Spin fluctuations and weak pseudogap behaviors in Na$_{0.35}$CoO$_2$ : renormalization of band structure

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Abstract. We analyze the normal electronic states of Na$_{0.35}$CoO$_2$ based on the multi-orbital Hubbard model using the FLEX approximation. The fundamental electronic property of this system is drastically changed by the presence or absence of the small hole pockets associated with the $\epsilon'_g$ orbital. This change of the Fermi surface topology may be caused by the crystalline electric splitting due to the trigonal distortion. When small hole pockets are absent, the weak pseudogap behaviors appear in the density of states and the uniform spin susceptibility, which are observed by recent experiments. We estimate the mass enhancement factor of quasiparticle $m^*/m \simeq 1.5 \sim 1.8$. This result supports ARPES measurements.

Keywords: FLEX, Na$_{0.35}$CoO$_2$, spin fluctuations, pseudogap
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Na$_{0.35}$CoO$_2$ · 1.3H$_2$O is the first Co-oxide superconductor with $T_c \sim 4.5K$ (1). While many theoretical and experimental studies are widely performed, the topology of Fermi surface (FS) and the low-energy electronic structure are still unresolved. To resolve these problems is very important to find out the mechanism of superconductivity.

In Na$_{0.35}$CoO$_2$, local density approximation (LDA) calculations (2) have predicted that Na$_{0.35}$CoO$_2$ has a large FS associated with the $a_{1g}$ band and six small hole pockets corresponding to the $\epsilon'_g$ band. However, such small pockets are not observed in recent ARPES measurements (3, 4). ARPES measurements also observed that renormalized quasiparticle bandwidth is approximately half of that calculated by band calculation. In the present work, we study the normal electronic states in Na$_{0.35}$CoO$_2$ using the fluctuation exchange (FLEX) approximation to elucidate Fermi surface topology and renormalized band structure. In Na$_{0.35}$CoO$_2$, the topology of the FS is sensitively changed by the $a_{1g}$ splitting $3V_t$, whose value can be modified by the trigonal distortion of crystal. In this work, we study the many body effect for various values of $3V_t$.

We have reported (5) that density of states (DOS) on the Fermi energy and uniform spin susceptibility increase as temperature decreases when small pockets exist. On the other hand, when small pockets are absent, both of them decrease at lower temperatures. It is a weak pseudogap behavior due to magnetic fluctuations. In this case, the degree of reduction of DOS is greater when the top of the $\epsilon'_g$ band is just below the Fermi level. In experimental measurements, both uniform spin susceptibility and DOS in the photoemission spectroscopy decrease at lower temperatures. These pseudogap behaviors are consistent with the latter result. As the pseudogap in the DOS is more prominent in bilayer hydrate samples than that in monolayer ones, the effect of intercalation of water is expected to raise the $\epsilon'_g$ band slightly as expected by the analysis based on the point charge model. As a result, we have concluded that the small Fermi pockets do not exist or very small if any.

In this paper, we report the band structure of Na$_{0.35}$CoO$_2$ at $3V_t = 0.12$. In this case, small hole pockets are absent; they sink just below the Fermi energy. We find that the quasiparticle band is renormalized by the electronic correlation, and mass enhancement factor $m^*/m \simeq 1.5 \sim 1.8$. It agrees with the result of ARPES measurements.

The model Hamiltonian used in the present study is as follows.

$$H = H_0 + H',$$

$$H_0 = \sum_{i,j,\sigma} i_{ij}^{\ell} \epsilon_{ij}^{\ell} \sigma \sum_{\ell' \sigma} i_{\ell\sigma}^{\ell'} c_{\ell'\sigma}^\dagger c_{\ell\sigma},$$

$$H' = \sum_{k,\sigma} i_{k\sigma}^{\ell} \epsilon_{k\sigma}^{\ell} c_{k\sigma}^\dagger c_{k\sigma},$$

where $\ell$ represents 3$d$ orbitals of Cobalt atoms (5 orbitals) and 2$p$ orbitals of Oxygen atoms (2 $\times$ 3 orbitals), and $i$ has the Slater-Koster’s matrix form. $H'$ is on-site Coulomb integrals in $t_{2g}(d_{xy}, d_{xz}, d_{yz})$ orbitals.

$$H' = H_U + H_{U'} + H_J + H_{J'},$$

where $U$ ($U'$) is the intra-orbital (inter-orbital) Coulomb interaction, $J$ is the Hund’s coupling and $J'$ represents the pair-hopping interaction. We put $U' = 1.3, J = J' = 0.13, U = U' + 2J = 1.56$ hereafter. In these parameters, deformation of the FS due to the interaction is very small.
In this case, we take care that both \( \hat{\epsilon}_k \) and 
\( \hat{\Sigma}_k \) cancel out the effect of damping of quasiparticle. By 
\( t \)-\( \text{tarded and advanced selfenergy on the selfenergy to} \)
matrices. Here we employed the mean value of re-
\( \text{lations (dot line) at } T = 0.01, 0.02, 0.04 \text{ and } 0.06 \text{ (eV) respectively. The mass enhancement factor would} \)
increase further if one take large \( U \). In the three bands we 
show in Fig. [II] the top band which across the Fermi 
energy is strongly renormalized in whole. The other two 
band dispersion decreases at lower temperatures. The 
mass enhancement factor at point A in Fig. II are 1.78, 
1.73, 1.60 and 1.47 at \( T = 0.02 \text{, } 0.04 \text{ and } 0.06 \text{ (eV)} \).

In summary, we analyzed the multi-orbital Hubbard 
model for \( \text{Na}_{0.35}\text{CoO}_2 \). Near the Fermi level, we notice that 
the electronic band is renormalized and the slope of 
band dispersion decreases at lower temperatures. The 
mass enhancement factor at point A in Fig. II are 1.78, 
1.73, 1.60 and 1.47 at \( T = 0.02 \text{, } 0.04 \text{ and } 0.06 \text{ (eV)} \).

We calculate the normal selfenergy \( \Sigma(k, \omega) \) in the FLEX 
approximation scheme. Then, the renormalized quasi-
particle band dispersion \( E_k \) is decided by the following 
equation.

\[
det(|E_k + \mu|)1 - \hat{\epsilon}_k - \left( \hat{\Sigma}^R(k, E_k) + \hat{\Sigma}^A(k, E_k) \right) / 2 = 0.
\]

In this case, we take care that both \( \hat{\epsilon}_k \) and 
\( \left( \hat{\Sigma}^R(k, E_k) + \hat{\Sigma}^A(k, E_k) \right) / 2 \) are complex Hermitian 
matrices. Here we employed the mean value of re-
tarded and advanced selfenergy on the selfenergy to 
cancel out the effect of damping of quasiparticle. By 
diagonalizing the Green function \( \hat{G} \), we can switch to 
band-representation. In the band-representation, mass 
enhancement factor \( m^*/m \) is determined by following 
equation.

\[
m_{\alpha}^* = \frac{dE_{\alpha}^g}{dk} \cdot \frac{dE_{\alpha}^g}{dk} \\
= \left( 1 + \frac{\partial \text{Re} \Sigma^\alpha(k, E_k^\alpha)}{\partial k} \right)^{-1}
\]

\[
\times \left( 1 - \frac{\partial \text{Re} \Sigma^\alpha(k, E_k^\alpha)}{\partial k} \right).
\]

where \( k = k \cdot n_\perp \) \( (n_\perp \text{ is a unit vector perpendicular to the} \)
FS), and \( \alpha \) indicates the band index. The first bracket in 
this equation is so-called \( k \)-mass and the second bracket is 
so-called \( \omega \)-mass. In strongly correlated electron sys-
tems, \( \omega \)-mass constitutes the main part of mass enhance-
ment and it makes the effective mass heavy.

In Fig. II we show the calculated band dispersion 
of \( \text{Na}_{0.35}\text{CoO}_2 \). Near the Fermi level, we notice that 
the electronic band is renormalized and the slope of 
band dispersion decreases at lower temperatures. The 
mass enhancement factor at point A in Fig. II are 1.78, 
1.73, 1.60 and 1.47 at \( T = 0.01, 0.02, 0.04 \) and 0.06 
(eV) respectively. The mass enhancement factor would 
increase further if one take large \( U \). In the three bands we 
show in Fig. II the top band which across the Fermi 
energy is strongly renormalized in whole. The other two 
band dispersion decreases at lower temperatures. The 
mass enhancement factor at point A in Fig. II are 1.78, 
1.73, 1.60 and 1.47 at \( T = 0.02 \text{, } 0.04 \text{ and } 0.06 \text{ (eV)} \).

In summary, we analyzed the multi-orbital Hubbard 
model for \( \text{Na}_{0.35}\text{CoO}_2 \) using the FLEX approximation, 
and we found the weak pseudogap behavior in the DOS 
and spin susceptibility when small hole pockets are ab-
sent. The electronic band is renormalized by the 
electronic correlation, and mass enhancement factor \( m^*/m \approx 
1.5 \sim 1.8 \). This result supports the ARPES measure-
ments.

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