The local density approximation (LDA) calculations have an important role in the unconventional superconductivity. It is believed that the topology of the Fermi surface (FS) plays an important role in the conventional superconductivity. The local density approximation (LDA) calculations have been shown to exhibit certain kind of anisotropy, which agrees qualitatively with the angle-resolved photoemission spectroscopy (ARPES) measurements. Moreover, the spectral function and density of states (DOS) in the normal state are calculated, with a weak pseudogap behavior being seen, which is explained as a result of the strong Coulomb correlations. Our results suggest that the large Fermi surface (FS) associated with the \( a_{1g} \) band plays a central role in the charge dynamics.

Based on a single band Hubbard model and the fluctuation exchange approximation, the effective mass and the energy band renormalization in \( \text{Na}_{0.33}\text{CoO}_2 \) is elaborated. The renormalization is observed to exhibit certain kind of anisotropy, which agrees qualitatively with the angle-resolved photoemission spectroscopy (ARPES) measurements. Moreover, the spectral function and density of states (DOS) in the normal state are calculated, with a weak pseudogap behavior being seen, which is explained as a result of the strong Coulomb correlations. Our results suggest that the large Fermi surface (FS) associated with the \( a_{1g} \) band plays a central role in the charge dynamics.

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The layered oxide \( \text{Na}_x\text{CoO}_2 \) has attracted much attention due to its possible connection to the high-\( T_c \) superconductivity and its role in the phenomenon of Anderson's resonating valence bond (RVB) state.\(^{1,2}\) By hydration, it becomes a superconductor with \( T_c \approx 5 \text{K} \) in \( \text{Na}_{0.33}\text{CoO}_2\cdot1.3\text{H}_2\text{O} \).\(^{3}\) The unhydrated compound \( \text{Na}_x\text{CoO}_2 \) exhibits a rich phase diagram: a paramagnetic metal \( (x < 0.5) \), a charge-ordered insulator \( (x = 0.5) \), a "Curie-Weiss metal" \( (x \sim 0.7) \), and a magnetic order state \( (x \geq 0.75) \).\(^{4}\)

Experimentally, it is indicated that \( \text{Na}_x\text{CoO}_2 \) seems to be strongly electronic correlated.\(^{5,6}\) Angle-resolved photoemission spectroscopy (ARPES) measurements show a strong mass renormalization.\(^{7,8}\) The effective mass is about 5-10 times larger than the bare mass.\(^{9}\) Decreasing the Na concentration to \( x = 0.3 \), the cobaltites appear to be less electron-correlated with a weaker but still apparent energy band renormalization factor \( \sim 2 \).\(^{10}\) For the hydrated compounds, the effective mass is estimated to be \( \sim 2-3 \).\(^{11}\) In addition, recent experiments reported that \( \text{Na}_{0.33}\text{CoO}_2\cdot1.3\text{H}_2\text{O} \) display certain pseudogap behaviors such as the decreasing of the Knight shift\(^{12}\) and the density of states (DOS) at the Fermi level below \( 300\text{K} \).\(^{13}\) Optical spectroscopy measurements for \( \text{Na}_x\text{CoO}_2 \) and \( \text{Na}_{y}\text{CoO}_2 \) also suggest the incipient formation of pseudogap.\(^{14}\) However, unlike the pseudogap effect observed in the high-\( T_c \) cuprates, the pseudogap behavior is rather weak. The renormalization of the energy band and the pseudogap formation are directly related to the electronic structure, such as the quasiparticle spectral function, the quasiparticle dispersion, and the Fermi surface topology. Therefore it is of importance and significance to study the normal state quasiparticle dynamics.

It is believed that the topology of the FS plays an important role in the unconventional superconductivity. The local density approximation (LDA) calculations suggest a large FS associated with the \( a_{1g} \) band and six pockets associated with the \( \epsilon_g \) band. However, intriguingly, the small pockets have not been observed in the ARPES measurements.\(^{15,16}\) The unexpected inconsistency of the topology of the FS between the LDA results and the ARPES measurements has aroused much controversy. One possibility might be due to the surface effect in the ARPES measurements. From another viewpoint, Zhou et al. suggested that the strong Coulomb interactions may induce significant renormalization of the band structure which pulls the \( \epsilon_g \) band down from the Fermi energy.\(^{17}\) Furthermore, the \( \epsilon_g \) band is suggested to be relevant to the spin-triplet superconductivity in some theoretical and numerical studies.\(^{17,18}\) On the other hand, the possibility of the spin-singlet superconductivity is also suggested according to recent Knight-shift measurements.\(^{19,20}\) Taking the above considerations into account, a single band model focusing on the \( a_{1g} \) band may be a starting point as a minimal model of \( \text{Na}_x\text{CoO}_2 \).

In this paper, we study the normal state electronic structure in \( \text{Na}_{0.33}\text{CoO}_2 \) on the basis of the single band Hubbard model and the fluctuation exchange (FLEX) approximation. Several experimental features, such as the band renormalization and the weak pseudogap behavior, are well reproduced, which suggests an important role of the holelike Fermi surface centered around the \( \Gamma \) point in the quasiparticle dynamics. We start with the two-dimensional single band Hubbard model given by,

\[
H = \sum_{ij,\sigma} (t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} \quad (1)
\]

where \( t_{ij} \) denotes the hopping term (in the following we will use \( t_1, t_2, t_3, t_4 \) to denote the hoppings along the nearest- to the fourth nearest-neighbors), \( U \) the on-site Coulomb repulsion and \( \mu \) the chemical potential. To reproduce the large FS around the \( \Gamma \) point, we set the parameters \( (t_1, t_2, t_3, t_4) \) of the bare dispersion \( \epsilon_k \) to be \((-1, 0, 0, 0.2)\), where \( t_1 \) is set to be the unit hereafter. According to the numerical result for the bandwidth,\(^{21}\)
one can get \( t_1 = 130 \) meV. We note that the main feature of the bare dispersion is similar to that of the band with an \( \alpha_{1g} \) character in the LDA calculation by Lee et al.\textsuperscript{14}

The FLEX approximation is employed in our study, which has been applied to the two dimensional Hubbard model in literatures\textsuperscript{22,23,24,25}. As a self-consistent approximation, the FLEX approximation solves the Dyson’s equation with a primarily RPA+ladder type effective interaction self-consistently. Based on the scenario of the FLEX approximation, the self-energy is given by,

\[
\Sigma(k) = \frac{T}{N} \sum_q V_{eff}(k - q)G(q),
\]

where

\[
V_{eff}(q) = \frac{3}{2} U^2 \chi_s(q) + \frac{1}{2} U^2 \chi_e(q).
\]

The spin susceptibility is

\[
\chi_s(q) = \frac{\bar{\chi}(q)}{1 - U \bar{\chi}(q)},
\]

and the charge susceptibility is

\[
\chi_e(q) = \frac{\bar{\chi}(q)}{1 + U \bar{\chi}(q)},
\]

with the irreducible susceptibility,

\[
\bar{\chi}(q) = -\frac{T}{N} \sum_k G(k + q)G(k).
\]

The electron Green’s function is give by,

\[
G(k) = \left[ i \omega_n - \epsilon_k - \Sigma(k) \right]^{-1}.
\]

In the above equations, \( k \equiv (\mathbf{k}, i \omega_n) \) and \( q \equiv (\mathbf{q}, i \nu_n) \) are used, \( T \) is the temperature. These equations are solved self-consistently, where \( N = 64 \times 64 \) \( k \)-point meshes and up to 2048 Matsubara frequencies \( \omega_n = (2n + 1)\pi T \) are taken. The electron density is determined by the chemical potential \( \mu \) from the equation \( \langle n \rangle = 1 - \frac{\pi T}{N} \sum_k G(k) \).

As an important physical quantity related closely to the strength of the electronic correlations, the effective mass \( m^* \) is given by

\[
\frac{m}{m^*} = Z(1 + \frac{m}{k_F} \frac{\partial}{\partial k} \text{Re} \Sigma(k, 0) \big|_{k=k_F}),
\]

where

\[
Z = (1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma(k_F, \omega) \big|_{\omega=0})^{-1}
\]

is the renormalization constant. The self-energy with real frequencies \( \Sigma(k, \omega) \) is obtained with the Padé approximants\textsuperscript{26} which analytically continue \( \Sigma(k, i\omega) \) from the Matsubara frequencies to the real-frequency axis. The ratio of the effective mass to the bare mass \( m^*/m \) with different on-site Coulomb repulsions \( U \) near the FS (point A in Fig. 1) is plotted in Fig. 2, where \( m^*/m \) increases monotonously with the increasing of \( U \). It is noticeable that when \( U \) is less than 4, the enhancement of the effective mass is inapparent (\( < 1.2 \)). With a strong Coulomb repulsion \( U \gtrsim 6 \approx 0.8 \text{ eV} \), the effective mass is enhanced significantly. Comparing the calculated effective mass with the ARPES measurements (\( \sim 2 \) for \( x \sim 0.3 \)), we set \( U \sim 6 \) in the present simple model to reflect the strong correlation effect in Na\(_{0.33}\)CoO\(_2\)\textsuperscript{27}. The strong electronic correlations are evident from Fig. 3 (a), where the sharp quasiparticle peak is suppressed with strong Coulomb repulsion. For \( U = 2 \) and \( T = 0.1 \), the spectral function shows a sharp peak near the Fermi energy. Increasing the Coulomb repulsion to \( U = 6 \), the spectral function is broadened and the spectral weight at the Fermi level is reduced greatly.

For \( U = 6 \) we now investigate the renormalization of the quasiparticle energy band. To do it, we need to evaluate the spectral function of quasiparticles defined as

\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega),
\]
where \( G(\mathbf{k}, \omega) \) is the dressed Green's function in real frequency, which is analytically continued from the dressed Green's function in imaginary-frequency via the Padé approximants. Then, the renormalized band dispersion is determined by the position of the peak of \( A(\mathbf{k}, \omega) \). The calculated result at \( T = 0.1 \) is shown in Fig. 3 (b), where the solid and the dotted lines denote the renormalized and the bare energy bands, respectively. One can see that the bandwidth is compressed obviously due to the strong Coulomb interactions. From Fig. 3 (b) we get the bandwidth of the bare band dispersion (7.7) and the renormalized bandwidth (5.0), which gives a band renormalization factor 1.54. This is consistent with the ARPES measurements for \( x = 0.3 \). Moreover, we find that the band renormalization shows an anisotropy along the Γ-K and Γ-M direction, namely the renormalization along the Γ-K direction is stronger than that along the Γ-M direction. The similar anisotropy has been found in the ARPES experiments for \( x = 0.6 \), though the experimental result seems stronger than what we disclosed here. We note that the compound \( \text{Na}_x\text{CoO}_2 \) with \( x = 0.6 \) is in fact in the range of the Curie-Weiss metal, in which the correlation is stronger than that in the paramagnetic metal with \( x = 0.3 \). So, a weaker anisotropy in the renormalization is expected. This anisotropy originates from the nesting of the Fermi surface along the Γ-K direction as shown in Fig. 1.

We now turn to address the weak pseudogap behavior. This is manifested in the suppression of the density of states at the Fermi level. We present the \( \omega \) dependence of the density of states at different temperatures in Fig. 4. With the decrease of temperature from \( T = 0.7 \) (dash dotted) through \( T = 0.5 \) (dotted) and \( T = 0.3 \) (dashed) to \( T = 0.1 \) (solid), a weak suppression of the density of states near the Fermi energy is evident, suggesting the opening of a weak pseudogap. The weak pseudogap behavior is also manifested in the quasiparticle spectral function \( A(\mathbf{k}, \omega) \) which measures the probability to find the quasiparticle at momentum \( \mathbf{k} \) and frequency \( \omega \). As shown in Fig. 5 (a), with the decrease of temperature (from the dashed line to the solid line), the spectral weight is transferred away from the region around \( \omega = 0 \), producing a weak secondary maximum at \( \omega < E_F \). Thus, a weak pseudogap is formed.

This weak pseudogap behavior is a consequence of strong Coulomb repulsion. To show this, we also present the results with a smaller \( U = 2 \) at \( T = 0.1, 0.3, 0.5, 0.7 \) in the insert of Fig. 4. Different from the \( U = 6 \) case, the density of states is not suppressed with the decreasing of temperature at all (in fact there is no appreciable difference between them, so only one line can be seen from the figure). For a more detailed discussion, we also present the spectral function for \( U = 2 \) (dotted), \( U = 4 \) (dash dotted) and \( U = 6 \) (solid) in Fig. 5 (a), where the secondary maximum shows up gradually with the increase of the Coulomb correlations. Note that since the secondary maximum disappears for \( U = 2 \), no pseudogap is expected for this case and what for \( U < 2 \). We refer to the depression of the spectral weight to be a weak pseudogap here based on the observation that the spectral function consists of a peak and a weak secondary maximum (not a peak). In fact, the real part of the denominator of the Green's function has only one pole, which can be seen from the real part of the self-energy shown in Fig. 5 (b). It is the extremum of the imaginary part of the self-energy around \( \omega = -4 \) that produces the weak maximum of the spectral function, as shown in Fig. 5 (c). In the case of a smaller Coulomb repulsion \( U \), such as \( U = 2 \), a usual Fermi-liquid form of the self-energy is preserved (The dotted lines in Fig. 5 (b) and (c)), so it gives a
well defined quasiparticle peak in the spectral function (The dotted line in Fig. 5 (a)). This secondary maximum might suggest a "shadow band"\textsuperscript{29} which occurs when a short-range spin correlation is developed with the increase of Coulomb repulsion. Therefore, the weak pseudogap behavior reported here may be due to the spin fluctuation in the strong correlated regime.\textsuperscript{29}

A similar weak pseudogap behavior was reported by Yada \textit{et al.}\textsuperscript{29} based on a multi-orbital model with the absence of small hole pockets. Our results based on the single band model provide further support for the sinking down of the small hole pockets. In our opinion, the agreement between the two models suggests that the multi-orbital effect may play a minor role in the mechanism of the pseudogap formation.

In summary, we have studied the quasiparticle band renormalization and the pseudogap behavior in Na\textsubscript{0.33}CoO\textsubscript{2} based on the single band Hubbard model in a two-dimensional triangle lattice. The renormalization of the band structure and its anisotropy of the $\Gamma$-$K$ and $\Gamma$-$M$ direction have been elaborated. The estimated effective mass is consistent with the ARPES measurements. In the meantime, a weak pseudogap behavior is reproduced, which is explained as the result of the strong spin fluctuations. Our results are qualitatively consistent with experiments as well as the theoretical calculations based on a multi-orbital model.

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