Spin-triplet f-wave pairing due to three-site cyclic-exchange ferromagnetic interactions

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Ferromagnetism and superconductivity in a two-dimensional triangular-lattice Hubbard model are studied using the density-matrix renormalization group method. We propose a mechanism of the f-wave spin-triplet pairing derived from the three-site cyclic-exchange ferromagnetic interactions. We point out that a triangular network of hopping integrals, which is required for the three-site cyclic hopping processes, is contained in the (possibly) spin-triplet superconducting systems, such as Bechgaard salts (TMTSF)$_2$X, cobalt oxide Na$_{0.35}$CoO$_2$·1.3H$_2$O, and layered perovskite Sr$_2$RuO$_4$.

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Symmetry of Cooper pairs give an invaluable information of our elucidating a superconducting mechanism. Both spin and angular momentum are good quantum numbers for describing the Cooper pairs. In the spin-triplet channel, the total spin is one and the pairing symmetry is of p- or f-wave. The long-standing quest for a new example of spin-triplet superconductivity has been pursued since the spin-triplet superfluid was discovered. Recently, three experimental candidates have been hand-running recognized to be likely spin-triplet superconductivity (see below). They provide an excellent chance for us to have productive insights into the nature of spin-triplet pairing, which is less understood than that of the spin-singlet pairing. Spin-triplet superconductivity is thus one of the hottest topics in the field of strongly-correlated electron systems.

From the theoretical aspect, spin-triplet Cooper pairs are considered to be formed simply by a ferromagnetic interaction. The realization of such pairs in a system of electrons interacting via spin-independent Coulomb interaction, namely the Hubbard model, is still a significant challenge. The Nagaoka-Thouless and flat-band mechanisms are well known as the origin of ferromagnetism. However, both of them are unsuitable for explaining the spin-triplet superconductivity since they lead not to Cooper pairs but to saturated magnetization. Then one may turn his eyes to the three-site cyclic-exchange ferromagnetic interaction which is only the remaining mechanism in the simple Hubbard model. It brings a couple of electrons to be locally ferromagnetic, so that applying the mechanism to the spin-triplet superconductivity seems to be a natural extension. In this letter, we propose a mechanism of the spin-triplet superconductivity derived from the three-site cyclic-exchange ferromagnetic interaction.

We are also highly motivated by the fact that all of the three experimental candidates contain a triangular network of hopping integrals which is required for the three-site cyclic-exchange mechanism. One of the candidates is Bechgaard salts (TMTSF)$_2$X. The crystal structure consists of well-separated sheets containing one-dimensional (1D) TMTSF stacks along the a-axis. The sheets are in the ab-plane and the hopping integrals along the b-axis are about 10 − 20% of those along the a-axis. The unique structure of the hopping integrals can be regarded as an anisotropic triangular lattice. In experiment, it has been widely concluded that the superconducting state is of the spin-triplet pairing: the spin susceptibility, from the NMR Knight shift measurement, remains unchanged through the superconducting transition ($T_c$) and the upper critical magnetic field exceeds substantially the Pauli limit in both a and b directions. Also, the enhancement of the spin-lattice relaxation ratio just below $T_c$, indicating the presence of line nodes in the superconducting order parameter, was found. In theory, we seem to have reached a consensus on the spin-triplet pairing; nevertheless, the pairing symmetry is still open issue.

Another experimental candidate is cobalt oxide Na$_{0.35}$CoO$_2$·1.3H$_2$O, which shows a superconducting transition at $T_c \approx 5$ K. The conductive ab planes consist of edge-sharing CoO$_6$ octahedra and each plane is strongly separated by Na$^+$ ions and H$_2$O molecules along c axis. The Co ions form a triangular lattice, and the system may be regarded as a two-dimensional (2D) triangular lattice doped with 35% electrons. Some experiments have suggested the possibility of an unconventional superconductivity with line nodes in the gap function. In particular, spin-triplet p- or f-wave pairing state has been argued based on an invariant behavior of the ab-plane Knight shift across $T_c$ and a $T^3$-dependence of 1/$T_1$ below $T_c$. On the other hand, a suppression of Knight shift across $T_c$ for both magnetic field parallel and perpendicular to the ab-plane suggesting a spin-singlet pairing state has also been reported. As described above,
experimental decision of the pairing symmetry is still controversial. Similarly, theoretical studies are not in agreement: the $d+id$- (or $p$-)wave spin-singlet pairing with a triangular-lattice $t−J$ model and the $f$-wave spin-triplet pairing with extended Hubbard model have been proposed. Also, the $p$-wave spin-triplet has been suggested phenomenologically.

The third candidate is Sr$_2$RuO$_4$, which is a tetragonal, layered perovskite system of stacking RuO$_2$-planes. No sooner was discovered the superconducting transition at $T_c \sim 1.5$ K, the possibility of spin-triplet pairing was pointed out. After that, the spin-triplet pairing state with $d$-vector perpendicular to the conducting plane has been confirmed by a NMR measurement.

In our previous works, we studied the ground-state properties of two-chain Hubbard model coupled with zigzag bonds. This system is equivalent to a 1D triangular-lattice Hubbard model. We argued that a cyclic hopping motion of two electrons in each triangle yields a ferromagnetic correlation in the strong-coupling regime; as a consequence, a spin-triplet superconducting state becomes dominant if the following conditions are satisfied: (i) The product of three hopping integrals in each triangle is positive. (ii) The zigzag bond is rather weaker than the intra-chain bond. (iii) The filling is substantially away from zero and half fillings. The three-site cyclic-hopping mechanism should work even in 2D system, and it is particularly worth noting that the above-mentioned three materials completely meet the conditions.

We employ the density-matrix renormalization group (DMRG) method to calculate the spin-spin and spin-triplet pair-correlation functions. It will thereby be confirmed that the spin-triplet pairing occurs predominantly in the $f$-wave channel for a simple 2D Hubbard model.

The Hamiltonian of the anisotropic triangular-lattice Hubbard model is given by

$$H = \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron with spin $\sigma$ at site $i$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is a number operator, and $t_{ij}$ is hopping integral between sites $i$ and $j$. The sum $\langle ij \rangle$ runs over nearest-neighbor pairs. We here include two kinds of nearest-neighbor hopping integrals $t$ in the $x$- ($y$-) direction and $t'$ otherwise, as shown in Fig. 1. Onsite Coulomb repulsion $U$ is set to be $10t$ as a typical value in the strongly-correlated electrons system. We take $t = 1$ as the energy unit hereafter.

Let us first demonstrate that the cyclic-hopping mechanism indeed leads to ferromagnetic correlation in the 2D system. We thus study a finite-size cluster of $l_x = 6$ and $l_y = 8$, where the periodic (open) boundary conditions are applied for the $x$- ($y$-) direction. This choice of the boundary conditions enables us to carry out sufficiently accurate calculations. We keep up to $m = 3400$ density-matrix eigenstates in the DMRG procedure. In this way, the maximum truncation error, i.e., the discarded weight, is less than $1 \times 10^{-5}$ and the maximum error in the ground-state energy is estimated to

![FIG. 1: (Color online) Schematic representation of the anisotropic triangular-lattice Hubbard model. Lattice drawn with bold lines is extracted for our calculation of the spin-triplet pair-correlation functions. The $f$-wave pair function is also shown.](image1)

![FIG. 2: (Color online) Average spin-spin correlations $\langle S_i^x S_j^x \rangle$ between sites bonded with $t'$, as a function of filling $n$.

$$\langle S_i^x S_j^x \rangle$$
We next turn to the long-range behavior and the spatial symmetry of spin-triplet pair-correlation functions

$$D(\theta, l) = \left\langle \Delta_l^\dagger \Delta_i \right\rangle$$

(2)

with a spin-triplet operator \(\Delta_i = c_i^\dagger c_{i+r}\) where \(i+r\) denotes the neighboring site of \(i\). As in Fig. 1, we extract a three-leg ladder from 2D lattice, which is a minimal model to generate all possible pairing symmetries. In Eq. (2), we remove a pair from sites \((i, i+r)\) and add the pair at sites \((i+l, i+l+r')\), whereby we rotate the pair by \(\theta\) degree from \(i \rightarrow r\) direction to \(i \rightarrow r'\) clockwise [see Fig. 3(a)]. Note that the same results must be expected even if we define the spin-triplet operator as \(\Delta_i = c_i^\dagger c_{i+l}\) or \(c_i^\dagger c_{i+l}\). We also restrict ourselves to the case at quarter filling, i.e., \(n = 0.5\). We calculate the pair-correlation functions \(D(\theta, l)\) of the three-leg ladder with the DMRG method. The OBC are applied in the \(x\)-direction so that the correlation functions will be calculated using distances taken about the midpoint. In the following, we study a ladder with 32 × 3 sites with keeping \(m = 4500\) density-matrix eigenstates to build the DMRG basis. The obtained ground-state energy is expected to be accurate to parts in \(10^{-2}\). In Fig. 3(b), the pair-correlation functions \(D(\theta, l)\) are plotted as a function of distance \(l\) for all possible \(\theta\) values with a fixed anisotropy \(t' = 0.5\). We can see that \(D(\theta, l)\) decay as \(\sim 1/\gamma\) \((1 < \gamma < 2)\) for all \(\theta\) values. The exponent \(\gamma\) smaller than 2 would imply an attractive interaction between electrons \([10]\). It is consistent with our previous results \([13]\). We also find that the values of \(D(\theta, l)\) are mostly positive for \(\theta = 0^\circ, 120^\circ, 240^\circ\) and, whereas, negative for \(\theta = 60^\circ, 180^\circ, 300^\circ\). In other words, the pair wave function changes its sign by \(\pi/3\) rotation.

In order to organize the angle dependence of \(D(\theta, l)\) more explicitly, we sum it up for pair separations \(l = 7 - 25\):

$$D(\theta) = \sum_{l=7}^{25} D(\theta, l).$$

The open-end effects are expected to be rather small for central 25 sites of the system \((l \leq 25)\). In Fig. 4, the results of \(D(\theta)\) with \(t' = 0.25\) and 0.5 are shown. For both parameters we can see that the sign of \(D(\theta)\) changes by \(\pi/3\) rotation, which clearly indicates the \(f\)-wave spatial symmetry of the pair correlation function. Since the spin-triplet pairs are formed mostly on the zigzag bond for \(t' = 0.25\) \([12]\), \(D(\theta)\) involving the on-leg pairs, namely, at \(\theta = 2\pi/3, 5\pi/3\) in the upper left panel, \(\theta = \pi/3, 4\pi/3\) in the upper right panel, and all of \(\theta\) in the lower panels, are relatively small. When \(t'\) is increased from 0.25 to 0.5, the pairing correlation on the zigzag bond is somewhat reduced and, whereas, that on the leg bond is enhanced. The situation is rather complicated: \(t'\) enhances the antiferromagnetic correlation on the zigzag bond by the di-

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**FIG. 3:** (Color online) (a) Definition of the rotation angle \(\theta\) and the distance \(l\). For a case that the pair is removed from a position \(i\) with dashed ellipse, the position of the pair created at \(i + l\) is denoted by solid ellipse for each \(\theta\). (b) \(\log |D(\theta, l)|\) with \(l\) at \(t' = 0.5\) for all possible \(\theta\). Filled (empty) symbol denotes a positive (negative) value of \(D(\theta, l)\).

be \(E_0/(\lambda_x\lambda_y) \sim 10^{-2}\). Figure 2 shows the average spin-spin correlations \(\left\langle S_i^+ S_{i+j}^- \right\rangle\) between the neighboring sites bonded with \(t'\), where \(\langle \cdot \cdot \cdot \rangle\) denotes the ground-state expectation value. We can see the enhancement of ferromagnetic correlation in a wide range of filling for \(t' = 0.25\) and 0.5. The suppression of the correlation around \(n = 0.7\) implies that the origin of ferromagnetism for \(n \gtrsim 0.7\) is different from that for \(n \lesssim 0.7\): it comes from the cyclic-hopping mechanism around \(n = 0.5\) and from the Nagaoka- Thouless mechanism near \(n = 1\). Those behaviors are qualitatively consistent with the results in the 1D triangular-lattice Hubbard model \([14]\). On the other hand, antiferromagnetic correlation is mostly dominant for \(t' = 1\) since the direct exchange interaction will exceed the ferromagnetic ones. We note that the correlation seems to be slightly ferromagnetic for \(n \lesssim 0.2\), where the nearly flat-band system may be realized. So we confirm that in the 2D triangular-lattice Hubbard model the ferromagnetic correlation induced by the cyclic-hopping mechanism can occur at \(n \sim 0.5\) if the anisotropy is rather strong.
rect exchange interaction (scaled as $\propto t'^2$), and also enhances the ferromagnetic correlation on each triangle by the three-site cyclic-hopping exchange interaction (scaled as $\propto tt'^2$). Consequently, the $f$-wave symmetry of the superconducting state becomes more isotropic. However, we note that the spin-triplet pair correlation becomes smaller as the system approaches to an isotropic triangle lattice.

In summary, the ground state of the 2D triangular-lattice Hubbard model is studied with the DMRG method. We find that the three-site cyclic-hopping mechanism really induces ferromagnetic correlation around quarter filling, which is mandatory for the spin-triplet pairing, provided that the anisotropy is rather strong. Slow decay of the pair-correlation functions with distance is indicative of the dominant spin-triplet superconductivity. The pair-correlation function changes its sign by $\pi/3$ rotation, indicating the $f$-wave rotational symmetry. Thus, we suggest a new mechanism of the $f$-wave spin-triplet superconductivity derived from the three-site cyclic-hopping ferromagnetic interactions. We also point out that the mechanism may be possibly relevant to the spin-triplet superconducting systems, such as Bechgaard salts (TMTSF)$_2$X, cobalt oxide Na$_{0.35}$CoO$_2$$\cdot$1.3H$_2$O, and layered perovskite Sr$_2$RuO$_4$.

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