Anomalous c-axis charge dynamics in copper oxide materials

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Within the t-J model, the c-axis charge dynamics of the copper oxide materials in the underdoped and optimally doped regimes is studied by considering the incoherent interlayer hopping. It is shown that the c-axis charge dynamics is mainly governed by the scattering from the in-plane fluctuations. In the optimally doped regime, the c-axis resistivity is a linear in temperatures, and shows the metallic-like behavior for all temperatures, while the c-axis resistivity in the underdoped regime is characterized by a crossover from the high temperature metallic-like to the low temperature semiconducting-like behavior, which are consistent with experiments and numerical simulations.

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The copper oxide materials are among the most complex systems studied in condensed matter physics. The complications arise mainly from (1) strong anisotropy in the properties parallel and perpendicular to the CuO$_2$ planes which are the key structural element in the whole copper oxide superconducting materials, and (2) extreme sensitivity of the properties to the compositions (stoichiometry) which control the carrier density in the CuO$_2$ plane. After over ten years of intense experimental study of the copper oxide materials, a significant body of reliable and reproducible data has been accumulated by using many probes, which indicates that the normal-state properties in the underdoped and optimally doped regimes are quite unusual in many aspects suggesting the unconventional metallic state realized. Among the striking features of the normal-state, the quantity which most evidently displays the anisotropic property in the copper oxide materials is the charge dynamics, which is manifested by the optical conductivity and resistivity. It has been shown from the experiments that the in-plane charge dynamics is rather universal within the whole copper oxide materials. The in-plane optical conductivity for the same doping is nearly materials independent both in the magnitude and energy dependence, and shows the non-Drude behavior at low energies and anomalous midinfrared band in the charge-transfer gap, while the in-plane resistivity $\rho_{ab}(T)$ exhibits a linear behavior in the temperature in the optimally doped regime and a nearly temperature linear dependence with deviations at low temperatures in the underdoped regime. By contrast, the magnitude of the c-axis charge dynamics in the underdoped and optimally doped regimes is strongly materials dependent, i.e., it is dependent on the species of the building blocks in between the CuO$_2$ planes. Although the c-axis charge dynamics is very complicated, some qualitative features seem to be common, such as (1) for the optimally doped YBa$_2$Cu$_3$O$_{6+x}$ and overdoped La$_{2-x}$Sr$_x$CuO$_4$ systems, the transferred weight in the c-axis conductivity decays as $\rightarrow 1/\omega$ at low energies, which is in accordance with the metallic-like c-axis resistivity $\rho_c(T)$ for all temperatures, and (2) for the lower doping the temperature dependent c-axis resistivity $\rho_c(T)$ is characterized by a crossover from the high temperature metallic-like behavior to the low temperature semiconducting-like behavior. The nature of the c-axis charge dynamics in the copper oxide materials is of great importance, as the superconducting mechanism is closely associated with the anisotropic normal-state properties.

Since the undoped copper oxide materials are antiferromagnetic Mott insulators, upon hole doping, the antiferromagnetic long-range-order is rapidly destroyed and the unusual metallic state emerges. In this case, many researchers believe that the essential physics is contained in the doped antiferromagnets, which may be effectively described by the 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. Within the two-dimensional (2D) t-J model, the in-plane charge dynamics of the copper oxide materials has been extensively studied theoretically as well as numerically. Since the understanding of the charge dynamics in the copper oxide materials is not complete without an understanding of the c-axis charge dynamics, therefore a number of alternative mechanisms for the c-axis charge dynamics have been proposed, and the most reliable results for the c-axis charge dynamics have been obtained by the numerical simulation. To shed light on this issue, we, in this paper, apply the fermion-spin approach to study the c-axis charge dynamics based on the t-J model by considering the interlayer coupling. Within each CuO$_2$ plane, the essential physics properties are described by the 2D t-J model as,

$$H_I = -t \sum_{\mathbf{i} \mathbf{j} \sigma} C_{\mathbf{i} \sigma}^\dagger C_{\mathbf{j} \sigma} + h.c. + \mu \sum_{\mathbf{i} \sigma} C_{\mathbf{i} \sigma}^\dagger C_{\mathbf{i} \sigma}$$
+ J \sum_{i\eta} \mathbf{S}_{li} \cdot \mathbf{S}_{li+\hat{\eta}}, \quad \text{(1)}

where \( \hat{\eta} = \pm a_0 \hat{x}, \pm a_0 \hat{y} \), \( a_0 \) is the lattice constant of the square planar lattice, which is set as the unit hereafter, \( i \) refers to planar sites within the \( l \)-th \( \text{CuO}_2 \) plane, \( C_{l\alpha\sigma} = (C_{l\sigma}) \) are the electron creation (annihilation) operators, \( \mathbf{S}_{li} = C_{l\sigma}^\dagger \sigma C_{l\sigma}/2 \) are the spin operators with \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) as the Pauli matrices, and \( \mu \) is the chemical potential. The Hamiltonian (1) is supplemented by the on-site local constraint, \( \sum_{\sigma} C_{li\sigma}^\dagger C_{l\sigma} \leq 1 \), i.e., there be no doubly occupied sites. For discussing the c-axis charge dynamics, the hopping between \( \text{CuO}_2 \) planes is considered as

\[
H = -t_c \sum_{i\eta_{\hat{\eta},i\sigma}} C_{l\sigma}^\dagger C_{l+i\eta_{\hat{\eta}},i\sigma} + \text{h.c.} + \sum_i H_i, \quad \text{(2)}
\]

where \( \hat{\eta}_c = \pm c_0 \hat{z}, c_0 \) is the interlayer distance, and has been determined from the experiments\(^{21} \) as \( c_0 > 2a_0 \). In the underdoped and optimally doped regimes, the experimental results\(^{8-8} \) show that the ratio \( R = \rho_c(T)/\rho_{ab}(T) \) ranges from \( R \sim 100 \) to \( R > 10^5 \), this large magnitude of the resistivity anisotropy reflect that the c-axis mean free path is shorter than the interlayer distance, and the carriers are tightly confined to the \( \text{CuO}_2 \) planes, and also is the evidence of the incoherent charge dynamics in the c-axis direction. Therefore the c-axis momentum cannot be defined\(^{22} \). Moreover, the absence of the coherent c-axis charge dynamics is a consequence of the weak interlayer hopping matrix element \( t_c \), but also of a strong intralayer scattering, i.e., \( t_c \ll t \), and therefore the common \( \text{CuO}_2 \) planes in the copper oxide materials clearly dominate the most normal-state properties. In this case, the most relevant for the study of the c-axis charge dynamics is the results on the in-plane conductivity \( \sigma_{ab}(\omega) \) and related single-particle spectral function \( A(k, \omega) \).

Based on the 2D \( t-J \) model, the self-consistent mean-field theory in the underdoped and optimally doped regimes has been developed\(^{20} \) within the fermion-spin approach\(^{19} \), which has been applied to study the photoemission, electron dispersion and electron density of states in the copper oxide materials, and the results are qualitatively consistent with the experiments and numerical simulations. Moreover, the in-plane charge dynamics in the copper oxide materials has been discussed\(^{14} \) by considering the fluctuations around this mean-field solution, and the results exhibits a behavior similar to that seen in the experiments\(^{3} \) and numerical simulations\(^{15} \).

In the fermion-spin theory\(^{19,20} \), the constrained electron operators in the \( t-J \) model is decomposed as

\[
C_{l\uparrow \dagger} = h_{l\uparrow}^\dagger S_{l\uparrow}^-, \quad C_{l\downarrow \dagger} = h_{l\downarrow}^\dagger S_{l\downarrow}^+, \quad \text{(3)}
\]

with the spinless fermion operator \( h_{\uparrow} \) keeps track of the charge (holon), while the pseudospin operator \( S_{\uparrow} \) keeps track of the spin (spinon), then it naturally incorporates the physics of the charge-spin separation. 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 (2) in the fermion-spin representation can be rewritten as\(^ {14} \),

\[
H = t_c \sum_{i\eta_{\hat{\eta},i\sigma}} h_{l\uparrow}^\dagger h_{l+i\eta_{\hat{\eta},i\sigma}} (S_{li\uparrow}^+ S_{l+i\eta_{\hat{\eta},i\sigma}}^- + S_{li\downarrow}^+ S_{l+i\eta_{\hat{\eta},i\sigma}}^+) + \sum_i H_i, \quad \text{(a)}
\]

\[
H_i = t \sum_{i\eta} h_{l\uparrow+i\eta} h_{li\uparrow} (S_{li\uparrow}^+ S_{li+i\eta\uparrow}^- + S_{li\downarrow}^+ S_{li+i\eta\uparrow}^+) - \mu \sum_i h_{l\uparrow}^\dagger h_{li\uparrow} + J_{eff} \sum_{i\eta} (\mathbf{S}_{li\uparrow} \cdot \mathbf{S}_{li+i\eta\uparrow}), \quad \text{(b)}
\]

where \( J_{eff} = J[(1 - \delta)^2 - \phi^2] \), the holon particle-hole parameter \( \phi = \langle h_{l\uparrow}^\dagger h_{li+i\eta\uparrow} \rangle \), and \( S_{li\uparrow}^+ \) and \( S_{li\downarrow}^- \) are the pseudospin raising and lowering operators, respectively. These pseudospin operators obey the Pauli algebra, i.e., they behave as fermions on the same site, and as bosons on different sites. It is shown\(^ {19} \) that the constrained electron operator in the \( t-J \) model can be mapped exactly onto the fermion-spin transformation defined with an additional projection operator. However, this projection operator is cumbersome to handle for the actual calculation possible in 2D, we have dropped it in Eq. (4). It has been shown in Ref.\(^ {19} \) that such treatment leads to the errors of the order \( \delta \) in counting the number of spin states, which is negligible for small doping \( \delta \).

In the framework of the charge-spin separation, an electron is represented by the product of a holon and a spinon, then the external field can only be coupled to one of them. Ioffe and Larkin\(^ {22} \) and Li et al.\(^ {24} \) have shown that the physical conductivity \( \sigma(\omega) \) is given by,

\[
\sigma^{-1}(\omega) = \sigma^{(h)-1}(\omega) + \sigma^{(s)-1}(\omega), \quad \text{(5)}
\]

where \( \sigma^{(h)}(\omega) \) and \( \sigma^{(s)}(\omega) \) are the contributions to the conductivity from holons and spinons, respectively. Within the Hamiltonian (4), the c-axis current densities of holons and spinons are given by the time derivative of the polarization operator using Heisenberg’s equation of motion as,

\[
\text{(h)} = 2t_c cE \sum_{i\eta_{\hat{\eta},i\sigma}} \hat{\eta}_c h_{l\uparrow}^\dagger h_{li\downarrow} \\
\text{(s)} = t_c cE \sum_{i\eta_{\hat{\eta},i\sigma}} \hat{\eta}_c (S_{li\uparrow}^+ S_{l+i\eta\uparrow\downarrow}^- + S_{li\downarrow}^+ S_{l+i\eta\uparrow\downarrow}^+),
\]

where \( t_c = t_c cE / \chi \) is the effective interlayer holon hopping matrix element, and the mean-field spinon and holon order parameters are defined\(^ {20} \) as \( \chi = \langle S_{li\uparrow}^\dagger S_{l+i\eta\uparrow\downarrow} \rangle \), \( \chi = \langle S_{li\downarrow}^\dagger S_{l+i\eta\downarrow\uparrow} \rangle \), and \( \phi_c = \langle h_{l\uparrow}^\dagger h_{li+i\eta\uparrow} \rangle \). As in the previous discussions\(^ {14} \), a formal calculation for the spinon part shows that there is no the direct contribution to the current-current correlation from spinons, but the strongly correlation between holons and spinons is considered through the spinon’s order parameters entering in the holon part of the contribution to the current-current correlation, therefore the charge dynamics in the copper oxide materials is mainly caused by the charged holons within the \( \text{CuO}_2 \) planes, which are strongly renormalized because of the strong interactions with fluctuations of the surrounding spinon excitations. In this case,
the c-axis optical conductivity is expressed\textsuperscript{25} as \( \sigma_c(\omega) = -\text{Im} \Pi_c^{(h)}(\omega)/\omega \) with the c-axis holon current-current correlation function \( \Pi_c^{(h)}(t-t') = \langle (j_c^{(h)}(t) j_c^{(h)}(t')) \rangle \). In the case of the incoherent charge dynamics in the c-axis direction, \( \bar{t}_c \ll t \), this c-axis holon current-current correlation function \( \Pi_c^{(h)}(\omega) \) can be evaluated in terms of the in-plane holon Green’s function \( g(k, \omega) \)\textsuperscript{14,18}, then we obtain the c-axis optical conductivity as\textsuperscript{14,18,26},

\[
\sigma_c(\omega) = \frac{1}{2} (4 t_c \chi_c(0)) \sum_k \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A_h(k, \omega' + \omega) \times A_h(k, \omega') \frac{n_F(\omega' + \omega) - n_F(\omega')}{\omega},
\]

where \( n_F(\omega) \) is the Fermi distribution functions, the in-plane holon spectral function \( A_h(k, \omega) = -2\text{Im} g(k, \omega) \), while the in-plane holon Green’s function \( g(k, \omega) \) has been obtained by considering the second-order correction for holons due to the antiferromagnetic fluctuations, and given in Ref.\textsuperscript{14}. As pointed in Ref.\textsuperscript{18}, the approximation assumption of the independent electron propagation in each layer has been used in the above discussions, and is justified for \( \bar{t}_c \ll t \), therefore the c-axis conductivity is essentially determined by the properties of the in-plane spectral function. We have performed a numerical calculation for the c-axis optical conductivity \( \sigma_c(\omega) \), and the results at the doping \( \delta = 0.12 \) (solid line), \( \delta = 0.09 \) (dashed line), and \( \delta = 0.06 \) (dot-dashed line) for the parameters \( t/J = 2.5, \bar{t}_c/t = 0.04 \), and \( c_0/a_0 = 2.5 \) at the temperature \( T = 0 \) are shown in Fig. 1, where the charge \( e \) has been set as the unit. From Fig. 1, it is found that \( \sigma_c(\omega) \) is composed of two bands separated at \( \omega \sim 0.4t \), the higher-energy band, corresponding to the “midinfrared band” in the in-plane optical conductivity \( \sigma_{ab}(\omega) \)\textsuperscript{4,14}, weighs a broad peak at \( \omega \sim 0.7t \), moreover, the weight of this band is strongly doping dependent, and decreasing rapidly with dopings, but the peak position does not appreciably shift to higher energies, which is consistent with the experimental results\textsuperscript{5,6}. On the other hand, the transferred weight of the lower-energy band forms a sharp peak at \( \omega < 0.4t \), which can be described formally by the non-Drude formula, and our analysis indicates that this peak decay is \( \sim 1/\omega \) at low energies as in the case of \( \sigma_{ab}(\omega) \)\textsuperscript{4,14}. In comparison with \( \sigma_{ab}(\omega) \)\textsuperscript{14}, the present results also show that the values of \( \sigma_c(\omega) \) are by 2 ~ 3 orders of magnitude smaller than those of \( \sigma_{ab}(\omega) \) in the corresponding energy range. For further understanding the property of \( \sigma_c(\omega) \), we have also discussed the finite temperature behavior of \( \sigma_c(\omega) \), and the numerical results at the doping \( \delta = 0.12 \) for the parameters \( t/J = 2.5, \bar{t}_c/t = 0.04 \), and \( c_0/a_0 = 2.5 \) with \( T = 0.2J \) (solid line) and \( T = 0.5J \) (dashed line) are plotted in Fig. 2, which show that \( \sigma_c(\omega) \) is temperature dependent for \( \omega < 1.2t \) and almost temperature independent for \( \omega > 1.2t \), while the higher-energy band is severely suppressed with increasing temperatures, and vanishes at higher temperature \( (T > 0.4J) \). These results are also qualitative consistent with the experimental results\textsuperscript{5,6} and numerical simulations\textsuperscript{18}.

The quantity which is closely related with the c-axis conductivity is the c-axis resistivity \( \rho_c(T) \), and can be expressed as,

\[
\rho_c = \lim_{\omega \to 0} \sigma_c(\omega).
\]

This c-axis resistivity has been evaluated numerically and the results at the doping \( \delta = 0.12 \) and \( \delta = 0.06 \) for the parameters \( t/J = 2.5, \bar{t}_c/t = 0.04 \), and \( c_0/a_0 = 2.5 \) are shown in Fig. 3(a) and Fig. 3(b), respectively. In the underdoped regime, the behavior of the temperature de-

FIG. 1. The c-axis optical conductivity at the doping \( \delta = 0.12 \) (solid line), \( \delta = 0.09 \) (dashed line), and \( \delta = 0.06 \) (dot-dashed line) for \( t/J = 2.5, \bar{t}_c/t = 0.04 \), and \( c_0/a_0 = 2.5 \) with the temperature \( T = 0 \).

FIG. 2. The c-axis optical conductivity at the doping \( \delta = 0.12 \) for \( t/J = 2.5, \bar{t}_c/t = 0.04 \), and \( c_0/a_0 = 2.5 \) with the temperature \( T = 0.2J \) (solid line) and \( T = 0.5J \) (dashed line).
pendence of $\rho_c(T)$ shows a crossover from the high temperature metallic-like $\left(\frac{d\rho_c(T)}{dT} > 0\right)$ to the low temperature semiconducting-like $\left(\frac{d\rho_c(T)}{dT} < 0\right)$, but the metallic-like temperature dependence dominates over a wide temperature range. In comparison with the in-plane resistivity $\rho_{ab}(T)^{14}$, it is shown that the crossover to the semiconducting-like range in $\rho_c(T)$ is obviously linked with the crossover from the temperature linear to the nonlinear range in $\rho_{ab}(T)$, and are caused by the pseudogap observed in the normal-state, but $\rho_{ab}(T)$ is only slightly affected by the pseudogap$^{14}$, while $\rho_c(T)$ is more sensitive to the underlying mechanism. Our results also show that there is the common origin for these crossovers. Therefore in this case, there is a general trend that the copper oxide materials show nonmetallic $\rho_c(T)$ in the underdoped regime at low temperatures. While in the optimally doped regime, $\rho_c(T)$ is a linear in temperatures, and shows the metallic-like behavior for all temperatures. These results are qualitative consistent with the experimental results$^{5-8}$ and numerical simulation$^{18}$. It has been shown from the experiments$^{27}$ that the charge dynamics in some strongly correlated ladder materials shows the similar behaviors.

In the above discussions, the central concerns of the c-axis charge dynamics in the copper oxide materials are the two dimensionality of the electron state and incoherent hopping between the CuO$_2$ planes, and therefore the c-axis charge dynamics in the present fermion-spin picture is determined by the in-plane charged holon fluctuations. In this case, the c-axis scattering rate is associated with the in-plane charge and spin dynamics, and can be roughly described by the imaginary part of the self-energy of the charged holons within the CuO$_2$ planes, which is consistent with the ”dynamical dephasing” theory proposed by Leggett$^{16}$.

In the fermion-spin theory$^{19}$, the charge and spin degrees of freedom of the physical electron are separated as the holon and spinon, respectively. Although both holons and spinons contributed to the charge and spin dynamics, but it has been shown that the scattering of spinons dominates the spin dynamics$^{28}$, while the results of the in-plane charge dynamics$^{14}$ and present c-axis charge dynamics shows that scattering of holons dominates the charge dynamics, therefore the notion of the charge-spin separation naturally accounts for all the qualitative features of the normal-state properties of the copper oxide materials. To our present understanding, the main reasons why the fermion-spin theory based on the charge-spin separation is successful in studying the normal-state property of the strongly correlated copper oxide materials are that (1) the electron single occupancy on-site local constraint is exactly satisfied in the analytic calculation. Since the anomalous normal-state property of the copper oxide materials are caused by the strong electron correlation in these systems$^{10,13}$, and can be effectively described by the $t$-$J$ model$^{10-13}$, but the strong electron correlation in the $t$-$J$ model manifests itself by the electron single occupancy on-site local constraint, then the satisfaction of this local constraint is equivalent to that the strong electron-electron interaction has been properly treated. This is why the crucial requirement is to treat this constraint exactly in the $t$-$J$ model in the analytic discussions. (2) Since the local constraint is satisfied even in the mean-field approximation within the fermion-spin theory$^{19}$, the extra gauge degree of freedom related to the common ”flux” phase problem occurring in the slave-particle approach$^{29}$ does not appear here, which is confirmed by our previous discussions within the mean-field theory$^{20}$, where the photoemission, electron dispersion and electron density of states in the copper oxide materials have been studied, and the results are qualitative similar to that seen in the experiments and numerical simulations. (3) As mentioned above, the dropping the projection operator in Eq. (4) will only lead to errors of the order $\delta$ in counting the number of spin states within the common decoupling approximation$^{29}$. This because that the constrained electron operators $C_{i\sigma}$ in the $t$-$J$ model can be also mapped onto the slave-fermion formulism$^{29}$ as $C_{i\sigma} = h_i^{\dagger} a_{i\sigma}$ with the local constraint $h_i^{\dagger} h_i + \sum_{i} a_{i\sigma}^{\dagger} a_{i\sigma} = 1$. We can solve this constraint by rewriting the boson operators $a_{i\sigma}$ in terms of the CP$^1$ boson operators $b_{i\sigma}$ as $a_{i\sigma} = (1 - h_i^{\dagger} h_i)^{1/2} b_{i\sigma} \approx (1 - h_i^{\dagger} h_i/2) b_{i\sigma}$ supplemented by the local constraint $\sum_{i\sigma} b_{i\alpha}^{\dagger} b_{i\sigma} = 1$. Since the CP$^1$ boson operators $b_{i\uparrow}$ and $b_{i\downarrow}$ with the local con-

**FIG. 3.** The c-axis electron resistivity at the parameter $t/J = 2.5$, $t_c/t = 0.04$, and $c_0/a_0 = 2.5$ for (a) the doping $\delta = 0.12$ and (b) $\delta = 0.06$. 
constraint can be identified with the pseudospin lowering and raising operators in the fermion-spin approach\textsuperscript{19}, respectively, then the spinon propagator in the restricted Hilbert space can be written as

$$D_p(i-j,t-t') = \langle [1 - h_i^1(t)h_i(t)/2] [1 - h_{i'}^1(t')h_{i'}(t')/2] \rangle D(i-j,t-t') \approx [1 - \delta - O(\delta^2)] D(i-j,t-t')$$

where $D(i-j,t-t')$ is the spinon propagator within the fermion-spin approach. In this case, the extra spin degrees of freedom in the fermion-spin theory only lead to the errors of the order $\delta$. This is why the theoretical results of the spin dynamics within the fermion-spin approach\textsuperscript{28} are qualitative consistent with the experiments and numerical simulations.

In summary, we have studied the $c$-axis charge dynamics of the copper oxide materials within the $t-J$ model by considering the incoherent interlayer hopping. Our results show that the $c$-axis charge dynamics is mainly governed by the scattering from the in-plane charged holon fluctuations. The $c$-axis optical conductivity and resistivity have been discussed, and the results are qualitative consistent with the experiments and numerical simulations.

Finally we also note that since the structure of the building blocks in between the CuO$_2$ planes for the chain copper oxide materials is different from these for the nochain copper oxide materials, some subtle differences between the chain and nochain copper oxide materials for the $c$-axis charge dynamics have been found from the experiments\textsuperscript{5,6}. It has been suggested\textsuperscript{8} that for the nochain copper oxide materials the doped holes may introduce the disorder in between the CuO$_2$ planes, contrary to the case of the chain copper oxide materials, where the increasing doping reduces the disorder in between the CuO$_2$ planes. It is possible that the disorder introduced by the doped holes residing between layers in the nochain copper oxide materials in the underdoped regime may modify the interlayer hopping elements, which leads to the subtle differences between the chain and nochain copper oxide materials for the $c$-axis charge dynamics. These and other related issues are under investigation now.

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