Normal-state pseudogap and electron flat dispersion in copper oxide materials

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The anomalous momentum and doping dependence of the electron spectral function and electron dispersion for copper oxide materials in the underdoped regime are studied within the $t$-$J$ model. It is shown that the electron spectrum is changed with dopings, and the electron dispersion exhibits a flat band around $(\pi,0)$ point in the Brillouin zone, which leads to the normal-state pseudogap formation. The theoretical results are consistent with the experiments and numerical simulations.

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The copper oxide materials are unusual in that the undoped materials are antiferromagnetic (AF) insulators, and changing the carrier concentration by ionic substitution or increase of the oxygen content turns these compounds into correlated metals leaving short-range AF correlations still intact \[1, 2\], where a central issue to clarify the nature of the anomalous properties is how the electronic structure evolves with hole dopings, since many of the unusual physical properties including the anomalously high superconducting transition temperature have often been attributed to particular characteristics of low energy excitations determined by the electronic structure \[1, 2, 3, 4\]. The experimental measurements from the angle-resolved photoemission spectroscopy \[5, 6, 7, 8\] show that electron spectrum \( A(k, \omega) \) in copper oxide materials is strongly momentum and doping dependent, and has an anomalous form as a function of energy \( \omega \) for \( \mathbf{k} \) in the vicinity of \((\pi,0)\) point in the Brillouin zone, which leadd to the flat band near momentum \((\pi,0)\) with anomalously small changes of electron energy as a function of momentum. This flat band around \((\pi,0)\) point reflects the underlying electronic structure near a band saddle point, and has a particular importance in the mechanism of the normal-state pseudogap formation, since in the underdoped regime the normal-state pseudogap starts growing first in the single-particle excitations around \((\pi,0)\) point, and then exists in a wide range of dopings \[6, 9, 10, 11\]. This flatted band also makes degenerate excitations and may cause various instabilities. It is believed that the broad feature in the spectrum around \((\pi,0)\) point in copper oxide materials in the underdoped regime is manifestation of a strong coupling between the quasiparticle and collective excitations \[12\]. On the other hand, it has been argued that there is the intriguing connection between the velocity scale \( v^* \ll v_F \) and the flat band \[13\], where \( v_F \) is the Fermi velocity, while \( v^* \) has been found from the inelastic neutron-scattering experiments that it is related to the superconducting transition temperature \( T_c \) by the simple relation as \( K_B T_c = h v^* \lambda \), where \( \lambda \) is the splitting of the incommensurate peaks or the peak width. Although this intriguing connection is not
unambiguously confirmed by experiments, we still believe that the flat band may be an essential element to understanding of the superconducting mechanism in copper oxide materials.

The electron spectrum and flat band in copper oxide materials have been extensively studied theoretically within some strongly correlated models \([14, 15, 16, 17, 18]\). The most striking aspect is the presence of the flat band that can not be explained by either of the band theory scenarios. The numerical calculation of the electron spectrum based on the two-dimensional (2D) large U Hubbard \([14, 15]\) model shows the flat band similar to those observed in experiments. In these calculation, the flat band arises from the large Coulomb interaction \(U\). The flat band has been also observed in the 2D \(t-J\) model \([16, 17, 18]\), where the quantitative agreement between the experiment and numerical simulation along the \((0,0)\) to \((\pi, \pi)\) direction is significant because it shows unambiguously that the energy scale of the insulating band is controlled by the magnetic interaction \(J\). Moreover, many authors \([19]\) suggest that the flat band is a consequence of spin and charge excitations. Although the exact origin of the flat band saddle point still is controversial, a strongly correlated many-body like approach may be appropriate to describe the electronic structure of copper oxide materials. To shed light on this issue, we, in this paper, try to study the momentum and doping dependence of the electron spectrum within the framework of the fermion-spin theory \([20]\). Our results show that the electron spectrum is changed with dopings, and the electron dispersion exhibits the flat band around \((\pi,0)\) point, which leads to the normal-state pseudogap formation.

Very soon after the discovery of copper oxide superconductors, many authors \([21]\) suggested that the essential physics of these materials is contained in doped Mott insulators, which may be effectively described by the 2D \(t-J\) model acting on the space with no doubly occupied sites. On the other hand, there is a lot of evidence from the experiments and numerical simulations in favour of the \(t-J\) model as the
basic underlying microscopic model \[22\]. The \( t-J \) model on a square lattice can be written as,

\[
H = -t \sum_{\langle ij \rangle} C_{i\sigma}^\dagger C_{j\sigma} + h.c. - \mu \sum_{i\sigma} C_{i\sigma}^\dagger C_{i\sigma} + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)
\]

supplemented by the on-site local constraint \( \sum_{\sigma} C_{i\sigma}^\dagger C_{i\sigma} \leq 1 \) to avoid the double occupancy, where \( C_{i\sigma}^\dagger (C_{i\sigma}) \) are the electron creation (annihilation) operators, \( \mathbf{S}_i = C_i^\dagger \sigma C_i/2 \) are spin operators with \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) as Pauli matrices, \( \mu \) is the chemical potential, and the summation \( \langle ij \rangle \) is carried over nearest nonrepeated bonds. Since the \( t-J \) model was originally introduced as an effective Hamiltonian of the large-\( U \) Hubbard model \[21\], where the on-site Coulomb repulsion \( U \) is very large as compared with the electron hopping energy \( t \), which leads to that electrons become strongly correlated to avoid double occupancy, therefore the strong electron correlation in the \( t-J \) model manifests itself by the electron single occupancy on-site local constraint. This is why the crucial requirement is to impose this electron on-site local constraint for a proper understanding of the physics of copper oxide materials \[23\]. To incorporate this local constraint, the fermion-spin theory based on the charge-spin separation has been proposed \[20\]. In the fermion-spin theory, the constrained electron operators in the \( t-J \) model are decomposed as,

\[
C_{i\uparrow} = h_i^\dagger S_i^- \quad \text{and} \quad C_{i\downarrow} = h_i^\dagger S_i^+, \quad (2)
\]

with the spinless fermion operator \( h_i \) keeps track of the charge (holon), while the pseudospin operator \( S_i \) keeps track of the spin (spinon). The main advantage of this approach is that the electron on-site local constraint can be treated exactly in analytical calculations. In this case, the low-energy behavior of the \( t-J \) model (1) in the fermion-spin representation can be written as,

\[
H = t \sum_{i\eta} h_{i+\eta}^\dagger h_i (S_i^+ S_{i+\eta}^- + S_i^- S_{i+\eta}^+) + \mu \sum_i h_i^\dagger h_i + J_{\text{eff}} \sum_{i\eta} (\mathbf{S}_i \cdot \mathbf{S}_{i+\eta}), \quad (3)
\]
where \( \hat{\eta} = \pm \hat{x}, \pm \hat{y} \), \( J_{\text{eff}} = J[(1 - \delta)^2 - \phi^2] \), the holon particle-hole parameter \( \phi = \langle h_i h_{i+\hat{\eta}} \rangle \), and \( S_i^+ \) and \( S_i^- \) are the pseudospin raising and lowering operators, respectively. As a consequence, the kinetic part in the \( t-J \) model has been expressed as the holon-spinon interaction in the fermion-spin representation, which dominates the physics in the underdoped and optimally doped regimes in copper oxide materials \([24, 25]\). In this paper, we hope to discuss the electronic structure of copper oxide materials, and therefore it needs to calculate the electron Green’s function \( G(i - j, t - t') = \langle\langle C_{i\sigma}(t); C^\dagger_{j\sigma}(t')\rangle\rangle \). According the fermion-spin transformation \( (2) \), the electron Green’s function is a convolution of the spinon Green’s function \( D(i - j, t - t') = \langle\langle S_i^+(t); S_j^-(t')\rangle\rangle \) and holon Green’s function \( g(i - j, t - t') = \langle\langle h_i h^\dagger_j(t')\rangle\rangle \), and can be formally expressed in terms of the spectral representation as,

\[
G(k, \omega) = \frac{1}{N} \sum_q \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} A_h(q, \omega') A_s(q + k, \omega'') \frac{n_F(\omega') + n_B(\omega'')}{\omega + \omega' - \omega''},
\]

where the holon spectral function \( A_h(q, \omega) = -2\text{Im}g(q, \omega) \), the spinon spectral function \( A_s(k, \omega) = -2\text{Im}D(k, \omega) \), and \( n_B(\omega) \) and \( n_F(\omega) \) are the boson and fermion distribution functions for spinons and holons, respectively. In this case, the electron spectral function \( A(k, \omega) = -2\text{Im}G(k, \omega) \) can be obtained as,

\[
A(k, \omega) = \frac{1}{N} \sum_q \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A_h(q, \omega') A_s(q + k, \omega' + \omega) [n_F(\omega') + n_B(\omega' + \omega)].
\]

Within the fermion-spin theory, the mean-field theory in the underdoped and optimally doped regimes without AF long-range-order (AFLRO) has been developed \([26]\), and the mean-field spinon and holon Green’s functions \( D^{(0)}(k, \omega) \) and \( g^{(0)}(k, \omega) \) have been evaluated as,

\[
D^{(0)}(k, \omega) = \frac{B_k}{2\omega_k} \left( \frac{1}{\omega - \omega_k} - \frac{1}{\omega + \omega_k} \right),
\]

\[
g^{(0)}(k, \omega) = \frac{1}{\omega - \xi_k},
\]
respectively, where \( B_k = \Lambda [(2\epsilon \chi + \chi)\gamma_k - (\epsilon \chi + 2\chi)] \), \( \gamma_k = (1/Z) \sum_{\eta} e^{i k \cdot \eta} \), \( \Lambda = 2 Z J_{eff} \), \( \epsilon = 1 + 2 t \phi/J_{eff} \), \( Z \) is the number of the nearest neighbor sites, while the mean-field spinon spectrum

\[
\omega_k^2 = \Lambda^2 \left( \alpha \epsilon [\chi \gamma_k + \frac{1}{2Z} \chi] - \alpha C_z + \frac{1}{4Z} (1 - \alpha) \right) (\epsilon \gamma_k - 1) \\
+ \Lambda^2 \left( \alpha \frac{1}{2} \chi \gamma_k + \frac{1}{Z} \chi_z - \frac{1}{2} \epsilon [\alpha C + \frac{1}{2Z} (1 - \alpha)] \right) (\gamma_k - \epsilon),
\]

(8)

and the mean-field holon spectrum \( \xi_k = 2 Z \chi t \gamma_k + \mu \), with the spinon correlation functions \( \chi = \langle S_i^+ S_{i+\eta}^- \rangle \), \( \chi_z = \langle S_i^z S_{i+\eta}^z \rangle \), \( C = (1/Z^2) \sum_{\eta, \eta'} \langle S_i^+ S_{i+\eta}^- \rangle \langle S_{i+\eta}^+ S_{i+\eta'}^- \rangle \), and \( C_z = (1/Z^2) \sum_{\eta, \eta'} \langle S_i^z S_{i+\eta}^z \rangle \langle S_{i+\eta}^z S_{i+\eta'}^z \rangle \). In order not to violate the sum rule of the correlation function \( \langle S_i^+ S_i^- \rangle = 1/2 \) in the case without AFLRO, the important decoupling parameter \( \alpha \) has been introduced in the mean-field calculation, which can be regarded as the vertex correction \[26\]. The mean-field order parameters \( \chi, C, \chi_z, C_z, \phi \) and chemical potential \( \mu \) have been determined by the self-consistent calculation. Based on this mean-field theory, the electron mean-field spectral function and electron dispersion have been discussed \[26\], where the most important feature is that the mean-field intensity peaks in the electron spectral function are qualitatively consistent with the numerical simulations. However, the detailed behaviors of the flat band near \((\pi,0)\) point and normal-state pseudogap related to this flat band should be studied beyond the mean-field approximation, since these behaviors are associated with fluctuations of holons and spinons (then electrons).

The spinon and holon may be separated at the mean-field level, but they are strongly coupled beyond the mean-field approximation due to many-body correlations. In this paper, we limit the spinon part to the first-order (mean-field level) since in the underdoped and optimally doped regimes without AFLRO, the spinon magnetic energy is much smaller than the holon kinetic energy, and some physical properties can be well described at this level. On the other hand, it has been shown that there is a connection between the charge dynamics (the anomalously temper-
ature dependence of the resistivity) and the saddle-point singularity around \((\pi,0)\) point and normal-state pseudogap \([4, 27, 28]\). We have discussed the charge dynamics of copper oxide materials within the fermion-spin theory, and found that there is no direct contribution to the charge dynamics from spinons, although the strongly correlation between holons and spinons has been considered through the spinon’s order parameters entering in the holon part of the contribution to the charge dynamics. Therefore we treat the holon part by using the loop expansion to the second-order correction as in the discussion of the charge dynamics. In this case, the holon self-energy due to the spinon pair bubble has been obtained \([24]\) as,

\[
\Sigma_h^{(2)}(k, \omega_n) = \left( Zt \right)^2 \frac{1}{N^2} \sum_{pp'} (\gamma_{p'-k} + \gamma_{p'+p-k}) \frac{B_{p'} B_{p+p'}}{4 \omega_p \omega_{p'}^2} \times \left( 2 n_F(\xi_{p+k}) [n_B(\omega_{p'}) - n_B(\omega_{p'+p'})] - n_B(\omega_{p'+p'}) n_B(-\omega_{p'}) \right) \frac{\omega + \omega_{p'+p'} - \omega_{p'} - \xi_{p+k}}{\omega + \omega_{p'+p'} - \omega_{p'} - \xi_{p+k}} + n_F(\xi_{p+k}) [n_B(\omega_{p'+p'}) - n_B(-\omega_{p'})] + n_B(\omega_{p'}) n_B(\omega_{p'+p'}) \right) \frac{\omega - \omega_{p'+p'} - \omega_{p'} - \xi_{p+k}}{\omega - \omega_{p'+p'} - \omega_{p'} - \xi_{p+k}},
\]

while the full holon propagator \(g(k, \omega_n)\) can be expressed in terms of the self-energy \((9)\) as,

\[
g(k, \omega) = \frac{1}{g^{(0)-1}(k, \omega) - \Sigma_h^{(2)}(k, \omega)} = \frac{1}{\omega - \xi_k - \Sigma_h^{(2)}(k, \omega)}. \tag{10}
\]

With the help of this full holon Green’s function \(g(k, \omega)\) and spinon Green’s function \(D^{(0)}(k, \omega)\) in Eq. (6), we obtain the holon and spinon spectral functions \(A_h(k, \omega)\) and \(A_s(k, \omega)\). Substituting these spectral functions into Eq. (5), we therefore can obtain the electron spectral function.

In the \(t-J\) model, the doubly occupied Hilbert space has been pushed to infinity as Hubbard \(U \rightarrow \infty\) and therefore the spectrum function only describes the lower Hubbard band. Although the particular details of the electron spectrum and dispersion may differ from compound to compound, some qualitative features, such as
the flat band near momentum \((\pi,0)\) point, seem common and have been universally observed in hole-doped copper oxide materials \[3\]. We have performed a numerical calculation for the electron spectral function at \((\pi,0)\) point, and the results at (a) the doping \(\delta = 0.06\) and (b) \(\delta = 0.10\) for the parameter \(t/J = 2.5\) in the zero temperature are plotted in Fig. 1 (solid line). For comparison, the corresponding self-consistent mean-field results \[26\] (dashed line) are also plotted in Fig. 1. These results indicate that at the mean-field level, the electron spectrum at \((\pi,0)\) point consists of two main parts, which comes from noninteracting particles. After including the fluctuation, the mean-field part is renormalized and the spectral weight has been spread to lower energies, in particular, the sharp mean-field peak at \((\pi,0)\) point near the chemical potential \(\mu\) has been split into two peaks, where the renormalization is strongest. Moreover, the low energy peaks are well defined at all momenta, and the positions of the dominant peaks in \(A(k,\omega)\) as a function of momentum in (a) the doping \(\delta = 0.06\) and (b) \(\delta = 0.10\) for the parameter \(t/J = 2.5\) are shown in Fig. 2 (solid line). In comparison with corresponding mean-field results \[26\] (dashed line) in Fig. 2, it is shown that in accordance with the property of the electron spectral functions in Fig. 1, the mean-field electron dispersion \(E_k^{(0)}\) in the vicinity of \((\pi,0)\) point has been split into two branches \(E_k^{(-)}\) and \(E_k^{(+)}\), and a pseudogap opens. The branch \(E_k^{(-)}\) has a very weak dispersion around \((\pi,0)\) point, and then the flat regime appears, while the Fermi energy is only slightly above this flat regime. This result is in agreement with those obtained within the concept of proximity of the underdoped regime to electronic topological transition \[17\]. The anomalous electron dispersion in the present theoretical framework is determined by the strong electron correlation which give rise to the local holon-spinon correlation, and is also consistent with the numerical simulations in low temperatures \[15\], \[16\]. The momentum dependence of the pseudogap is in qualitative agreement with the experiments \[3\], \[3\], \[4\], \[8\] in that its value, which is of the order of the magnetic exchange energy \(J\), occurs around \((\pi,0)\) point. On the
other hand, our results also indicate that although the electron spectrum is changed with dopings in the underdoped regime, the flat band near ($\pi,0$) point and pseudogap still exist in a wide range of dopings. We emphasize that the simplest $t$-$J$ model can not be regarded as the complete model for the quantitative comparison with copper oxide materials, but our present results only are in qualitative agreement with the experiments.

Although the nature of the pseudogap is different in different theories, the present results show that the pseudogap near ($\pi,0$) point is closely related to the spinon fluctuation, since the full holon Green’s function (then the holon and electron spectral function) is obtained by considering the second-order correction due to the spinon pair bubble, where the single-particle hopping is strongly renormalized by the short-range AF order resulting in a bandwidth also of order of (a few) $J$, this renormalization is then responsible for the anomalous dispersion around ($\pi,0$) point and normal-state pseudogap. It has been shown that an remarkable point of the pseudogap is that it appears in both of spinon and holon excitations. We [24, 25] have found that this saddle-point singularity at ($\pi,0$) point and normal-state pseudogap also lead to the holon pseudogap, which is responsible for the metallic to semiconducting crossover in the c-axis resistivity $\rho_c$ and the deviation from the temperature linear behavior in the in-plane resistivity $\rho_{ab}$ in the underdoped regime in copper oxide materials. In other words, the unconventional normal-state transport properties in the underdoped regime are attributed to the presence of the saddle-point singularity around ($\pi,0$) point and the normal-state pseudogap.

In summary, we have discussed the anomalous momentum and doping dependence of the electron spectrum and electron dispersion of copper oxide materials in the underdoped regime within the $t$-$J$ model. It is shown that the electron spectrum is changed with dopings, and the electron dispersion exhibits the flat band around ($\pi,0$) point, which leads to the pseudogap formation. Our theoretical results are consistent
with the experiments and numerical simulations.

Finally, we note that the angle-resolved photoemission spectroscopy has been carried out \[29\] on \((La_{1.28}Nd_{0.6}Sr_{0.12})CuO_4\), a model system of the charge- and spin-ordered state, or stripe phase, where the electron dispersion also exhibits a flat band around \((\pi,0)\) point. This behavior is consistent with \((La_{2-x}Sr_x)CuO_4\) near the metal-insulator transition region \[29\] of \(x \sim 0.05\) to 0.07. In this doped regime, the holon kinetic energy is much smaller than the spinon magnetic energy, \(i.e., \delta t \ll J\), then it is possible that the flat band behavior is dominated by the strong magnetic fluctuation with AFLRO. This and other related issues are under investigation now.

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Figures

FIG. 1. Spectral function $A(k, \omega)$ at $(\pi,0)$ point for (a) the doping $\delta = 0.06$ and (b) $\delta = 0.10$ for the parameter $t/J = 2.5$ in the zero temperature. The dashed line is the result at the mean-field level.

FIG. 2. Position of the the dominant peaks in $A(k, \omega)$ as a function of momentum at (a) the doping $\delta = 0.06$ and (b) $\delta = 0.10$ for the parameter $t/J = 2.5$. The dashed line is the result at the mean-field level.
$A(k, \omega)$ (arb. units)

$(\omega - \mu)/t$
