Unconventional Spin Density Waves in Dipolar Fermi Gases

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The conventional spin density wave (SDW) phase \[\text{SDW}_\sigma\] as found in antiferromagnetic metal for example \[\text{SDW}_\sigma\] can be described as a condensate of particle-hole pairs with zero angular momentum, \(\ell = 0\), analogous to a condensate of particle-particle pairs in conventional superconductors. While many unconventional superconductors with Cooper pairs of finite \(\ell\) have been discovered, their counterparts, density waves with non-zero angular momenta, have only been hypothesized in two-dimensional electron systems \[\text{ESDW}_\sigma\]. Using an unbiased functional renormalization group analysis, we here show that spin-triplet particle-hole condensates with \(\ell = 1\) emerge generically in dipolar Fermi gases of atoms \[\text{He}^3\] or molecules \[\text{He}^4\] on optical lattice. The order parameter of these exotic SDWs is a vector quantity in spin space, and, moreover, is defined on lattice bonds rather than on lattice sites. We determine the rich quantum phase diagram of dipolar fermions at half-filling as a function of the dipolar orientation, and discuss how these SDWs arise amidst competition with superfluid and charge density wave phases.

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The lattice is aligned along the nearest neighbor hopping \( t \) briefly further down. The characteristic scale for \( V_t \) is \( V_t = d^2/a^3 \), with \( a \) the lattice spacing. \( V_t \) depends also sensitively on the orientation of the dipoles labelled by angles \((\theta, \phi)\). (a) The conventional antiferromagnetic spin density wave (SDW\(_s\)). (b) Checkerboard charge density wave (CDW\(_s\)), where "charge" is defined as the total density. (c) An example of \( p\)-wave spin density waves (SDW\(_p\)) with modulation of \( y \) bond variables. (d) An example of mixed (extended) \( s\)- and \( d\)-wave spin density waves (SDW\(_{s+d}\)). Red arrows in (c) and (d) indicate the direction of the spin vector \( \mathbf{S} \) defined on the bonds (yellow ellipsoids).

Dipolar Fermi gas \cite{24,26} in an optical square lattice at half filling. The two pseudo-spin states can be two hyperfine states of Dy atoms, or two rovibrational states of KRb molecules. This provides a tunable platform for quantum simulation of interacting fermions with long-range interactions \cite{21,22}, beyond the Fermi-Hubbard model. The system is described by the Hamiltonian

\[
\hat{H} = -\sum_{\langle i,j \rangle, \sigma} t \hat{a}_{j, \sigma}^\dagger \hat{a}_{i, \sigma} + \frac{U}{2} \sum_{i, \sigma} \hat{n}_{i, \sigma} \hat{n}_{i, -\sigma} + \sum_{i \neq j} V_{ij} \hat{n}_i \hat{n}_j. \tag{1}
\]

The lattice is aligned along the \( x \)- and \( y \)-directions, with nearest neighbor hopping \( t \) and on-site interaction \( U \). \( U \) contains contributions from the bare short range interaction \( U_{\text{short}} \), and the on-site dipolar interaction \( V_{ij}^d \), defined below. We assume that all dipoles are aligned in the same direction \( \mathbf{d} = d(\hat{d}, \theta, \phi) \) by an external magnetic (or electric) field. In general, the off-site dipole-dipole interaction can be decomposed into equal- and unequal-spin components, labeled by \( \parallel \) and \( \perp \), respectively, \( V_{ij}^{\parallel/\perp} \hat{n}_{i, \sigma} \hat{n}_{j, \sigma} + V_{ij}^{\perp/\parallel} \hat{n}_{i, \sigma} \hat{n}_{j, -\sigma} \), and depends on \( \hat{d} \) and \( \mathbf{r} = \mathbf{r}_i - \mathbf{r}_j \) via \( V_{ij}^{\parallel/\perp}(\hat{d}) \equiv V_{ij}^{\parallel/\perp}(\hat{d}) = \langle ij | V_{\text{dd}}^{\parallel/\perp}(\hat{d}) | ij \rangle = V_{dd}^{\parallel/\perp}(1 - 3(\hat{r} \cdot \hat{d})^2)/r^3 \). We will mostly assume \( V_{d}^{\parallel}(\hat{d}) = V_{d}^{\perp}(\hat{d}) \equiv V_{d}(\hat{d}) \) as in Eq. 1, which arises naturally when the two states are associated with the same hyperfine manifold. The \( V_{d}^{\parallel}(\hat{d}) \neq V_{d}^{\perp}(\hat{d}) \) case will be discussed briefly further down.

To give a heuristic argument about possible orders of the system, we consider a simplified version of model \( \mathbb{1} \) retaining only the nearest and next-nearest neighbor dipolar interactions, denoted \( V_{\hat{d}(\hat{y})} \) and \( V_{\hat{x}+\hat{y}} \) respectively, see Fig. 1. First, for \( \hat{d} = \hat{z} \), dipolar interactions are purely repulsive. For \( U \gg V_d \), the Hamiltonian reduces to the Fermi-Hubbard model, implying a ground state with SDW\(_s\) order at half-filling, Fig. 1(a). For \( U \ll V_d \), the dipolar energy is reduced by placing same-spins on diagonally opposite sites, while opposite spins share the same site with only a small energy cost \( U \). This implies a checkerboard modulation of the total density \( n_i = \langle \hat{n}_i \rangle \), i.e. CDW\(_s\), shown in Fig. 1(b).

As \( \hat{d} \) is tilted away from \( \hat{z} \) towards the \( \hat{x} \)-direction, there exists a region of tilting direction for which the nearest neighbor interaction \( V_{\hat{d}} \) 

As \( \hat{d} \) is tilted away from \( \hat{z} \) towards the \( \hat{x} \)-direction, there exists a region of tilting direction for which the nearest neighbor interaction \( V_{\hat{d}} \) becomes attractive while \( V_{\hat{y}} \) and \( V_{\hat{x}+\hat{y}} \) remain repulsive. For instance, for \( \phi = 0 \), this region is bounded by two critical values of \( \theta \): \( \theta_{c1} = \cos^{-1}((\sqrt{2}/3) \approx 35^\circ \) and \( \theta_{c2} = \sin^{-1}((\sqrt{2}/3) \approx 54^\circ \). In the simpler case of spinless dipolar fermions, a checkerboard bond order solid is formed \( \mathbb{3} \) in this region. Then it is plausible that for the spin 1/2 case, unconventional SDWs of non-s wave symmetry may be stabilized by interaction-induced correlated hopping either along the \( \hat{x}, \hat{y} \), or the diagonal \( \hat{x}+\hat{y} \) direction. The spatial symmetry of these SDWs depends on the value of \( \phi \). This scenario is illustrated in Figs. 1(c) and 1(d).

Finally, for large dipole tilting angles, e.g., \( \theta > \theta_{c2} \)
for $\phi = 0$, the dominant dipolar interaction is attractive. The leading instability is towards formation of Cooper pairs. Again, the precise orbital symmetry of the BCS phase is determined by the value of $\phi$.

We now determine the phase diagram of these intricate competing orders in the weak coupling limit, $\{U, V_d\} < t$. In particular, we prove the existence of unconventional SDW phases for intermediate tilting angles. We use the functional renormalization group (FRG) technique, which takes an unbiased approach (without any a priori guess) to isolate the most dominant instability among all possible orders $[8, 27–30]$. The FRG used here is an SU(2) symmetric version of that previously applied to treat non-interacting Fermi surface, satisfying momentum conservation $k_1 + k_2 = k_3 + k_4$, and $l$ is the renormalization group flow parameter. The flow of equal spin vertex, $U_l^1$, is related to that of $U_l^1$ via the spin-rotation symmetry of $H$. (2) We project out the interaction channels of interest at each RG step,

\begin{align*}
U_l^{\text{CDW}}(k_1, k_2) &= (2 - \hat{X})U_l^1(k_1, k_2, k_1 + Q), \\
U_l^{\text{SDW}}(k_1, k_2) &= -\hat{X}U_l^1(k_1, k_2, k_1 + Q), \\
U_l^{\text{BCS}}(k_1, k_2) &= U_l^1(k_1, -k_1, k_2, -k_2),
\end{align*}

where the exchange operator $\hat{X}$ interchanges the incoming momenta. (3) Finally we identify the most dominant instability of the Fermi surface from the most divergent eigenvalue of the interaction matrix. The corresponding eigenvector provides information about the orbital symmetry of the incipient order parameter. The phase diagram is shown in Fig. 2.

The phase diagram displays three types of phases: CDW, SDW, and BCS superfluid. We first focus on the case $U < V_d$ in the vicinity of $\phi = 0$ as shown in Fig. 2(a). Consistent with our heuristic argument above, FRG confirms a checkerboard CDW (CDW$_s$) for small $\theta$, and a spin-triplet, $p$-wave BCS (BCS$_p$) superfluid at large $\theta$. For the intermediate regime, roughly between $|\theta|_1$ and $|\theta|_2$, the flow for the SDW channel diverges rapidly, dominating over the CDW and BCS instabilities on either side. The SDW phase shows $p$-wave orbital symmetry, i.e. the eigenvector of the SDW$_p$ phase (shown in Fig. 2) is essentially of the form $\sin k_y$. This admits an interpretation of SDW$_p$ as a particle-hole analog of triplet superconductivity/superfluidity within Nayak’s classification $[8]$ for generalized SDW$_p$. The SDW$_p$ phase found here corresponds to the class with $\langle \hat{a}_{\alpha}^\dagger(k + Q)\hat{a}_{\beta}(k) \rangle = S(k) \cdot \sigma_{\alpha\beta}$, by identifying $S(k) \propto \hat{s}\sin k_y$ where $Q = (\pm \pi, \pm \pi)$. The position space representation implies the checkerboard pattern of hopping amplitudes, $\langle \hat{a}_{l,\alpha}^\dagger \hat{a}_{j,\beta} \rangle; r_j - r_i = \hat{y}$, depicted in the schematic of Fig. 1(c).

Additional unconventional orders with $l \neq 0$ occur in the vicinity of $\phi = 45^\circ$, where the nearest-neighbor interaction along the lattice vectors $\hat{x}$ and $\hat{y}$ is nearly equal. FRG predicts three more phases, CDW$_{s+d}$, SDW$_{s+d}$,
and BCS\textsubscript{s+d}, all of which contain a $d_{xy}$-wave as well as s-wave components. The contributions of the isotropic s-wave, extended s-wave, and d-wave components are inferred by fitting the FRG wavefunctions using function $c_0 + c_1 \cos k_x \cos k_y + c_2 \sin k_x \sin k_y$, with $\{c_0, c_1, c_2\}$ as fitting parameters. As a general trend, for increasing $\theta$, the magnitude of isotropic s-wave $c_0$ reduces, while the magnitudes of $c_1$ and $c_2$ are comparable and increase. The CDW\textsubscript{s+d} phase can be viewed as the natural continuation of the CDW\textsubscript{s} as $c_1$ and $c_2$ become appreciable. The two representative points shown in Fig. 2(a) for the SDW\textsubscript{s+d} and BCS\textsubscript{s+d} are fit by $0.05 - 0.16 \cos k_x \cos k_y - 0.18 \sin k_x \sin k_y$ and $0.01 + 0.23 \cos k_x \cos k_y - 0.19 \sin k_x \sin k_y$, respectively. Since $c_0$ is small, the real space modulation pattern for such SDW\textsubscript{s+d} takes the form of Fig 1(d): atoms delocalize across a plaquette, in the diagonal direction perpendicular to the dipole tilting direction. In contrast to the triplet BCS\textsubscript{p} phase at small $\phi$, the BCS\textsubscript{s+d} phase is a superfluid of singlet Cooper pairs with mixed orbital symmetry, $\ell = 0, 2$.

Next we illustrate how the phase diagram changes as the model approaches the repulsive Fermi-Hubbard model ($U > 0, V_d = 0$). We calculate the FRG flows for increased on-site interaction, $U = 0.5$, while keeping $V_d$ fixed at 0.5. The phase diagram is shown in Fig. 2(b). Since the on-site interaction $U$ favors antiferromagnetism, the SDW\textsubscript{p} phase shrinks, while the SDW\textsubscript{s+d} phase extends to cover a broader region, including that previously occupied by BCS\textsubscript{s+d}. Note that the d-wave component of SDW, even though diminished, is always present since the dipole interaction is kept finite. When $U$ is further increased such that $U \gg V_d$, only the isotropic component ($c_0$) will survive, indicating the SDW\textsubscript{s+d} crosses over to SDW\textsubscript{s}, the conventional antiferromagnetic ordering of spins in Fig. 1(a).

To corroborate the FRG prediction of the unconventional spin density waves, we use self-consistent mean field theory. For a square lattice of finite size $N \times N$, we impose periodic boundary conditions and retain the dipole interactions up to a distance of 12 lattice constants. We define the various normal and anomalous averages, $\langle \hat{a}_{j,\sigma} \hat{a}_{j,\sigma}' \rangle$ and $\langle \hat{a}_{j,\sigma}^\dagger \hat{a}_{j,\sigma}'^\dagger \rangle$. The corresponding mean field Hamiltonian is solved self-consistently by starting from an initial guess of the generalized density matrix, and iterating until desired convergence is reached. At each step the chemical potential is tuned to maintain half filling. The results are checked to be size-independent by varying $N > 24$. In Fig. 2(b) $N$ is set to 28. Although mean field results are only suggestive, they provide an independent confirmation of the FRG results and unveil the real space patterns of $\mathcal{S}$ directly in the SDW\textsubscript{p} phases. They can also be used to investigate the direction of $\mathcal{S}$ for the generalized model with $V_d^\perp (d) \neq V_d^\parallel (d)$. We search for unconventional SDW phases with homogeneous spin density, $n_{i,\sigma} = 1/2$. In and around the SDW\textsubscript{p} region predicted by FRG, we indeed find solutions with order parameter $S^y = \langle \hat{a}_{i,\sigma}^\dagger \hat{a}_{i,\sigma}' \rangle$, $r_y - r_i = y$. Further, the mean field energy for $S^z$ order is identical to that for $S^y$ and $S^z$, due to the SU(2) symmetry of $\hat{H}$ imposed by $V_d^\parallel (d) \neq V_d^\perp (\bar{d})$. This degeneracy is lifted for $V_d^\perp (d) \neq V_d^\parallel (\bar{d})$. In Fig. 3 we compare the mean-field energies of the SDW\textsubscript{p} solution with order parameter $S^z$ and $S^x$. The $z(x)$- polarized order $S^x$ ($S^z$) is energetically favored for $V_d^\parallel > V_d^\perp$ ($V_d^\parallel < V_d^\perp$). However, the degeneracy between $S^x$ and $S^y$ remains. The mean field results support our interpretation of the SDW\textsubscript{p} order as schematically shown in Fig. 1(c). A similar analysis can be performed for the SDW\textsubscript{s+d} phase.
In conclusion, we have established the emergence of unconventional spin density wave orders, SDW_p and SDW_s+id, along with other exotic phases with non-zero angular momentum, within ultra-cold spin-1/2 dipolar fermions on the square lattice. These phases occupy a sizable region of the phase diagram mapped out via the functional renormalization group approach. Furthermore, the self-consistent mean field estimation for the energy gaps of SDW_p, shown in Fig. 3(c), indicates a critical temperature $T_c \approx 0.08T_F$ for $V_d/t = 1.5$. Considering the currently reported temperature of degenerate dysprosium $T \approx 0.27T_F$ [4], this suggests experimental accessibility of these emergent phases in the near future.

Our study thus articulates the dipolar Fermi system as an intriguing and novel test bed for exotic many-body effects. They provide a fresh perspective on systems with competing orders.

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