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Low Energy Electronic States and Triplet Pairing in Layered Cobaltate

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The structure of the low-energy electronic states in layered cobaltates is considered starting from the Mott insulating limit. We argue that the coherent part of the wave functions and the Fermi-surface topology at low doping are strongly influenced by spin-orbit coupling of the correlated electrons on the t_{2g} level. An effective t-J model based on mixed spin-orbital states is radically different from that for the cuprates, and supports unconventional, pseudospin-triplet pairing.

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The layered cobalt oxides Na_xCoO_2 exhibit a number of remarkable properties with potential applications. At large x, they are unconventional metals showing a large thermopower (suppressed by magnetic field [1]) and also signatures of localized magnetic states. Such a mixture of itinerant transport and Curie-Weiss magnetism ("Curie-Weiss metal" [2]) is not easy to reconcile, and there is growing evidence that special charge/orbital ordering correlations are at work at large x [3]. Static charge ordering is observed at $x = 0.5$ [2]. These observations are not totally unexpected, as a rich interplay between spin/charge/orbital degrees of freedom is a common phenomenon in transition metal oxides. Yet a real surprise and new challenge for theory was the recent discovery [4] of superconductivity at $T_c \sim 5$ K in water-intercalated cobaltates with low sodium content about $x \sim 0.3$. It is believed that the superconductivity of the cobaltates emerges from a correlated metallic state with enhanced electronic mass [5,6], and it may have an unconventional, possibly spin-triplet [7–9] pairing symmetry.

Theoretically, regarding Na_xCoO_2 as spin 1/2 Mott insulator doped by spinless charge carriers, a t-J model similar to that for the high-T_c cuprates has been considered [10–13]. However, the predicted time-reversal violating $d_1 + id_2$ singlet state is not supported by experiment [6,9], and other proposals employing Fermi-surface nesting and/or charge-density fluctuations have been discussed [14,15] in favor of spin-triplet pairing.

In this Letter, we show that the relevant t-J model for the cobaltates is in fact qualitatively different from its simplest version used in Refs. [10–13]. The key point is that the low-energy electronic states of the CoO_2 layer are derived from the Kramers pseudospin doublets of the Co^{4+} ion with *mixed spin and orbital* quantum numbers. The projection of the (initially spin-antiferromagnetic) J interaction on the pseudospin states has nontrivial consequences for the internal structure of the Cooper pairs, leading to novel *pseudospin-triplet* pairing.

The basic structural elements of Na_xCoO_2 are CoO_2 layers, which consist of edge sharing CoO_6 octahedra slightly compressed along the trigonal axis [16]. The Co ions form a 2D triangular lattice, sandwiched by oxygen layers. Sodium doping is believed to introduce spinless Co^{3+} states into the spin 1/2 Co^{4+} background.

A minimal model for the cobaltates should include the orbital degeneracy of the Co^{4+} ion [17], where a hole in the $d^5(t_{2g})$ shell has the freedom to occupy one out of three orbitals $a = d_{yz}$, $b = d_{xz}$, $c = d_{xy}$. The degeneracy is partially lifted by trigonal distortion, which stabilizes the A_{1g} electronic state $(a + b + c)/\sqrt{3}$ over the E'_g doublet $(e^{\pm i\phi}a + e^{\mp i\phi}b + c)/\sqrt{3}$ (hereafter $\phi = 2\pi/3$): $H_\Delta = \Delta[n(E'_g) - 2n(A_{1g})]/3$. The value of Δ is not known; Ref. [17] estimates it ~25 meV, while the band structure calculations for a related structure give ~100 meV [18].

In terms of the effective angular momentum $l_{eff} = 1$ of t_{2g} shell [19], the functions A_{1g} and E'_g correspond to the $|l_z = 0\rangle$ and $|l_z = \pm 1\rangle$ states, respectively. Therefore, a hole residing on the E'_g orbital doublet will experience an unquenched spin-orbit interaction $H_\lambda = -\lambda(\vec{l} \cdot \vec{s})$. The constant λ for Co^{4+} is about 640 $cm^{-1} \approx 80$ meV [20]. Although λ is somewhat smaller than the bare hopping matrix element $t \sim 0.1$ eV in cobaltates (inferred from

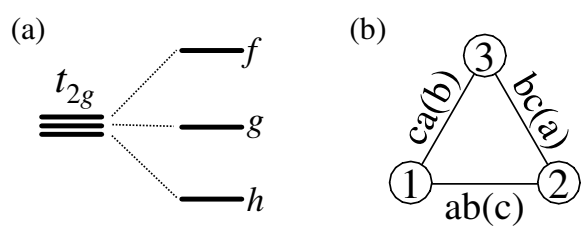

FIG. 1. (a) The t_{2g}-orbital degeneracy of $Co^{4+}(d^5)$ ion is lifted by trigonal distortion and spin-orbit interaction. A hole with pseudospin one-half resides on the f level. Its wave function contains both E'_g and A_{1g} states mixed up by spin-orbit coupling. (b) The hopping geometry on the triangular lattice of Co ions. $\alpha\beta(\gamma)$ on bonds should read as $t_{\alpha\beta} = t$, $t_{\gamma\gamma} = -t'$, and $\alpha, \beta, \gamma \in \{a, b, c\}$ with $a = d_{yz}$, $b = d_{xz}$, $c = d_{xy}$. The t hopping stems from the charge-transfer process via oxygen ions, while t' stands for the direct d-d overlap.

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the free-electron bandwidth ~1 eV [21]), the spin-orbit coupling strongly affects the coherent motion of the fermions when the quasiparticle bandwidth is reduced by correlation effects to much smaller values ~0.1 eV [22].

At $x = 0$, $H = H_\Delta + H_\lambda$ is diagonalized by a transformation:

$$\alpha_\sigma = i[c_\theta e^{-i\sigma\psi_\alpha} f_{-\bar{\sigma}} + i s_\theta f_{\bar{\sigma}} + e^{i\sigma\psi_\alpha} g_{\bar{\sigma}} + s_\theta e^{-i\sigma\psi_\alpha} h_{-\bar{\sigma}} - i c_\theta h_{\bar{\sigma}}]/\sqrt{3}, \quad (1)$$

where $c_\theta = \cos\theta$, $s_\theta = \sin\theta$, $\alpha = (a, b, c)$, and $\psi_\alpha = (\phi, -\phi, 0)$, correspondingly. The angle θ is determined from $\tan 2\theta = 2\sqrt{2}\lambda/(\lambda + 2\Delta)$. As a result, one obtains three levels, $f_{\bar{\sigma}}, g_{\bar{\sigma}}, h_{\bar{\sigma}}$ [see Fig. 1(a)]; each of them are Kramers doublets with pseudospin one-half $\bar{\sigma}$. The highest, f level, which accommodates a hole in the t_{2g} shell, is separated from the g level by $\varepsilon_f - \varepsilon_g = \lambda + \frac{1}{2} \times (\lambda/2 + \Delta)(1/\cos 2\theta - 1)$. This splitting is $\sim 3\lambda/2$ at $\lambda \gg \Delta$, and $\sim\lambda$ in the opposite limit. It is important to observe that the pseudospin $f_{\bar{\sigma}}$ states

$$|\bar{\uparrow}\rangle_f = i c_\theta |+1\rangle|\downarrow\rangle - s_\theta |0\rangle|\uparrow\rangle, \quad |\bar{\downarrow}\rangle_f = i c_\theta |-1\rangle|\uparrow\rangle - s_\theta |0\rangle|\downarrow\rangle \quad (2)$$

are coherent mixtures of different orbital and spin states, and this will have important consequences for the symmetry of the intersite interactions, as we see below.

We model the band motion by the following Hamiltonian suggested by the edge-shared structure [17]:

$$H_t^{ij} = t(\alpha_{i\sigma}^\dagger \beta_{j\sigma} + \beta_{i\sigma}^\dagger \alpha_{j\sigma}) - t' \gamma_{i\sigma}^\dagger \gamma_{j\sigma} + \text{H.c.}, \quad (3)$$

where $t = t_{pd}^2/\Delta_{pd}$ originates from the d-p-d process via the charge-transfer gap Δ_{pd}, and $t' > 0$ is the direct d-d hopping. On each bond, there are two orbitals (α, β) active in d-p-d process, while the third one (γ) is transferred via the direct d-d channel [Fig. 1(b)]. The hopping geometry in real situation could, of course, be more complicated (e.g., include p-p hoppings). The t, t' model is the simplest possibility chosen for illustrative purposes.

The quasiparticle band structure is obtained within a slave-boson approach, where the electron operator is represented as $\alpha_{i\sigma} \Rightarrow e_i^\dagger \bar{\alpha}_{i\sigma} \Rightarrow \sqrt{x}\bar{\alpha}_{i\sigma} + \textit{incoherent part}$. The last equation implies that we consider a Fermi-liquid regime, where holons (described by the $e_i^\dagger$ operator) are condensed, while the $\bar{\alpha}_{i\sigma}$ operators represent coherent fermionic quasiparticles. On the mean-field level (the incoherent part being discarded), this leads to $t \to t_{\text{coh}} \simeq xt$, and one obtains a renormalized hopping Hamiltonian $H_t^{\text{coh}} \simeq xH_t$. While such a Gutzwiller-type approximation fails to capture high-energy electronic processes far from the Fermi level, it is believed to provide a qualitatively correct description of the low-energy states.

Under the transformation (1), the hopping Hamiltonian obtains a rather complicated matrix structure in the full spin/orbital space, and the elements of this matrix sensitively depend on the angle θ. The Hamiltonian $H_\Delta + H_\lambda + H_t^{\text{coh}}$ has been diagonalized in momentum space numerically. The obtained quasiparticle dispersion curves are shown in Fig. 2(a). The first point to notice is that even for a substantial doping level, $x = 0.3$, there is a clear separation of bands that can be traced back to the on-site level structure discussed above. In particular, we find at small doping that the states near the Fermi level are derived dominantly from the f-pseudospin states; therefore, they are dispersive modes with mixed spin-orbital quantum numbers. The "f" band has the bottom at the Γ point [23] and shows flat portions near the K points in the Brillouin zone of the triangular lattice, which lead to a singular density of quasiparticle states near the Fermi level [Fig. 2(a) and 2(b)]. An interesting doping evolution of the Fermi surface (FS) [Fig. 2(c)] is also related to the presence of those flat portions. The overall energy window, covered by three quasiparticle bands, is reduced to $\sim 3t$ by correlation effects. The high-energy, incoherent electronic states, extending up to a free-electron scale $\sim 9t$, are beyond the present approximation. The consideration of the incoherent part of the electronic motion, which is a difficult task in correlated models in general, is further complicated here because of the additional orbital degrees of freedom.

As far as the low-energy physics at small doping is concerned, we arrived in fact at a single-band picture for states near the FS. However, this band has little to do with a conventional single-orbital band of A_{1g} symmetry suggested by free-electron band calculations [21] and taken in Refs. [10–13] as a starting point to develop t-J model physics for cobaltates. The crucial difference here is that

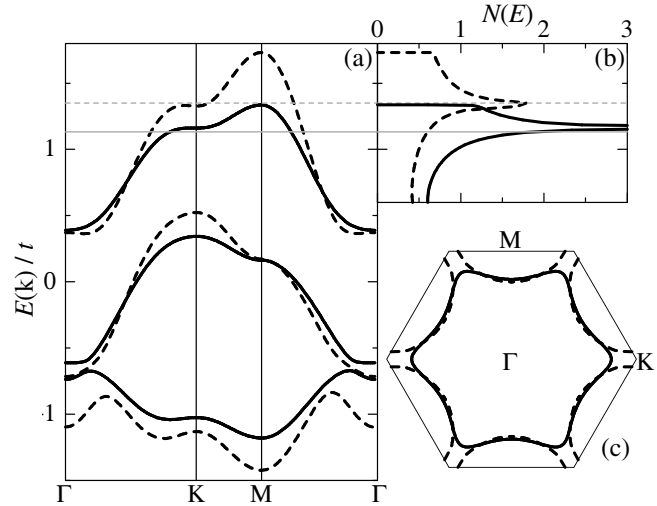

FIG. 2. (a) Quasiparticle dispersion curves in a slave-boson mean-field approximation. (b) Density of states (in units of $1/t$) near the Fermi level. The latter is indicated by thin gray lines. (c) Fermi surface in the Brillouin zone. $\Gamma = (0, 0)$, $M = (0, 2\pi/\sqrt{3})$, $K = (4\pi/3, 0)$. In all the panels, solid (dashed) lines correspond to the doping level $x = 0.2$ ($x = 0.3$). Parameters used: $t'/t = 0.8$, $\lambda/t = 0.7$, $\Delta/t = 1.0$.

the quasiparticle wave functions are made of states that do not conserve neither spin nor orbital angular momentum separately; rather, they are build on eigenstates of the total angular momentum, as reflected in Eq. (2). This unusual situation results from the interplay between strong spin-orbit coupling of Co^{4+} ion and the quasiparticle kinetic energy reduced by correlation effects. The main message is that spin-orbit coupling becomes increasingly effective near the Mott insulating limit and is thus essential for the formation of the quasiparticle bands, and hence for the FS topology. This implies that the FS shape at low doping may *not necessarily be similar* to that given by a free-electron picture, as one would expect in single-band systems like the cuprates. In a more general context, the outlined picture might be relevant also to other transition metal oxides, where narrow quasiparticle bands are derived from (quasi)degenerate t_{2g} states with strong spin-orbit coupling, such as compounds based on late-$3d$, $4d$ and $5d$ ions.

Now we turn to the superexchange interactions which, in analogy with high-T_c cuprates, could be one of the relevant interactions responsible for superconducting pairing. When the FS states are derived from pseudospin states with mixed spin and orbital quantum numbers, an important question arises about implications of such a mixing for the pairing symmetry. Projected on the pseudospin states, the superexchange interactions may in fact give nontrivial pairing channels, which were not present in the original, pure-spin Heisenberg model.

A superexchange Hamiltonian in orbitally degenerate systems reads in general as $H_J = J[(\vec{S}_i \cdot \vec{S}_j)\hat{A}_{ij} + \hat{K}_{ij}]$ [24]. The energy scale is $J = 4t^2/E$, where the virtual charge excitation energy E is determined either by the on-site Coulomb U_d or the charge-transfer energy Δ_{pd}, depending on which one is lower. The operators $\hat{A}_{ij}$, $\hat{K}_{ij}$ represent the orbital degrees of freedom. Without orbital degeneracy (e.g., in the cuprates), $\hat{A}_{ij} = 1$, $\hat{K}_{ij} = -1/4$, and H_J supports uniquely singlet pairing. In the present situation, one has to: (i) derive a full structure of the orbital operators $\hat{A}_{ij}$ and $\hat{K}_{ij}$ (which usually depends on the $\langle ij\rangle$-bond orientation in crystal via the hopping geometry [24]), and (ii) project the obtained H_J onto the active pseudospin $f_{\bar{\sigma}}$ subspace given by Eq. (2). Details of this lengthy derivation [25] will be presented elsewhere; for our purpose, the result can conveniently be represented in the following form:

$$H_J^f(ij) = -J_f \kappa_s s_{ij}^\dagger s_{ij} - J_f \kappa_t T_{ij}^\dagger T_{ij}. \tag{4}$$

Here, $J_f = J/9$ with $J = 4t^2/\Delta_{pd}$. In Eq. (4), the interactions are separated into pseudospin singlet and triplet channels, namely, $s_{ij} = (f_{i\bar{\uparrow}} f_{j\bar{\downarrow}} - f_{i\bar{\downarrow}} f_{j\bar{\uparrow}})/\sqrt{2}$, while

$$T_{ij} = a_z t_{ij,0} + a_{xy}(e^{i\phi_\delta} t_{ij,1} + e^{-i\phi_\delta} t_{ij,-1})/\sqrt{2}, \tag{5}$$

with $t_{ij,0} = i(f_{i\bar{\uparrow}} f_{j\bar{\downarrow}} + f_{i\bar{\downarrow}} f_{j\bar{\uparrow}})/\sqrt{2}$, $t_{ij,1} = f_{i\bar{\uparrow}} f_{j\bar{\uparrow}}$, and $t_{ij,-1} = f_{i\bar{\downarrow}} f_{j\bar{\downarrow}}$. The phase ϕ_δ in Eq. (5) and below depends on the $\langle ij\rangle$-bond direction δ: $\phi_\delta = (0, \phi, -\phi)$ on $\delta = (12, 23, 13)$ bonds [see Fig. 1(b)], respectively. The relative weights of the different components ($M = 0, \pm 1$ projections of the total pseudospin of the pair) are controlled by the angle θ, defined above, via $a_z = (1 + \cos 2\theta)/2$ and $a_{xy} = \sin 2\theta$. Finally, a constant

$$\kappa_s = \frac{1}{2}\left(\frac{3\cos 2\theta - 1}{2}\right)^2 + \frac{\Delta_{pd}}{U_d}\left(\frac{3\cos 2\theta - 1}{2} + \frac{t'}{t}\right)^2, \tag{6}$$

while for the triplet channel one has $\kappa_t = 3/2$.

In general, the interaction (4) supports both singlet and triplet pairings on the Fermi surface. Certainly there are also some other pairing forces in the cobaltates, yet it is interesting to explore the outcome of the superexchange interactions alone. We have therefore calculated the mean-field superconducting transition temperatures as functions of the parameters involved in our effective t-J model for the "f"-pseudofermion band.

In the singlet channel, it is known [10–13] that pairing on the triangular lattice is optimized by a complex order parameter $\langle s_{ij}\rangle = De^{i\phi_\delta}$ (the degenerate conjugate state is obtained by $\phi_\delta \to -\phi_\delta$). In momentum space, the gap function is determined by $\gamma_d(\vec{k}) = \gamma_1(\vec{k}) + i\gamma_2(\vec{k})$, where $\gamma_1 = \cos k_x - \cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}$ and $\gamma_2 = \sqrt{3}\sin\frac{k_x}{2}\sin\frac{\sqrt{3}k_y}{2}$. This state breaks the time-reversal symmetry.

As suggested by the very form of Eq. (5), the bond dependence of the triplet order parameter is best parametrized according to the projection M of the Cooper-pair pseudospin. Namely, a positive interference among the different M channels is achieved by

$$\langle t_{ij,0}\rangle = d_z, \qquad \langle t_{ij,\pm 1}\rangle = d_{xy} e^{\mp i\phi_\delta}. \tag{7}$$

The pairing amplitudes d_z, d_{xy} are proportional to a_z and a_{xy}, respectively. The bond arrangement of the phases $e^{-iM\phi_\delta}$ translates in momentum space into the form factors $\gamma_z(\vec{k})$ and $\gamma_{xy}^{\pm}(\vec{k}) = \pm\gamma_x(\vec{k}) + i\gamma_y(\vec{k})$, where

$$\gamma_z(\vec{k}) = \sin k_x - 2\sin\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}, \tag{8}$$

$$\gamma_x(\vec{k}) = \sqrt{3}\cos\frac{k_x}{2}\sin\frac{\sqrt{3}k_y}{2}, \tag{9}$$

$$\gamma_y(\vec{k}) = \sin k_x + \sin\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}. \tag{10}$$

The gap function has no nodes (apart from the Γ and M points), and the superconducting gap anisotropy is given by $\Delta(\vec{k}) \propto \sqrt{|a_z\gamma_z|^2 + |a_{xy}\gamma_{xy}^{\pm}|^2}$, which depends on angle θ. Remarkably, the pseudospin-triplet state is nondegenerate and thus *respects* the time-reversal symmetry. This is because the orbital currents associated with $M = +1$ and $M = -1$ components flow in opposite directions

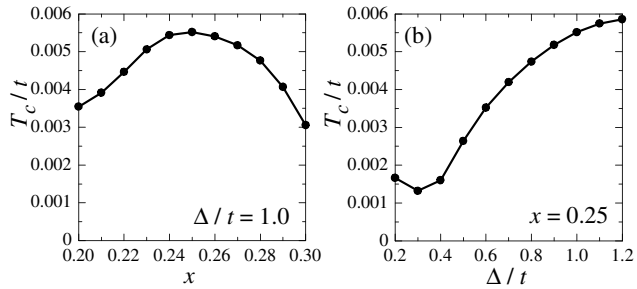

FIG. 3. (a) Doping x and (b) trigonal field splitting Δ dependences of the mean-field superconducting transition temperature T_c. Parameters used: $t'/t = 0.8$, $\lambda/t = 0.7$, $J_f/t = 0.05$.

(observe $\pm$ signs in above equations), and the orbital angular momentum of the Cooper pair is quenched.

The mean-field T_c for the triplet state (assuming the holons are already condensed) is obtained from

$$1 = J_f \sum_{\vec{k}} \frac{|a_z \gamma_z|^2 + |a_{xy} \gamma_{xy}^{\pm}|^2}{2\xi_{\vec{k}}} \tanh\frac{\xi_{\vec{k}}}{2T_c}, \qquad (11)$$

where $\xi_{\vec{k}}$ is a "f"-quasiparticle energy. To obtain T_c in the singlet channel, one simply has to replace the numerator in this equation by $[\frac{2}{3}\kappa_s|\gamma_d(\vec{k})|^2]$.

Numerical calculations show that for $t' < t$ and $\Delta_{pd}/U_d < 1$ (relevant for cobalt oxides [26]), the triplet state is always favored. Shown in Fig. 3 are some plots for T_c, calculated for an effective exchange parameter $J_f = 0.05t$ (implying $\sim$5 meV for $t \sim 0.1$ eV). Nonmonotonic dependences of T_c on doping and the orbital splitting (induced by c-axis compression) are due to sensitive variations of the quasiparticle band near the K points of Brillouin zone (Fig. 2). We note that the obtained T_c values ($\sim$5 K for $t \sim 0.1$ eV) and their dependences are qualitatively consistent with experimental data [4,16].

The superexchange driven triplet state is interesting on its own. This state is stabilized by spin-orbit coupling acting on the low-energy states of doped Mott insulator with t_{2g} orbital degeneracy. Its basic features (no time-reversal symmetry breaking, only partial Khight-shift drop below T_c, high critical fields H_{c2}, *etc.*) are reminiscent to reported data in cobaltates. However, a specific comparison with (ongoing and still controversial) experiments would require that some other relevant physics (electron-phonon coupling, charge-ordering tendencies that are enhanced by orbital-polaron effects [27], phase separation, *etc.*), may need to be included in a more realistic theory. We believe that the present work should be a proper starting point for such a theory.

To conclude, the low-energy Fermi-surface states in the underdoped cobaltates are strongly influenced by spin-orbit interaction intrinsic to the t_{2g} electrons of Co^{4+} ions. This leads to nontrivial symmetry of the superexchange interactions and to a novel pseudospin-triplet paired state, qualitatively different from that in the high-T_c cuprates. Rather, there might be some common physics between cobaltates and ruthenates [28] and also the recently discovered superconductors KOs_2O_6 [29], where Ru($4d$) and Os($5d$) electrons with strong spin-orbit coupling reside on nearly degenerate t_{2g} levels.

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