Time-Reversal-Breaking and $d$-Wave Superfluidity of Ultracold Dipolar Fermions in Optical Lattices

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We describe possible superfluid phases of ultracold dipolar fermions in optical lattices for two-dimensional systems. Considering the many-body screening of dipolar interactions at larger filling factors, we show that several superfluid phases with distinct pairing symmetries naturally emerge in the singlet channel: local $s$-wave ($sl$), extended $s$-wave ($se$), $d$-wave ($d$) or time-reversal-symmetry breaking ($sl + se + 2id$)-wave. The temperature versus filling factor phase diagram indicates that $d$-wave is favored near half-filling, that ($sl + se$)-wave is favored near zero or full filling, and that time-reversal-breaking ($sl + se + id$)-wave is favored in between. When a harmonic trap is included a sequence of phases can exist in the cloud depending on the filling factor at the center of the trap. Most notably in the region where the ($sl + se + id$)-wave superfluid exists, spontaneous currents are generated, and may be detected using velocity sensitive Bragg spectroscopy.

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Ultracold heteronuclear molecules are very interesting quantum systems to study because they possess electric dipole moments. This internal degree of freedom adds richness to the nature of interactions between molecules in comparison to interactions between atoms in purely atomic systems. Dipolar molecules can be either fermionic or bosonic in nature depending on their constituent atoms, and dipolar interactions allow for the emergence of quantum phases which may be extremely difficult to be realized in condensed matter. Recently, ultracold dipolar molecules were produced optically \cite{1} followed by their production from Bose-Fermi mixtures of ultracold atoms first in the vicinity of Feshbach resonances \cite{2}, and later brought into their roto-vibrational ground state \cite{3}. The production of these heteronuclear molecules in harmonic traps has paved the way for studies of the quantum phases of interacting dipolar bosonic or fermionic molecules. In the case of trapped clouds, a few quantum phases have been proposed for dipolar bosons including ferroelectric superfluids \cite{4}, Wigner crystals \cite{5}, while for dipolar fermions phases such as ferroelectric \cite{6} or ferro-nematic \cite{7} Fermi liquids and Berezinskii-Kosterlitz-Thouless \cite{8} or $j$-triplet \cite{9} superfluids have been suggested. In the case of optical lattices, additional phases such as supersolids \cite{10} or micro-emulsions \cite{11} have been proposed for dipolar bosons, while studies for dipolar fermions in optical lattices are just beginning.

A natural next step for experiments is the loading of dipolar (heteronuclear) molecules in optical lattices. In anticipation of these experiments, we discuss here the quantum phases of dipolar fermions in harmonically confined optical lattices, paying particular attention to the emergence of superfluid phases that break time reversal symmetry spontaneously, as there are no confirmed analogues in condensed matter physics \cite{11}. By including the effects of screening at intermediate and high filling factors, we argue that quantum phases of dipolar fermions in harmonically confined optical lattices (two-dimensional square geometry) can be approximately described by an extended Hubbard model, with local on-site and a few neighbor interactions. For attractive local and nearest neighbor interactions, we derive the phase diagram and establish all accessible phases in the singlet channel, the most important of which corresponds to $d$-wave superfluidity and a superfluid phase that breaks time reversal symmetry spontaneously and involves a superposition of $s$-wave and $d$-wave components of the order parameter. In the broken time-reversal symmetry phases, spontaneous currents flow and can be detected using velocity sensitive Bragg spectroscopy \cite{12,13}.

The bare Hamiltonian for dipolar fermions in optical lattices for a two-dimensional system ($xy$-plane) is

$$H_b = -t \sum_{\langle ij \rangle} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow} + \sum_{i<j, \sigma \sigma'} V_{ij} n_{i \sigma} n_{j \sigma'},$$

where $\langle \ldots \rangle$ indicates nearest neighbors, and $n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma}$ is the local particle number operator. The on-site interaction $U = U_s + U_{dip}$ contains two contributions. The first is from $s$-wave scattering $U_s = (4\pi \hbar^2 a_s/m) \int d \mathbf{r} |w(\mathbf{r})|^4$ and the second is from the on-site dipole-dipole interaction $U_{dip} = \int d \mathbf{k} w_F^2(\mathbf{k}) V_{dip}(\mathbf{k})$, where $a_s$ is the $s$-wave scattering length, $w_F(\mathbf{r})$ is the Wannier function, $w_F^2(\mathbf{k})$ and $V_{dip}(\mathbf{k})$ are the Fourier transforms of $|w(\mathbf{r})|^2$ and of the dipole-dipole potential $V_{ij}$, respectively. The long-range part of the dipole-dipole interaction is $V_{ij} \approx D^2 (\mathbf{e}_i \cdot \mathbf{e}_j - 3 (\mathbf{e}_i \cdot \mathbf{r}_{ij}) (\mathbf{e}_j \cdot \mathbf{r}_{ij}) ||\mathbf{r}_i - \mathbf{r}_j||^{-3}$, where $D$ is the magnitude of the dipole moments located at $\mathbf{r}_i$ and $\mathbf{r}_j$, $\mathbf{e}_i$ is the direction of the dipole moment at $\mathbf{r}_i$, and $\mathbf{r}_{ij}$ is the direction of the line connecting dipoles, while $||\mathbf{r}_i - \mathbf{r}_j||$ is the distance between dipoles, with $\mathbf{r}_j = (j a, j a)$ being the lattice vector, and $a$ being the lattice spacing.

The bare Hamiltonian is now transformed into an effective many-body Hamiltonian which includes the ef-
fects of screening, as the dipole interaction between two bare dipoles is renormalized (reduced) by the dielectric function $\varepsilon_d(r, r')$, leading to an effective screened dipole-dipole interaction $\tilde{V}(r) = \sum r \cdot V(r')\varepsilon_d^{-1}(r, r')$. Although this effect is negligible at small filling factors, it may be substantial for filling factors $\nu > 1/3$ as the dielectric function becomes sufficiently large to reduce the range of the interaction to a few neighbors.

Since we are interested in superfluid phases, we choose to tune the experimental parameters to generate mostly attractive interactions. For the off-site dipolar interactions, we choose to have all dipoles aligned along the same direction $(\alpha, \phi)$ of an external electric field, where $\alpha$ $(\phi)$ is the polar (azimuthal) angle with respect to the $z$ $(x)$ axis. The interaction becomes $\tilde{V}_{ij} = V_\alpha \delta_{ij} \tilde{V}_{ij} = V_\alpha \delta_{ij}$ along the $x$ $(y)$ axis. Here, $V_x = D^2(1 - 3 \sin^2 \phi)/(a^2 e_\alpha(a))$, $V_y = D^2(1 - 3 \sin^2 \phi)/(a^2 e_\alpha(a))$, and $\delta_{ij} = 1$ for nearest neighbors and zero otherwise. For the angles $\phi = \pm \pi/4, \pm 3\pi/4$, the interactions are $V_x = V_y = V = D^2(1 - 3 \sin^2 \phi)/(a^2 e_\alpha(a))$, and become negative when the condition $\sin^2 \alpha > 2/3$ is satisfied. For the on-site interaction, we choose to adjust the scattering length $a_\alpha$ to produce $U = |U| < 0$.

To study the physics discussed above, we use the effective two-dimensional model hamiltonian

$$H = -\sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} - |U| \sum_i n_{i\uparrow} n_{i\downarrow} - |V| \sum_{\langle ij \rangle} n_{i\sigma} n_{j\sigma}$$

on a square lattice. In order to establish the quantum phases as a function of filling factor $\nu$, we start by constructing the partition function $Z = \int Dc^\dagger Dc e^{S}$ for the action

$$S = \int_0^{\beta} d\tau \left[ \sum_{i\sigma} c^\dagger_{i\sigma}(\tau)(-\partial_\tau + \mu)c_{i\sigma}(\tau) - H(c^\dagger, c) \right].$$

(1)

By symmetry, the singlet order parameters for superfluidity correspond to local s-wave $\Delta_s$, extended s-wave $\Delta_{se}$ and d-wave $\Delta_d$ pairing [14]. Upon integration of the fermionic degrees of freedom the action becomes

$$S = -\frac{N_s}{T} \sum_{q, \alpha} |\Delta_\alpha(q)|^2 + \text{Tr} \ln \left( G_{\alpha}^{-1} - \frac{V}{T} \right) + \frac{\mu N_s}{T},$$

(2)

where $N_s$ is the total number of sites, $\alpha = sl, se, d$, the interactions $V_{ij} = |U|, V_{se} = V_{d} = |V|$, and the four-vector $q = (i\omega_n, q)$. The inverse free fermion propagator matrix is

$$G_{\alpha}^{-1}(k, k') = \begin{pmatrix} \xi_k + \xi_{k'} & \Delta_\alpha(k - k') \\ \Delta_\alpha(k - k')^* & \xi_{k} + \xi_{k'} \end{pmatrix} \delta_{k, k'},$$

(3)

with kinetic energy $\xi_k = \epsilon_k - \mu$, band dispersion $\epsilon_k = -2t[\cos(k_x a) + \cos(k_y a)]$, chemical potential $\mu$, four-vector $k = (i\omega_n, k)$, and unit cell length $a$. The additional matrix appearing in Eq. (2) is

$$V(k, k') = \begin{pmatrix} 0 & \Delta_\alpha(k - k') \\ \Delta_\alpha^*(k - k') & 0 \end{pmatrix} \lambda_\alpha(k, k'),$$

(4)

where the Einstein summation over $\alpha$ is understood, and $\lambda_\alpha(k, k')$ are the symmetry factors for the order parameters, which in the limit of zero momentum pairing $(k = k')$ become $\lambda_{sl}(k, k) = 1$, $\lambda_{se}(k, k) = \cos(k_x a) + \cos(k_y a)$, $\lambda_d(k, k) = \cos(k_x a) - \cos(k_y a)$.

In terms of the quasiparticle $(\gamma = 2)$ or quasihole $(\gamma = 1)$ energies $E_{k, \gamma} = (-)^{\gamma} \xi_k + |\Delta_\alpha\lambda_\alpha(k)|^2$, where the symmetry function $\lambda_\alpha(k) = \lambda_\alpha(k, k)$, the effective action becomes

$$S = -\frac{N_s}{|U/T|} |\Delta_s|^2 - \frac{N_s}{V/T} (|\Delta_{se}|^2 + |\Delta_d|^2) + S_2 + \frac{\mu N_s}{T}.$$  

(5)

Here, the second term in the action is $S_2 = \sum_{k, \gamma} \ln[1 + \exp(-E_{k, \gamma}/T)]$. Notice that there are three possible pure phases: local s-wave $(sl)$; extended s-wave $(se)$ and d-wave $(d)$. In addition, there are several possible binary mixed phases $sl \pm se$, $sl \pm d$ and $se \pm d$, which do not break time-reversal symmetry, and there are also those that do, such as $sl \pm ise$, $sl \pm id$ and $se \pm id$. Lastly, several possible ternary mixed phases involving all three symmetries $sl$, $se$ and $d$ may also exist.

**General Case:** The order parameter equations can be obtained by minimization of the action with respective to each order parameter. By taking $\delta S/\delta \Delta_\alpha^* = 0$, with $\alpha = sl, se, d$, we obtain

$$\Delta_\alpha = \frac{V_\alpha}{N_s} \sum_k \tan\left(\frac{E_{k, 2}/2T}{2E_{k, 2}}\right) \Lambda_\alpha(k),$$

(6)

with symmetry factors $\Lambda_\alpha(k) = \lambda_\alpha(k) [\Delta_\alpha^* \lambda_{\alpha'}(k)]$, where repeated indices $\alpha'$ indicate summation.

The number equation that fixes the chemical potential is obtained through the thermodynamic relation $N = -\partial \Omega/\partial \mu$, where $\Omega = -T \ln Z$ is the thermodynamic potential. In the present approximation $\Omega = -TS$, and the number equation reduces to

$$\nu = \frac{1}{N_s} \sum_k \left[ 1 - \frac{\xi_k}{E_{k, 2}/2T} \tanh(\xi_E/2T) \right],$$

(7)

where $\nu = N/N_s$ is the filling factor.

Using the amplitude-phase representation, we write the order parameter as $\Delta_{sl} = |\Delta_{sl}|e^{i\phi_{sl}}$ for the local s-wave symmetry, $\Delta_{se} = |\Delta_{se}|e^{i\phi_{se}}$ for the extended s-wave symmetry, and $\Delta_d = |\Delta_d|e^{i\phi_d}$ for the d-wave symmetry. The filling factor dependence of the critical temperature $T_c(\nu)$ and the critical chemical potential $\mu_c(\nu)$ can be obtained for pure $sl$, $se$, $d$-wave symmetries by setting the order parameters $\Delta_{sl} = 0$, $\Delta_{se} = 0$, and $\Delta_d = 0$ in Eqs. (6) and (7). The solutions for $T_c(\nu)$ are shown in Fig. 4 for two cases $|U|/t = 0$ and $|V|/t = 3,$
and \(|U|/t = 2\) and \(|V|/t = 3\), where the corresponding superfluid phases are also indicated. The phase diagram is symmetric about \(\nu = 1\), since the Helmholtz free energy \(F = \Omega + \mu N\) is invariant under the global particle-hole transformation \(\mu \rightarrow -\mu\) and \(\nu \rightarrow 2 - \nu\). Notice that \(s\)-wave phases are favored at lower filling factors, while the \(d\)-wave phase is favored near half-filling, and this is directly correlated with the higher effective density of states in this vicinity. The time-reversal-symmetry-breaking phases occur at filling factors between the \(s\)-wave and \(d\)-wave phases. Generally, when \(|U|/t = 0\), the only accessible phases are \(se\), \(d\) and \((se \pm id)\)-wave, however when \(|U|/t \neq 0\) the only accessible phases are \((sl + se)\), \(d\) and \((sl + se \pm id)\)-wave.

**FIG. 1:** Critical temperature \(T_c/t\) versus filling factor \(\nu\) at fixed interaction \(|U|/t = 0\) in (a) or \(|U|/t = 2\) in (b) and \(|V|/t = 3\). Notice the tetracritical point where the normal and all superconducting phases meet.

Given that on-site interactions can be experimentally controlled, we focus our discussion at \(|U|/t = 0\), which already contains the essential physics of superfluid phases that spontaneously break time reversal symmetry and have a \(d\)-wave component. The Ginzburg-Landau theory near \(T_c\) is obtained by expanding the action of Eq. (5) in terms of the order parameters \(\Delta_{se}, \Delta_d\) and their complex conjugates. From the thermodynamic potential \(\Omega = -TS\), we can calculate the Helmholtz Free energy \(F = \Omega + \mu N\). The free energy per site \(F/N_s\) takes the simple form

\[
F = a_{se}|\Delta_{se}|^2 + a_d|\Delta_d|^2 + b_{se}|\Delta_{se}|^4 + b_d|\Delta_d|^4 + 2b_{sd} \left[ 1 + \frac{1}{2}\cos(2\phi_d) \right]|\Delta_{se}|^2|\Delta_d|^2 + \mu(\nu - 1).
\]

The coefficients \(a\) and \(b\) depend explicitly on the parameters of the model used and \(\phi_d = \phi_d - \phi_{se}\). In the present case the possible phases \(se\pm d\) are not accessible, and a tetracritical point exists where the normal and superconducting phases with \(se, d\) and \(se \pm id\) symmetries meet. In addition, the free energy depends only on \(\cos(2\phi_d)\) and does not distinguish between the phases \(se + id\) and \(se - id\), which are thus degenerate. In the \(se \pm id\) phases, time-reversal symmetry is broken but not chirality.

**Harmonic Trap:** The essential effect of an underlying harmonic trap \(V_h(\mathbf{r}) = kr^2/2\) is to allow for the emergence of non-uniform solutions. In particular, the harmonically confining potential allows for the emergence of all accessible phases \(se\), \(d\) and \((se \pm id)\)-wave for \(|U|/t = 0\) and \(sl + se\), \(d\) and \((sl + se \pm id)\)-wave for \(|U|/t \neq 0\). Within the local density approximation, we solve the order parameter Eq. (6) and number Eq. (7) with \(\mu \rightarrow -V_h(\mathbf{r})\). In Fig. 2, we show the spatial profiles of the filling factor and order parameters as a function of dimensionless position \(\eta = (t/\epsilon_h)^{1/2}(r/a)\) measured from the center of the trap, where \(\epsilon_h = k_o^2/2\). The parameters used are \(|U|/t = 0, |V|/t = 3, T/t = 0.1\), assuming that \(\nu = 1\) (half-filling) at the center of the trap. Notice that as the filling factor decreases from the center of the trap to its edge, all accessible phases emerge: \(d\)-wave superfluid at the center of the trap, followed sequentially by regions of \((se \pm id)\) and \(se\)-wave superfluids, and the normal state. Similarly, in the case of \(|U|/t \neq 0\) at low temperatures and assuming that \(\nu = 1\) at the center of the trap, the sequence of phases from the center of the trap is \(d\)-wave, \((sl + se \pm id)\), \((sl + se)\)-wave superfluid followed by a normal region at the edge. The interesting qualitative aspect here is the emergence of regions where time-reversal symmetry is spontaneously broken: \((se \pm id)\) for \(|U|/t = 0\) and \(sl + se \pm id\) for \(|U|/t \neq 0\). This is very important in a very broad sense, because there are no confirmed examples in condensed matter physics of superfluid that spontaneously break time-reversal-symmetry.

**FIG. 2:** Spatially resolved filling factor \(\nu\) in (a) and superfluid order parameters \(\Delta_\alpha (\alpha = se, d)\) in (b) as a function of \(\eta = (t/\epsilon_h)^{1/2}(r/a)\), assuming that \(\nu(0) = 1\) (half-filling) at the center of the trap. The parameters used are \(|U|/t = 0, |V|/t = 3,\) and \(T/t = 0.1\).

**Spontaneous Currents:** In order to keep the discussion simple, we continue to focus on the case of \(|U|/t = 0\), and discuss the spontaneous current flow in the shell corresponding to the \((se \pm id)\)-wave superfluid. Consider for example that either the \(se + id\) phase or the \(se - id\) phase is realized in the example of Fig. 2. Given that either chiral phase spontaneously break time-reversal symmetry, it is expected that within the boundaries of the \(se + id\) \((se - id)\) phase spontaneous currents circulate clockwise (counter-clockwise) near the outer boundary, and counter-clockwise (clockwise) near the inner boundary. To visualize the spontaneously generated currents, we perform a long-wavelength expansion of the action in Eq. (11), which leads to the effective Free energy density.
The first term is
\[ \mathcal{F}_{\text{di}} = \nabla \Delta^*_s \frac{\gamma_{se}}{2m} \nabla \Delta_{se} + \nabla \Delta^*_d \frac{\gamma_{se}}{2m} \nabla \Delta_d, \]
the second term is non-diagonal in the indices \(se\) and \(d\)
\[ \mathcal{F}_{\text{nd}} = \left[ \partial_x \Delta^*_s \frac{\gamma_{se,d}}{2m} \partial_x \Delta_{se} - \partial_y \Delta^*_s \frac{\gamma_{se,d}}{2m} \partial_y \Delta_d + C.C. \right], \]
the third term is \( \mathcal{F}_h = \gamma_{se} V_h(r) |\Delta_{se}|^2 + \gamma_d V_h(r) |\Delta_d|^2 \),
while the last term \( \mathcal{F} \) is given in Eq. 3.

Adding a current source term \( -i \partial_m - a_m \) and considering the phase difference \( \delta \phi = \phi_d - \phi_{se} = \pm \pi/2 \), we obtain within the \( se \pm id \) phase the particle current density \( J_i = J_i,\phi + J_i,|\Delta|^2 \) in Cartesian representation \((i = x, y)\). Here, \( J_i,\phi = \frac{2}{m} [ |\Delta|^2 c_{d,d} + |\Delta_{se}|^2 c_{se,se} ] \partial \phi_d \)
which breaks time reversal symmetry spontaneously. We calculated the spatially-dependent profiles of filling factor and order-parameter for various superfluid phases,

\[ J_{\text{d},\phi} = \frac{1}{m} \left| \partial_x \Delta_{se} c_{se,d} \partial_x \Delta_{se} - \partial_y \Delta_{se} c_{se,d} \partial_y \Delta_{se} \right|, \]

\[ J_{\text{d},|\Delta|^2} = \frac{2}{m} |\Delta_{se}|^2 c_{se,se} \partial |\Delta_{se}|^2, \]
\[ J_{\text{d},\phi} = \frac{2}{m} |\Delta_{se}|^2 c_{se,se} \partial \phi_d. \]

Given the existence of the harmonic potential, we transform the currents to polar coordinates \((r, \theta)\), and require the radial current \( J_r \) to vanish \((J_r = \hat{r} \cdot \mathbf{J} = 0)\) at the boundaries between the \( se \pm id \) and \( se \) occurring at \( r = R_s \) and at the boundaries between \( se \pm id \) and \( d \) phases occurring at \( r = R_d \). At these boundaries spontaneous currents flow only within the \( se \pm id \) phase limits, since these are the only phases that break spontaneously time-reversal symmetry. Under these conditions, a simple solution of the form \( \phi_d = \chi (|\pi/2 + f(r)\theta| \phi_{se} = \chi f(r)\theta) \phi_{se} = \chi f(r)\theta \) with \( f(r = R_s) = +1, f(r = R_d) = -1, \) and \( df(r)/dr|_{R_s} = df(r)/dr|_{R_d} = 0 \) is possible.

The spontaneous currents at the interface boundaries are tangential, have the simple forms \( J_\theta(r = R_s) \approx (2\chi/m)|\Delta|^2 c_{d,d}/R_s \) and \( J_\theta(r = R_d) \approx -2(\chi/m)|\Delta_{se}|^2 c_{se,se}/R_d \), and can be detected via Bragg spectroscopy as discussed next.

**Detection of time-reversal-symmetry-breaking:** A detection scheme of spontaneous currents using velocity sensitive Bragg spectroscopy \([12,13]\) is shown in Fig. 3 with right- (left-) going beam of frequency \( \omega \) (\( \omega' \)) and linear momentum \( \mathbf{k} \) (\( \mathbf{k}' \)). In Fig. 3, circulating currents are shown at the boundaries of the region for \((se + id)\) superfluidity, due to spontaneous breaking of time reversal symmetry at lower temperatures. The case of a normal region (higher temperatures), where no spontaneous currents exist, is shown in Fig. 3 for comparison.

**Conclusions:** We discussed screened dipolar fermions in harmonically confined optical lattices modeled by an extended attractive Hubbard model, where both interactions and filling factors can be controlled. We established the superfluid phases in the singlet channel and indicated that accessible phases have not only pure \( s \)-wave or \( d \)-wave characters, but also mixed \((s \pm id)\)-wave character and proposed a Bragg spectroscopy experiment to detect the time-reversal symmetry breaking phase, which contains spontaneously circulating supercurrents.

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