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Phonon-mediated unconventional superconductivity in $Na_xCoO_2{\cdot}yH_2O$ compounds

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Abstract

We investigate the symmetry of the superconducting gap induced by dominant small-**q** phonon scattering in a triangular lattice. Using the energy band appropriate for $Na_xCoO_2{\cdot}yH_2O$ and solving the BCS-like gap equation within the weak coupling theory self-consistently, we find that an f-wave pairing state is favored in this system. It is a consequence of the combined effects of the momentum decoupling due to the small-**q** phonon scattering, the anisotropy of the local density of states (DOS) in the momentum space and the sufficient effective Coulomb repulsion. We propose that this scenario may provide a new picture for the superconductivity in $Na_xCoO_2{\cdot}yH_2O$ compounds.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The superconductivity found in CoO_2-layered material, $Na_xCoO_2{\cdot}yH_2O$ [1], has attracted much attention. This material consists of two-dimensional (2D) CoO_2 layers where Co atoms form a 2D triangular lattice and are separated by a thick insulating layer of Na^+ ions and H_2O molecules. Increasing sodium content x corresponds to adding x electrons to the CoO_2 plane which is otherwise a spin-1/2 lattice. Thus, this compound shares some similarities with the extensively studied high-T_c cuprates and an unconventional superconductivity has been proposed [2–6].

To understand the superconductivity of this material it is essential to determine its superconducting pairing symmetry. Though an extensive study has been carried out, experimental results on the pairing symmetry in $Na_xCoO_2{\cdot}yH_2O$ are still controversial. Some experiments suggest the possible occurrence of conventional superconductivity [7]. Others suggest the possible occurrence of unconventional pairing [8–12]. In particular, an unchanged Knight shift across T_c found in some experiments [9] suggests spin-triplet pairing. On the other hand, several quite different theoretical proposals for its pairing symmetry [2–6], such as the spin-singlet $d + id'$-wave and the spin-triplet $p_x + ip_y$-wave or f-wave, have been put forward. Kuroki *et al* propose a possible spin-triplet f-wave pairing due to disconnected Fermi surfaces in $Na_xCoO_2{\cdot}yH_2O$ [13]. Johannes *et al* propose odd-gap superconductivity in $Na_xCoO_2{\cdot}yH_2O$ based on nesting of Fermi surfaces and spin fluctuations [14]. These theories are all based on magnetically mediated pairing. However, there is substantial experimental evidence to suggest that phonons may be crucial for the pairing in $Na_xCoO_2{\cdot}yH_2O$. Structural instabilities have been reported in the non-hydrated compound [15], suggesting the possibility of a related soft mode and thus strong electron–phonon coupling. The existence of a strong electron–phonon interaction in $Na_xCoO_2{\cdot}yH_2O$ is also indicated by various optical measurements [16–18]. In particular, the quasiparticle dispersion for the a_{1g}-band observed by angle-resolved photoemission spectroscopy (ARPES) measurement has a prominent kink structure around 70 meV below the Fermi level [19], which is expected to originate from phonons because the energy of the optical phonon is also ∼70 meV. Some electronic Raman experimental results also support strong electron–phonon interaction in this compound [20]. In addition, the role of the electron–phonon interactions in the superconductivity and charge dynamics has been theoretically studied in this compound recently [21, 22].

Based on the above analysis, we will in this paper consider a phonon-mediated pairing mechanism for the superconductivity in $Na_xCoO_2{\cdot}yH_2O$. From the conventional viewpoint, the phonon-mediated interaction is considered to induce only an isotropic SC gap. This is true when

the electron–phonon interactions are momentum independent. However, if the phonon-mediated interactions are momentum dependent, an anisotropic superconducting gap may be induced. In fact, an anisotropic superconducting gap induced by a momentum-dependent phonon interaction has been considered in high-T_c superconductors [23–25] and other unconventional superconductor such as the layered organic salt κ-(BEDT-TTF)$_2$X [26]. It has also been shown that d-wave superconductivity could be induced by the screened phonon interactions with the assistance of a contribution from antiferromagnetic fluctuations [27, 28]. Here, we show that small-**q** phonon scattering will lead to an f-wave SC gap symmetry in $Na_xCoO_2{\cdot}yH_2O$. The small-**q** phonon interaction is characterized by a strongly **q**-dependent attraction which is peaked at small momenta, and therefore leads to momentum decoupling [24–26]. As a result, the magnitude of the SC gap tends to match the local DOS at the Fermi momentum $\mathbf{k}_F$ (defined as $N(\mathbf{k}) = 1/|\nabla_{\mathbf{k}}\varepsilon_k|$ with ε_k the quasiparticle dispersion). By using an energy band appropriate for the $Na_xCoO_2{\cdot}yH_2O$, the local DOS $N(\mathbf{k})$ shows six maxima at the crossings of the Fermi surface with the Γ–M direction. Thus, it will give rise to an anisotropic gap function. In the meantime, considering that $Na_xCoO_2{\cdot}yH_2O$ is a strongly correlated system in which a sufficient residual Coulomb repulsion is unavoidable, with this residual interaction we find that the f-wave SC symmetry is favored.

2. Formalism

The main physics related to superconductivity in $Na_xCoO_2{\cdot}yH_2O$ is believed to occur in the 2D CoO_2 layers where Co atoms form a 2D triangular lattice. In this triangular lattice, the dispersion of quasiparticles is given by

$$\begin{aligned}\varepsilon_{\mathbf{k}} = &-2t_1\cos k_y - 4t_1\cos\frac{\sqrt{3}}{2}k_x\cos\frac{1}{2}k_y\\ &-2t_2\cos\sqrt{3}k_x - 4t_2\cos\frac{\sqrt{3}}{2}k_x\cos\frac{3}{2}k_y\\ &-2t_3\cos 2k_y - 4t_3\cos\sqrt{3}k_x\cos k_y\\ &-4t_4\cos\frac{5}{2}k_y\cos\frac{\sqrt{3}}{2}k_x - 4t_4\cos\sqrt{3}k_x\cos 2k_y\\ &-4t_4\cos\frac{1}{2}k_y\cos\frac{3\sqrt{3}}{2}k_x - \mu, \end{aligned} \tag{1}$$

where t_i denotes the hopping terms from the nearest-neighbor t_1 to the fourth-nearest-neighbor t_4. To reproduce the observed Fermi surface by ARPES [29], we set parameters (t_1, t_2, t_3, t_4) of the bare dispersion $\varepsilon_{\mathbf{k}}$ to be $(-1, 0, 0, 0.2)$. μ is the chemical potential which is chosen to make the electron doping density $\delta = 0.3$.

To obtain the gap function in the SC state, we will solve the BCS-like gap equation:

$$\lambda\Delta(\mathbf{k}) = -\frac{1}{N}\sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}')W(\mathbf{k}')\Delta(\mathbf{k}'), \tag{2}$$

where $W(\mathbf{k}') = \frac{\tanh(\beta\varepsilon_{\mathbf{k}'}/2)}{2\varepsilon_{\mathbf{k}'}}$ with $\beta = 1/k_BT$ and T the temperature. We note that we have assumed that the pairing interaction is instantaneous in equation (2). Consequently $V(\mathbf{k}-\mathbf{k}')$ has no frequency dependence. This approximation is expected to grasp the physical essence of the pairing symmetries [30, 31]. In the conventional s-wave superconductor the pairing potential $V(\mathbf{k}-\mathbf{k}')$ due to the interaction between electrons and phonons is almost constant around the Fermi surface and this gives rise to an isotropic SC gap. When Coulomb correlations are screened to be short range, the system may show electron–phonon interaction dominated by forward scattering in a general way. In this way, we take the following form for the interaction [24–26, 32]

$$V(\mathbf{k}-\mathbf{k}') = -\frac{V}{q_c^2 + |\mathbf{k}-\mathbf{k}'|^2} + U \tag{3}$$

where the cutoff momentum q_c selects those phonons with a small wavevector in the phonon spectrum, V is the strength of election–phonon interaction and U is an effective Coulomb repulsion which prevails at large momentum. This form of interaction is found to occur in the scattering of electrons off phonons when the electronic system is close to the phase separation instability and has been examined by many authors for high-T_c and organic superconductors [23–28]. Due to the existence of the cutoff momentum q_c in the interaction form of equation (3), the dominant transfer momenta in the pairing interaction are basically limited to small momenta. Therefore, when q_c is small compared to the characteristic momentum of the variations of the local DOS $N(\mathbf{k})$ for the electronic state, there is a tendency for decorrelation between pairing couplings at different regions of the Fermi surface. Therefore, an anisotropic SC gap will be expected in this case.

3. Numerical results and discussions

We have solved the gap equation (2) self-consistently to obtain the SC gap function. In the numerical calculation, we decrease the temperature T gradually to search for the SC state: when the eigenvalue $\lambda = 1$ the SC state is reached. The results for different cutoff momenta q_c with a fixed $U/V = 0.145$ are presented in figure 1. One can see that the magnitude of $\Delta(\mathbf{k})$ shows six maxima sitting along the Γ–M direction, the nearest two maxima of $\Delta(\mathbf{k})$ have a π phase difference and this gives rise to six gap nodes which right lie at the crossings of the Fermi surface with the Γ–K line. This shows that the solution for the gap function has an f-wave symmetry. We find that the f-wave gap symmetry is robust for a range of cutoff momenta, as shown in figure 1 for $q_c = 0.05\pi, 0.18\pi$ and 0.5π. We note that the local DOS in the momentum space $N(\mathbf{k})$ of the energy band equation (1) exhibits a local maximum at the crossings of the Γ–M line with the Fermi surface and a local minimum at the crossings of Γ–K with the Fermi surface. Thus, the characteristic momentum of $N(\mathbf{k})$ variations on the Fermi surface is about $\frac{\pi}{\sqrt{3}}$. On the other hand, the strongly **q**-dependent pairing potential $V(\mathbf{q})$ is peaked at small momenta(its characteristic momentum is q_c). Therefore, if q_c is sufficiently smaller than $\frac{\pi}{\sqrt{3}}$, a momentum decoupling occurs so that the modulus of the gap function tends to match the local DOS $N(\mathbf{k})$ of the system. This leads to the local DOS

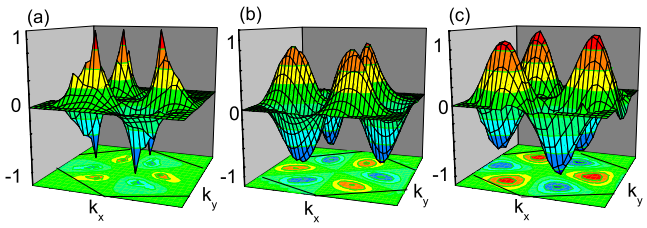

Figure 1. Self-consistent solution of the superconducting gap $\Delta(\mathbf{k})$ as a function of momentum $\mathbf{k}$ for several choices of the cutoff momentum q_c with $U/V = 0.145$: (a) $q_c = 0.05\pi$; (b) $q_c = 0.18\pi$; (c) $q_c = 0.5\pi$.

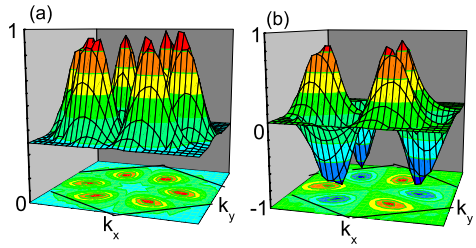

Figure 2. Self-consistent solution of the superconducting gap $\Delta(\mathbf{k})$ as a function of momentum $\mathbf{k}$ for (a) $U/V = 0.03$ and (b) $U/V = 0.94$ with $q_c = 0.18\pi$.

induced gap anisotropy. A quantitative difference between the results in figure 1 is that the peaks of the gap magnitude become sharper and sharper with the decrease of q_c, which indicates a stronger momentum decoupling with the decrease of q_c.

However, the momentum decoupling alone does not necessarily lead to the f-wave gap function, though it indeed gives rise to an anisotropic gap. As shown in figure 2(a), when we decrease the repulsive Coulomb potential U, such as $U/V = 0.03$, there is no π shift in the phase of the gap function and no gap nodes, though it is still anisotropic. In fact, now the gap function is an anisotropic s-wave, while for a larger U the f-wave gap function remains, as shown in figure 2(b) for $U/V = 0.94$. In fact, a repulsive Coulomb potential besides the attractive part in equation (3) is necessary for the formation of the f-wave SC gap because there is a sign change in this gap function.

Thus, an explanation of the above results is as follows. First because the cutoff momentum q_c is less than the characteristic momentum of the local DOS in the momentum space $N(\mathbf{k})$, the attractive potential is peaked at small momentum as shown in figure 3 and this leads to a momentum decoupling which means a tendency for the strong pairing between quasiparticles situating in the nearby k-points where $N(\mathbf{k})$ is maximum. Second, the energy band equation (1) has a feature that there are six maxima in $N(\mathbf{k})$ at the crosses of the Fermi surface with the Γ–M direction which is shown schematically as six shaded regions (labeled as 1–6) in figure 4. The momentum decoupling leads the quasiparticles at one of the six maxima (for example in the region 1 in figure 4) to be paired mainly to the quasiparticles at the other five maxima (in the regions 2–5 in figure 4). Thus, an anisotropic SC gap

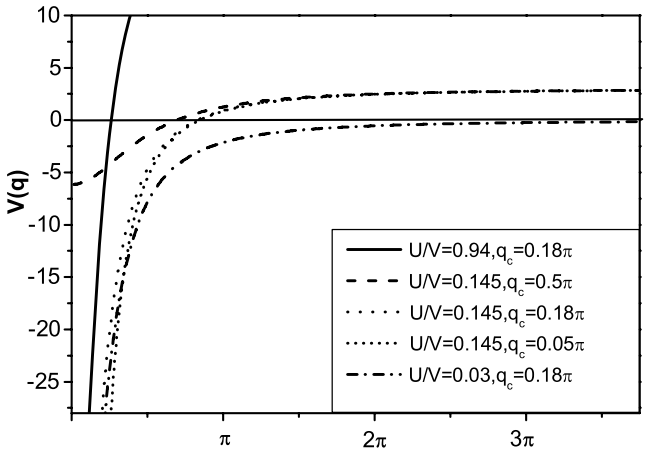

Figure 3. The pairing potential $V(q)$ for different parameters U/V and q_c (see equation (3)).

is formed. Thirdly, for the formation of an f-wave SC gap, an effective Coulomb repulsive potential plays an essential role. As shown in figure 3, where the variation of the pairing potential $V(\mathbf{q})$ with the repulsive Coulomb potential U and the cutoff momentum q_c is presented, $V(\mathbf{q})$ will change sign from a negative attractive potential at small momenta to a positive repulsive one at large momenta due to the presence of U. For a fixed cutoff momentum ($q_c = 0.18\pi$), one sees that the momentum q_0 at which $V(\mathbf{q}) = 0$ decreases with the increase of U/V. When U/V is increased to be larger than 0.14, the momentum q_0 is decreased to be about the characteristic momentum of $N(\mathbf{k})$, i.e. the momentum between the nearest two shaded regions. In this case, the pairing potential is attractive between the quasiparticles at the nearby shaded regions and positive between the next nearest shaded regions, so an f-wave SC gap is formed. When we decrease the Coulomb repulsive potential, such as $U/V = 0.03$, the momentum q_0 will increase to be larger than the reciprocal lattice vector. In this case, the pairing potential between two quasiparticles in any shaded regions will be negative, so no π shift of the gap phase will be caused and an anisotropic s-wave gap is produced by the momentum decoupling and the feature of the local DOS in the momentum space.

From the above analysis it is clear that the f-wave solution is the favorite gap symmetry of the SC phase in our model as long as a sufficient effective Coulomb repulsion U is presented. For $q_c = 0.18\pi$, we find that the lower limit of U for the appearance of the f-wave solution is $U/V = 0.14$. Below this critical value the anisotropic s-wave solution is obtained.

We note that the Coulomb correlation in Na_xCoO_2 is large. In particular, it is estimated from the ARPES measurement that the bare on-site Coulomb interaction is about 3.5–5 eV in $Na_xCoO_2{\cdot}yH_2O$ [33], which is comparable with that in high-T_c superconductors. Notice that a value of $U/V = 0.7$ has been chosen in a similar model; when it is applied to high-T_c superconductors [32], we believe that the presence of a sizable $U/V > 0.14$ in $Na_xCoO_2{\cdot}yH_2O$ is acceptable. Therefore, a small-$\mathbf{q}$ phonon-mediated pairing in the strongly correlated $Na_xCoO_2{\cdot}yH_2O$ may lead to an f-wave symmetry.

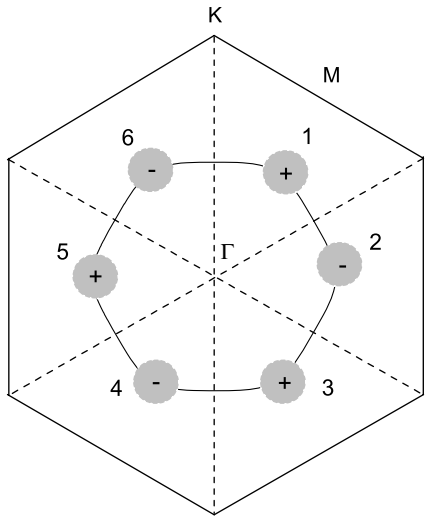

Figure 4. A schematic illustration of the formation of the f-wave superconducting gap. The shaded regions indicate the k-points where the local density of states $N(\mathbf{k})$ is maximum (see text).

In conclusion, we have shown that based on the phonon-mediated pairing dominated by the small-**q** phonon, an f-wave pairing solution in a triangular lattice with an energy band applying to $Na_xCoO_2{\cdot}yH_2O$ is favored. The f-wave superconductivity is a consequence of the combined effects of the momentum decoupling due to the small-**q** phonon scattering, the anisotropy of the local density of states in the momentum space and sufficient effective Coulomb repulsion. Our results suggest that the phonon-mediated interaction may play an important role in the superconductivity in $Na_xCoO_2{\cdot}yH_2O$.

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