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# Spin-resonance peak in $Na_xCoO_2 \cdot yH_2O$ superconductors: A probe of the pairing symmetry

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Spin dynamics in the superconducting state of the newly discovered $Na_xCoO_2 \cdot yH_2O$ superconductor with three possible pairing symmetries ($p_x+ip_y$, $d+id'$, and $f$ wave) is studied theoretically on a two-dimensional triangular lattice. We find that a spin resonance peak, which is found to have a close relevance to the relative phase of the gap function and the geometry of the Fermi surface, appears in both the in-plane and the out-of-plane components of the spin susceptibility for the spin-singlet $(d+id')$-wave pairing, while only in the out-of-plane (in-plane) component for the spin-triplet $(p_x+ip_y)$-wave ($f$-wave) pairing. We also indicate that there is no spin resonance for an $s$-wave pairing. These distinct features may be used to probe or determine the pairing symmetry in this compound unambiguously.

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Recently, superconductivity with $T_c \sim 5$ K was discovered in the $CoO_2$-layered material, $Na_xCoO_2 \cdot yH_2O$.[1] This compound consists of two-dimensional (2D) $CoO_2$ layers, with Co atoms forming a 2D triangular lattice and being separated by a thick insulating layer of $Na^+$ ions and $H_2O$ molecules. Although its $T_c$ is relatively low, this superconductor has still attracted much attention because it shares some similarities with high-$T_c$ cuprates; in particular, it may be another unconventional superconductor in a family of the doped Mott insulators. Therefore, the investigation of this compound is expected to give insight on the mechanism of the unconventional superconductivity. So far, several quite different theoretical proposals[2–7] for its pairing symmetry, such as the spin-singlet $d+id'$ wave and the spin-triplet $p_x+ip_y$ wave (or even $f$ wave[6,8]), have been put forward. On the other hand, experimental results on the pairing symmetry reported by different groups are also controversial, even with the same experimental method.[9–12]

In unconventional $d$-, $p$-, and $f$-wave superconductors, the gap function $\Delta_{\mathbf{k}}$ changes the sign (phase) around the Fermi surface and thus would lead to zeros (nodes) in the superconducting (SC) energy gap $|\Delta_{\mathbf{k}}|$. Therefore, one can in principle determine the pairing symmetry, by measuring the distribution of the phase and/or node positions. In practice, it is the node position rather than the phase that can be inferred in usual thermodynamic, transport, and NMR experiments. Therefore, the probe of the node position has been mostly used in the clarification of the pairing symmetry in unconventional superconductors.[13] However, the much debated pairing symmetries so far proposed for $Na_xCoO_2 \cdot yH_2O$ are the broken-time-reversal symmetry $d+id'$ and $p_x+ip_y$ waves. In this case, the energy gap $|\Delta_{\mathbf{k}}| = \sqrt{[\Delta_{\mathbf{k}}^d]^2+[\Delta_{\mathbf{k}}^{d'}]^2}$ is nodeless. So, a probe that is directly related to the phase is of special importance for the determination of the pairing symmetry in this compound as well as in other unconventional superconductors, as seen from the fact that the phase-sensitive experiments played a key role in the determination of the pairing symmetry in high-$T_c$ superconductors.[14] In this paper, by noting that a spin resonance peak appears in the different components of the dynamical spin susceptibility $\chi$ for all possible unconventional pairing symmetries in the 2D triangular lattice with the nearest-neighbor (NN) pairing interaction, we show that the identification of the spin resonance peak in the SC state, which can be carried out by neutron scattering experiments, may also provide an unambiguous clue to probe or determine the pairing symmetry in this compound. We elaborate that the occurrence of the spin resonance peak in a specific component of $\chi$ exclusively corresponds to a *definite* change of the phase of $\Delta_{\mathbf{k}}$.

To address both the spin-singlet and the spin-triplet superconductivity in the same model as well as to capture the essential physics of electron correlation, we employ a phenomenological $t$-$U$-$V$ model[15,16] on a 2D triangular lattice, in which an effective NN pairing interaction ($V$) is responsible for superconductivity and an on-site Hubbard $U$ for the electron correlation. Choosing the mean-field parameter $\Delta_{ij}^{(\pm)} = V(\langle c_{i\uparrow}c_{j\downarrow}\rangle \pm \langle c_{i\downarrow}c_{j\uparrow}\rangle)/2$, we can write the effective Hamiltonian as

$$H_{eff} = -\sum_{\langle ij\rangle,\sigma}[tc_{i\sigma}^{\dagger}c_{j\sigma} + \text{H.c.}] + U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{\langle ij\rangle}[\Delta_{ij}^{(\pm)} \times (c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger} \pm c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}) + \text{H.c.}], \quad (1)$$

where the upper sign is for the spin-triplet pairing state and the lower sign for the spin-singlet pairing state.

In the 2D triangular lattice, the dispersion relation of quasiparticles is

$$\epsilon_k = -2t\left[\cos k_x + 2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}\right] - \mu. \quad (2)$$

For the NN SC pairing interaction, $(d_{x^2-y^2} \pm id_{xy})$-wave, $(p_x \pm ip_y)$-wave, and $f$-wave pairing states may exist on a 2D triangular lattice:[17] (i) $\Delta_k^{d+id'} = \Delta_0\{\cos(k_x) - \cos(k_x/2) \times \cos(\sqrt{3}k_y/2) + i\sqrt{3}\sin(k_x/2)\sin(\sqrt{3}k_y/2)\}$, (ii) $\Delta_k^{p_x+ip_y} = \Delta_0 \times \{\sin(k_x) + \sin(k_x/2)\cos(\sqrt{3}k_y/2) + i\sqrt{3}\cos(k_x/2)\sin(\sqrt{3}k_y/2)\}$, and (iii) $\Delta_k^f = \Delta_0\{\sin(k_x) - 2\sin(k_x/2)\cos(\sqrt{3}k_y/2)\}$. Given the attractive interaction $V$ and with $t<0$,[2,4,16] the mean-field calculation of Eq. (1) shows that nearly degenerate singlet $(d+id')$- and triplet $f$-wave solutions are favored at $n=0.4$, while the triplet $p_x+ip_y$ wave is stable at $n=1.35$, where $n$ is the average electron number per site.[16,18] In order to compare the results for different pairing symmetries with roughly the same SC gap, we have chosen $V=0.75t$ for $n=0.4$ and $V=1.7t$ for $n=1.35$, which gives $\Delta_0=0.015t$ for the $f$ wave, $\Delta_0=0.014t$ for the $d+id$ wave $(n=0.4)$, and $\Delta_0=0.015t$ for the $p+ip$ wave $(n=1.35)$. The effective on-site Hubbard interaction is assumed to be $U=2.3t$.[19]

The bare spin susceptibility is given by

$$\chi^0_{ij}(\mathbf{q},\omega) = \frac{1}{4N}\sum_k \left[ \frac{C^-_{ij}(k,q)(F^+_{k,q}-1)}{\omega-\Omega^+_{k,q}+i\Gamma} - \frac{C^-_{ij}(k,q)(F^+_{k,q}-1)}{\omega+\Omega^+_{k,q}+i\Gamma} + \frac{2C^+_{ij}(k,q)F^-_{k,q}}{\omega+\Omega^-_{k,q}+i\Gamma}\right], \tag{3}$$

where the coherence factors are

$$C^\pm_{ij}(k,q) = \left[1 \pm \frac{\epsilon_k\epsilon_{k+q}+\mathrm{Re}(\Delta_k\Delta^*_{k+q})}{E_{k+q}E_k}\right] \tag{4}$$

for the spin-singlet pairing and if $ij=zz$ (the out-of-plane component of $\chi$) for the spin-triplet pairing, and

$$C^\pm_{ij}(k,q) = \left[1 \pm \frac{\epsilon_k\epsilon_{k+q}-\mathrm{Re}(\Delta_k\Delta^*_{k+q})}{E_{k+q}E_k}\right] \tag{5}$$

if $ij=+-$ (the in-plane component of $\chi$) for the spin-triplet pairing. $F^\pm_{k,q}=f(E_{k+q})\pm f(E_k)$ and $\Omega^\pm_{k,q}=E_k\pm E_{k+q}$, with $E_k=\sqrt{\epsilon_k^2+|\Delta_k|^2}$ and $f(E_k)$ the Fermi distribution function. Near $T=0$, only the first term in Eq. (3) with the coherence factor $C^-$, involving the creation of quasiparticle pairs, contributes to the spin susceptibility. An essential difference in the coherence factors between the spin-singlet pairing (or the component $\chi_{zz}$ for the spin-triplet pairing) and the component $\chi_{+-}$ for the spin-triplet pairing is the sign difference in front of $\mathrm{Re}[\Delta_k\Delta^*_{k+q}]$. This sign difference is a key point for our later discussions.

We may include the many-body correction to the spin susceptibility by the random phase approximation.[19] In this way, the renormalized spin susceptibility is given by,

$$\chi_{ij}(\mathbf{q},\omega) = \chi^0_{ij}(\mathbf{q},\omega)[1-U\chi^0_{ij}(\mathbf{q},\omega)]^{-1}. \tag{6}$$

The momentum dependences of the dynamical spin susceptibility for $\omega=0.02t$ in the SC state $(T=0.0001t)$ are presented in Fig. 1. For the $(p_x+ip_y)$-wave pairing, a peak near $\mathbf{Q}_1=0.94(2\pi/3,2\pi/\sqrt{3})$ can be seen, while for the $f$-wave and $(d+id')$-wave pairings, a peak near $\mathbf{Q}_2=(0,\sqrt{3}\pi/2)$ appears. An obvious feature, seen from the figure, is that these peaks depend only on the doping density and is irrespective of the symmetry of the pairing state and the components of $\mathrm{Im}\,\chi$. This is due to the fact that these peaks arise from the nesting of the Fermi surface, which is determined only by the doping density. We note that a much sharper peak occurs around $\mathbf{q}=(0,0)$ for $\mathrm{Im}\,\chi_{+-}$ in the case of the spin-triplet pairing. This peak already presents in the normal state (not shown here) and reflects an enhanced ferromagnetic fluctuation that may arise from the substantial density of state at the

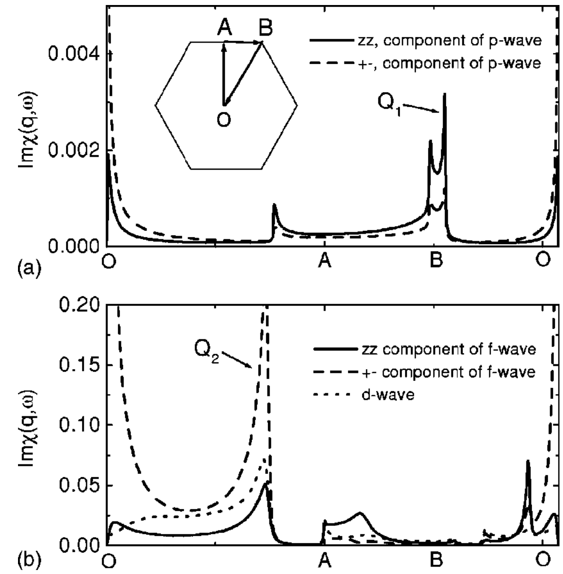


FIG. 1. Momentum dependence of $\mathrm{Im}\,\chi$ with $\omega=0.02t$ for (a) $p_x+ip_y$ wave at $n=1.35$, and (b) $f$ and $d+id'$ waves at $n=0.4$. The momentum is scanned along the path shown in the inset of (a).

Fermi level. However, it is highly suppressed for the spin-singlet pairing and for $\mathrm{Im}\,\chi_{zz}$ in the spin-triplet pairing as shown in Fig. 1.

In Fig. 2(a), we present the frequency dependence of $\mathrm{Im}\,\chi$ at $\mathbf{Q}_1$ for the spin-triplet $(p_x+ip_y)$-wave pairing. It is seen that a spin resonance peak occurs near $\omega=0.05t$ for the out-of-plane component $\mathrm{Im}\,\chi_{zz}$, but it is absent for the in-plane component $\mathrm{Im}\,\chi_{+-}$. However, in sharp contrast, the spin resonance peak appears in the in-plane component rather than in the out-of-plane component for the spin-triplet $f$-wave pair-

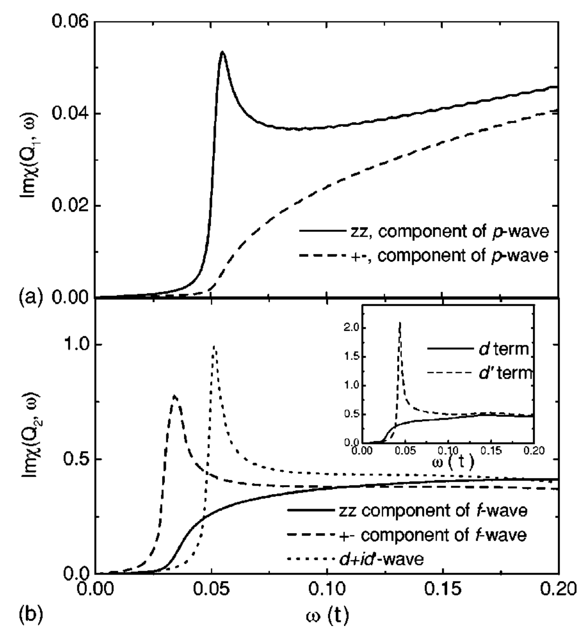


FIG. 2. Frequency dependence of $\mathrm{Im}\,\chi$ in the SC state $(T=0.0001t)$: (a) for the $p_x+ip_y$ wave at $n=1.35$ and $\mathbf{Q}_1$; (b) for the $f$ and $d+id'$ waves at $n=0.4$ and $\mathbf{Q}_2$. The inset of (b) shows the results for the pure $d$ and $d'$ waves, respectively.

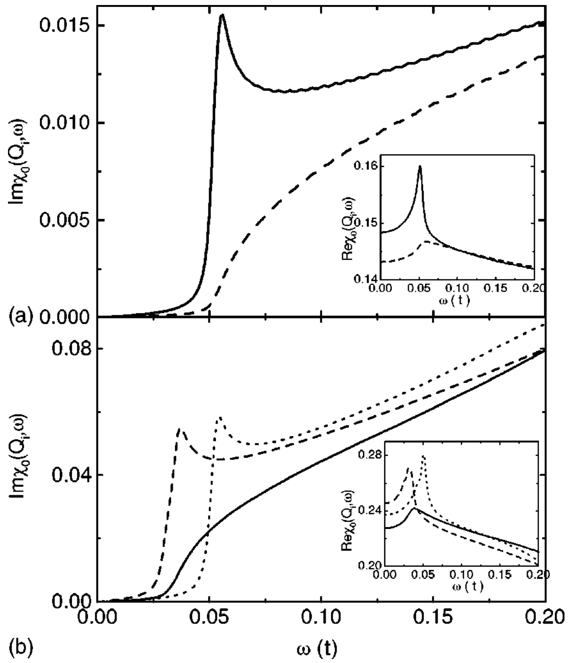


FIG. 3. Frequency dependence of the bare spin susceptibility $\chi_0$ in the SC state ($T=0.0001t$): (a) the $p_x+ip_y$ wave at $n=1.35$ and $\mathbf{Q}_1$, where the solid line indicates Im $\chi^0_{zz}$ and the dashed line Im $\chi^0_{+-}$; (b) the $f$ and $d+id'$ waves at $n=0.4$ and $\mathbf{Q}_2$, where the solid line indicates Im $\chi^0_{zz}$ of the $f$ wave, the dashed line Im $\chi^0_{+-}$ of the $f$ wave, and the dotted line the $d+id'$ wave.

ing [Fig. 2(b)]. Moreover, the spin resonance peak can be found in both components for the $d+id'$ pairing,[20] via the relation $\mathrm{Im}\,\chi_{+-}=2\,\mathrm{Im}\,\chi_{zz}$, which holds for a spin-singlet state. The quite different features in the spin response for all three possible pairing states are significant, and may be used as an unambiguous clue to probe or determine experimentally the pairing symmetry in this compound.

To understand our observation, we plot the bare spin susceptibility Im $\chi_0$ in Fig. 3. It is clear that a peak is evident at the spin gap edge following by a steplike decrease just below the gap edge in the channel where there is a spin resonance peak. Using the Kramers-Kroenig relation, we will obtain a logarithmic singularity in its real part Re $\chi_0$ (the inset of Fig. 3). Thus, the RPA correction will further magnify this effect and leads to a sharp peak near the gap edge. This indicates that a peak just above the spin gap edge is the source of the spin resonance. According to the BCS theory, the density of states (DOS) is divergent just above the SC gap edge, and this divergence is expected to show up in some physical properties. However, the effect is limited by the coherence factor which is either $\sim 0$ or $\sim 1$, depending on the relative sign of $\Delta_k$ and $\Delta_{k+q}$, when $E_k$ and $E_{k+q}$ are near the gap edge. Specifically, $C^-$ is negligible unless $\Delta_k$ and $\Delta_{k+q}$ are of opposite signs for the spin-singlet pairing[21] and for Im $\chi_{zz}$ in the spin-triplet pairing, or of the same sign for Im $\chi_{+-}$ in the spin-triplet pairing. With these general considerations, let us now address the origin of the above observation.

In Fig. 4, we plot the phase (+ sign denotes the phase 0, − sign the phase $\pi$) and node position (dotted lines) for various terms of the three possible pairing symmetries. The

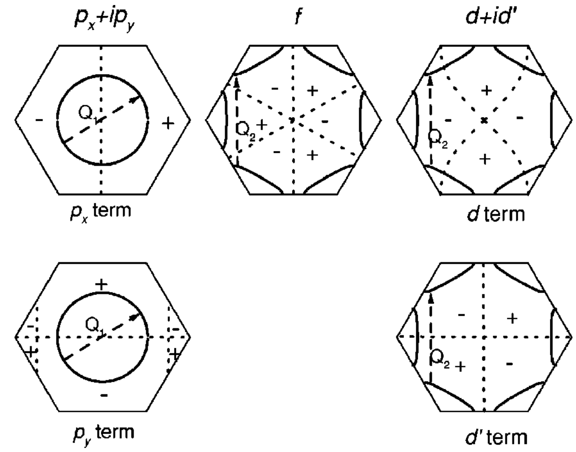


FIG. 4. Fermi surface (thick lines) and phase ($\pm$) of the gap functions for three possible pairing symmetries. The dotted lines denote the node positions that separate the regions with different phases, and the dashed lines with arrows represent the transition wave vectors $\mathbf{Q}_1$ and $\mathbf{Q}_2$ as indicated in Fig. 1.

Fermi surface for $n=1.35$, where the $p_x+ip_y$ wave is favored, is a circle centered at (0,0) point. For either the $p_x$ or $p_y$ term, the two half circles separated by the line node will have the opposite (different) signs (phases) of the gap function $\Delta_k$. Therefore, for the wave vector $\mathbf{Q}_1=0.94(2\pi/3,2\pi/\sqrt{3})$, $\Delta_k$ and $\Delta_{k+Q_1}$ have opposite signs. According to Eqs. (4) and (5), the coherence factor $C^-$ is appreciable for $ij=zz$ and vanishes for $ij=+-$. As a result, the DOS peak shows up in Im $\chi^0_{zz}$ and does not in Im $\chi^0_{+-}$, as shown in Fig. 3(a). But for the $f$-wave pairing state, $\Delta_k$ and $\Delta_{k+Q_2}$ connected by $\mathbf{Q}_2=(0,\sqrt{3}\pi/2)$ are of the same sign (phase). Therefore, the DOS peak exists in Im $\chi^0_{+-}$, instead of in Im $\chi^0_{zz}$ [Fig. 3(b)]. The most definite demonstration of this argument can be found in the case of the $d+id'$ wave, where an appreciable coherence factor $C^-$ requires that $\Delta_k$ and $\Delta_{k+q}$ have the opposite signs. However, from Fig. 4 one can see that, though the $\Delta_k$'s connected by the wave vector $\mathbf{Q}_2$ satisfy the requirement for the $d'$ term, those for the $d$ term do not. To see their effect, we have calculated the results for $d$ and $d'$ terms, separately. As shown in the inset of Fig. 2(b), we find no peak for the $d$-wave term, but a sharp peak for the $d'$-wave term. Remembering that the term $\mathrm{Re}[\Delta_k^{d+id'}\Delta_{k+q}^{d+id'*}]=\Delta_k^d\Delta_{k+q}^d+\Delta_k^{d'}\Delta_{k+q}^{d'}$, one will expect that the effect of $d'$ term is dominant for the $d+id'$ wave. The only relevant difference between the $d$- and $d'$-wave pairings is the sign (phase) of their gap function. So, the spin resonance peak depends *uniquely* on the relative phase of the gap functions connected by the transition wave vector. Therefore, its identification may be taken as a phase-sensitive method to probe the pairing symmetry of $Na_xCoO_2\cdot yH_2O$ superconductors. The spin susceptibility can be measured by the inelastic neutron scattering, as done for high-$T_c$ cuprates where a spin resonance was observed around $\mathbf{q}=(\pi,\pi)$.[22] Note that a similar procedure had also been applied to high-$T_c$ cuprates with a dominant $d_{x^2-y^2}$ pairing state.[23] In that case, $\Delta_k$ and $\Delta_{k+q}$ with $\mathbf{q}=(\pi,\pi)$ have the opposite sign and therefore the spin resonance appears. Moreover, we can also conclude from the above analysis that there should be no spin resonance peak for an $s$-wave pairing, because the coherence factor $C^{-}$ is negligible due to the same sign in $\Delta_k$ and $\Delta_{k+q}$ for any wave vector $\mathbf{q}$ in the case of the spin-singlet *s*-wave pairing. This feature is distinctly different from those for the above-addressed three unconventional pairing symmetries.

Before concluding the paper, let us use the above argument to address the anisotropic suppression of the spin response at $\mathbf{q}=(0,0)$ shown in Fig. 1. At $\mathbf{q}\sim(0,0)$, the two gap functions connected by $\mathbf{q}$ will surely have the same phase. So, the coherence factor $C^{-}$ is negligible for the spin-singlet pairing and Im $\chi_{zz}$ of the spin-triplet pairing, but it is not for Im $\chi_{+-}$. Thus, the spin response around $\mathbf{q}\sim(0,0)$ in the former case is strongly suppressed.

In conclusion, we have found that the spin resonance peak exists in quite different ways for all possible pairing symmetries proposed for the newly discovered $Na_xCoO_2 \cdot yH_2O$ superconductor, and suggested to use it as an unambiguous clue to probe or determine the pairing symmetry in future inelastic neutron scattering experiments. Moreover, we have elaborated that the spin resonance peak has a close relevance to the relative phase of the gap function and the geometry of the Fermi surface.

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[18] In the case of the electron doping, the average electron number $n=1.35$ ($n=0.4$) corresponds roughly to the experimental value in $Na_xCoO_2 \cdot yH_2O$ with $x=0.35$ ($x=0.6$) for $t<0$ ($t>0$).

[19] We also tried other values in the range of $U=0.75t-2.6t$, in which the random phase approximation (RPA) is still valid, and find no qualitaive change. We note that the weak coupling approach (RPA) can still give accurate results for the spin susceptibility even for the intermediate coupling if an effective (reduced) $U$ is used, as shown by N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. B **47**, 2742 (1993).

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