Pairing symmetry of superfluid state in three-component repulsive fermionic atoms in optical lattices

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We investigate the pairing symmetry of the superfluid state in repulsively interacting three-component (colors) fermionic atoms in optical lattices. When two of the three color-dependent repulsions are much larger than the other, pairing symmetry is an extended $s$ wave although the superfluid state appears adjacent to the paired Mott insulator in the phase diagram. As the difference between the three repulsions is decreased in square optical lattices, the extended $s$-wave pairing changes into a nodal $s$-wave pairing and then into a $d$-wave pairing. This change in pairing symmetry is attributed to the competition among the density fluctuations of unpaired atoms, the quantum fluctuations of the color-density wave, and those of the color-selective antiferromagnet. This phenomenon can be studied using existing experimental techniques.

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The cold atoms in optical lattices are well known for their high controllability. Recently, highly symmetric systems have been realized such as $^{173}$Yb atoms with SU(6) symmetry [1,2] and mixtures of $^{171}$Yb atoms and $^{173}$Yb atoms with SU(2)×SU(6) symmetry [3]. These features mean that the cold fermionic atoms in optical lattices constitute a quantum simulator for studying the correlation effects of multicomponent lattice fermions. Currently, one of the most attractive research fields in condensed-matter physics is superconductivity in strongly correlated multiorbital systems. For instance, superconductivity mediated by orbital fluctuations has been discussed as a possible mechanism of the heavy-fermion superconductivity of PrOs$_4$Sb$_{12}$ [4–6] and PrTi$_2$Al$_{20}$ [7,8]. For iron-based superconductors, it has been pointed out that the effects of electron correlation in the multiorbital system play a key role in the appearance of superconductivity. As regards pairing symmetry, both the spin fluctuation-mediated $s_{++}$ wave [9–13] and the orbital fluctuation-mediated $s_{++}$ wave [14, 16] have been proposed theoretically. In the former state, the sign between the hole pocket and the electron pocket reverses, while in the latter state, the sign between them is the same. Pairing symmetry and its origin have been actively debated. As discussed later, in three-component repulsive fermionic atoms in optical lattices two kinds of quantum fluctuations related to the long-range order compete with each other, leading to a change in the superfluid pairing symmetry depending on the dominant quantum fluctuations. We can regard these two kinds of quantum fluctuation as spin fluctuations and orbital fluctuations. Thus, three-component repulsive fermionic atoms in optical lattices act as a minimal model for discussing the change in the Cooper-pairing symmetry of multicomponent repulsive fermions. Our findings provide an insight into the Cooper-pairing mechanism and the symmetry of, for instance, multiorbital correlated electron systems.

We have already investigated repulsively interacting three-component (color degrees of freedom) fermionic atoms in optical lattices with a balanced population [17–21]. We have shown that characteristic Mott states can appear in spite of half filling, where the average atom number per site is the noninteger 3/2: the paired Mott insulator (PMI) appears when two of the three color-dependent repulsions are stronger than the other, while the color-selective Mott state (CSM) appears when two of the three repulsions are weaker than the other [18]. In the ground state at half filling, two kinds of the ordered states appear in both parameter regions: a color-density wave (CDW) and a color-selective antiferromagnet (CSAF) [17]. These results suggest that a superfluid state appears in a Fermi liquid state at close to half filling and at half filling in the ‘color paramagnetic’ sector where the CDW and the CSAF are not taken into account. Using a dynamical mean-field theory (DMFT) combined with a modified iterated perturbation theory we have shown that a superfluid state appears at close to half filling in the parameters for the CDW [20,21]. We have also shown that a superfluid appears at close to the PMI transition point at half filling by using a self-energy functional approach [20,21]. In these superfluid states, atoms with the weakest repulsion form Cooper pairs while atoms with the remaining color stay a Fermi liquid. Quite recently, a superfluid in the ‘color paramagnetic’ sector at half filling has been obtained using a DMFT combined with a continuous-time quantum Monte Carlo method [22]. These calculations are based on a DMFT, thus making it difficult to discuss pairing symmetry.

In this Letter, we investigate superfluid pairing symmetry in repulsively interacting three-component fermionic atoms in optical lattices by using an Eliashberg equation. We show that when two of the three repulsions are sufficiently strong pairing symmetry is an extended $s$...
wave, although the superfluid state appears adjacent to the PMI in the phase diagram. As the difference between the three repulsions decreases, the extended s-wave pairing changes into a nodal s-wave pairing, a $d_{xy}$-wave pairing, and then into a $d_{x^2-y^2}$-wave pairing in square optical lattices. From our calculations of the effective interaction and the Fourier transform of the superfluid order parameter, we show that this change in pairing symmetry can be attributed to the change in the dominant quantum fluctuations among the density fluctuations of unpaired atoms, the quantum fluctuations of the CDW, and those of the CSAF.

The low-energy properties of the ultracold atoms in an optical lattice are well described by the following Hubbard-type Hamiltonian [23]:

$$
\hat{H} = -t \sum_{\langle i,j \rangle} a_{i\alpha}^\dagger a_{j\alpha} - \sum_i \mu_\alpha \hat{n}_{i\alpha} + \frac{1}{2} \sum_i \sum_{\alpha \neq \beta} U_{\alpha\beta} \hat{n}_{i\alpha} \hat{n}_{i\beta},
$$

where $t$ is the nearest-neighbor hopping integral, and $\hat{a}_{i\alpha}^\dagger$ is the creation operator of a fermion of color $\alpha$. The on-site repulsive interactions between color-$\alpha$ and $\beta$ are denoted as $U_{\alpha\beta}$. For convenience we set $U_{12} \equiv U$ and $U_{23} = U_{31} \equiv U'$, which yield $\mu_1 = \mu_2 \equiv \mu$ and $\mu_3 \equiv \mu'$. We discuss pairing symmetry by solving the following Eliashberg equation for the superfluid order parameter $\Delta(k)$ within a weak-coupling theory:

$$
\lambda \Delta(k) = -\frac{1}{M} \sum_{k'} \hat{U}(k-k') \frac{\tanh(\beta \epsilon_{k'} / 2)}{2\epsilon_{k'}} \Delta(k'),
$$

where $M$ is the number of $k$-point meshes, $\beta = 1/(k_B T)$ and $\epsilon_k$ is the bare energy dispersion of the color-1 and 2 atoms measured from the chemical potential. The eigenvalue $\lambda$ is a measure of the dominant pairing symmetry and it reaches unity at the transition point. The effective pairing interaction between color-1 and 2 atoms is calculated by collecting random-phase-approximation-type bubble diagrams and ladder-type diagrams, and is given as

$$
\hat{U}(q) = U + \frac{3}{2} U^2 \chi_s(q) - \frac{1}{2} U^2 \chi_c(q),
$$

where

$$
\chi_s(q) = \frac{\chi_1(q)}{1 - U \chi_1(q)},
$$

and

$$
\chi_c(q) = \frac{\chi_1(q)}{1 - U \chi_1(q)}.
$$

FIG. 1: (Color online) (a) Superfluid order parameter $\Delta(k)$, (b) effective pairing interaction $\hat{U}(q)$, and (c) $\chi_s(q)$ and (d) $\chi_c(q)$ in square optical lattices for $U/U' = 0.1$, $U'/W = 0.15$, $N \sim 1.35$, and $T/W = 0.00125$. Momentum satisfy $q = k - k'$. Here, $\chi_1(q) = \chi_2(q) = \frac{1}{M} \sum_k \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\epsilon_{k+q} + \epsilon_k}$ is the bare susceptibility of color $\alpha = 1, 2$ atoms, and $\chi_3(q) = \frac{1}{M} \sum_k \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\epsilon_{k+q} + \epsilon_k}$ is the bare susceptibility of color $\alpha = 3$ atoms with $\epsilon_k$ being the bare energy dispersion of the color-3 atoms measured from the chemical potential, and $f(x)$ is the Fermi distribution function. We consider the system in square optical lattices. Thus, $\epsilon_k = -2t [\cos(k_x) + \cos(k_y)] - \mu$ and $\epsilon'_k = -2t [\cos(k_x) + \cos(k_y)] - \mu'$. We set the system is close to half filling: $N \sim 1.35$. We employ $256 \times 256$ $k$-point meshes in the numerical calculations.

In Fig. 1(a), we show the numerical results for the order parameter $\Delta(k)$ at $U'/W = 0.15$, $U/U' = 0.1$, $N \sim 1.35$, and $T/W = 0.00125$ with $W$ being a bandwidth. The parameters $U/U' \sim 0.1$ and $N \sim 1.35$ correspond to the condition for the appearance of the superfluid state in Ref. [20], where color-1 and 2 atoms form Cooper pairs. We find that $\Delta(k)$ is nodeless and has large amplitudes at $k = (\pm \pi, 0), (0, \mp \pi)$. The results indicate that pairing symmetry is an extended s wave. We discuss the origin of the large amplitude of $\Delta(k)$ in terms of the effective pairing interaction $\hat{U}(q)$, where $q = k - k'$. As shown in Fig. 1(b), $\hat{U}(q)$ is negative in the entire $q$ region, meaning that the effective interaction between color-1 and 2 atoms is attractive. We also find a peak at $q \sim (\pi, \pi)$. Note that $\hat{U}(q)$ has peaks at $q \sim (\pm \pi, \pm \pi)$ and $(\pm \pi, \mp \pi)$. As shown in Eq. (3), $\hat{U}(q)$ is described by two susceptibilities $\chi_s(q)$ and $\chi_c(q)$. Figure 1(c) and (d) show that both $\chi_c(q)$ and $\chi_s(q)$ have peaks at $q \sim (\pi, \pi)$. Because of the third term in the denominator of Eq. (5), $\chi_c(q)$ has the possibility of showing a divergent peak. For $U' = 0$ the third term in the denominator of Eq. (5) disappears and $\chi_c(q)$ is reduced to the charge susceptibilit
ity of the conventional two-component Hubbard model, which never diverges. Therefore, the divergent peak in $\chi_c(q)$ is characteristic of the three-component repulsive fermionic atoms in optical lattices.

Since the momentum $q = (\pi, \pi)$ describes the perfect nesting condition in square optical lattices at half filling, we consider that the peak in $\chi_c(q)$ at $q \sim (\pi, \pi)$ is caused by quantum fluctuations of the staggered CDW, which appears at half filling for $U/U' < 1$ [17,21]. On the other hand, $\chi_s(q)$ in Eq. (4) is the same form as the spin susceptibility of the conventional two-component Hubbard model. Therefore, the peak in $\chi_s(q)$ at $q \sim (\pi, \pi)$ is caused by quantum fluctuations of the staggered CAF and is inherent to the repulsively interacting fermionic system. For $U/U' = 0.1$, $\chi_c(q)$ overcomes $\chi_s(q)$ in the entire $q$ region, leading to the strong attractive peak in $\tilde{U}(q)$. To gain these strong attractive interactions at $q \sim (\pm \pi, \pm \pi)$ and $(\pm \pi, \mp \pi)$, $\Delta(k)$ has a large amplitude at $k = (\pm \pi, 0)$ and $(0, \pm \pi)$, yielding an extended $s$-wave pairing.

We perform a Fourier transform of $\Delta(k)$ and obtain the Fourier components $\Delta(r)$. As shown in Fig. 2 (a), $\Delta(r)$ has the largest weight $\Delta(r = 0) \sim 3.79 \times 10^{-3}$, the second largest weights $\Delta(\pm 1, \pm 1) \sim \Delta(\pm 1, \mp 1) \sim 4.52 \times 10^{-4}$, the third largest weights $\Delta(\pm 2, \pm 2) \sim \Delta(\pm 2, \mp 2) \sim 1.36 \times 10^{-5}$, and so on. The most dominant $\Delta(r = 0)$ represents the local component, which yields the uniform $s$-wave superfluid gap, while others represent the nonlocal components yielding the $k$-dependence of $\Delta(k)$. Therefore, the extended $s$-wave superfluid gap mainly consists of the local component, although the strong attractive peak caused by CDW fluctuations appears in $\tilde{U}(q)$. In other words, the local correlation effects play an important role in the appearance of this superfluid state. To confirm this consideration we investigate a superfluid state in triangular optical lattices, where quantum fluctuations induced by long-range orders are suppressed owing to geometrical frustration.

We use $c_k = -2t \cos(k_x) + \cos(k_y) + \cos(k_x + k_y) - \mu$ and $c_k' = -2t \cos(k_x) + \cos(k_y) + \cos(k_x + k_y) - \mu'$ for the triangular optical lattices. In Fig. 3 we show $\Delta(k)$ and $\tilde{U}(q)$ for the same parameters as those used in Fig. 1. We find that $\Delta(k)$ is nodeless and has six satellite peaks characteristic of triangular lattices in addition to the central peak. Therefore, the pairing symmetry in triangular optical lattices is also an extended $s$-wave for these parameters. The Fourier components $\Delta(r)$ shown in Fig. 2 (b) have the largest weight $\Delta(r = 0) \sim 3.90 \times 10^{-3}$, the second largest weights $\Delta(\pm 1, \pm 1) \sim \Delta(\pm 1, 0) \sim \Delta(0, \pm 1) \sim 3.83 \times 10^{-5}$, the third largest weights $\Delta(\pm 1, \mp 1) \sim \Delta(\pm 2, \pm 1) \sim \Delta(\pm 1, \pm 2) \sim 3.48 \times 10^{-5}$, and so on. The local component is the most dominant as is expected. We evaluate the ratio of the largest weight ($\Delta_0$) to the second largest weight ($\Delta_1$). In triangular optical lattices the ratio is $|\Delta_0/\Delta_1| \sim 102$, which is about one order larger than that in square optical lattices $|\Delta_0/\Delta_1| \sim 8.37$. This means that the local component is more dominant in triangular optical lattices. We thus argue that the local correlation effects in triangular optical lattices play a more important role as regards the appearance of the superfluid state than those in square optical lattices. As shown in Fig. 3 (b) we can see no conspicuous peak in $\tilde{U}(q)$, which indicates the absence of quantum fluctuations induced by long-range orders. This is because long-range orders at half filling disappear owing to geometrical frustration.

We have shown that for $U/U' < 1$ the superfluid state with an extended $s$-wave pairing appears at close to half filling, where the local correlation effects play an important role. We consider that in this superfluid, the effective attractive interaction is mainly caused by local density fluctuations of unpaired atoms. This situation is similar to the system dealt with the DMFT, where only local correlation effects are included precisely. Thus, the phase diagrams obtained based on the DMFT [20] qualitatively are adequate for the superfluid state in three-component fermionic atoms with $U/U' < 1$, in particular, in triangular optical lattices.

We next investigate the pairing symmetry in square optical lattices, when the difference in the repulsive interactions is reduced ($U/U'$ is increased). For $U/U' = 0.28$ shown in Fig. 4 (a) and (d), we see a nodal circle round $k = 0$ in $\Delta(k)$. This feature signifies a nodal $s$-wave pairing. In $\tilde{U}(q)$ the attractive peak appears at $q \sim (\pi, \pi)$,
although its strength is reduced compared to that for \( U/U' = 0.1 \) shown in Fig. 2(b). In addition, the repulsive region appears except for \( q \sim (\pi, \pi) \) in \( \tilde{U}(q) \). This is because CDW fluctuations are suppressed as \( U/U' \) is increased. To make use of the attractive peak and the repulsive \( \tilde{U}(q) \), \( \Delta(k) \) has large amplitudes with the same sign at \( k \sim (\pm \pi, 0) \) and \( (0, \pm \pi) \), and its sign changes around \( k \sim 0 \) from those of \( \Delta(\pm \pi, 0) \) and \( \Delta(0, \pm \pi) \). As shown in Fig. 2(c) the largest weights of the Fourier component in this nodal s-wave pairing appear in non-local \( \Delta(\pm 1, \pm 1) \sim \Delta(\pm 1, \mp 1) \sim -1.75 \times 10^{-3} \), the absolute values of which are slightly larger than the local component \( \Delta(r = 0) \sim 1.36 \times 10^{-3} \). This means that local density fluctuations of unpaired color-3 atoms are suppressed with increasing \( U/U' \).

For \( U/U' = 0.4 \) shown in Fig. 2(b) and (e), we find two nodal lines: \( k_y = 0 \) and \( k_z = 0 \) in \( \Delta(k) \). Thus, the pairing symmetry is a \( d_{xy} \) wave. The attractive peak in \( \tilde{U}(q) \) at \( q \sim (\pi, \pi) \) is more strongly suppressed and the strength of the repulsive \( \tilde{U}(q) \) is more effectively enhanced than those for \( U/U' = 0.28 \), since CDW fluctuations are more suppressed with increasing \( U/U' \). To make use of the large repulsive \( \tilde{U}(q) \) at \( q \sim (\pm \pi, 0) \) and \( (0, \pm \pi) \) and the small but nonzero attractive peak, \( \Delta(k) \) has large positive amplitudes at \( k \sim (\pm \pi/2, \pm \pi/2) \) and negative ones at \( k \sim (\pm \pi/2, \mp \pi/2) \), yielding the two nodal lines \( k_y = 0 \) and \( k_x = 0 \). Although the \( \tilde{U}(q) \) values show qualitatively similar \( q \) dependences for both \( U/U' = 0.26 \) and \( U/U' = 0.4 \), the pairing symmetry changes between them. As shown in Fig. 3 the \( d_{xy} \)-wave pairing spreads in a wider \( U/U' \) than the nodal s-wave pairing. This may be related to the fact that the nodal lines in the \( d_{xy} \)-wave pairing cross the Fermi energy, which yields an energy gain larger than that in the nodal s-wave pairing. For \( U/U' = 0.8 \) shown in Fig. 3 and (f), we find two nodal lines: \( k_y = \pm k_x \) in \( \Delta(k) \). Thus, the pairing symmetry is a \( d_{x^2-y^2} \) wave. Actually, \( \tilde{U}(q) \) is positive in the entire \( q \) region and has a repulsive peak at \( q \sim (\pi, \pi) \). This behavior is attributed to the fact that \( \chi_L(q) \) overcomes \( \chi_E(q) \), because the CDW fluctuations are suppressed and the CSAF fluctuations become dominant.

Our results demonstrate that the pairing symmetry of a superfluid changes as the difference between the repulsions changes in three-component fermionic atoms in optical lattices. Recently, s-wave superconductivity was found in the paramagnetic sector of the Kondo lattice model by using a DMFT [24]. This superconductivity is driven by local spin fluctuations caused by Kondo exchange coupling. In Ref. [24], a question arose concerning the pairing symmetry driven by the competition or cooperation between local and nonlocal fluctuations. Our results provide an answer to this question.

We summarize the results in Fig. 5. We show the largest eigenvalue \( \lambda \) for given \( U/U' \) and \( T/W \) values when \( U/W = 0.15 \). When the temperature is reduced, \( \lambda \) increases towards unity in the extended s-wave pairing for \( U/U' \lesssim 0.2 \) and the \( d_{xy} \)-wave pairing for \( U/U' \gtrsim 1.0 \). Between both pairings, superfluid states with a nodal s-wave pairing and a \( d_{xy} \)-wave pairing appear with eigenvalues of only \( \lambda \lesssim 0.2 \) at the lowest temperatures that we can achieve. The results suggest that the nodal s-wave and the \( d_{xy} \)-wave superfluid states are unstable and appear at extremely low temperatures. Thus, for the corresponding \( U/U' \) regime a Fermi liquid may be observed in experiments instead of these superfluid states. The present results capture the essentials of the superfluid state in repulsively interacting three-component fermionic atoms in square optical lattices.
When the higher-order corrections of correlation effects are included, we consider that the quantitative features are refined but the qualitative features remain.

We discuss the relationship between our theoretical results and the experiments. When we consider hyperfine states to be the color degrees of freedom, we realize a three-component $^6$Li fermionic gas. As shown in Fig. 2(c) in Ref. [23], the magnetic Feshbach resonance of $^6$Li allows us to control the color dependent repulsions. Furthermore, a very small three-body loss was observed in the repulsive region under a magnetic field from 550G to 600G [23]. We thus expect the $^6$Li atoms in optical lattices to be a possible candidate for observing the change in the pairing symmetry of this superfluid. Another candidate is a mixture of different isotopes, such as $^{173}$Yb atoms and $^{171}$Yb atoms, in optical lattices [3]. A three-component system can be realized by, for example, choosing two hyperfine states of $^{171}$Yb and one state of $^{173}$Yb. In this system, the color-dependent interactions are naturally induced and can be controlled by the optical Feshbach resonance [27].

State-of-the-art experimental techniques such as rf-spectroscopy [28] can allow us to detect momentum-resolved single-particle excitation spectra. This quantity provides useful information for detecting a superfluid transition and its pairing symmetry. On the basis of the obtained results, we discuss the features of momentum-resolved single-particle excitation spectra at the special momentums $k = (0,0), (\pi, 0)$, and $(\pi/2, \pi/2)$. In the extended $s$-wave pairing, the full spectral gap opens. On the other hand, in the nodal $s$-wave pairing, the spectral gap closes at $k \sim (\pi/2, \pi/2)$. In the $d_{x^2-y^2}$-wave pairing, the spectral gap closes at $k \sim (0, 0)$ and $(\pi, 0)$, while in the $d_{x^2-y^2}$-wave pairing, the spectral gap closes at $k \sim (0, 0)$ and $(\pi/2, \pi/2)$. Thus the superfluid gap of each pairing symmetry exhibits characteristic behavior at these three momentums, which makes it possible to probe the change in pairing symmetry experimentally. When three-component repulsive fermionic atoms in optical lattices are realized and the $U/U'$ values is changed, we expect, at least, to observe the superfluid states with the extended $s$-wave pairing and the $d_{x^2-y^2}$-wave pairing. As discussed above the nodal $s$-wave pairing state and the $d_{x^2-y^2}$-wave pairing state are probably difficult to observe, and instead the Fermi liquid may be observed. We have shown that three-component repulsive fermionic atoms in optical lattices can act as a quantum simulator for controlling the pairing symmetry of a superfluid. We hope to confirm these fascinating phenomena experimentally.

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