Competing phases in dipolar quantum gas

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Fermi gas of polar molecules: KRb, NaK

$T \sim 400nK \sim 3T_F$

$d \sim 0.5$ Debye

D. S. Jin and J. Ye, Physics Today 64, 5(2011)

Chemically stable. $d \sim 0.8$ Debye.
Life time > 2.5s; $T \sim 500nK \sim 2T_F$

Wu et al, PRL 109, 085301 (2012)
Degenerate Fermi gas of magnetic atoms: \(^{161}\text{Dy},^{167}\text{Er}\)

Sympathetic cooling of \(^{161}\text{Dy}\) with bosonic \(^{162}\text{Dy}\)

\[
\frac{T}{T_F} = 0.2 \quad T_F = 300 \text{ nK}
\]


Aikawa et al, PRL 112, 010404 (2014)
Science 345, 1484 (2014)
Quantum phases of dipolar fermi gases

Q: What are the many-body phases of fermions with dipole-dipole interaction? Are they all “boring,” i.e., known and understood in condensed matter physics?

For dipoles pointing in the same direction:

$$V_{dd} = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3\cos^2\theta}{r^3} \rightarrow P_2(\cos\theta) \text{ anisotropic}$$

$$\rightarrow \text{long-ranged}$$
Comparing to other Fermi systems

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Candidate phases of dipolar fermions:

- ★ anisotropic Fermi liquid
- ★ charge density waves (CDW)
- ★ $p$-wave superfluid
- ★ stripes, quantum liquid crystals?
- ★ supersolid? ...

Outline of this talk

1. Dipolar Fermi gas on square lattice @ half filling:
   phase diagram from functional renormalization group

2. Continuum gas of dipolar fermions:
   trying to go beyond Hartree-Fock and RPA

3. Frustrated magnetism of localized (deeply trapped) dipoles:
   hints from exact diagonalization on a small lattice

The common theme of the 3 problems is competing order.

Wish: treat (all) orders on the same footing, without a priori bias.
1. Dipolar fermions on lattice

Collaborators:
Satyan Bhongale (GMU)
Ludwig Mathey (Hamburg)
Shan-Wen Tsai (UC Riverside)
Charles Clark (NIST/JQI)
Dipolar fermions on square lattice: model Hamiltonian

\[ H = -t \sum_{\langle ij \rangle} a_i^\dagger a_j + \frac{1}{2} \sum_{i \neq j} V_{dd}(r_{ij}) n_i n_j, \]

★ Half filling: on average, one fermion every two sites.
★ Zero temperature; Neglect collapse instability.
The Fermi surface is just a square (half filling)

In the absence of dipole-dipole interaction:

- Perfect Nesting: \( \mathbf{Q} \) couple \( \mathbf{k} \) points on the opposite sides of the FS.
- We will discretize the Fermi surface into \( N \) patches.
- The Fermi surface may become unstable when \( V_{dd} \) is turned on.
Interactions for dipoles tilting in the x direction

\[ V_x \]

\[ V_y \]

\[ \theta_F \]

\[ \phi_F \]

\[ \hat{x} \]

\[ \hat{y} \]

\[ \hat{z} \]

\[ d \]

\[ \theta_{c1} \approx 35^\circ \]

\[ \theta_{c2} \approx 54^\circ \]

\[ V_{x+y} \]

\[ V_x \]

\[ V_y = V_d \propto \frac{d^2}{a^3} \]

\[ \theta_F \left( ^\circ \right) \]
Two limits easy to understand

1. Small tilting angle ($\theta_F < \vartheta_{c1}$): all interactions are repulsive.

**Density wave (CDW):**
Periodic modulation of on-site density.

$$\langle a_i^+ a_i \rangle$$

In \textbf{k} space, this is an instability of FS in the particle-hole channel with $Q$.

2. Large tilting angle ($\theta_F > \vartheta_{c2}$): $V_x$ and $V_{x+y}$ attractive, but $V_y$ repulsive.

**Anisotropic p-wave pairing (BCS):**
The pairing order parameter

$$\langle a_i a_{i+\hat{x}} \rangle = -\langle a_i a_{i-\hat{x}} \rangle \quad \langle a_i a_{i\pm y} \rangle = 0$$

In \textbf{k} space, this is an instability of FS in the particle-particle channel.
How about the intermediate tilting angle

$V_x$ and $V_y$ opposite in sign and comparable in magnitude. What do the fermions do?

Settle to BCS or CDW? Neither? Both?

$\vartheta_{c1} \approx 35^\circ$ $\vartheta_{c2} \approx 54^\circ$
Competing orders in interacting dipolar fermions

Three possible scenarios:

★ Direct (1st order) transition from CDW to p-wave BCS superfluid.
★ Coexistence: density modulation + pairing = supersolid.
★ Or, some other completely different animal.

The problem of competing order is at the heart of the many-body physics of dipolar fermions.

Simple mean field theories or perturbation theories, such as single-channel Renormalization Group or Random Phase Approximation, are insufficient/unreliable to treat competing orders in the regime of intermediate tilting angle.

We need a theory that can treat all ordering instabilities on equal footing, without any a priori assumptions about dominant orders.
Functional Renormalization Group (FRG)

★ Separate the low-energy modes and high energy modes with scale $\Lambda$.  
★ At each scale $\Lambda$, there is an effective theory description, including the effective interaction (vertex function) $U$ between the low energy modes.  
★ As $\Lambda$ is reduced, the evolution of $U$ obeys the exact “flow equation.”  
★ For weak coupling, the infinite hierarchy of flow eqns can be truncated and solved numerically by discretizing $\mathbf{k}$.

See e.g. Metzner et al, Rev. Mod. Phys. 84, 299–352 (2012); And reference therein.
FRG applied to interacting dipolar fermions

\[ U_\ell(k_1, -k_1, k_2), \quad U_\ell(k_1, k_2, k_1 + Q), \]

\( \text{BCS Channel} \quad \text{CDW Channel} \)

FRG keeps track of all effective interactions as the high energy modes are traced out, including the p-p and p-h channel, as well as their subtle interplay. Especially, we are interested in the BCS and the CDW channel.

The most dominant instability can be inferred from the most diverging eigenvalue of \( U \), which is a matrix of \( k_1 \) and \( k_2 \). The corresponding eigenvector indicates the symmetry of the incipient order.
Instability analysis within FRG

Eigenvector

\[ \chi \]

\[ \theta_F = 30^\circ \]

\[ \theta_F = 70^\circ \]

Eigenvalue

CDW Channel

\[ \lambda \]

BCS Channel

\[ \lambda \]

\[ 0 \]

\[ \pi \]

\[ 2\pi \]
**Bond order solid (BOS)**

Such p-wave instability in the CDW channel corresponds to a spatial modulation of “bonds”, more precisely, the average of hopping

\[ \langle a_i^{\dagger} a_{i+y} \rangle \]

How can such bond order save energy?

A mean field perspective:

\[ n_i n_j = -a_i^{\dagger} a_j a_j^{\dagger} a_i + n_i \]

\[ \rightarrow a_i^{\dagger} a_j \rho_{ji} + \rho_{ij} a_j^{\dagger} a_i - |\rho_{ij}|^2. \]

with \( \rho_{ij} = \langle a_i^{\dagger} a_j \rangle \)

\[ \rho_{i,x \pm x} = \chi_x, \rho_{i,y \pm y} = \chi_y \pm \delta \]

★ Opening up a gap at the Fermi surface.

★ Ground state energy: \( E_{\text{GS}} = -2(\chi_x + \chi_y)(t + V_x + V_y) - 2V_y \delta^2 \)

finite bond modulation \( \delta \) is energetically favored
Phase diagram ($T=0$, half-filling, $\phi_F=0$)

$$\langle a_i^\dagger a_j \rangle$$

- BCS
- $BOS_p$
- $cb$-CDW

Phase diagram for general dipole tilting

\[ V_d = 0.5t. \]

Density waves (condensate of particle-hole pairs):

\[
\langle f_{\alpha}^{\dagger}(k + Q)f_{\beta}(+k) \rangle = \Phi(k) \delta_{\alpha\beta}
\]

\[
\langle f_{\alpha}^{\dagger}(k + Q)f_{\beta}(+k) \rangle = \Phi(k) \cdot \sigma_{\alpha\beta}
\]

- s-wave CDW (checkerboard)
- p-wave CDW
- d-wave CDW (DDW)...

They show up in dipolar Fermi gas!
Observation of d-wave density waves?

Observation of d-form factor density waves (in BSCCO and Na-CCOC)

Theory: Metlitski & Sachdev, PRB 82, 075128 (2010); PRL 111, 027202 (2013); etc.

\[ P_{ij} = \left\langle c_{i\alpha}^\dagger c_{j\alpha} \right\rangle \text{ for } i = j, \text{ and } i, j \text{ nearest neighbors.} \]

\[ P_{ij} = \left[ \int_k \mathcal{P}(k)e^{ik\cdot(r_i-r_j)} \right] e^{iQ\cdot(r_i+r_j)/2} + c.c. \]

\[ \mathcal{P}(k) = e^{i\phi} [\cos(k_x) - \cos(k_y)] \quad \text{and} \quad Q = 2\pi(1/4, 0) \]
Beyond weak coupling

Bond order is most robust for intermediate interaction, $V_d \sim 2.5t$, where the mean field gap is $0.23t$, or $0.05 E_F$.

Exact diagonalization (ED) yields the hopping correlation function

$$C(i, j) = \langle K_{i,i+y} K_{j,j+y} \rangle - \langle K_{i,i+y} \rangle \langle K_{j,j+y} \rangle$$

$K_{i,j} \equiv (a_i^\dagger a_j + h.c.)$

It approaches $4\delta^2$ in the limit of large $|i-j|$. 
where the exchange operator FRG calculation are: (1) Derive and solve the renormalization group equation for each RG step, $H$ is related to that of the non-interacting Fermi surface, satisfying momentum conservation.

As the on-site interaction is increased from $U=0.1$ to $U=0.5$, the phase diagram of unconventional orders for dipolar fermions on a square lattice at half filling obtained from FRG is shown in Fig. 2. The SDW phase shows the $d$ wave component of SDW $\langle t\rangle$ in each phase is shown. The pattern of hopping amplitudes, position space representation implies the checkerboard pattern of hopping amplitudes, which is nearly equal. Possible orders for fixed interactions $V_d=0.5, U=0.1$ and $V_d=0.5, U=0.5$ are shown in Fig. 2(a) and (b), respectively.

The $p$-wave spin density wave phase is sandwiched between the CDW and BCS superfluid phases. Its phase boundary depends on $U$.

S. G. Bhongale, L. Mathey, S.-W. Tsai, C. W. Clark, EZ, PRA 87, 043604 (2013).
Quadrupolar Fermi gas

\[ V^{qq} = V(3 - 30 \cos^2 \theta + 35 \cos^4 \theta)/r^5 \]

2. Functional renormalization group analysis of continuum dipolar gas in 2D

Collaborator:
Ahmet Keles (Pitt and GMU)
2D dipolar Fermi gas, mean field and RPA predictions

Tightly confined in z direction

Sieberer and Baranov, PRA 84, 063633 (2011)
See also: Babadi & Demler, PRB 2011;
Zhao et al (Pu’s group) PRA, 2010;
Bruun and Taylor PRL 2008; and many others.

Technical slide 1: Flow of effective action

Add infrared regulator $R_k$ to the action $S$, $k$ being the sliding momentum scale, e.g.,

$$R_k(p) = \left[ \frac{k^2}{2m} \text{sgn}(\xi(p)) - \xi(p) \right] \theta\left( \frac{k^2}{2m} - |\xi(p)| \right)$$

Wetterich’s flow equation:

$$\partial_k \Gamma_k = -\frac{1}{2} \tilde{\partial}_k \text{Tr} \ln \left[ \Gamma^{(2)} + R_k \right]$$


Expand $\Gamma$ to quartic order, $\Gamma_k = \bar{\psi}_1 [G_0^{-1} - \Sigma_k + R_k] \psi_2 + \Gamma^{(4)} \bar{\psi}_1 \psi_2 \psi_3 \psi_4 + ...$

Truncate the flow equation,

$$\partial_k \Gamma_k = \tilde{\partial}_k \left( \begin{array}{c} p \\ \text{loop} \end{array} \right)$$

Discretize $|q|$ and decompose $\Gamma$ into angular momentum channels $\{m\}$.

$$\Gamma_k(p; q, q') = \sum_m \Gamma_m(p; |q|, |q'|) e^{im(\phi-\phi')}$$

In the limit of large $k >> k_F$, $\Gamma$ is the bare interaction.

$$\Gamma_{k \to \Lambda}(q, q') = V(q - q') \quad V(p) = 2\pi p[\cos^2 \phi \sin^2 \theta - \cos^2 \theta] d^2$$

$\Gamma_k$ at the end of the flow $k \to 0$ contains information about the instability and $T_c$. 

Technical slide 2: parametrize the flow
Flow in the particle-particle channel: p-wave superfluidity

Divergence of $\Gamma$ (i.e. zero of $1/\Gamma$) signals the transition to superfluid.

$$\left[ \Gamma_{k=0}^{(4)}(p=0) \right]^{-1} = 0 \text{ at } T = T_c.$$ 

$g = 0.5 \quad m = 1, \quad \theta = 0.375\pi, \quad q_1 = q_2 = 1$

$q_1, q_2$ and $k$ are in units of $p_F$

- Neglected the self energy correction;
- Neglected the particle-hole channel.
The superfluid transition temperature

Remaining questions:

1. How about the particle-hole channel?
2. Self energy corrections (Fermi surface distortion, nematic phase…).
3. Solving the full flow equation numerically.
3. Magnetism of confined dipoles on lattice (preliminary results, very speculative)

Collaborator:
Zhenyu Zhou (Pitt and GMU)
Quantum spin liquid in frustrated spin model: J1-J2 model

\[ H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j \]

Hong-Chen Jiang, Hong Yao, and Leon Balents, PRB 86, 024424 (2012)
Experiments

Observation of dipolar spin-exchange interactions with lattice-confined polar molecules,
B. Yan, S. A. Moses, B. Gadway, J. P. Covey, K. R. A. Hazzard, A. M. Rey, D. S. Jin & J. Ye,

Nonequilibrium quantum magnetism in a dipolar lattice gas.
A. de Paz, A. Sharma, A. Chotia, E. Maréchal, J. H. Huckans, P. Pedri, L. Santos, O. Gorceix, L. Vernac, and B. Laburthe-Tolra,
Lattice spin model: 2d, square lattice

\[ H_d = \frac{J}{2} \sum_{i \neq j} f(r_i - r_j)(s_i^x s_j^x + s_i^y s_j^y + \eta s_i^z s_j^z). \]

Here \( s_i = (s_i^x, s_i^y, s_i^z) \) is the spin at site \( i \), \( \eta \) describes the anisotropy depending on the detailed implementation (e.g., \( \eta = 0 \) for the KRb experiment), \( f(r) = [1 - 3 \cos^2(\hat{r} \cdot \hat{d})](a/r)^3 \) characterizes the long range, anisotropic spin exchange due to dipolar interaction, and \( a \) is the lattice constant.

Consider \( S=1/2, \eta=1 \), and truncate exchange interactions to next nearest neighbor.
Competing exchange interaction

$\phi = 0$

$\phi = 22^\circ$

$\phi = 45^\circ$

Sweet spots?

$J_x \sim J_y \sim 2J_1 \sim 2J_2$
Benchmarking the exact diagonalization: J1-J2 model

16 sites, our calculation.

16 sites, with J1=2.
Dagotto and Moreo, PRL 1989

State of the art: 40 sites, # of basis: 430 909 650
An example of the energy spectrum $\phi = 35^\circ$
Excitation (spin) gap

\[ \phi = 45^\circ \]

\[ \text{Theta (degrees)} \]

\[ E_1 - E_0 \]

Graph showing the excitation gap as a function of theta degrees with different lines for 30°, 35°, and 40°.
\[ M(Q) = \sum_{i,j} \langle s_i \cdot s_j \rangle e^{i Q \cdot (r_i - r_j)} \]

\( \theta = 15^\circ \)

\( \theta = 50^\circ \)

\( \theta = 35^\circ \)
Speculations

- This model can be highly, even maximally, frustrated;
- It is closely related to J1-J2 model; but the physics is even richer;
- Our numerical study (for small lattice) suggests a gaped quantum paramagnetic phase between the Neel and collinear ordered phase;
- Numerics on larger size systems is required to resolve the phase diagram.