Possible spin-triplet $f$-wave pairing due to disconnected Fermi surfaces in $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$

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We propose that spin-triplet pairing mechanism due to disconnected Fermi surfaces proposed in our previous study [Phys. Rev. B 63 174507 (2001)] may be at work in a recently discovered superconductor $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$. We introduce a single band effective model that takes into account the pocket-like Fermi surfaces along with the van Hove singularity near the K point found in the band calculation results. Applying fluctuation exchange method and solving the linearized Eliashberg equation, the most dominant pairing is found to have spin-triplet $f$-wave symmetry, where the nodes of the gap function do not intersect the pocket Fermi surfaces. Presence of finite $T_c$ is suggested in sharp contrast with cases when the gap nodes intersect the Fermi surface.

Recent discovery of superconductivity in $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ has attracted much attention. One reason why the material is of great interest is that it is a $d$-electron system having a quasi-two-dimensional lattice structure, which resembles the high $T_c$ cuprates. On the other hand it differs from the cuprates in that the Co ions form a triangular lattice, and also there are several bands intersecting the Fermi level, all of which are quite away from half-filling. Another interesting point concerning this material is that some experiments suggest possible occurrence of an unconventional superconductivity, although there are also experiments suggesting conventional pairing. In particular, an unchanged Knight shift across $T_c$ found in some experiments suggests spin-triplet pairing, while absence of broken time reversal symmetry may exclude possibility of chiral $p$-wave or $d$-wave pairing states, leaving spin triplet $f$-wave pairing as a good candidate.

Theoretically, although importance of multiband effects has been proposed, number of studies have considered a single band model on a triangular lattice, and in particular focused on the band filling (number of electrons per site) $n = 1.33$, corresponding to the nominal number of $t_{2g}$ holes (0.67 holes) per Co in the case of $\text{Na}_{0.33}\text{CoO}_2$. Several of these theories have indeed proposed possible occurrence of spin-triplet superconductivity, and in particular $f$-wave pairing.

In fact, the presence of ferromagnetic spin fluctuations observed experimentally indirectly support the spin-triplet pairing scenario. Couple of years ago, however, two of the present authors showed that $T_c$ of spin triplet superconductivity due to ferromagnetic spin fluctuations should in general be very very low (much lower than the $T_c$ in $\text{Na}_x\text{CoO}_2$) or does not even exist. A similar conclusion has been reached by Montheoux and Lonzarich. This is because the triplet pairing interaction in the spin-fluctuation scenario is proportional to $\chi/2$ (in contrast with $3\chi/2$ for the singlet case), where $\chi$ is the spin susceptibility, while the effective interaction (denoted as $V^{(1)}$) that enters the normal self-energy overpowers the pairing effect. Succeedingly, we have then shown that this difficulty for spin-fluctuation-mediated triplet pairing may be eased in systems having disconnected Fermi surfaces', where the nodal lines of the odd-parity gap can run in between the Fermi surfaces to open up a full gap on the Fermi surfaces. Since one of the reasons that degrade pairing with high angular momentum is the presence of gap nodes on the Fermi surface, opening a full gap may result in an enhanced pairing. As an example, we have considered the Hubbard model on a triangular lattice, where the Fermi surface becomes disconnected into two pieces centered around the K point and the K' point (see Fig 1(a)) when there are a small number of holes (or electrons, depending on the sign of the hopping integral). Using fluctuation exchange approximation and solving the linearized Eliashberg equation, we have shown that a finite $T_c$ for spin-triplet $f$-wave pairing may be obtained at a $T_c$ of order 0.001$t$ ($t$ is the hopping integral), which is much higher than the $T_c$ obtained by the same method, if any, for systems having enhanced ferromagnetic spin fluctuations but with connected Fermi surfaces.

If we look at the band calculation results of $\text{Na}_x\text{CoO}_2$ from this point of view, we find that the pocket-like Fermi surfaces near the K and K' points (as in the bottom figure of Fig 1(b)), originating from the band having $e_2'$ character to some extent in the notation of ref. 21 (denoted by the thick line in Fig 2(a)),
are disconnected in a similar sense as in the triangular lattice, namely the nodes of the \( f \)-wave gap do not intersect the Fermi surfaces (although they do intersect the large Fermi surface around the \( \Gamma \) point originating from the bands having \( a_{1g} \) character). This viewpoint has motivated us to investigate possible occurrence of \( f \)-wave superconductivity due to these pocket-like Fermi surfaces.

Another reason to focus on the pocket Fermi surfaces is the presence of van Hove singularity (vHS) near the \( K \) point. Namely, as can be seen from the band structure shown in Fig.2, there exist saddle points at points denoted as SP, where the density of states (DOS) takes a large value. Since this large DOS lies close to the Fermi level, it is likely that the band structure around the \( K \) and \( K' \) points strongly affects the low energy properties of this material. In particular, ferromagnetic spin fluctuations may arise due to this high DOS near the Fermi level.

To our knowledge, the effect of the pocket Fermi surfaces and the vHS has not been properly considered in previous studies. Although it is necessary to consider a multiband model in order to strictly take into account these effects, we believe that a good starting point for the present purpose is to separate out the portion of the bands [22] which has \( e'_{g} \) character to some extent (we will call these bands \( e'_{g} \) bands for simplicity), and in particular focus on the upper \( e'_{g} \) band, which contributes to the formation of the pocket Fermi surfaces and to the large DOS at the vHS, while neglecting the lower \( e'_{g} \) band, which has only small DOS near the Fermi level due to the linear dispersion at the band top. Although this portion of the band, shown by the thick curves in Fig.2(a), is disconnected between \( M \) and \( \Gamma \) points due to \( a_{1g}-e'_{g} \) hybridization, it originally comes from a single band having \( e'_{g} \) character, as can be understood from the inset of Fig.2(a), where a tight binding band dispersion is given for a case when large \( a_{1g}-e'_{g} \) level offset is introduced. In fact, we have found that the thick portion of the band in Fig.2(a) (apart from the missing part between \( M \) and \( \Gamma \) points) can be roughly reproduced by a single band tightbinding model on a triangular lattice with hopping integrals up to 4th nearest neighbor. Namely, the dispersion of the tight binding model on an isotropic triangular lattice with only nearest neighbor hoppings takes its maximum at the \( K \) point (Fig.1(a)), while the band top moves towards the \( \Gamma \) point when 4th neighbor hopping is introduced (Fig.1(b)), resulting in a pocket like Fermi surface that lies between the \( K \) and \( \Gamma \) points when small amount of holes are present. Moreover, the band structure around the \( K \) point resembles that of the actual

**FIG. 1:** Band dispersion (top) along with the Fermi surfaces (schematic) for a small number of holes and the \( f \)-wave gap (bottom) are shown for a tight binding model on a triangular lattice with (a) only nearest neighbor hopping, and (b) when 4th nearest neighbor hopping \( t_{4} = 0.2 \) is introduced. \( +\)\(−\) denote the sign of the gap function, while the dashed lines represent the nodal lines.

**FIG. 2:** (a) A schematic plot of the band structure of Na\(_{x}\)CoO\(_{2}\) following the calculation results of ref.[21]. The thick line denotes the portion of the upper part of the bands which has \( e'_{g} \) character to some extent. Bottom inset: dispersion of a three band tight binding model, where large \( a_{1g}-e'_{g} \) level offset as well as third nearest neighbor hoppings between same orbitals is introduced in addition to the hoppings considered in ref.[8]. (b) Brillouin zone is shown in the extended zone scheme. The points denoted as SP are saddle points since the energy of the thick band at SP is lower than those around the gray circles, while it is higher than those around the open circles.
material (compare Fig.1b) and the thick curve in Fig.2, so the vHS at points SP in Fig.2 is also reproduced by this effective model. As for the electron-electron interaction, here we consider the Hubbard model, where we take into account only the on-site repulsion.

In standard notations, the Hamiltonian considered in the present study is given in the form,

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

where $t_{ij} = t_1, t_2, t_3$, and $t_4$ for the nearest, 2nd nearest, 3rd nearest and 4th nearest neighbors, respectively. We take $t_1 = -1$ throughout the study. We apply the fluctuation exchange (FLEX) approximation[23,24,25], where (i) Dyson’s equation is solved to obtain the renormalized Green’s function $G(k)$, where $k \equiv (k,\nu_n)$ denotes the 2D wave-vectors and the Matsubara frequencies, (ii) the effective electron-electron interaction $V^{(1)}(q)$ is calculated by collecting RPA-type bubbles and ladder diagrams consisting of the renormalized Green’s function, namely, by summing up powers of the irreducible susceptibility $\chi_{\text{irr}}(q) = -\frac{1}{N} \sum_k G(k + q)G(k)$ ($N$: number of $k$-point meshes), (iii) the self energy is obtained as $\Sigma(k) \equiv \frac{1}{N} \sum_q G(k - q)V^{(1)}(q)$, which is substituted into Dyson’s equation in (i), and the self-consistent loops are repeated until convergence is attained. Throughout the study, we take up to 64 × 64 $k$-point meshes and the Matsubara frequencies $\epsilon_n$ from $(-2N_c - 1)\pi T$ to $(2N_c - 1)\pi T$ with $N_c$ up to 65536 in order to ensure convergence at low temperatures.[26]

To obtain $T_c$, we solve the linearized Eliashberg equation for the gap function $\phi(k)$,

$$\lambda \phi(k) = -\frac{T}{N} \sum_{k'} \phi(k')|G(k')|^2 V^{(1)}(k - k'),$$

where the pairing interaction $V^{(2)}$ is given as $V^{(2)}_t(q) = -\frac{1}{2} \left[ \frac{U^2 \chi_{\text{irr}}(q)}{1 - U^2 \chi_{\text{irr}}(q)} \right] - \frac{1}{2} \left[ \frac{U^2 \chi_{\text{irr}}(q)}{1 + U^2 \chi_{\text{irr}}(q)} \right]$ for triplet pairing. The tendency toward singlet pairing is weak in the present case, so we focus only on the triplet pairing. $T_c$ is the temperature at which the maximum eigenvalue $\lambda$ reaches unity.

We now move onto the results. In Fig.3 we present contour plots of $|G(k, i\pi k_BT)^2|$, $\chi(k, 0)$, $\phi(k, i\pi k_BT)$ for $(t_2, t_3, t_4) = (0, 0, 0.2)$ (the band dispersion for $U = 0$ is shown in the upper panel of Fig.1b)), $U = 4.5$, number of holes per site $n_h = 0.2$ and $T = 0.01$. Note that we do not focus on $n_h \sim 0.65$ as in previous theories because the number of holes in the $c'_g$ band is small. It can be seen that pocket-like Fermi surfaces, represented by the ridge of $|G|^2$, lie between the K and $\Gamma$ points. Moreover, the presence of saddle points in $|G|^2$ at points corresponding to SP in Fig.4 indicates the presence of vHS just below the Fermi level as expected. The spin susceptibility takes large values around the $\Gamma$ point indicating presence of ferromagnetic spin fluctuations. The ferromagnetic fluctuation originates from the large density of states near the Fermi level. The gap function having the largest eigenvalue has spin-triplet $f$-wave symmetry, where the nodes of the gap do not intersect the Fermi surfaces.

In Fig.4(b), we show $\lambda$ as a function of temperature (solid curve). As can be seen, $\lambda$ tends to unity at low temperatures. As we have mentioned in the introductory part, were it for a system with connected Fermi surfaces, $T_c$ of spin triplet superconductivity due to ferromagnetic spin fluctuations (estimated by the present method) would be, if any, too low to be detected in a feasible calculation. Thus we attribute the present result.
to the disconnectivity of the Fermi surface and the absence of gap nodes on the Fermi surfaces. To show that large values of $\lambda$ is not restricted to a special choice of the hopping integral values, we show in Fig.4(b) a result for another choice of parameter set which also roughly reproduces the $\epsilon'_g$ band structure. It can be seen that $\lambda$ again tends to unity at low temperatures.

In order to reinforce our argument, we finally consider a case where the $f$-wave pairing dominates over other pairing symmetries, but the nodes of the gap intersect the Fermi surfaces. In Fig.5 we present a plot similar to Fig.3 for $(t_2, t_3, t_4) = (-0.25, 0.0), U = 4.5, n_h = 0.2$, and $T = 0.01$. We have chosen these parameter values so that the spin susceptibility is ferromagnetic and has roughly similar maximum values as in the case considered above. It can be seen that the nodes of the $f$-wave gap now intersect the Fermi surfaces. As a result, $\lambda$ becomes much smaller as seen in Fig.4 (dashed curve). 27

From this result, we can also say that the enhancement of triplet pairing obtained in the previous cases (solid lines in Fig.4(a)) is not simply due to large DOS at the Fermi level in the BCS sense because DOS near the Fermi level is also large in the present case.

Now let us comment on the relation between the present theory and experiments. Several experiments suggest presence of gap nodes, 5, 6 which may seem to contradict with the present scenario. In the actual Na$_2$CoO$_2$, however, there is also the large Fermi surface around the $\Gamma$ point, which is not taken into account in the present study. Then we can propose a possible scenario where the ‘active’ Fermi surfaces for superconductivity are the pockets, while the large Fermi surface is a ‘passive’ one, in which superconductivity is induced by the ‘active’ band via interband interactions. 28 Since the $f$-wave gap intersects the large Fermi surface, this can account for the experimental results suggesting the existence of gap nodes. In fact, it has recently been found that a $\mu$SR data can be well explained by taking this view. 5

Another point to be mentioned in relation with the experiments is that the pocket Fermi surfaces are not observed in ARPES experiments 24, 30 up to date. However, since these experiments are done for materials with relatively large Na content, (i.e., large number of electrons in CoO layers) it is likely that the Fermi level lies above the $\epsilon'_g$ bands. 31 In fact, an experimental result that maximum $T_c$ is reached only when the content of Na decreases sufficiently 32 can be considered as an indirect support for scenario in which the $\epsilon'_g$ band plays an important role for superconductivity.

Theoretically, there are some remaining problems. In the FLEX method adopted here, vertex corrections are not taken into account. Then, one may wonder whether the present conclusion holds even if vertex corrections are considered since in some cases it is known that such corrections suppress unconventional superconductivity 33. However, we have recently performed dynamical cluster approximation study on a triangular lattice, which automatically takes into account the vertex correction effects, and have found that the $f$-wave pairing susceptibility is strongly enhanced upon lowering the temperature. 34 Thus, the present conclusion should hold even if we take into account the vertex corrections.

Secondly, we have neglected the off-site repulsions in our model. The study on the effect of off-site repulsion is now underway, where we find that for moderate values of off-site repulsions, $f$-wave pairing still dominates, while for larger off-site repulsions, $f$-wave gives way to singlet pairings. In particular, we have surprisingly found that singlet $i$-wave (which belongs to $A_2$ symmetry and changes sign 12 times around the $\Gamma$ point) pairing, which does not break time reversal symmetry as contrasted with $d$-wave pairing (which belongs to $E_2$ symmetry and takes the form $d + id$ below $T_c$), may dominate due to the peculiar disconnectivity of the pocket Fermi surfaces considered here. So there may be a close competition between triplet $f$-wave and singlet $i$-wave pairings, which might be related to the fact that Knight shift is found to decrease below $T_c$ in some cases 3, while not in other cases. 8 Details on this point will be published elsewhere.

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conductivity is induced by interband interaction effects.

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[26] In the lowest temperatures, we could not strictly check the convergence of the results with respect to number of sites since a large number of Matsubara frequencies is required. Nevertheless, the tendency that large values of $\lambda$ are obtained at low temperatures should in any case be correct.

[27] In fact, this is similar to the case considered in a third order perturbation study ref.17, where a finite $T_c$ for $f$-wave superconductivity is obtained even though the gap intersects the Fermi surface, in contrast to FLEX results. Such a discrepancy between perturbational studies and FLEX seems to be a general trend. Concerning this trend, we have recently performed quantum Monte Carlo calculation on a square lattice (K.Kuroki, Y. Tanaka, T. Kimura, and R. Arita, cond-mat/0307553), where we have found results supporting FLEX studies.

[28] After completion of the present study, this scenario has quite recently been supported by a multiband FLEX study by M. Mochizuki and M. Ogata, which takes into account both the pockets and the large Fermi surface (unpublished).

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[31] This view may be further supported by a recent study by Karppinen et al. (cond-mat/0402484), which shows that the actual Co valence can be smaller (the Fermi level can be higher) than expected from the composition $\text{Na}_x\text{CoO}_2$ due to oxygen vacancy.

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