse. This gives the largest possible attractive pairing interaction, before the system collapses. We see that the effective pairing interaction increases monotonically with $g$ and can become very large. Thus, one can produce a strongly paired gas without the system collapsing. This should be compared with the 3D trapped case where recent results indicate that the system is superfluid and stable only in a narrow range in phase space where the pairing is relatively weak [13]. Solving the gap equation in the weak coupling regime yields $\Delta_0(\Theta) = \epsilon_F e^{-1/2} \sqrt{x} e^{1/2g_s}$ for $g_s < 0$. The resulting superfluid phase transition is infinite order in the sense that $\partial g_0 |_{\Theta = 0} = 0$ for all $n$.

At finite temperatures, long-range order is destroyed by phase fluctuations in 2D, and the superfluid phase transition is infinite order in the sense that $\partial g_0 |_{\Theta = 0} = 0$ for all $n$. The superfluid density remains finite, however, descri-
ing a Berezinskii-Kosterlitz-Thouless (BKT) superfluid of bound vortex-antivortex pairs [11]. The critical temperature \( T_{BKT} \) for this phase is the temperature at which the free energy of a single unbound vortex vanishes [12],

\[
T_{BKT} = \frac{\pi \hbar^2}{8 m^2 k_B \rho_s}.
\]  

Here, \( \rho_s = (\rho_{s,xx} + \rho_{s,yy})/2 \) is the average of the diagonal components of the superfluid mass density tensor \( \rho_{s,ij} \). In estimating the energy \( E = \frac{1}{2} \int d^2 r \rho_{s,ij} v_i v_j \approx \frac{\pi k_i^2}{4m} \ln \left( \frac{L}{a} \right) \rho_s \) of a single vortex of radius \( a \) in a 2D box with sides of length \( L \), we have assumed that the contribution from the off-diagonal component \( \rho_{s,xy} v_x v_y \) due to the anisotropy of the vortex velocity field is small. Generalizing the usual expression for \( \rho_{s,ij} \) [13] to allow for the effects of Fermi surface deformation, one finds

\[
\rho_{s,ij} = mn\delta_{ij} - \frac{\beta}{4} \sum_k \text{sech}^2 \left( \frac{\beta E_k}{2} \right) k_i k_j.
\]

As shown in the inset of Fig. 4 rotational symmetry is broken by the external field and \( \rho_{s,xx} > \rho_{s,yy} \). The \( g \) component of the superfluid density tensor is suppressed since the quasiparticle spectrum is gapless in the direction perpendicular to the field.

Since \( \rho_s \) depends on \( T \), (13) has to be solved self-consistently. We determine \( \rho_s(T) \) from (13) using a \( T \)-dependent gap \( \Delta_k(T) \) calculated by including the usual Fermi functions in the gap equation. The critical temperature determined this way is plotted in Fig. 4 for \( g = 0.2 \). We also plot the mean field transition temperature \( T^* \) obtained from the gap equation. Phase fluctuations suppress \( T_{BKT} \) below \( T^* \). For weak coupling, \( T_{BKT} \approx T^* \). Since \( T^* \propto \sqrt{\epsilon_F \hbar \omega_c} \) and \( n_{2D} \propto \epsilon_F \), we have \( T_{BKT} \propto n_{2D}^{1/2} \). This suggests that one can cross the critical temperature by adiabatically expanding the gas keeping \( T/\epsilon_F \) constant so that \( T/T_{BKT} \propto n_{2D}^{-1/2} \) decreases [13]. For stronger interactions, \( T_{BKT} \) quickly approaches its upper bound \( T_{BKT} \propto T/16 \propto n_{2D} \).

Let us consider the experimental requirements for observing the effects discussed in this letter. Recently, a gas of \(^{40}\text{K}\)-\(^{87}\text{Rb}\) polar molecules was created with a density of \( n \sim 10^{12}\text{cm}^{-3} \) at a temperature \( T/T_F \gtrsim 2 \) [3]. These molecules have dipole moments of 0.57 Debye in their vibrational ground state. Writing \( g \approx 2\pi^2 a^{-1} N_A/100 \), where \( d = d/1\text{Debye} \) is the dipole moment in Debyes, \( a = a/1\mu\text{m} \) is the interparticle spacing measured in \( \mu\text{m} \), and \( N_A = m/m_n \) is the mass of the dipole in atomic mass units, the experimental parameters of Ref. [8] give \( g \approx 0.8 \). Also, the creation of 2D systems has already been achieved for bosons [10]. The observation of the effects discussed in this letter is therefore within experimental reach once further cooling has been achieved.

In conclusion, we studied the quantum phases of a dipolar Fermi gas in 2D aligned by an external field. We demonstrated that by partially orienting the dipoles into the 2D plane, they can experience a strong \( p \)-wave pairing attraction without the system collapsing. This makes the system a promising candidate to study quantum phase transitions and pairing with unconventional symmetry. We also analyzed the BKT transition to the normal state at non-zero \( T \). Stimulating discussions with S. Stringari are acknowledged.

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