Exotic $p$-wave superfluidity of single hyperfine state Fermi gases in optical lattices

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We consider $p$-wave (triplet) pairing of single hyperfine state ultracold atomic gases trapped in quasi-two-dimensional optical lattices. We find that the critical temperatures in the lattice model is considerably higher and experimentally attainable around half-filling in contrast to the predictions of continuum model for $p$-wave superfluids. In tetragonal lattices, we show that the atomic compressibility and spin susceptibility have a peak at low temperatures exactly at the half-filling, but this peak splits into two in the orthorhombic lattices. These peaks reflect the $p$-wave structure of the order parameter for superfluidity and they disappear as the critical temperature is approached from below. We also calculate the superfluid density tensor, and show that for the orthorhombic case there is no off-diagonal component, however in the tetragonal case an off-diagonal component develops, and becomes a key signature of the exotic $p$-wave state.

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Tunable optical lattices have been extensively used to study phase transitions in bosonic atomic gases \cite{1,2}, because they allow the controlled manipulation of the particle density $n$, and of the ratio between the particle transfer matrix element $t$, and the interparticle interaction strength $V \gtrsim t$. This kind of control is not fully present in standard fermionic condensed matter systems, and has hindered the development of experiments that could probe systematically the effects of strong correlations as a function of $n$ and $t/V$. However, fermionic atomic gases like $^6$Li and $^{40}$K have been successfully trapped, and their normal state and superfluid properties are beginning to be studied \cite{12,13,14,15,16}. Since superfluid phases are more easily accessible in the experiments involving ultracold atomic gases, spin-polarized ultracold atomic systems are ideal candidates for the observation of novel triplet superfluid phases and for testing theoretical models that were proposed earlier. Thus, it is only natural to propose that optical lattices could be used to study the normal state and superfluid properties of ultracold fermionic systems as a function of $n$, $t/V$ and lattice symmetry. This systems are of a broad interest not only for the atomic physics community but also for the nuclear, condensed matter and more generally for the many-body physics communities where superfluidity models have been investigated in various contexts.

Presently there is only experimental evidence that $^{40}$K (Ref. \cite{12,11}) and $^6$Li (Ref. \cite{12,13,14,15,16}) can form weakly and tightly bound atom pairs, when the magnetic field is swept through an $s$-wave Feshbach resonance. However, the properties of $p$-wave spin-polarized ultracold fermions and their possible superfluid behaviour are beginning to be investigated \cite{17,18}. When identical fermionic atoms are trapped in a single hyperfine state (SHS) the interaction between them is strongly influenced by the Pauli exclusion principle, which prohibits $s$-wave scattering of atoms in identical spin states. As a result, in SHS degenerate Fermi gases, two fermions can interact with each other at best via $p$-wave scattering. Thus, one expects that the superfluid ground state of such SHS Fermi gases to be $p$-wave and spin triplet.

In the $p$-wave channel, if the atom-atom interactions are effectively attractive then the onset for the formation of Cooper pairs in three dimensions occurs at a temperature $T_c \approx E_F \exp[-\pi/(2 k_F a_{sc})^3]$, where $E_F$ is the Fermi energy and $a_{sc}$ is the $p$-wave scattering length. Unfortunately, this temperature is too low to be observed experimentally. However, in the presence of the Feshbach resonances \cite{17,18}, $p$-wave interactions can be enhanced, and the critical temperature for superfluid is expected to increase to experimentally accessible values. One the other hand, we show that the spin triplet ($p$-wave) weak coupling limit in optical lattices (like in the singlet cases \cite{3}) is sufficient to produce a superfluid critical temperature that is accessible experimentally.

In this manuscript, we consider quasi-two-dimensional optical lattices with a periodic trapping potential of the form $U(r) = \sum_i U_{0,i} \cos^2(k_i x_i)$, with $U_{0,z} \gg \min\{U_{0,x},U_{0,y}\}$, which strongly suppresses tunneling along the $z$ direction. This is a non-essential assumption, which just simplifies the calculations, but still describes an experimentally relevant situation. Here $x_i = x, y$, or $z$ labels the spatial coordinates, $k_i = 2\pi/\lambda_i$ is the wavelength, and $U_{0,i}$ is the potential well depth along direction $x_i$, respectively. The parameters $U_{0,z}$ are proportional to the laser intensity along each direction, and it is typically several times the one photon recoil energy $E_R$ such that tunneling is small and the tight-binding approximation can be used.

Thus, in the presence of magnetic field $\mathbf{h}$, we consider the following quasi-two-dimensional lattice Hamiltonian (already in momentum space) for an SHS Fermi gas

$$H = \sum_k \xi(k) a_{k\uparrow}^\dagger a_{k\uparrow} + \frac{1}{2} \sum_{k,k',q} V(k,k') b_{k,q}^\dagger b_{k',q'}, \quad (1)$$

where the pseudo-spin $\uparrow$ labels the trapped hyperfine state represented by the creation operator $a_{k\uparrow}$, and $b_{k,q}^\dagger = a_{k+q/2,\uparrow}^\dagger a_{-k+q/2,\uparrow}^\dagger$. Furthermore, $\xi(k) =$
\[ \varepsilon(\mathbf{k}) - \tilde{\mu} \] describes the tight-binding dispersion \[ \varepsilon(\mathbf{k}) = -t_x \cos k_x a_x - t_y \cos k_y a_y - t_z \cos k_z a_z, \] with \( \tilde{\mu} = \mu + g q \hbar \beta \), and \( \min\{t_x, t_y\} \gg t_z \). \( V(\mathbf{k}, \mathbf{k'}) = \pi \hbar |\mathbf{v}(\mathbf{k})| \mathbf{v}(\mathbf{k'}) | \) is the \( p \)-wave pairing interactions with matrix elements \( V_{ij} = -2 V_0 \delta_{ij} \) and \( \pi \hbar \mathbf{v}(\mathbf{k}) = (\sin k_x a_x, \sin k_y a_y) \). Here, \( V_{0,i} > 0 \) is the effective interaction and \( a_i \) is the corresponding lattice length along the \( i^{th} \) direction.

Using the functional integration formalism \( \int \mathcal{D}\mathbf{\sigma} \) \( (\beta = 1/T \) and units \( \hbar = k_B = 1) \), we obtain the saddle point effective action

\[
\frac{S_0}{\beta} = \Delta_0^2 \frac{\mathbf{V}^{-1}}{2} \Delta_0 + \sum_p \left( \frac{\xi(k)}{2} - \frac{1}{\beta} \text{Tr} \ln \frac{G^{-1}(p)}{2} \right),
\]

where we use \( p = (p, i v_i) \) with \( v_i = (2l + 1) \pi / \beta \) and define stationary vector field \( \Delta_0^i = (\Delta_{0,x}, \Delta_{0,y}) \). Here \( G^{-1}(p)/\beta = i v_i \sigma_0 - \xi(k) \sigma_3 + \Delta_0^i \mathbf{w}(k) \sigma_3 + \pi \hbar \mathbf{v}(k) \Delta_0 \sigma_3 \) is the inverse Nambu propagator and \( \sigma_\pm = (\sigma_0 \pm 2 \sigma_3)/2 \) and \( \sigma_3 \) is the Pauli spin matrix. The condition \( \delta S_0/\beta \Delta_0^* = 0 \) leads to the order parameter equation

\[
\Delta_0 = M \Delta_0
\]

where \( M \) has matrix elements \( M_{ij} = \sum_k V_{0,i} \sin k_x a_x \sin k_y a_y \tanh(\beta E(k)/2) / E(k) \). Here, \( E(k) = (\xi^2(k) + |\Delta(k)|^2)^{1/2} \) is the quasi-particle energy and the scalar order parameter \( \Delta(k) = \pi \hbar \mathbf{v}(k) \Delta_0 \) is separable in temperature \( T \) and momentum \( \mathbf{k} \).

Within the irreducible representations of the \( D_{4h} \) (or \( D_{2h} \)) group in the tetragonal (orthorhombic) lattices, \( \{2\} \) our exotic \( p \)-wave state corresponds to the \( ^3E_u(n) \) representation with a \( d \)-vector given by

\[
d(k) = f(k)(1, i, 0),
\]

where \( f(k) = AX + BY, \) and \( X \) and \( Y \) are \( \sin k_x a_x \) and \( \sin k_y a_y \), respectively. Notice that, this state also breaks time reversal symmetry, as expected from a fully spin-polarized state. In the tetragonal lattice, the stable solution for our model corresponds to the case \( A = B \neq 0 \), and thus to the \( ^3E_u(d) \) representation, where spin-orbit symmetry is preserved, but both spin and orbit symmetries are independently broken. In the orthorhombic lattice, the stable solutions correspond to either \( A \neq 0, B = 0 \) or \( A = 0, B \neq 0 \), thus leading to the \( ^3E_u(b) \) representation.

Our main interest is in tetragonal (square) lattices, however, we also want to investigate the effects of small anisotropies in optical lattice lengths. For definiteness, we set \( a_y = a \) constant and investigate square and orthorhombic lattices where \( a_x = a \) and \( a_y = a (1 - \delta) \) with \( \delta \ll 1 \), respectively. In the case of square lattices, we choose the parameters \( t_x = t_y = t \) and \( V_{0,x} = V_{0,y} = V_0 = 0.3t \) and change \( V_{0,x} \) and \( t_y \) accordingly as we vary \( a_x \). Using exponentially decaying on-site Wannier functions and the WKB approximation, we obtain that the tunneling and interaction matrix elements along the \( x \)-direction are proportional to \( \exp(2\delta \sqrt{V_{0,x} / E_0}) \). In the present calculation, we take \( t_y = t \exp(10\delta) \) and \( V_{0,x} = V_0 \exp(10\delta) \). As we increase (decrease) the ratio \( \delta \), both interactions and tunneling rate increase (decrease) in \( \hat{x} \) direction. A different choice of on-site Wannier functions does not change our general conclusions, the only qualitative difference is that \( t_x \) and \( V_{0,x} \) are different functions of \( \delta \). Depending on the lattice anisotropy, there are three distinct solutions: (1) \( \Delta_{0,x} \neq 0, \Delta_{0,y} = 0 \) \( (A \neq 0, B = 0) \); (2) \( \Delta_{0,x} = 0, \Delta_{0,y} \neq 0 \) \( (A = 0, B \neq 0) \); and (3) \( \Delta_{0,x} = \Delta_{0,y} = 0 \) \( (A = B \neq 0) \). In a square lattice both directions are degenerate (case 3), but even a small anisotropy in the lattice spacings or in the lattice potential lifts the degeneracy and throws the system into either case (1) or (2).

The critical temperature, \( T_c = \max\{T_{c,x}, T_{c,y}\} \), is determined from the condition \( \det M = 1 \) in Eq. \( \{2\} \), and can be written as

\[
0 = \prod_{i=x,y} \left( 1 - V_{0,i} \sum_k \sin^2 k_x a_x \tanh \frac{\xi(k)}{2 T_{c,i}} \right).
\]

But, this equation has to be solved simultaneously with the saddle point number equation \( N = -\partial \Omega_0 / \partial \tilde{\mu} \) where \( \Omega_0 = S_0(\Delta(0))/\beta \) is the saddle point thermodynamic potential. This leads to \( N = \sum_k n(k) \) where

\[
n(k) = \frac{1}{2} \left[ 1 - \frac{\xi(k)}{E(k)} \tanh \frac{\beta E(k)}{2} \right]
\]

is the momentum distribution. These equations are approximately valid for all temperatures \( T \leq T_c \) in the limit of weak interactions (BCS limit). Plots of

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{(Colour online) Plot of a) critical temperature \( T_r = T_c/E_0 \) and b) chemical potential \( \mu_r = \tilde{\mu}/E_0 \) versus filling \( N_c \) for the square case \( a_x = a \) (red); and the orthorhombic case \( a_x = 0.99 a \) (blue).}
\end{figure}

\( T_r = T_c/E_0 \) and \( \mu_r = \tilde{\mu}/E_0 \) as a function of number of atoms per unit cell \( (N_c) \) are shown in Fig. 1 for the cases of square and orthorhombic lattices. Here, \( E_0 = 2t \) is the half-filling Fermi energy for the square lattice. Notice that \( T_r \) is maximal at half-filling, and that it has a
value 0.01, which is much higher than the theoretically predicted $T_c$, from the continuum model, and comparable to experimentally attainable $T_c/T_F \approx 0.01$. This implies that the superfluid regime of spin-polarized fermion gases may be observed experimentally in a lattice, even in the limit of weak interactions. The observability of a superfluid transition in spin-polarized fermion systems is clearly enhanced when the system is driven through a Feshbach resonance (in a lattice or in the continuum), as $T_c$ is expected to increase further in this case, however our calculations indicate that the weak interaction (BCS) limit may be sufficient in the lattice case.

Notice that the order parameter symmetry dramatically effects $T_c$ as can be seen by rewriting Eq. 6 as

$$1 = \prod_{i=x,y} V_{0,i} \int_{-t_x - t}^{t_x + t} \frac{\tanh \frac{\sqrt{2} \mu - \epsilon}{2(\epsilon - \mu)}}{D_{p,i}(\epsilon)},$$

where we define an effective density of states (EDOS) $D_{p,i}(\epsilon) = \sum_k \delta(\epsilon - \epsilon(k))(\sqrt{2} \sin k_i a_i)^2$ which is plotted in Fig. 2 for $a_x = a$ (black), $a_x = 0.99a$ (red), and $a_x = 0.95a$ (blue). Here, $\sqrt{2} \sin k_i a_i$ are symmetry factors related to the order parameter. For instance in the $s$-wave case, this symmetry factor is 1 and EDOS becomes $D(\epsilon) = \sum_k \delta(\epsilon - \epsilon(k))$, which is the density of states (DOS) of normal fermions. For the $p$-wave symmetry discussed, $D_{p,i}(\epsilon)V_{0,i}$ plays the role of a dimensionless coupling parameter which controls the critical temperature. Notice that, EDOS and $T_c$ are maximal at half-filling in square lattices ($a_x = a$). Additionally, EDOS decreases and finally vanishes at the band edges where a small ratio of $T_c/T_F$ was predicted from continuum models. However, this is not the case around half-filling and we expect weak interactions to be sufficient in observing superfluidity. In the orthorhombic lattices, EDOS and $T_c$ are considerably increased and are maximal around half-filling with a small anisotropy ($a_x = 0.99a$) in the lattice spacings. Notice, however, that further anisotropy in the lattice spacings ($a_x = 0.95a$) leads to a decrease in EDOS and $T_c$ around half-filling with respect to the case with $a_x = 0.99a$.

Next we discuss the atomic compressibility and the spin susceptibility of the system. The isotropical atomic compressibility is given by $\kappa = -(1/N_c^2)\partial^2 \Omega/\partial \tilde{\mu}^2 = (1/N_c^2)\partial N_c/\partial \tilde{\mu}$ where

$$\frac{\partial N_c}{\partial \tilde{\mu}} = \sum_k \Delta^2(k) \tanh \frac{\beta E(k)}{2} + \sum_k Y(k) \frac{\epsilon^2(k)}{E^2(k)},$$

and $Y(k) = (\beta/4) \text{sech}^2[\beta E(k)/2]$. Plots of $\kappa_r = \kappa/\kappa_0$, where normalization $\kappa_0$ is evaluated at $T = 0$ and half-filling, is shown in Fig. 3 for the square and orthorhombic lattices. In the square lattice case, $\kappa$ has a peak at half-filling and low temperatures, and a hump at $T_c$. The same qualitative behavior is obtained in the case of orthorhombic lattices, with the additional feature that the central peak (hump) splits into two due to degeneracy lifting.

![FIG. 2: (Colour online) Plot of a) normal state DOS $D(\epsilon)$ and b) $p$-wave EDOS $D_{p,x}(\epsilon)$ versus energy $\epsilon/E_0$ in units of $t$ for $a_x = a$ (black) and $a_x = 0.99a$ (red), and $a_x = 0.95a$ (blue) in two dimensions.](image)

The peaks at $T \approx 0$, can be understood by noting that $N_c^2 \kappa$ can be written as $\sum_k g(k)/E(k)$ for $T = 0$, where $g(k) = 2n(k)[1 - n(k)]$. Therefore, the peaks are due to non-vanishing $g(k)$ in regions of $k$-space where $E(k)$ vanishes and $n(k)$ is rapidly changing. In tetragonal lattices, the integrand $g(k)/E(k)$ has 4 $k$-space points $(0, \pm \pi)$, and $(\pm \pi, 0)$ in the first Brillouin zone (1BZ) where it diverges only when the chemical potential $\mu = 0$ ($N_c = 0.5$). Similarly in orthorhombic lattices, the integrand diverges at 2 $k$-space points $(\pm \pi, 0)$ in the 1BZ when $\mu = t_x - t = 0.021$ ($N_c = 0.548$). Furthermore, the integrand diverges at 2 $k$-space points $(0, \pm \pi)$ when $\mu = -t_x + t = -0.021$ ($N_c = 0.452$). For every other $\mu$ the integrand is well-behaved resulting in a smooth $\kappa$ in both cases. At $T = T_c$, the humps are not related to the order parameter, but are due to the peaks appearing in DOS (Fig. 2a).

![FIG. 3: (Colour online) Plot of compressibility $\kappa_c = \kappa/\kappa_0$ versus filling $N_c$ at $T = 0.004T_F^{\text{max}}$ for a) $a_x = a$ (red) and b) $a_x = 0.99a$ (blue). Notice that the compressibility peaks disappears at $T = T_c$ and turns into humps (black) in both cases.](image)
divergence at half-filling in the tetragonal case, it has two peaks in the case of orthorhombic lattices which leads to two humps.

Furthermore, for a magnetic field $h = h\hat{y}$ applied along an arbitrary $\eta$-direction, the spin susceptibility tensor component is $\chi_{\eta\eta} = -\partial^2\Omega/\partial h^2 = g^2\mu_B^2\partial N_c/\partial h^2$. Therefore, in spin-polarized systems, $\chi_{\eta\eta}$ is directly related to the atomic compressibility and is given by $[N_c^2/(g\mu_B)^2]k$.

Next we discuss the superfluid density of the system. Generally speaking, there are two components to the reduction of the superfluid density at non-zero temperatures, one coming from fermionic (quasi-particle excitations) and the other bosonic (collective modes) degrees of freedom. The fermionic component comes from phase twists of the order parameter and the temperature dependence of its components is given by

$$\rho_{ij} = \frac{1}{2V} \sum_{\mathbf{k}} [n(\mathbf{k})\partial_i\partial_j\xi(\mathbf{k}) - Y(\mathbf{k})\partial_i\xi(\mathbf{k})\partial_j\xi(\mathbf{k})],$$

where $n(\mathbf{k})$ is the momentum distribution, and $\partial_i$ denotes the partial derivative with respect to $k_i$. Here, we will not discuss the bosonic contribution, except to say that at low temperatures the dominant terms come from Goldstone modes associated with the phase of the order parameter, which are underdamped in our case due to sub-critical Landau damping. Furthermore, in the case of tetragonal symmetry, Goldstone modes do not contribute to the off-diagonal component of the superfluid density, which is the main focus of the analysis that follows.

In summary, we considered $p$-wave pairing of single-hyperfine-state Fermi gases in quasi-two-dimensional optical lattices. We found that the critical temperatures in tetragonal and orthorhombic optical lattices are considerably higher than the continuum model predictions, and therefore, experimentally attainable. At low temperatures, we found a peak in the atomic compressibility (and similarly in the spin susceptibility) exactly at half-filling for the tetragonal lattice. This peak splits into two smaller peaks in the orthorhombic case. These peaks reflect the $p$-wave structure of the order parameter at low temperatures, and they decrease in size as the critical temperature is approached from below. Furthermore, in the orthorhombic lattices, the off-diagonal component $\rho_{xy}$ of the superfluid density tensor vanishes identically, while the diagonal components $\rho_{xx}$ and $\rho_{yy}$ are different. However, in the square lattices, we showed that $\rho_{xy} \neq 0$, while $\rho_{xx} = \rho_{yy}$. The presence of non-zero $\rho_{xy}$ is a key signature of our exotic $p$-wave triplet state.

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