Counterflow Superfluidity of Two-Species Ultracold Atoms in a Commensurate Optical Lattice

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In the Mott-insulator regime, two species of ultracold atoms in an optical lattice can exhibit the low-energy counterflow motion. We construct effective Hamiltonians for the three classes of the two-species (fermion-fermion, boson-boson, and boson-fermion–type) insulators and reveal the conditions when the resulting ground state supports super-counter-fluidity (SCF), with the alternative being phase segregation. We emphasize a crucial role of breaking the isotopic symmetry between the species for realizing the SCF phase.

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A recent pioneering experiment by Greiner *et al.* [1] (proposed in Ref. [2]) on the superfluid Mott-insulator transition in the optical lattice of ultracold atoms has opened up a new era of strongly correlated atomic systems. Now it is possible to experimentally study a Mott phase of ultracold atoms. As shown in Ref. [3], the spinor ($S = 1$) bosons in the lattice can exhibit a very rich and exotic phase diagram.

In the Mott phase of *single* species of atoms, any low-energy transport is suppressed [4]. The situation may change dramatically if the Mott phase includes at least *two* species. While the net number-of-atoms transport is still suppressed, the counterflow (when the currents of the two species are equal in absolute values and are in opposite directions), generally speaking, survives, and, at certain conditions, it can be nondissipative (super-counterflow). Note, the counterflow in optical lattice is analogous to motion of impurities—impuritons—in quantum crystals (see, e.g., Refs. [5]).

In this Letter, we discuss typical cases of counterflow dynamics in the two-species Mott phase. We consider three classes of the commensurate systems: fermion-fermion (FF), boson-boson (BB), and boson-fermion (BF) mixtures (assuming that each of the species does not possess internal degrees of freedom). We confine our analysis to the strong-coupling limit, when the effective counterflow Hamiltonian is readily obtained in the second order perturbation theory in the parameter $t/U \ll 1$, where t is the hopping amplitude and U is the on-site repulsion. For the same-statistics (BB or FF) mixtures, the effective Hamiltonian can be written in terms of $s = \nu/2$ isospin operators (the integer ν is the filling factor). We show that the FF case maps on to $s = 1/2$ antiferromagnetic, and the BB case maps on to ferromagnetic effective Hamiltonians, respectively. Depending on the particular means of breaking the isotopic SU(2) symmetry in the original Hamiltonian, either the effective Hamiltonian is of the easy-axis type, which means phase segregation, or it is of the easy-plane type resulting in the SCF ground state. In the BF case, it is possible to eliminate bosonic variables and obtain a spinless fermionic model with nearest-neighbor interaction. The sign of the interaction depends on the parameters of the original Hamiltonian, and how they deviate from the exact fermion-boson symmetry. In particular, the p-wave Cooper pairing is possible which results in the SCF.

Our lowest-order effective Hamiltonians will involve only on-site and nearest-neighbor interactions. Hence, to derive them it is sufficient to consider a system consisting of two strong traps, 1 and 2, between which weak tunneling is allowed. Only the lowest one-particle state φ_σ for the species $\sigma =\uparrow, \downarrow$ (we use pseudospin notation) in each trap is taken into account. We introduce the creation and annihilation fermionic/bosonic operators $a^\dagger_{b\sigma}$, $a_{b\sigma}$, respectively, where $b = 1, 2$ labels the trap (site). Our original two-site Hamiltonian then reads

$$H_{12} = H^{(0)}_{12} + V_{12}, \tag{1}$$

$$H^{(0)}_{12} = \frac{1}{2} \sum_{b\ \sigma\sigma'} U_{\sigma\sigma'} {:}n_{b\sigma} n_{b\sigma'}{:}, \tag{2}$$

$$V_{12} = -\sum_{\sigma} (t_\sigma a^\dagger_{1\sigma} a_{2\sigma} + \text{H.c.}), \tag{3}$$

where $n_{b\sigma} = a^\dagger_{b\sigma} a_{b\sigma}$, $U_{\sigma\sigma'} = g_{\sigma\sigma'} \int d\mathbf{x} |\varphi_\sigma|^2 |\varphi_{\sigma'}|^2$, $g_{\sigma\sigma'}$ is the interaction constant between species σ and σ', and $:(\ldots):$ denotes normal form of the product of the creation-annihilation operators. We consider the tunneling matrix element t_σ as real and positive and depending on the component index.

At commensurate total filling $n_b = \sum_\sigma n_{b\sigma} = \nu$ on each site, and in the limit $|t_\sigma| \ll U_{\sigma\sigma'}$, single particle jumps change the total on-site populations, and, therefore, require high energy. In contrast, exchanging two different particles does not require such an energy. In order to describe these processes, the single particle jumps should be eliminated in the second order with respect to the ratio t/U. Thus, we choose $H^{(0)}_{12}$ in Eq. (2) as the zeroth order part, while V_{12} is the perturbation. The basis in our effective Hilbert space is given by the states $|\mathrm{eff}\rangle = |n_{1\uparrow}, n_{1\downarrow}; n_{2\uparrow}, n_{2\downarrow}\rangle$, where $n_1 = n_2 = \nu$; the virtual excited states $|\mathrm{ex}\rangle$ (where $n_1 = n_2 \pm 1$) are excluded in the second order. The effective Hamiltonian V'_{12} can be represented in terms of the matrix elements of the original Hamiltonian as

$$(V'_{12})_{\alpha\beta} = -\sum_{\gamma} \frac{V_{\alpha\gamma}V_{\gamma\beta}}{E_\gamma - (E_\alpha + E_\beta)/2}, \qquad (4)$$

where α, β label $|\mathrm{eff}\rangle$, and γ denotes $|\mathrm{ex}\rangle$; E are the eigenenergies of $H^{(0)}$ in Eq. (2).

FF case.—This case is the easiest for calculation. The only possible filling factor is $\nu = 1$ and the only possible intermediate virtual state γ is the state with two different fermions on one site. The only relevant interaction vertex is $U_{\uparrow\downarrow} = U$. The Hamiltonian of the system is the standard Hubbard model [6] widely used for electrons in metal, the only specific feature being the dependence of the hopping amplitude on the "spin" index. The effective Hamiltonian is readily obtained from Eq. (4), in terms of isospin operators,

$$\mathbf{S}_b = (1/2) \sum_{\sigma\sigma'} a^\dagger_{b\sigma} \vec{\sigma}_{\sigma\sigma'} a_{b\sigma}, \qquad (5)$$

where $\sigma^j_{\sigma\sigma'}$ ($j = 1, 2, 3$) are the Pauli matrices. The operators S^j_b obey the standard spin commutation relation at the same site and commute with each other on different sites. The resulting effective two-site Hamiltonian $H'_{12} = 2J\mathbf{S}_1\mathbf{S}_2 + 2J'S_{1z}S_{2z}$ extended to a lattice is

$$H_{FF} = \sum_{\langle ij\rangle} [J\mathbf{S}_i\mathbf{S}_j + J'S_{iz}S_{jz}] - \sum_i BS_{iz}, \qquad (6)$$

$$J = 2t_\uparrow t_\downarrow/U, \qquad J' = (t_\uparrow - t_\downarrow)^2/U. \qquad (7)$$

where $\langle\cdots\rangle$ stands for the pairs of nearest neighbors; $B = \mu_\uparrow - \mu_\downarrow$, and μ_σ is the chemical potential of the σth component. The ground state of this system at $|B| > B_c \approx \sqrt{J'(2J + J')}$ (see, e.g., [7,8] for more details) is the spin-1/2 easy-plane (canted) antiferromagnet. It is important to stress that, in our situation—in contrast to the case of a real easy-plane antiferromagnet—the Néel vector fundamentally cannot be attached to any direction in the easy plane due to the exact conservation of the atoms of each component. This guarantees the exact U(1) symmetry. The easy-plane U(1) symmetry can be broken only *spontaneously* by forming the superfluid counterflow vacuum.

BB case.—In this case, we also introduce the site isospin operators according to Eq. (5) with bosonic creation-annihilation operators. The expression for the effective Hamiltonian in a general case of nonequal interactions is rather cumbersome. It becomes much simpler in two important particular cases: (i) when $U_{\sigma\sigma'} = U + \delta U_{\sigma\sigma'}$, with $|\delta U_{\sigma\sigma'}| \ll U$; and (ii) when $\nu = 1$. We start with the former case in the limit $|\delta U_{\sigma\sigma'}|/U \to 0$. Then, the denominators in Eq. (4) are the same and equal to U. Hence, the intermediate virtual states γ do not involve any projection operators, and the answer for the two sites can be written as a bilinear form of $s = \nu/2$ isospin operators as $H'_{12} = -J\mathbf{S}_1\mathbf{S}_2 - J'S_{1z}S_{2z} - B_{12}(S_{1z} + S_{2z})$, $B_{12} = (\nu + 1)(t^2_\uparrow - t^2_\downarrow)/U$, where the expressions for J and J' are given by Eqs. (7). When $|\delta U_{\sigma\sigma'}| \ll U$, the parameters J, J', and B_{12} remain, to the first order in $|\delta U_{\sigma\sigma'}|/U$, the same. The main correction to the Hamiltonian is associated with the term $H^{(0)}_{12}$ (1). Then, extending the two-sites Hamiltonian $H'_{12} + H^{(0)}_{12}$ to the lattice and omitting trivial constant terms, we find

$$H_{\mathrm{BB}} = -\sum_{\langle ij\rangle}[J\mathbf{S}_i\mathbf{S}_j + J'S_{iz}S_{jz}] + \sum_i[(D/2)(S_{iz})^2 - BS_{iz}], \qquad (8)$$

$$B = \mu_\uparrow - \mu_\downarrow - 2(\nu - 1)(U_{\uparrow\uparrow} - U_{\downarrow\downarrow}) + pB_{12}, \qquad (9)$$

$$D = U_{\uparrow\uparrow} + U_{\downarrow\downarrow} - 2U_{\uparrow\downarrow}, \qquad (10)$$

with p being the number of close neighbors on the lattice. Note that in contrast to the FF case, the minus sign now stands in front of J and J'. That is, if the D term in Eq. (8) is ignored, we arrive at the easy-axis ferromagnetic model, that implies a phase segregation. However, for large enough D in Eqs. (8) and (10), the easy-plane ground state can be realized. The mean field condition for this (in the case $B = 0$) is $D \gtrsim pJ'$ [9].

The effective Hamiltonian for the BB situation at $\nu = 1$ can readily be found for arbitrary $U_{\sigma\sigma'}$. The summation over γ in Eq. (4) in this case is very simple because, for any different states α and β in Eq. (4), there is no more than one state γ for which matrix elements differ from zero. In the diagonal terms $\alpha = \beta$, if two sites are both occupied by the same isospin σ bosons, the energy change due to jumping of either boson is $U_{\sigma\sigma}$; when the bosons have opposite spins, the energy change becomes $U_{\uparrow\downarrow}$. The final result acquires the form Eq. (8), with the parameters J, J', and B being

$$J = 2t_\uparrow t_\downarrow/U_{\uparrow\downarrow}, \qquad (11)$$

$$J' = -(t_\uparrow + t_\downarrow)^2/U_{\uparrow\downarrow} + 2t^2_\uparrow/U_{\uparrow\uparrow} + 2t^2_\downarrow/U_{\downarrow\downarrow}, \qquad (12)$$

$$B_{12} = 2(t^2_\uparrow/U_{\uparrow\uparrow} - t^2_\downarrow/U_{\downarrow\downarrow}). \qquad (13)$$

At certain conditions, one obtains the easy-plane situation $J' < 0$, that is the SCF. A solution for this can, in principle, be found exactly. We will, however, analyze it in a simplified situation when the system is almost SU(2) symmetric (like ^{87}Rb [10]), which means $U_{\uparrow\uparrow} \approx U_{\downarrow\downarrow} \approx U_{\uparrow\downarrow}$, $t_\downarrow \approx t_\uparrow$, and will choose chemical potentials to have $B = 0$. We represent $U_{\uparrow\uparrow} = U + U' + D/2$ $U_{\downarrow\downarrow} = U - U' + D/2$, $U_{\uparrow\downarrow} = U$, $t_\uparrow = t + t'$, $t_\downarrow = t - t'$, with $|U'|/U \ll 1$, $|D|/U \ll 1$, $|t'/t| \ll 1$. Then, $J' < 0$ yields

$$|t'/t| < \sqrt{D/2U}, \qquad D > 0. \tag{14}$$

The easy-plane state is equivalent to the SCF.—Now let us focus on why the easy-plane ground state of the models (6) and (8) can support the superfluid counterflow of the components. First, we note that, according to Holstein and Primakoff [11], spin lattice is equivalent to the lattice bosons, with the spin commutation relation being essentially equivalent to the Bose commutation relation. Then, the site operators $\hat{S}_i^+ = S_i^x + iS_i^y$ are proportional to the effective boson annihilation operators $\hat{b}_i$ [11], and the operator $\hat{S}_{zi} = (\nu/2) - \hat{b}_i^\dagger \hat{b}_i$. Accordingly, the formation of the easy-plane order parameter $S_i^+ = \langle S_i^x + iS_i^y \rangle = |S'| \exp(i\varphi) \sim \langle \hat{b}_i \rangle$, where $|S'| \approx \text{const} \neq 0$, is equivalent to the formation of the Bose-Einstein condensate (BEC) $\langle \hat{b}_i \rangle \neq 0$ of the Holstein-Primakoff boson $\hat{b}_i$. As long as the global invariance with respect to the phase φ of the bosons holds, which is ensured by the conservation of the original species, and the bosons are interacting, the system is (counter)superfluid.

Let us obtain an expression for the superfluid countercurrent density $\mathbf{I}$, which is the difference of the currents of each component. To be specific, we will discuss the BB case and keep in mind that the result for the FF case is, qualitatively, the same. In the long wave limit, the conservation law of the components takes the form $\dot{S}_z + \nabla \mathbf{I} = 0$, where $S_z = S_i^z/\Omega$ is the difference of the densities of the species, with Ω standing for the unit cell volume. This continuity equation follows from the Heisenberg equation of motion $i\dot{S}_i^z = [S_i^z, H_{BB}]$ after performing the commutations and taking the long wave limit. Finally, replacing the operators by c numbers, we find

$$\mathbf{I} = n_{\text{scf}} \nabla \varphi, \qquad n_{\text{scf}} = Jp\, d^2 |S'|^2/(12\ \Omega), \tag{15}$$

where d denotes the nearest-neighbor distance; n_{scf} has a meaning of the effective superfluid density, with $\nabla\varphi$ being the corresponding velocity. Thus, the easy-plane ground state of the models (6) and (8) supports a supercounterflow of the two components. The general condition for this is that the intrinsic symmetry [i.e., SU(2)] between the components is broken down to the U(1) group.

BF case.—Now we turn to the Bose-Fermi mixture on the lattice. The Hamiltonian (1) of two sites becomes

$$H_{12}^{(0)} = \sum_{b=1,2} [(U_0/2) n_b (n_b - 1) + U_1 n_b m_b], \tag{16}$$

$$V_{12} = -(t_B a_2^\dagger a_1 + t_F c_2^\dagger c_1 + \text{H.c.}), \tag{17}$$

where $a_b^\dagger$, a_b and $c_b^\dagger$, c_b stand for the site creation and annihilation operators of the bosons and the fermions, respectively; $n_b = a_b^\dagger a_b$, $m_b = c_b^\dagger c_b$; $U_0 > 0$, $U_1 > 0$. Below, we will see that the SCF is possible, if (formal) symmetry between bosons and fermions (when $U_0 = U_1$, $t_B = t_F$) is broken.

The effective two-site Hamiltonian can be written in terms of the fermionic operators only. The elimination of the bosonic operators is possible because the truncated Hilbert space is exhausted by different fermionic occupations, the bosonic occupations being unambiguously defined by the constraint $n_b + m_b = \nu$. Hence, bosonic matrix elements in Eq. (4) can be expressed in terms of fermionic operators only.

Finally, we find the effective lattice Hamiltonian as

$$H_{BF} = \sum_{\langle ij \rangle} [-\kappa c_i^\dagger c_j + (\lambda/2) m_i m_j] - \mu_F \sum_i m_i, \tag{18}$$

where $\mu_F = \mu + p\,\mu_{12}$ denotes the resulting fermionic chemical potential, with μ being the difference of the bare fermion and boson chemical potentials (adding one fermion to the lattice implies simultaneous removal of one boson); the notations are

$$\kappa = 2\nu t_B t_F / U_1, \tag{19}$$

$$\lambda = 2t_B^2 \left(\frac{\nu^2}{U_1} + \frac{\nu^2 - 1}{2U_0 - U_1} - \frac{2\nu^2}{U_0} \right) + \frac{2t_F^2}{U_1}, \tag{20}$$

$$\mu_{12} = \frac{t_F^2 + t_B^2 \nu^2}{U_1} + \frac{t_B^2(\nu^2 - 1)}{2U_0 - U_1} - \frac{2t_B^2 \nu(\nu + 1)}{U_0}, \tag{21}$$

and it is assumed that $2U_0 - U_1 > 0$ [12].

Note that in the case of the exact boson-fermion symmetry (in the meaning defined above), $\lambda = 0$ and SCF is not possible, because the problem maps on the ideal one-component fermion gas. Thus, the symmetry must be broken. From Eq. (20), it is seen that there is a region where $\lambda < 0$. At, e.g., $U_1 = U_0$, we find $\lambda = 2(t_F^2 - t_B^2)/U_0$, and $\lambda < 0$ when $t_B > t_F$. Thus, we obtain one-component lattice fermions with the nearest-neighbor attraction. This leads to the Cooper pairing (see, e.g., [13]), which in our case implies the SCF. As our fermions are effectively spinless (spin polarized), the pairing takes place in the p channel; that is, the superconducting order parameter is characterized by broken inversion symmetry, and can exhibit broken time-reversal symmetry (see [14]). The particular structure depends on the lattice.

Experimental realization and detection of the SCF.—The essential condition for the SCF is that the system is in the MI regime with respect to the net-atomic transport. It is exactly the same condition formulated for the one-component case [2]. In the FF case at $T = 0$ and $|B| > B_c$, the system will be in the SCF state. In the BB case, the three interaction constants $U_{\sigma\sigma'}$ must be tuned in order to avoid the phase separation. This can be achieved by creating slightly displaced lattice potentials [2] for the species in order to reduce the overlap of the states $\uparrow$, $\downarrow$ on each site, so that the value $U_{\uparrow\downarrow}$ is reduced and the parameter D (10) becomes positive and large enough to ensure the condition (14) for, e.g., ^{87}Rb.

It is important to note that in the cases FF and BB, once $T \neq 0$ the phase transition from the ordered (SCF) phase into the "paramagnetic" (i.e., normal with respect to the counterflow) state may occur. A typical critical (Néel or Curie) temperature T_c is given by the effective exchange constant as $T_c \approx pJ$. For the experimental parameters, this gives $T \leq 1$ nK. To put it differently, observation of the SCF does not require temperatures significantly lower than those actually achieved in the experiment of Ref. [1].

The SCF could be detected by observing nondissipative exchange of the components through the optical lattice. One of the possibilities consists of separating the components initially. Then, the species will be exchanging their position in the oscillating manner. Raising T above T_c will result in the abrupt increase of the damping of these oscillations.

The existence of the phase φ (15) implies that the countervortex can be supported in the SCF phase. Then, the winding of the phase in the SCF, which has a boundary with the regular BEC phase of the BB components, will imprint this winding on the BEC phases, resulting in regular BEC vortices. Detecting these vortices will, then, signal a presence of the SCF vortex.

The order associated with the SCF is revealed in the *two*-particle density matrix (TPDM). Its detection can be done by atomic scattering of fast atoms off the lattice [15]. This method for measuring the one-particle density matrix can also be employed for detecting the TPDM. Specifically, the cross section of the process, when an incoming fast particle of, e.g., sort $\uparrow$ strikes the atoms in the lattice and "transforms" into the outcoming particle $\downarrow$, is exactly given by the TPDM of the atoms in the lattice. This issue will be considered in greater detail elsewhere.

Finally, let us discuss a formation of the SCF vortex in a rotating lattice containing the BB mixture. The rotation can induce such vortices, if the components have different masses M_σ. Indeed, the total mass current can be expressed as $\mathbf{I}^{(M)} = (M_\uparrow - M_\downarrow) n_{\rm scf} \boldsymbol{\nabla}\varphi$, where $n_{\rm scf}$, φ define the countercurrent (15). External rotation of the lattice at some angular velocity ω changes the energy of the countervortex $\sim n_{\rm scf} L \ln(L/d)$, where L stands for a typical system size, by $\sim \pm (M_\uparrow - M_\downarrow) n_{\rm scf} L^3 \omega$. The formation of the vortex becomes energetically favorable at [13]

$$|\omega| \geq \omega_c \approx L^{-2} \ln(L/d)/|M_\uparrow - M_\downarrow|. \qquad (22)$$

Note that differences in masses can result in the phase separation induced by gravity/rotation. However, if the atomic magnetons of different species are different, the corresponding linear and oscillator fields can be compensated by adding nonuniform magnetic field.

In summary, we have demonstrated that there is a large variety of strongly correlated ground states in the two-component system of ultracold atoms in an optical lattice, even if the system is in the Mott-insulator regime with respect to the net number-of-atoms transport. The most dramatic effect that may occur is the so-called super-counter-fluidity, when the system supports a nondissipative counterflow of the two components. In the strong-coupling limit, the effective Hamiltonian for the super-counterfluids corresponds to: (i) easy-plane antiferromagnet (in the case of fermion-fermion mixture); (ii) easy-plane ferromagnet (in the case of boson-boson mixture); and (iii) p-wave superconductor (in the case of boson-fermion mixture). The experimental conditions and means of detecting the super-counter-fluidity are outlined.

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