Reentrant Superfluidity and Pair Density Wave in Single Component Dipolar Fermi Gases

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We study the superfluidity of single component dipolar Fermi gases in three dimensions within a pairing fluctuation theory. The transition temperature $T_c$ for the dominant $p_x$ wave superfluidity exhibits a remarkable re-entrant behavior as a function of the pairing strength induced by the dipole-dipole interaction (DDI), which leads to an anisotropic pair dispersion. The anisotropy and the long range nature of the DDI cause $T_c$ to vanish for a narrow range of intermediate interaction strengths, where a pair density wave state emerges as the ground state. The superfluid density and thermodynamics below $T_c$, along with the density profiles in a harmonic trap, are investigated as well, throughout the BCS-BEC crossover. Implications for experiments are discussed.

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Recent experimental realization of quantum degenerate Fermi gases of magnetic atoms \[1\] and the rapid progress toward creating degenerate polar molecules \[2, 3\] have opened a new frontier for exploring novel phases of quantum gases, where dipole-dipole interaction (DDI) plays a central role. A lot of attentions have been paid to unconventional $p$-wave superfluids \[4, 5\] in three dimensions (3D) and topological superfluid phases \[6\] in two dimensions (2D). The latter has been associated with Majorana fermions and can be used for topological quantum computation \[7\]. Such exotic superfluid phases emerge from the long-range DDI with a strong anisotropy, which is different from the widely studied contact potential in dilute atomic gases. Moreover, the relative DDI strength can be tuned by changing the fermion number density $n$ (or Fermi wavevector $k_F$) and, in the case of polar molecules \[3\], by varying an external electric field strength.

Of particular interest is the intermediate pairing strength regime, where complex physics beyond the weak coupling BCS theory arises and the superfluid transition temperature $T_c$ is relatively high, making it more practical to access the superfluid phase experimentally. For a contact potential, the entire BCS–Bose-Einstein condensation (BEC) crossover from weak to strong coupling regimes has been studied intensively in two-component Fermi gases of $^6$Li or $^{40}$K. In contrast, such a crossover in dipolar Fermi gases, where richer physics may arise, is yet to be explored. Existing theoretical studies in this aspect mostly focus on the ground state, based on mean field treatments \[4, 5, 8, 10\], which are inadequate in addressing moderate and strong coupling regimes at finite temperature.

In this Letter, we address the superfluidity and pairing phenomena of single component dipolar Fermi gases in 3D, with an emphasis on the finite temperature and interaction effects. Built on previous work \[11, 12\] that has been applied successfully to address various BCS-BEC crossover phenomena in two-component Fermi gases with a contact interaction \[12, 13\], here we construct a pairing fluctuation theory for the superfluidity of one-component dipolar fermions, in which thermally excited pairs naturally give rise to a pseudogap in the fermion excitation spectrum. We find that (i) the DDI leads dominantly to a $p_x$-wave superfluid, and the superfluid $T_c$ curve exhibits a re-entrant behavior as a function of the DDI strength; in the intermediate regime of the BCS-BEC crossover, $T_c$ vanishes and the ground state becomes a pair density wave (PDW), similar to the PDW state studied in underdoped high $T_c$ superconductors \[14, 15\]. (ii) In the fermionic regime, the temperature dependence of superfluid density and low $T$ thermodynamic quantities exhibit power laws, in stark contrast to the contact interaction case \[16\]. (iii) Within a local density approximation (LDA), the density profile in an isotropic harmonic trap exhibits a similar qualitative behavior to its $s$-wave counterpart, despite the different pairing symmetry.

We consider an ultracold gas of one-component dipolar fermions of mass $m$ in unit volume, with dipole moment $d = d\hat{z}$, polarized in the $\hat{z}$ direction. The many-body Hamiltonian is given by $\hat{H} = \hat{H}_0 + \hat{H}_I$, where $\hat{H}_0 = \sum_k \xi_k c_k^\dagger c_k$ is the non-interacting term, with fermion energy $\xi_k = k^2/(2m) - \mu$ measured with respect to the chemical potential $\mu$. (we take $\hbar = k_B = 1$). The field operator $c_k^\dagger$ ($c_k$) creates (annihilates) a dipolar fermion with momentum $k$ \[17\]. The interaction Hamiltonian $\hat{H}_I$ reads

$$\hat{H}_I = \frac{1}{2} \sum_{k,k',q} V_{k,k'} c_{k+q/2}^\dagger c_{-k-q/2}^\dagger c_{-k+q/2} c_{k-q/2},$$

We shall write the pairing interaction $V_{k,k'}$ into an effective separable form \[18\], i.e., $V_{k,k'} = g\varphi_k \varphi_{k'}^\ast$, where $g$ is the pairing strength, $\varphi_k$ is the symmetry factor with an odd parity and will be determined by the DDI.

Following previous work \[13, 20\], a sequence of equations of motion for the $n$-particle Green’s function (or propagator) $G_n$, with $n = 1, 2, 3, \ldots$, are obtained from the real space representation of the many-body Hamiltonian \[19\]. For the pairing problem, 2-particle correlations are of primary interest, and thus the sequence is truncated at the $G_3$ level, with
\[ \Sigma_{pg} = \begin{array}{c|c}
| & \\
\hline
\tau & t \\
\end{array} + \begin{array}{c|c}
| & \\
\hline
\tau & t \\
\end{array} \]

Figure 1. (Color online) Feynman diagrams for the pairing fluctuation self-energy \( \Sigma_{pg} \) and \( T \)-matrix. The thin solid, thick solid and dashed lines represent the bare propagator \( G_0 \), dressed propagator \( G \) and DDI, respectively.

fully connected 3-particle diagrams dropped [22]. The result can be naturally cast into a diagrammatic \( T \)-matrix approximation, with a \( G_0 G \) scheme for the pair susceptibility, i.e., \( \chi = G_0G \), where \( G_0 \) \((G)\) is the bare (full) fermion Green's function. The \( T \) matrix \( t \) represents connected 2-particle diagrams, as shown in Fig. 1 consisting of particle-particle scattering ladders. Noncondensed pairs are treated on an equal footing with single particle propagators. In contrast to the \( s \)-wave singlet pairing, an extra exchange diagram has now been retained in the self energy, as shown in Fig. 1. Finally, we obtain in the momentum space the fermion self-energy from noncondensed pairs

\[ \Sigma_{pg}(K) = \Sigma^{\text{direct}}_{pg}(K) + \Sigma^{\text{exchange}}_{pg}(K) = \sum_{Q \neq 0} t(Q)G_0(Q - K)\bar{\varphi}_{k - \mathbf{q}/2}^*\bar{\varphi}_{k - \mathbf{q}/2} - \sum_{Q \neq 0} t(Q)G_0(Q - K)\bar{\varphi}_{k - \mathbf{q}/2}^*\bar{\varphi}_{k - \mathbf{q}/2 - \mathbf{k}}, \]

where \( t(Q) = 1/[g^{-1} + \chi(Q)] \), with \( \chi(Q) = \sum_K G(K)G_0(Q - K)|\varphi_{k - \mathbf{q}/2}|^2 \). Here we use a four vector notation, \( K \equiv (i\omega_n, \mathbf{k}) \), \( Q \equiv (i\omega_l, \mathbf{q}) \), \[ \sum_{Q} = T\sum_i\sum_{\mathbf{q}}, \] etc., with \( \omega_n \) and \( \Omega_l \) being odd and even Matsubara frequencies, respectively. Note that \( \varphi_{k} \) may be complex in general, with

\[ |\varphi_{k}^2| = \varphi_{k}^*\varphi_{k} \]

where \( \varphi_{k} \) is the Bogoliubov quasiparticle.

At and below \( T_c \), a superfluid condensate develops at \( Q = 0 \), with \( t^{-1}(0, 0) = 0 \), which is called the Thouless criterion. The condensate self-energy is \( \Sigma_{sc}(K) = -\Delta^2_{sc}G_0(-K)|\varphi_{k}|^2 \), as in BCS theory [21], with the superfluid order parameter \( \Delta_{sc} \). Furthermore, the finite \( \mathbf{q} \) pair propagator \( t_{pg}(Q) \) can be expanded as \( t_{pg}(Q) = Z(i\Omega_l - \Omega_q + \mu_{\text{pair}} + iD\Omega_{l\mathbf{q}}) \), with an effective pair dispersion \( \Omega_q = \sqrt{\Omega^2_{l\mathbf{q}}/(2M^*_l)} + q^2_0/(2M^*_l) \) and an effective pair chemical potential \( \mu_{\text{pair}} \). Here the inverse residue \( Z \) and the (anisotropic) effective pair mass \( M^*_l = M^*_s = M^*_l \) and \( M^*_l \) can be determined in the process of Taylor expansion. Note that the pair mass anisotropy is a consequence of the anisotropic DDI. For \( T \leq T_c \), the BEC condition requires \( \mu_{\text{pair}} = 0 \). For small \( \Omega_q \), \( \Gamma_{l\mathbf{q}} \ll \Omega_q \). Therefore, \( t_{pg}(Q) \) is strongly peaked at \( Q = (0, 0) \), so that \( \Sigma_{pg} \) can be approximated as \( \Sigma_{pg}(K) \approx -\Delta^2_{pg}G_0(-K)|\varphi_{k}|^2 \). With the odd parity \( \varphi_{-\mathbf{k}} = -\varphi_{\mathbf{k}} \), we have defined the pseudogap \( \Delta_{pg} \) as

\[ \Delta^2_{pg} = -\sum_{Q} t_{pg}(Q) \approx 2Z^{-1} \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}}), \]

where \( b(x) \) is the Bose distribution function. This leads to the BCS form of the total self-energy, \( \Sigma(K) = \Sigma_{sc}(K) + \Sigma_{pg}(K) = -\Delta^2G_0(-K)|\varphi_{k}|^2 \), with a total excitation gap \( \Delta = \sqrt{\Delta^2_{sc} + \Delta^2_{pg}} \). Then the Green’s function \( G \) is given by the Dyson’s equation, \( G^{-1}(K) = G_0^{-1}(K) - \Sigma(K) \). After evaluating the sum over Matsubara frequencies, the Thouless criteria \( t^{-1}(0) = 0 \) gives the gap equation

\[ 1 + g \sum_{k} \frac{1 - 2f(E_k)}{2E_k}|\varphi_{k}|^2 = 0, \]

where \( E_k = \sqrt{\xi^2_k + \Delta^2_k} \) is the Bogoliubov quasiparticle dispersion and \( f(x) \) is the Fermi distribution function. In addition, we have the fermion number equation

\[ n = \sum_{K} G(K) = \sum_{k} \left[ \psi^2_k + \frac{\xi_k}{E_k} f(E_k) \right], \]

where \( \psi^2_k = \frac{1}{2}(1 - \frac{\xi_k}{E_k}) \) is the BCS coherence factor.

Now we determine the symmetry factor \( \varphi_{k} \) from the DDI,

\[ V_d(r) = d^2 \frac{1 - 3\cos^2\theta}{r^3}, \]

where \( d^2 = 2D/m \) is the DDI strength, with the dipole length \( D = md^2/2 \), and \( \theta_r \) is the polar angle of \( r \). \( V_d(r) = V(r)Y_{2,0}(\theta_r, \phi_r) \), where \( V(r) = -\frac{16\pi x}{d^2/3} \) is the radial part and the angular part \( Y_{2,0}(\theta_r, \phi_r) \) is the spherical harmonic \( Y_{lm}(r) \) with \( l = 2 \) and \( m_l = 0 \). So the DDI breaks \( SO(3) \) symmetry and mixes the odd partial waves. Now we expand \( V_{k,k'} \) in terms of partial waves as

\[ V_{k,k'} = \sum_{l' l} \sum_{m_{lm}} g_{lm_{lm'}}(k, k')Y_{lm}(k)Y^{*\text{lm'}}_{l'm'}(k'), \]

with

\[ g_{lm_{lm'}}(k, k') = \left\{ \begin{array}{cc} \frac{1}{2} & l \neq l' \ \text{or} \ |m| = |m'| \\text{and} \ \Delta_{lm} \neq \Delta_{l'm'}; \\
-\frac{1}{2} & l = l' \ \text{and} \ |m| = |m'|; \\
\frac{1}{4} & l' = l \ \text{and} \ |m| \neq |m'|; \\
\frac{1}{4} & \text{other cases}; \end{array} \right. \]

and \( w_{l,l'}(k, k') = \int_0^\infty r^2 dr j_{|l|}(kr)V(r)j_{|l'|}(kr'), \) where \( j_{|l|}(kr) \) is the spherical Bessel function.

Note that for a single component Fermi gas, only odd \( l \) and \( l' \) are allowed, with \( l' = l, \pm 2 \). The \( r^{-3} \) dependence of the DDI leads to a \( k \)-independent \( w_{l,l'}(k, k) \). Detailed analyses show that the dominant attractive channel in \( V_{k,k} \) is the \( l = 1, m_l = 0 \), i.e., \( p_z \), wave, where \( g_{10}(k, k) < 0 \) is the leading order term, with \( g_{00}(k, k) \approx 0.1g_{10}(k, k) \) being the next leading order term. The leading hybridization terms with \( l = 1, l' = 3 \) are repulsive. Therefore in our numerical calculation we concentrate on the leading channel with a \( p_z \) wave symmetry.

To remove the ultraviolet divergence in the momentum integral of the gap equation, caused by the \( k \) independence of \( w_{l,l'}(k, k) \), we regularize the DDI by multiplying a convergence factor \( F(r/r_0) \), where \( r_0 \) is the typical radius beyond which the DDI becomes dominant. We choose \( F(x) = \frac{1}{1 - e^{-x^2}(1 + x^2)} \), similar to that used in Ref. 23 but here the regularized DDI approaches a finite negative value as \( r \to 0 \), as shown in Fig. 2a. This regularization is justified in that the actual interaction necessarily deviates from the strict DDI at a distance closer than or comparable to the size of the atoms...
(or molecules). Finally, we arrive at a modified $p_z$ wave symmetry factor

$$ |\varphi_k|^2 = \frac{1}{2\eta^2} \left[ 1 - \frac{\ln(1 + 4\eta^2)}{4\eta^2} \right] \cos^2 \theta_k, \quad (7) $$

where $\eta = k/k_0 = kr_0$ and $\theta_k$ is the polar angle of $k$. Note that here $\varphi_k$ is real. Interestingly, the $k$ dependence of this $\varphi_k$ is quantitatively very close to a rescaled $s$-wave Lorentzian symmetry factor used in Ref. [18], $|\varphi_k|^2_{\text{NSR}} = \frac{1}{1 + (k/k_0)^2}$, as can be seen from Fig. 2(b). For comparison, we also plot the $k$ dependence of the $p$-wave symmetry factor, $|\varphi_k|^2 = \frac{(k/k_0)^2}{1 + (k/k_0)^2}$, induced by a short-range interaction $V_{\text{short}}$ [23, 24]. The partial wave scattering amplitude $f_k^l \sim V_{kk} \sim |\varphi_k|^2$ in the low energy limit. For a short-range interaction, $f_k^l \sim a_k/k^2$ as $k \to 0$, where, for $l = 1$, $a_l$ is the scattering volume. In contrast, for the present DDI, even though the angular dependence is in the $p$-wave channel, the scattering amplitude behaves similar to the short range $s$-wave case, giving rise to a well-defined scattering length rather than scattering volume. Indeed, the strict $V(r)$ gives rise to a completely $k$ independent scattering amplitude [5, 25], as is the $k_0 \to +\infty$ limit of Eq. (7).

Now with the symmetry factor given by Eq. (7), Eqs. (3), (4) and (5) form a close set, which can be solved self-consistently for $T_c$ as a function of $g = -24\pi D/(5m)$, as well as for gaps below $T_c$ as a function of $T$. The unitary limit corresponds to the critical coupling strength $g_c = -18\pi m k_0$, at which the scattering length diverges and a bound state starts to form, as determined by the Lippmann-Schwinger equation [22, 26] $g_c^{-1} = \sum_k |\varphi_k|^2$ with $\epsilon_k = k^2/(2m)$. Thus $g/g_c = 4k_0D/15 = 4\lambda k_FD/15$ with $\lambda = k_0/k_F$. In our numerical calculations we take $\lambda = 20$, corresponding to a dilute case.

We first present in Fig. 3(a) the calculated $T_c$ and corresponding $\mu$ and pseudogap $\Delta_{\text{pg}}$ at $T_c$ as a function of pairing strength, which are obtained by setting $\Delta_{ac} = 0$. For comparison, the mean-field solution $T_{c\text{MF}}$ is also shown in Fig. 3(a) (red dashed curve). In the weak coupling regime, $T_c$ follows the mean-field BCS result. It starts to decrease after it reaches a maximum around unitarity $g/g_c = 1$, due to the shrinking Fermi surface. Remarkably, it exhibits a re-entrant behavior. For a range of intermediate pairing strength, $T_c$ shuts off completely, before it recovers at stronger couplings, where the system has entered the BEC regime, with $\mu < 0$. In the BEC regime, all fermions are paired. With $M^*$ approaching $2m$ and $n_{\text{pair}} = n/2$, $T_c$ approaches the BEC asymptote, $0.137T_F$, from below. The pseudogap at $T_c$ increases monotonically with $g/g_c$.

In order to understand the re-entrant $T_c$ behavior, we plot the inverse pair masses in the lower inset of Fig. 3(b). It reveals that, when $T_c$ vanishes at the intermediate pairing strength, the effective pair mass in the dipole direction, $M^*$, at zero momentum becomes negative, so that the pair dispersion $\Omega_q$ in the $\hat{z}$-direction becomes roton-like [27], with a minimum at a finite $q_z$, as shown schematically in the lower left inset of Fig. 3(b) (solid curve). The pair mass in the $xy$-plane remains positive. This corresponds to a pair density wave ground state, with a crystallization wavevector $q_z$ in the $z$-direction. Similar PDW states were extensively investigated in high $T_c$ superconductors in the quasi-2D context [14, 15].

We note that the emergence of the PDW state has to do with the long range nature of the DDI, which essentially put the
system in the high density regime. At the same time, due to the $p_z$ symmetry, the coherence length $\xi \sim v_F/\Delta_k$ diverges in the nodal $xy$-plane (i.e., $k_z = 0$) so that the order parameter $\Delta \varphi_k$ exhibits a non-local effect similar to the case of a $d_{x^2-y^2}$-wave superconductor [28]. (Here $v_F$ is the Fermi velocity). Such a diverging coherence length makes it difficult for the pairs to move in the $k_z$ direction. At certain intermediate interaction strength, pairing is strong while the pair size is large, so that the strong interaction between pairs (as reflected in the effective pair mass) may dominate the kinetic energy of the pairs, in favor of forming a Wigner-like crystal structure.

In the absence of an underlying lattice potential, this PDW state is distinct from a Mott state. Instead, it may exhibit behaviors of a Bose metal [22, 29]. The presence of the PDW manifests a Bose “surface” for pair excitations [31], whose energy vanishes at a finite momentum $q_z$ (with $q_x = q_y = 0$). While the pair dispersion remains positive in the $xy$ plane, the two dimensionality destroys the long range superfluid order, leading to a metallic ground state with a density wave of Cooper pairs in the $k_z$ direction. The nature of the PDW state deserves further systematic investigations [32].

It should be mentioned that the chemical potential $\mu$ changes sign within the PDW regime. In the fermionic transition [23, 33]. The anisotropy in the pair mass is a consequence of the DDI. We emphasize that the re-entrant behavior of $T_c$ is robust against changes of $k_0$ and independent of the regularization scheme. It is also present in the next leading order, $f_z$-wave channel.

Next we investigate the transport and thermodynamics behavior in the superfluid phase. The superfluid density can be derived using a linear response theory. Following Ref. [11], we obtain

\[
n_s = \frac{m \Delta^2}{3} \sum_k \left[ \frac{1}{2} \frac{1 - f(E_k)}{E_k} + f'(E_k) \right] \times \left[ (\nabla_k \varphi_k)^2 |\varphi_k|^2 - \frac{1}{4} (\nabla_k \varphi_k)^2 \cdot (\nabla_k |\varphi_k|^2) \right], \tag{8}
\]

where $f'(x) = df(x)/dx$. It can be shown that $n_s(0) = n$. At $0 < T < T_c$, both Bogoliubov quasiparticles (with energy $E_k$) and pair excitation (with energy $\Omega_q$) contribute to the thermodynamics. This leads to the specific heat $C_v = \sum_k E_k \partial f(E_k)/\partial(E_k) + \sum_q \Omega_q \partial f(\Omega_q)/\partial(\Omega_q)$.

Shown in Fig. 4 are the $T$ dependencies of (a) $n_s$ and (b) $\gamma = C_v/T$, for $g/g_c = 0.85, 1.0, and 1.5$, corresponding to BCS, unitary and BEC regimes, respectively. These two quantities are sensitive to the spectrum of the elementary excitations. Due to the line node on the Fermi surface of the $p_z$-wave superfluid, the low energy density of states $N(E)$ is linear in $E$. Therefore, the low $T$ superfluid density and specific heat exhibit power laws in contrast to the exponential behavior of an $s$-wave superfluid. In the BCS regime, both the low

Figure 4. (Color online) Transport and thermodynamic behavior. (a) $n_s/n$ and (b) $\gamma(T)/\gamma(T_c)$ as a function of $T/T_c$ for $g/g_c = 0.85$ (BCS), 1.0 (unitary), and 1.5 (BEC), and log-log plot of (c) $1-n_s/n$ and (d) $\gamma(T)/\gamma(T_c)$ vs $T/T_c$.

Finally, we consider the effect of a 3D isotropic harmonic trap of frequency $\omega$ with a trapping potential $V_{\text{trap}}(r) = \frac{1}{2}m\omega^2 r^2$. We assume that $E_F$ is large enough to justify the use of LDA [34, 35]. Then $\mu$ is replaced by $\mu(r) = \mu_0 - E_{\text{trap}}(r)$, where the global chemical potential $\mu_0$ is determined by the total fermion number constraint, $N = \int_{\text{trap}} n(r)d^3r$, with local density $n(r)$. Outside the superfluid core, a non-vanishing $\mu_{\text{pair}}(r)$ is included so that the gap and the pseudogap equations are extended as $t^{-1}(0,0) = Z\mu_{\text{pair}}$ and $\Delta^{2}_{\mu_q} = 2Z^{-1}\sum_q b(\Omega_q - \mu_{\text{pair}})$, respectively. Shown in Fig. 5 is the evolution of the density profile from low to high $T$, throughout the BCS-BEC crossover. Despite the anisotropic pairing interaction, the density profile remains isotropic under LDA. It broadens with increasing temperature whereas it shrinks with increasing DDI strength, similar to its $s$-wave counterpart with a contact potential [35].

Recent studies [36–38] based on Hartree-Fock theory suggest that the normal state 3D dipolar Fermi gas is subject to collapse and phase separation instabilities in the high density and strong DDI regime. For the dilute case considered in the present work, the Hartree-Fock self-energy, proportional to $n^2$, is relatively weak. Our calculations show that the compressibility for paired superfluid phase at $T \leq T_c$ remains positive definite throughout the BCS-BEC crossover, ensuring a stable superfluid state.

In summary, our study of single-component dipolar Fermi
gases reveals a re-entrant behavior of a \( p_z \)-wave superfluid transition \( T_c \) and a PDW state in a range of intermediate DDI strength. Such a PDW state as well as the \( p_z \)-wave superfluid phase may be detected using local density measurements, Bragg spectroscopy and momentum resolved rf spectroscopy.

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\[ T_{TF} \]

\[ T / T_F = 0.01, 0.15 \text{ and } 0.25 \]

\[ g/g_c = 0.85 \text{ (BCS), } 1.0 \text{ (unitary) and } 1.5 \text{ (BEC).} \]

Here \( R_{TF} \) is the Thomas-Fermi radius and the density \( n \) is in units of \( k_F^{-3} \).

Figure 5. (Color online) Comparison of density profiles in an isotropic harmonic trap at \( T / T_F = 0.01, 0.15 \) and 0.25 and pairing strengths \( g/g_c = 0.85 \) (BCS), 1.0 (unitary) and 1.5 (BEC). Here \( R_{TF} \) is the Thomas-Fermi radius and the density \( n \) is in units of \( k_F^{-3} \).

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