Fermionic superfluidity and spontaneous superflows in optical lattices

Shi-Jie Yang and Shiping Feng
Department of Physics, Beijing Normal University, Beijing 100875, People’s Republic of China
E-mail: yangshijie@tsinghua.org.cn

Abstract. We studied the superfluidity of strongly repulsive fermionic atoms in optical lattices. Atoms are paired through a correlated tunneling mechanism, which induces superfluidity when repulsive nearest-neighbor interactions are included in the Hubbard model. This paired superfluid is a metastable state, which persists for a long time as the pair-broken process is severely suppressed. The mean-field phase diagram and low-energy excitations are investigated in a square lattice system. Intriguingly, spontaneous superflows may appear in the ground state of a triangular optical lattice system due to antiferromagnetic frustration.

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1 Author to whom any correspondence should be addressed.
1. Introduction

Recently, the strongly correlated properties of ultracold atoms in optical lattices have attracted the interest of physicists [1]–[3]. The high tunability of the interaction strength between atoms and the easy manipulation of optical lattices make the system realistically viable to implement a quantum simulator [4]. The quantum atomic gases in optical lattices make it possible to build a model system so that we can explore correlated properties in many-body physics, such as superconductivity, quantum magnetism, quantum criticality, etc, and examine related theoretical models [5]–[7].

A recent experiment [8] showed that a couple of strongly repulsive atoms occupying the same site of an optical lattice can be stabilized by damping the single-particle tunneling. The lifetime of the pair increases significantly with the on-site repulsion $U$ of the Hubbard model, which is quite intriguing as intuitively an attractive force between particles is required to obtain a bound state. In the presence of a periodic spatial potential, the energy of a particle does not vary continuously but is restricted to particular ranges of values. A pair of strongly repelling particles can be stable, because if it fell apart, the two isolated atoms would ensure kinetic energies that fall in a forbidden band [9]. Another experiment directly observed that for a pair of strongly repulsive atoms in the optical lattice, single-particle tunneling is severely suppressed by the requirement of energy conservation while atom-pair co-tunneling is permitted through the second-order quantum process [10]. Although these experiments were performed on bosonic atoms, it is conceivable that they can be applied to fermionic atoms since no quantum statistics is involved.

The formation of a metastable atom pair with repulsive interactions was first proposed by A F Andreev in his study of diffusion of impurities in a quantum crystal [11, 12]. The quantum liquid of repulsive particle pairs in optical lattices has been discussed by several authors [13]–[17]. In a recent paper, Rosch et al [18] studied the metastable superfluidity of repulsive fermionic atoms in optical lattices. Other authors attempted to explore the possibility of counterflow superfluidity and to control the spin exchange interaction of two-species ultracold atoms in a commensurate optical lattice [19]–[22]. In fermionic superconductivity and superfluidity, a central concept is pairing. In Bardeen–Cooper–Schrieffer (BCS) theory, electrons pair up by an attractive interaction mediated by phonons of underlying crystals. The attraction between ultracold fermionic atoms is provided by Feshbach resonances. Another pairing mechanism comes from correlated hopping, which occurs in fermionic tight-binding models. It has been suggested as a possible explanation for high-$T_c$ superconductivity [23]–[25].

In this paper, we explore the fermionic superfluid (SF) in a system consisting of repulsive atom pairs in optical lattices. We deal with a system partially filled by couples of spin-up and spin-down fermionic atoms. The lattice site is either occupied by two atoms or empty in the one-band Hubbard model. In the limit of strong on-site repulsion $U \gg t$, pair-breaking tunneling is suppressed, as is revealed by the experiment [8]. On the other hand, atom pairs may transport across the lattice through the second-order quantum transition [10]. As a result, the atoms always move in pairs. The effective Hamiltonian is obtained by quantum perturbation theory, which is mapped to an anisotropic antiferromagnetic (AF) model instead of the usual ferromagnetic model in the Bose–Hubbard model. The system exhibits superfluidity when nearest-neighbor (NN) repulsive interactions are included. This paired SF is a metastable state because the pair-breaking process is severely suppressed. We investigate the mean-field (MF) phase diagram and
low-energy excitations for a square lattice system. It exhibits a gapless mode in the SF state and a gapful mode in the solid state.

The AF feature of the effective Hamiltonian may lead to an interesting phenomenon when the underlying optical lattice is triangular. As is well known, the ground state has a long-range 120° Néel order. The variation of azimuthal angles between NN spins corresponds to the phase modulation of the SF state, which leads to spontaneous superflow in the ground state due to AF frustration. As a result, the system exhibits a pattern of convection consisting of vortex–antivortex pairs.

The paper is organized as follows. In section 2, we obtain an effective Hamiltonian for strong on-site interactions by the second-order quantum perturbation approximation. In section 3, we demonstrate the superfluidity of paired fermionic atoms by mapping the system to the pseudospin-1/2 AF model. The phase diagram and low-energy excitations are calculated in the MF approximation. In section 4, we explore the possible phenomenon of spontaneous superflows of paired atoms in a triangular lattice. A summary is included in section 5.

2. Effective Hamiltonian

We focus on the partial pair-filling system with \( \nu < 1 \). For sufficient low temperature and strongly repulsive on-site interaction, atoms will be confined to the lowest band, which is described by the Hubbard model [5],

\[
\hat{H} = - \sum_{\langle ij \rangle \sigma} t_{\sigma} (f_{i \sigma}^\dagger f_{j \sigma} + f_{j \sigma}^\dagger f_{i \sigma}) + U \sum_i n_{i \uparrow} n_{i \downarrow} + V \sum_{\langle ij \rangle} n_i n_j, \tag{1}
\]

where \( f_{i \sigma} (f_{i \sigma}^\dagger) \) is the annihilation (creation) spin-\( \sigma \) fermionic operator, \( n_i = n_{i \uparrow} + n_{i \downarrow} \) is the number operator with \( n_{i \sigma} = f_{i \sigma}^\dagger f_{i \sigma} \) and \( t_{\sigma} \) is the tunneling matrix element. \( U > 0 \) is the on-site interacting energy and \( V > 0 \) is the NN interaction. In this paper, we confine our discussions to the case of \( U \gg t_{\sigma} \).

Since pair-breaking processes are suppressed, single-particle hopping is eliminated in the second-order quantum perturbation theory. The on-site Hubbard term is considered as the unperturbed Hamiltonian \( H_0 \). The hopping term is treated as perturbation \( H_1 \), which should be calculated to the second order of \( t_{\sigma}/U \) to avoid pair breaking. The NN interaction term commutes with the Hubbard term and will be included in the effective Hamiltonian later. Using a generalization of the Schriffer–Wolf transformation [26],

\[
\hat{H} = H_0 + \frac{1}{2} [S, H_1] + \frac{1}{2} [S, [S, H_1]] + \cdots, \tag{2}
\]

where \( [S, H_0] = -H_1 \) and \( S^\dagger = -S \). Suppose \( |\alpha\rangle \) are the degenerate paired states of unperturbed \( H_0 \) with energy \( E_0 \) and \( |\beta\rangle \) are the pair-breaking intermediate states of \( H_0 \) with \( H_0 |\beta\rangle = E_1 |\beta\rangle \). Then \( E_1 = E_0 - U \). It should be emphasized that in the initial states \( |\alpha\rangle \) all atoms are paired in the lattice sites, while in the intermediate states \( |\beta\rangle \) only one pair of atoms is breaking. We have \( \langle \alpha | H_1 | \alpha' \rangle = \langle \beta | H_1 | \beta' \rangle = 0 \) and \( \langle \alpha | S | \beta \rangle = \langle \alpha | H_1 | \beta \rangle / U \). Disregarding intermediate states with more breaking of atom pairs, which will involve higher order of \( t_{\sigma}/U \), the second-order quantum perturbation Hamiltonian is then

\[
\langle \alpha | H^{(2)} | \alpha' \rangle = \frac{1}{U} \sum_{\beta} \langle \alpha | H_1 | \beta \rangle \langle \beta | H_1 | \alpha' \rangle. \tag{3}
\]

An alternative method of quantum perturbation theory can be found in [19, 27].
The effective Hamiltonian is then

\[
\hat{H}_{\text{eff}} = \frac{4t_\uparrow t_\downarrow}{U} \sum_{\langle ij \rangle} (f_{i \uparrow} \dagger f_{j \uparrow} + f_{i \downarrow} \dagger f_{j \downarrow}) + \left( V - \frac{t_\uparrow^2 + t_\downarrow^2}{U} \right) \sum_{\langle ij \rangle} n_i n_j + \frac{z(t_\uparrow^2 + t_\downarrow^2)}{U} \sum_{i} n_i, \tag{4}
\]

where \( z \) is the number of NN sites. In second-order quantum perturbation, the intermediate virtual state \( |\beta\rangle \) that breaks the atom pair has a lower energy \((-U)\) than the initial and final states \(|\alpha\rangle\), which induce an attractive NN interaction. In order to prevent the atom pairs from congregation, a moderate repulsive NN interaction \( V \) is introduced in the original Hamiltonian (1) to overcome the induced attractive interaction. The first term describes pair hopping, implying that the spin-up and spin-down atoms are transported together across the lattice. The composite object behaves like a hard-core bosonic molecule because the fermion pairs always hop together to their nearest-neighboring site, and for each site only one pair of atoms is allowed. It should be noted that the pairing in our work is of s-wave type, where only the lowest single-particle band is considered in the Hubbard model.

To study the MF properties of the system, it is convenient to map the effective Hamiltonian (4) to the spin representation [19, 28] by defining \( S_i \) as \( S_{ix} = (f_{i \uparrow} \dagger f_{i \downarrow} + f_{i \downarrow} \dagger f_{i \uparrow})/2 \), \( S_{iy} = (f_{i \uparrow} \dagger f_{i \downarrow} - f_{i \downarrow} \dagger f_{i \uparrow})/2i \) and \( S_{iz} = [S_{ix}, S_{iy}]/i = (n_i - 1)/2 \),

\[
\hat{H}_{\text{eff}} = \frac{8t_\uparrow t_\downarrow}{U} \sum_{\langle ij \rangle} (S_{ix} S_{jx} + S_{iy} S_{jy}) + 4 \left( V - \frac{t_\uparrow^2 + t_\downarrow^2}{U} \right) \sum_{\langle ij \rangle} S_{iz} S_{jz} + 2zV \sum_{i} S_{iz}. \tag{5}
\]

The NN interaction \( V \) also acts as an external magnetic field exerting on the spins.

In contrast to the ferromagnetic model [29, 30] in the usual hard-core Bose–Hubbard model, the effective Hamiltonian (5) represents an anisotropic AF model, where there are several competitive phases dependent on the pair-filling \( \nu \) as well as on \( V \) and \( t_\sigma \). Rosch et al [18] obtained a ferromagnetic model by making a particle–hole transformation for the down spins. At the MF level, we minimize the energy at fixed \( z \)-polarization or pair filling. Suppose the classical spins \( S_i \) are in the X–Z-plane with an angle \( \theta_i \) to the z-axis; then a bipartite structure with sublattices A and B is employed to describe the possible periodicity in the ground state [37]–[39]. Candidate states include an easy-plane AF phase (\( \theta_A = -\theta_B \)) or paired SF with a non-vanishing order parameter \( \langle f_{i \uparrow} f_{i \downarrow} \rangle \neq 0 \) and a canted AF phase (\( \cos \theta_A \neq \cos \theta_B \)), which is actually a checkerboard solid with a non-vanishing \( \langle f_{i \uparrow} f_{i \downarrow} \rangle \) in one sublattice and a vanishing \( \langle f_{i \uparrow} f_{i \downarrow} \rangle \) in another sublattice. In addition, there is a phase separation (PS) regime caused by attractive NN interactions. The easy-plane ferromagnetic phase (\( \theta_A = \theta_B \)) is proved to have higher energy than the easy-plane AF phase and does not appear in this system.

3. MF results in a square lattice

We are now ready to explore the superfluidity of fermionic atoms in a square optical lattice \((z = 4)\). Hereafter, we use the units of \( U = 1 \). Figure 1 displays the \( V – \nu \) phase diagram for hopping integrals \( t_\uparrow = 0.1 \). We take, for example, the ratio \( t_\uparrow/t_\downarrow = 1.1 \). The other choice of \( t_\uparrow/t_\downarrow \) does not alter the conclusion qualitatively. We compare the MF energies of each candidate phase to determine the ground state. Generally, the canted AF phase with \( \cos \theta_A \neq \cos \theta_B \neq 0, 1 \) is a supersolid. But in the square lattice, we find \( \theta_B = 0 \) or \( \pi \), implying the supersolid order degenerates to an ordinary solid. We will re-examine this issue through low-energy excitations.
Figure 1. $V$–$\nu$ phase diagram for a square optical lattice system with $t_\downarrow = 0.1$ and $t_\uparrow = 1.1t_\downarrow$.

Figure 2. Condensate density versus pair-filling $\nu$ for the SF state (dashed curve) and the solid state (solid curves). For the solid state, the two branches correspond to sublattices A and B.

The solid phase takes place in the regime of $0.4 \lesssim \nu \lesssim 0.6$. For SF order, there is a $\pi$-phase difference between the two sublattices (cant AF order). The phase diagram is symmetrical with respect to the pair-filling $\nu = 0.5$, which results from particle–hole symmetry of the effective Hamiltonian (4).

We discuss superfluidity in terms of the condensate density $\rho_\nu = |\langle S^- \rangle|^2 = |\langle f_\uparrow f_\downarrow \rangle|^2$. The SF phase has a uniform condensate density $\rho_s = \nu(1 - \nu)$ for a given pair filling, independent of the value of $V$. In figure 2, we plot the condensate density for the SF state (dashed curve) as well as for the solid state (solid curves) versus the filling $\nu$ for $V = 0.1$. At the MF level, the condensate density vanishes in one sublattice but does not vanish in another sublattice. This indicates that this phase is a usual checkerboard solid instead of a supersolid. More accurate calculations such as quantum Monte Carlo simulations have demonstrated that supersolid states indeed do not exist in a square lattice system [31, 32].

Superfluidity can also be investigated through low-energy excitations, which provide an accurate probe for the nature of the quantum phase. We study low-energy excitations by introducing pseudo-spin operators $a_i^\dagger (a_i)$ for sublattice A and $b_i^\dagger (b_i)$ for sublattice B. We define $a_i^\dagger = S_i^+ = f_{i\downarrow}^\dagger f_{i\uparrow}^\dagger$ for sublattice A. After making a rotation to align the local spins along the

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Figure 3. Excitation energies of (a) the SF state at $\nu = 0.2$ and (b) the solid state at $\nu = 0.45$ for momentum along the $x$-direction. $t_\downarrow = 0.1, t_\uparrow = 1.1 t_\downarrow$ and $V = 0.1$.

In the $z$-direction, we obtain the spin-wave-type Hamiltonian in momentum space as

$$H_{sw} = \sum_k \left\{ \frac{\gamma_k}{2} (2 \tilde{t} \cos \theta_A \cos \theta_B + \tilde{U} \sin \theta_A \sin \theta_B)(a_k^\dagger b_{-k}^\dagger + a_k b_{-k} + a_{-k}^\dagger b_k + a_k b_k^\dagger) \\
- \tilde{t} \gamma_k (a_k^\dagger b_{-k}^\dagger + a_k b_{-k} - a_{-k}^\dagger b_k - a_k b_k^\dagger) \\
- (2 \tilde{t} \sin \theta_A \sin \theta_B + \tilde{U} \cos \theta_A \cos \theta_B)(a_{-k}^\dagger a_k + b_k^\dagger b_k) \\
- \frac{\tilde{H}_z}{2} (\cos \theta_A a_k^\dagger a_k + \cos \theta_B b_k^\dagger b_k) \right\} + H_{linear},$$

(6)

where $\gamma_k = (\cos k_x + \cos k_y)/2$, the renormalized parameters $\tilde{t} = 4 t_\downarrow t_\uparrow / U$, $\tilde{U} = 4[V - (t_\downarrow^2 + t_\uparrow^2) / U]$ and $\tilde{H}_z = 2(z V - \mu)$, and the summation for momentum $k$ is restricted to half the Brillouin zone. $H_{linear}$ includes the linear term in operators $a_k$ and $b_k$. With $H_{linear} = 0$, $\theta_A$ and $\theta_B$ are determined and the above MF result is recovered. This Hamiltonian (6) can be diagonalized in terms of the Bogoliubov transformation to obtain the low-energy excitation spectrum. For the SF state, we have

$$\omega_k^2 = 4 \tilde{t} (1 - \gamma_k)[\tilde{t}(1 - \gamma_k) + 2 \nu(1 - \nu)(\tilde{U} + 2 \tilde{t}) \gamma_k].$$

(7)

Figure 3 exhibits excitation energies versus momentum along the $x$-direction for $t_\downarrow = 0.1, t_\uparrow = 1.1 t_\downarrow$ and $V = 0.1$. For the SF state in figure 3(a) with $\nu = 0.2$, the energy spectrum is linear at small momenta, which reveals a gapless mode. At larger momenta, a energy dip plays the role of a roton as in the $^4$He SF. The excitations of the solid state in figure 3(b) with $\nu = 0.45$ reveal a gapful mode. No gapless low-energy excitation mode is found in this parameter regime, which justifies that this phase is a usual checkerboard solid rather than a supersolid.

4. Spontaneous superflow in a triangular lattice

We now study an intriguing phenomenon of spontaneous superflow of fermionic superfluidity for a triangular optical lattice system. Although there are some debates on the possible disordered ground state in a triangular AF model because of geometric frustration as well as quantum fluctuations, the current consensus is that the ground state has a long-range Néel order [33]–[36]. We consider the classical spins $S_i$ and use the 120° XY-Néel order for three
Figure 4. Spontaneous superflows of the paired SF in the optical triangular lattice. (a) The azimuthal angles between spins correspond to the phase difference between SFs on neighboring sites and a Josephson superflow spontaneously occurs along the edge. (b) The arrowed circles represent vortex–antivortex pairs, which form the superflow convection.

sublattices A, B and C. Let $\theta_A$, $\theta_B$ and $\theta_C$ be the corresponding polar angles that reflect the spatial density variations [37]–[39]. Then the MF energy of the system is written as

$$E_{MF} = \frac{3}{2} \left( V - \frac{t^2_1 + t^2_2}{U} \right) \left( \cos \theta_A \cos \theta_B + \cos \theta_B \cos \theta_C + \cos \theta_C \cos \theta_A \right)$$

$$- \frac{3t_1 t_2}{2U} \left( \sin \theta_A \sin \theta_B + \sin \theta_B \sin \theta_C + \sin \theta_C \sin \theta_A \right)$$

$$+ \left( V - \frac{\mu}{3} \right) \left( \cos \theta_A + \cos \theta_B + \cos \theta_C \right),$$

where $\mu$ is the Lagrangian multiplier that controls the total pair-filling. In formula (8), the $2\pi/3$ azimuthal angle difference between spins in the three sublattices has been incorporated.

The MF energy should be minimized with respect to angles $\theta_A$, $\theta_B$ and $\theta_C$ at a given polarization $\langle S_z \rangle = v - \frac{1}{2}$. It has a form similar to that in [40] except that the first term may become negative. In that case, the system is phase separated. Generally, there is a supersolid phase with $\theta_A = \theta_B \neq \theta_C$. For $V < (t^2_1 + t^2_2)/U$, the ground state is a uniform SF. We focus on the uniform SF phase ($\theta_A = \theta_B = \theta_C = \cos^{-1}(v - \frac{1}{2})$), which is implemented at a moderate NN interaction $V > (t^2_1 + t^2_2)/U$. We explore the implications of this $120^\circ$ Néel state and its possible consequence in the paired SF.

According to the spin mapping $\langle f_{i \uparrow} f_{i \downarrow} \rangle = \langle S^- \rangle = \frac{1}{2} \sin \theta_i e^{-i\phi_i}$, the paired SF has an order parameter phase similar to that of the azimuthal angle $\phi_i$ of the spin. Therefore, the $2\pi/3$ azimuthal angle difference of the spins implies a $\Delta \phi_{ij} = 2\pi/3$ phase difference between neighboring sites of the SF. The Néel order of the AF model thus corresponds to a periodic phase modulation in the SF. In the theory of Josephson tunneling, two weakly connected SFs or superconductors will induce a current as a result of their phase difference as $J \propto \sin \Delta \phi$. Consequently, the ground state SF spontaneously flows along the link of neighboring sites, as shown in figure 4(a). In the triangular lattice system, SF flows form a closed ring-like vortex.
Figure 4(b) schematically displays a regular convection pattern of superflows, which contains a sequence of vortex–antivortex pairs.

Similar cellular superflows and periodic textures were suggested in the $^3$He–A SF when a perpendicular magnetic field is applied to a sample slab [41]. The coupling between SF velocity and the orbital axis favors spontaneous superflows. Early theoretical discussions of possible superflow in solid $^4$He involved quantum tunneling through ground-state vacancies as well as Bose–Einstein condensation and quantum exchanges within the lattice [12, 42, 43]. In 2004, Kim and Chan reported the observation of unusual superflow without resistance from frictional forces in crystalline helium [44, 45]. This remarkable finding has now been confirmed [46]–[48]. Latest experiments indicate that, rather than being an intrinsic property of a perfect quantum solid, superflows owe their existence to macroscopic defects or extended disorder in the structure of solid helium.

In a mismatched Josephson junction of ultracold fermionic atomic gases, Kulić [49] proposed an oscillating SF amplitude inside the weak link and as a result the so-called $\pi$-junction. If the junction is a part of the closed ring, then spontaneous and dissipationless SF current can flow through the ring.

5. Summary and discussions

We have studied the superfluidity of strongly repulsive fermionic atoms from a correlated pairing mechanism. The SF is a metastable state with optical lattice sites either doubly occupied or empty. The composite objects are transported in the optical lattice through the second quantum processes via virtual pair-breaking states. The system exhibits superfluidity below a critical temperature. Phase diagrams and low-energy excitations in the square optical lattice system are investigated. Due to AF frustration, correlated pairs may result in a spontaneous superflow phenomenon in the triangular optical lattice system.

Some authors explored the possibility of formation of the non-s-wave BEC through Feshbach resonance in a nonzero angular momentum channel on a lattice with double occupation [50]–[52]. Varying the detuning of non-s-wave resonance can lead to various quantum phase transitions between the phases: s-wave BEC, non-s-wave BEC, conventional Mott insulator and orbital Mott insulator (with broken lattice symmetries). This becomes possible when the atoms are confined in the p-orbital Bloch band of an optical lattice rather than the usual s-orbital band. The new condensate simultaneously forms an order of transversely staggered orbital currents, reminiscent of orbital antiferromagnetism or d-density waves in correlated electronic systems but different in fundamental ways.

NN interaction depends on the overlap of Wannier functions between the NN sites. A moderate value of $V \sim (t_{↓}^2 + t_{↑}^2)/U$ is sufficient to create superfluidity in the system. An alternative way of generating NN interaction by long-range dipolar interaction is also possible [53, 54]. In order to detect the superfluidity of correlated pairs, photoassociation spectroscopy may be used [55]. Interference of matter waves released from the lattice has been used to probe the superfluidity of single atom condensation [56]. By tuning the interaction from repulsive to attractive, fermionic atom pairs are converted into molecules. Sharp peaks will appear in the interference pattern of released bosonic molecules due to the presence of an SF fraction.
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