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Unconventional Spin Density Waves in Dipolar Fermi Gases

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The conventional spin density wave (SDW) phase \[, as found in antiferromagnetic metal for example \[, can be described as a condensate of particle-hole pairs with zero angular momentum, \[. This analogy is quite robust and extends to particle-hole pairing with higher angular momenta, \[, respectively \[. The SDW \[ constitutes SDW, whereas SDW is the particle-hole analogue of the spin-triplet \[ wave component, and its order parameter is defined similarly with \[ and \[ respectively.

In contrast, the conventional SDW and CDW are described by on-site order parameters \[ and \[ respectively. The key insight of this paper is that fermions in a 2D lattice with dominant dipole-dipole interaction have the right ingredients to stabilize p- and d-wave SDWs. They emerge between the CDW and the BCS regime in the phase diagram, as a result of the competition between the short-ranged inter-atomic and the anisotropic long-ranged dipolar interaction.

In a new generation of experiments, ultra-cold gases of dipolar fermions have become accessible in the quantum degenerate limit. Fermionic atoms of dysprosium 161, with a large magnetic moment of 10 Bohr magnetic quantum, have been successfully trapped and cooled well below quantum degeneracy \[. The fermionic polar molecule 40K\(^{87}\)Rb has been cooled near quantum degeneracy \[ and loaded into optical lattices. Recently, the formation of ultra-cold fermionic Feshbach molecules of 23Na\(^{40}\)K has been achieved \[. On the theory side, many-body physics of single-species (spinless) dipolar Fermi gases have been explored by many groups. Numerous quantum phases are predicted: charge density wave \[, p-wave superfluid \[, liquid crystalline \[, supersolid \[, and bond-order solid \[.

Here we consider a two-component (pseudo-spin 1/2)
The lattice is aligned along the nearest neighbor hopping \(t\) and on-site interaction \(U\). \(U\) contains contributions from the bare short range interactions, \(U_{ij}\), defined on the bonds (yellow ellipsoids). In general, the off-site dipole-dipole interaction can be decomposed into equal- and unequal-spin components, labeled by \(\parallel\) and \(\perp\), respectively, and on-site dipolar interaction \(V^\perp_{dd}\), defined below. We assume that all dipoles are aligned in the same direction \(d = \hat{d}d = (d, \theta, \phi)\) by an external magnetic (or electric) field. In the simpler case of spinless dipolar fermions, a checkerboard bond order solid is formed [8] in this region. Then \(V_{dd}\) becomes attractive while \(V_{\hat{x}\hat{y}}\) remains repulsive. For instance, for \(\phi = 0\), this region is bounded by two critical values of \(\theta\): \(\theta_{c1} = \cos^{-1}(\sqrt{2/3}) \approx 45^\circ\) and \(\theta_{c2} = \sin^{-1}(\sqrt{2/3}) \approx 54^\circ\). In this region, we consider a simplified version of model [11] retaining only the nearest and next-nearest neighbor dipolar interactions, denoted \(V_{\hat{x}\hat{y}}\) and \(V_{\hat{x}+\hat{y}}\) respectively, see Fig. 1. First, for \(d = \hat{x}\), 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 \(d\) is tilted away from \(\hat{x}\) towards the \(\hat{x}\)-direction, there exists a region of tilting direction for which the nearest neighbor interaction \(V_x\) becomes attractive while \(V_{\hat{x}\hat{y}}\) and \(V_{\hat{x}+\hat{y}}\) remain repulsive. For instance, for \(\phi = 0\), this region is bounded by two critical values of \(\phi\): \(\phi_{c1} = \cos^{-1}(\sqrt{2/3}) \approx 35^\circ\) and \(\phi_{c2} = \sin^{-1}(\sqrt{2/3}) \approx 54^\circ\). In this case, spinless dipolar fermions, a checkerboard bond order solid is formed [8] 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., \(\theta > \theta_{c2}\)
where the exchange operator \( \hat{X} \) group flow parameter. The flow of equal spin vertex, \( U \{ k_1, k_2, k_3 \} \) between unequal spins, \( U \{ k_{1,2}, k_{3,4} \} \) are incoming (outgoing) momenta in the vicinity of the flow at each RG step, \( U \{ k_1, k_2, k_3 \} \) are incoming (outgoing) momenta in the vicinity of the 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, \( U \{ k_1, k_2 \} \), is related to that of \( U \{ k_1, k_2 \} \) via the spin-rotation symmetry of \( H \). (2) We project out the interaction channels of interest at each RG step,

\[
\begin{align*}
U^\text{CDW}_{\phi} (k_1, k_2) &= (2 - \hat{X}) U^\phi (k_1, k_2, k_1 + Q), \\
U^\text{SDW}_{\phi} (k_1, k_2) &= -\hat{X} U^\phi (k_1, k_2, k_1 + Q), \\
U^\text{BCS}_{\phi} (k_1, k_2) &= U^\phi (k_1, -k_1, k_2, -k_2),
\end{align*}
\]

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_{\alpha}) for small \( \theta \), and a spin-triplet, \( p \)-wave BCS (BCS_{\rho}) superfluid at large \( \theta \). For the intermediate regime, roughly between \( \theta_{1,2} \), the flow for the CDW 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_{\rho} phase (shown in Fig. 2) is essentially of the form \( \sin k_y \). This admits an interpretation of SDW_{\rho} as a particle-hole analog of triplet superconductivity/superfluidity within Nayak’s classification for generalized SDW_{\rho}. The SDW_{\rho} 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 \( S(k) \propto \sin k_y \) where \( Q = (\pm \pi, \pm \pi) \). The position space representation implies the checkerboard pattern of hopping amplitudes, \( \langle \hat{a}_{\alpha}^\dagger (i,j) \hat{a}_{\beta} (i,j) \rangle \); \( r_j - r_i = \hat{y} \), depicted in the schematic of Fig. 1(c).

Additional unconventional orders with \( \ell \neq 0 \) occur in the vicinity of \( \phi = 45^\circ \), where the nearest-neighbor interaction along the lattice vectors \( z \) and \( \hat{y} \) is nearly equal. FRG predicts three more phases, CDW_{s+d}, SDW_{s+d},
Preferred direction of the spin polarization vector $\mathbf{S}$ as a function of the ratio $V_d^\parallel/V_d^\perp$. It is along the $z$-direction for $V_d^\perp < V_d^\parallel$ and lies in the $x$-$y$ plane for $V_d^\perp > V_d^\parallel$. The energy difference between the mean field states with $S^\parallel$ and $S^\perp$ order. The inset shows the magnitude of the corresponding order parameter. The parameters are $U = 0.1$, $V_d^\parallel = 1.0$, $\theta = 47^\circ$, $\phi = 0$. All energies are in units of $t$. (c) The mean field energy gap of the SDW$_d$ phase, in units of the Fermi energy, as a function of the inter-site long-range dipolar interaction $V_d^\perp$ for $\theta = 47^\circ$ and $\phi = 0$. For the SU(2) symmetric case plotted in (c), the energy gaps for different vector polarizations are degenerate.

and BCS$_{s+d}$, 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$_{s+d}$ phase can be viewed as the natural continuation of the CDW$_s$ as $c_1$ and $c_2$ become appreciable. The two representative points shown in Fig. 2(a) for the SDW$_{s+d}$ and BCS$_{s+d}$ 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$_{s+d}$ 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$_p$ phase at small $\phi$, the BCS$_{s+d}$ 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$_p$ phase shrinks, while the SDW$_{s+d}$ phase extends to cover a broader region, including that previously occupied by BCS$_{s+d}$. 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$_{s+d}$ crosses over to SDW$_s$, 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, $\langle \hat{a}_{i,\sigma}^\dagger \hat{a}_{i,\sigma}' \rangle$ and $m_{i,\sigma,j,\sigma'} = \langle \hat{a}_{i,\sigma}^\dagger \hat{a}_{j,\sigma'} \rangle$. 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. 3, $N$ 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 $\mathbf{S}$ directly in the SDW$_p$ phases. They can also be used to investigate the direction of $\mathbf{S}$ for the generalized model with $V_d^\perp (\hat{d}) \neq V_d^\parallel (\hat{d})$. We search for unconventional SDW phases with homogeneous spin density, $n_{i,\sigma} = 1/2$. In and around the SDW$_p$ region predicted by FRG, we indeed find solutions with order parameter $S^\parallel = \langle \hat{a}_{i,\sigma}^\dagger \hat{a}_{i,\sigma}' \rangle$, $r_j - r_i = \hat{y}$. Further, the mean field energy for $S^\parallel$ order is identical to that for $S^\parallel$ and $S^\perp$, due to the SU(2) symmetry of $H$ imposed by $V_d^\parallel (\hat{d}) = V_d^\parallel (\hat{d})$. This degeneracy is lifted for $V_d^\parallel (\hat{d}) \neq V_d^\parallel (\hat{d})$. In Fig. 3 we compare the mean-field energies of the SDW$_p$ solution with order parameter $S^\parallel$ and $S^\perp$. The $z(x)$-polarized order $S^\parallel$ ($S^\perp$) is energetically favored for $V_d^\parallel > V_d^\perp$ ($V_d^\parallel < V_d^\perp$). However, the degeneracy between $S^\parallel$ and $S^\perp$ remains. The mean field results support our interpretation of the SDW$_p$ order as schematically shown in Fig. 1(c). A similar analysis can be performed for the SDW$_{s+d}$ phase.
critical temperature $T_c$ and energy gaps of SDW.

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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