

Low-frequency chain and in-plane optical conductivities of detwinned $\text{YBa}_2\text{Cu}_3\text{O}_y$: Slave-boson mean-field analysis of the t - J model

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Based on a scenario in which the CuO_2 plane and CuO chain is coupled together, we study theoretically the low-frequency chain and in-plane optical conductivities of detwinned $\text{YBa}_2\text{Cu}_3\text{O}_y$. Using the slave-boson mean-field approach to the t - J model and including the antiferromagnetic spin fluctuations in the plane, we elaborate that the chain is superconducting for $y > 6.67$ while insulating for $y < 6.67$ due to the competition between the plane-chain coupling and the antiferromagnetic order in the chain, corresponding to a superconductor-insulator transition. Stemming also from the coupling between the plane and chain, a new peak emerges at a low frequency in the in-plane spectra in the superconducting state, while it disappears in the normal state. These results are consistent with very recent experiments.

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I. INTRODUCTION

$\text{YBa}_2\text{Cu}_3\text{O}_y$ (YBCO) is one of the most studied high- T_c superconducting materials. A primary distinction between this system and other cuprates is the presence of the quasi-one-dimensional CuO chain. Though it is widely believed that the main physics in this material is within the CuO_2 plane, the study of electronic properties in the chain and their influence on the superconducting plane may enable us to have a detail understanding on superconductivity in the present system.¹⁻⁴ One of powerful tools to detect the electronic structure is the measurement of optical conductivity. It was reported that a pronounced a - b axis anisotropy exists in the spectra,⁵⁻¹¹ which are strongly enhanced in the chain direction. By subtracting the a -axis spectra from the b -axis (the chain direction) spectra, one can obtain experimentally the spectra contributed by the chain. In this way, the chain electronic structure revealed by the optical experiments shows some unusual features. Several experiments showed that the optical conductivity in the CuO chain exhibits a peak at a finite frequency⁵⁻⁷ and approaches to zero in the dc limit, implying that the chain is insulating though the CuO_2 plane is still in the superconducting state. On the other hand, it was also reported that the chain spectra are characterized as a Drude-like peak located at the zero frequency, demonstrating the chain superconductivity.⁸⁻¹⁰

Recently, a detail investigation of the infrared response in the detwinned YBCO (Ref. 11) provided us a systematic doping dependence of the electrodynamic in the CuO chain. The optical spectra contributed by the chain display a dominant Drude-like peak in the $y=6.75$ sample. While as y decreases to 6.65, the Drude-like peak will shift to a narrow resonance peak at the finite frequency, indicating that the superconductor-insulator transition occurs in the CuO chain. In fact, the appearance of this transition around $y=6.65$ may also be inferred from the doping dependence of the superfluid density.¹⁰ A theoretical explanation of the chain superconductivity based on the plane-chain coupling was given by

Morr and Balatsky,¹² however, an elaboration of the observed superconductor-insulator phase transition and the insulating nature of the chain is still awaited. In the meantime, another important issue is how the in-plane spectra are influenced by the chain. Very recently, an experiment on the detwinned ortho-II phase $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ observed an extra strong peak at 180 cm^{-1} (about 20 meV) in the a -axis optical conductivity in addition to the usually observed Drude-like peak and the mid-infrared (MIR) component in twinned samples.¹³ Therefore a consistent accounting for the optical response in both the plane and chain of the detwinned system is appealing.

In this paper, we demonstrate that the competition of the plane-chain coupling and the antiferromagnetic (AF) order in the chain gives rise to the superconductor-insulator transition in the CuO chain, namely, the proximity superconductivity in the chain is induced by the plane-chain coupling when there is no AF order or it is very weak, while the insulating gap in the optical conductivity is caused by the AF order when its magnitude is appreciable. Starting from a self-consistent mean-field treatment for both the planar and chain Hamiltonian, we extend a simple existing model^{14,15} of the plane-chain coupling to include the emergence of the AF order in the chain at low doping. Interestingly, we find a steplike rise of the AF order at the oxygen content $y=y_c=6.67$ which is almost the same as the superconductor-insulator transition point observed experimentally.¹¹ In the meantime, the chain optical conductivity shows an insulating gap below y_c ; while above y_c , the chain optical conductivity rapidly acquires a Drude-like peak at the dc limit and shows a proximity-induced superconductivity. On the other hand, we find that a new peak occurs at a low frequency ($0.18J \approx 23 \text{ meV}$ with J the AF exchange integral) in the in-plane optical conductivity due to the coupling between the plane and chain. These results agree with the recent experimental measurements,^{11,13} and thus give a consistent picture of the chain and in-plane optical conductivity in the detwinned YBCO.

The paper is organized as follows. In Sec. II, we introduce the model and work out the formalism. In Sec. III, we per-

form numerical calculations and discuss the obtained results. Finally, we give a brief summary in Sec. IV.

II. MODEL AND FORMALISM

We start with a Hamiltonian which describes a system with a plane and a chain per unit cell,

$$H = H_p + H_c + H_I, \quad (1)$$

where H_p represents the CuO₂ plane and is described by the two-dimensional t - t' - J model,

$$H_p = -t_p \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{p\dagger} c_{j\sigma}^p + \text{H.c.} - t'_p \sum_{\langle ij \rangle', \sigma} c_{i\sigma}^{p\dagger} c_{j\sigma}^p + \text{H.c.} + J \sum_{\langle ij \rangle} \left(\mathbf{S}_i^p \cdot \mathbf{S}_j^p - \frac{1}{4} n_i^p n_j^p \right). \quad (2)$$

H_c represents the y -direction CuO chain and is described by the one-dimensional t - J model,

$$H_c = -t_c \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{c\dagger} c_{j\sigma}^c + \text{H.c.} + J_c \sum_{\langle ij \rangle} \left(\mathbf{S}_i^c \cdot \mathbf{S}_j^c - \frac{1}{4} n_i^c n_j^c \right), \quad (3)$$

and H_I is the coupling between the plane and chain:

$$H_I = -t_{\perp} \sum_{ij\sigma} (c_{i\sigma}^{p\dagger} c_{j\sigma}^c + \text{H.c.}). \quad (4)$$

Here $\langle ij \rangle$ denotes the nearest-neighbor (NN) bond and $\langle ij \rangle'$ the next NN bond.

First, we use the slave-boson mean-field theory to decouple the Hamiltonians (2) and (3). Then, the coupling of the planar fermions to spin fluctuations are included via the random phase approximation (RPA). In the slave-boson approach, the creation operators of the planar and chain electrons $c_{i\sigma}^{p(c)\dagger}$ are expressed by slave bosons $b_i^{p(c)}$ carrying the charge and fermions $f_{i\sigma}^{p(c)}$ representing the spin, $c_{i\sigma}^{p(c)\dagger} = f_{i\sigma}^{p(c)\dagger} b_i^{p(c)}$. Then, the constraint of no double occupancy is $b_i^{p(c)\dagger} b_i^{p(c)} + f_{i\sigma}^{p(c)\dagger} f_{i\sigma}^{p(c)} = 1$, which will be satisfied averagely at the mean-field level. The mean-field order parameters are defined as $\Delta_{ij}^p = \langle f_{i\uparrow}^p f_{j\downarrow}^p - f_{i\downarrow}^p f_{j\uparrow}^p \rangle = \pm \Delta_p$, (\pm depend on if the bond $\langle ij \rangle$ is in the \hat{x} or the \hat{y} direction), $\chi_{ij}^{p(c)} = \langle f_{i\sigma}^{p(c)\dagger} f_{j\sigma}^{p(c)} \rangle = \chi_{p(c)}$. Notice that we do not assume any superconducting pairing in the chain at the mean-field level. The AF order in the chain is represented by the staggered magnetization $m_c = (-1)^i \langle S_{iz}^c \rangle$. At low temperatures we are concerned with, the boson condensation is assumed $b_i^{p(c)} \rightarrow \langle b_i^{p(c)} \rangle = \sqrt{\delta_{p(c)}}$, where $\delta_{p(c)}$ is the hole density in the plane (chain).

After Fourier transformation, the mean-field Hamiltonian of the planar and chain fermions can be written as

$$H_p = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}^p f_{\mathbf{k}\sigma}^{p\dagger} f_{\mathbf{k}\sigma}^p - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^p (f_{\mathbf{k}\uparrow}^{p\dagger} f_{-\mathbf{k}\downarrow}^{p\dagger} + \text{H.c.}) + 2N_p J'_p (\chi_p^2 + \Delta_p^2), \quad (5)$$

$$H_c = \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}}^c f_{\mathbf{k}\sigma}^{c\dagger} f_{\mathbf{k}\sigma}^c + \varepsilon_{\mathbf{k}+\mathbf{Q}_c}^c f_{\mathbf{k}+\mathbf{Q}_c, \sigma}^{c\dagger} f_{\mathbf{k}+\mathbf{Q}_c, \sigma}^c) - 2J_c m_c + \sum_{\mathbf{k}\sigma} \sigma (f_{\mathbf{k}\sigma}^{c\dagger} f_{\mathbf{k}+\mathbf{Q}_c, \sigma}^c + \text{H.c.}) + 2N_c J_c (\chi_c^2 + m_c^2), \quad (6)$$

where the summation over \mathbf{k} in the chain Hamiltonian is in the magnetic Brillouin zone (MBZ) due to the AF order, i.e., $-\pi/2 < k_y \leq \pi/2$. \mathbf{Q}_c is the one-dimensional AF wave vector with $\mathbf{Q}_c = \pi/2$. $\varepsilon_{\mathbf{k}}^{p(c)}$ are given by $\varepsilon_{\mathbf{k}}^p = -2(\delta_p t_p + J'_p \chi_p)(\cos k_x + \cos k_y) - 4\delta_p t'_p \cos k_x \cos k_y - \mu_p$ and $\varepsilon_{\mathbf{k}}^c = -2(\delta_c t_c + J_c \chi_c) \cos k_y - \mu_c$, respectively. Correspondingly, the coupling of the planar and chain fermions can be written as

$$H_I = \tilde{t}_{\perp} \sum_{\mathbf{k}\sigma} (f_{\mathbf{k}\sigma}^{p\dagger} f_{\mathbf{k}\sigma}^c + \text{H.c.}), \quad (7)$$

with $\tilde{t}_{\perp} = t_{\perp} \sqrt{\delta}$.

The renormalized Green's functions for the planar fermions \hat{G}_p due to the coupling to spin fluctuations are calculated by Dyson's equation in the Nambu representation:

$$\hat{G}_p(\mathbf{k}, i\omega)^{-1} = \hat{G}_{p0}(\mathbf{k}, i\omega)^{-1} - \hat{\Sigma}_p(\mathbf{k}, i\omega), \quad (8)$$

where the self-energy can be obtained from¹⁴

$$\hat{\Sigma}_p(\mathbf{k}, i\omega) = \frac{1}{\beta N_p} \sum_q \sum_{ig a_m} J^2(\mathbf{q}) \chi_p(\mathbf{q}, i\omega_m) \times \hat{\sigma}_3 \hat{G}_{p0}(\mathbf{k} - \mathbf{q}, i\omega - i\omega_m) \hat{\sigma}_3, \quad (9)$$

\hat{G}_{p0} is the bare Green's function obtained from the mean-field Hamiltonian and $\chi_p(\mathbf{q}, i\omega_m \geq \omega_m + i\delta)$ is the RPA-type spin susceptibility which can be found in Ref. 14, $J(\mathbf{q}) = J(\cos q_x + \cos q_y)$, and $\hat{\sigma}_3$ the Pauli matrix. The Green's function for the chain fermions \hat{G}_c in the Nambu representation is obtained directly from the above mean-field Hamiltonian.

The real part of the optical conductivity $\sigma_1(\omega)$ is given by $\sigma_{1\alpha\alpha}(\omega)_{p(c)} = -\text{Im} \Pi_{\alpha\alpha}(\omega)_{p(c)}/\omega$ ($\alpha = \hat{x}, \hat{y}$). Here the imaginary part of the current-current correction function $\text{Im} \Pi_{\alpha\alpha}(\omega)_{p(c)}$ is expressed as¹⁶

$$\text{Im} \Pi_{\alpha\alpha}(\omega)_{p(c)} = \sum_{\mathbf{k}} \frac{\pi e^2}{N_{p(c)}} \int d\omega' [v_{\alpha}(\mathbf{k})_{p(c)}]^2 \times [f(\omega + \omega') - f(\omega')] \times \text{Tr}[\hat{A}_{p(c)}(\mathbf{k}, \omega + \omega') \hat{A}_{p(c)}(\mathbf{k}, \omega')], \quad (10)$$

where the vertex corrections have been neglected as usually done,¹⁷⁻²² v_{α} is the α -component of the quasiparticle group velocity, $\hat{A}_{p(c)}(\mathbf{k}, \omega)$ the spectral function [$\hat{A}_{p(c)}(\mathbf{k}, \omega) = -(1/\pi) \text{Im} \hat{G}_{p(c)}(\mathbf{k}, \omega)$], and $f(\omega)$ the Fermi distribution function.

In order to investigate the doping dependence of the optical conductivity, we need to determine the planar and chain

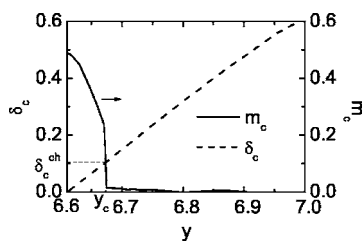


FIG. 1. The hole density δ_c (dashed line) and AF order m_c (solid line) in the chain vs the oxygen content y in $\text{YBa}_2\text{Cu}_3\text{O}_y$.

doping density $\delta_{p(c)}$ for a given oxygen content y in $\text{YBa}_2\text{Cu}_3\text{O}_y$. We determine δ_p vs y by using an empirical relation proposed recently by Liang *et al.*²³ On the other hand, in the parent compound ($y=6$), the valence of Cu ion in the CuO chain is +1, and thus the electron density in the chain is 2. As y increases, i.e., the compound is doped with holes, the holes reside either in the planes or in the chains. By counting the electron density, we find that a conservation condition $2-n_c+2\delta_p=2(y-6)$ is satisfied, which relates the chain electron density n_c and the planar doping density δ_p with y . From this condition, we can derive the chain doping density $\delta_c=|1-n_c|$ as a function of y , as shown in Fig. 1. With the hole doping density, we can then solve the set of self-consistent equations for mean-field parameters $\chi_{p(c)}$, Δ_p , m_c , and $\mu_{p(c)}$. The input parameters are $t_c=t_p=2J$, $t'_p=-0.45t_p$, $J_c=J'_p=3J/8$, $\tilde{t}_\perp=0.1J$ (we have checked numerically that our results are not sensitive to slight changes of the input parameters). The AF coupling constant J in the plane is used as the energy unit ($J\approx 130$ meV). The chain AF order m_c as a function of y at temperature $T\approx 0$ is shown as the solid line in Fig. 1. We can see that the chain AF order m_c emerges with the decrease of the oxygen content y and reaches its maxima value at $y=y_m=6.61$ where the chain doping density is zero (half filled).²⁴ In addition, we note from Fig. 1 that the AF order has a steplike rise from a negligible value to about a half of its maxima at $y=y_c=6.67$.

III. RESULTS AND DISCUSSION

A. Chain spectra

The chain optical conductivity for different oxygen content y is plotted in Fig. 2. As y is increased to exceed $y_c=6.67$ [Fig. 2(a)], a prominent Drude-like peak at the dc limit shows up in the spectra, which indicates that the chain is superconducting, while, when the oxygen content y is below $y=6.67$, the Drude-like peak disappears and a finite frequency peak at $0.35J\approx 46$ meV occurs, leaving an excitation gap between this peak and the dc limit. This indicates that the system becomes insulating at this doping density. With further decrease of the oxygen content (we limit our discussion to the range $y>6.61$, i.e., the chain is in the hole-doped range as will be discussed following), the finite frequency peak will move to a higher energy, leading to a larger excitation gap. Meanwhile, the intensity of the spectra is suppressed heavily as shown in the inset of Fig. 2(b). This

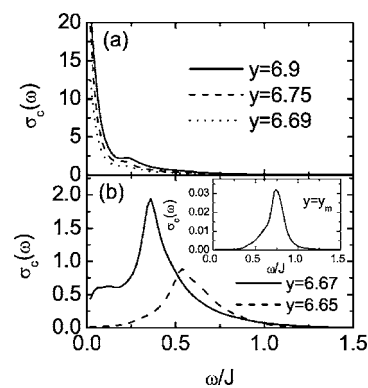


FIG. 2. The chain optical conductivity as a function of frequency in $\text{YBa}_2\text{Cu}_3\text{O}_y$ for different oxygen content y . The inset of (b) shows the spectra at $y=y_m=6.61$ where the calculated chain doping density is zero (half filled).

shows that a superconductor-insulator transition occurs at $y=6.67$, and the corresponding critical doping density in the chain is about $\delta_c^h\approx 0.11$. This result is consistent with the recent experimental measurement on the superconductor-insulator transition observed by optical conductivity.¹¹

From Fig. 1, one can see that the AF order is negligible or disappears (for $y>6.69$) in the doping range where a Drude-like peak in the optical spectra is observed and has an appreciable value when the optical spectra show an insulating behavior. More importantly, at $y=y_c=6.67$ where the insulator-superconductor transition occurs, the magnitude of the AF order has a step like increase, i.e., it rises from a negligible value to nearly a half of its maximum. This shows clearly that the transition is associated with the emergence of the AF order. The occurrence of the AF order leads to a gap $2J_c m_c\approx 24.4$ meV in the single-particle energy band of the chain, i.e., a 48.8-meV excitation gap in the particle-hole excitations. This excitation gap suppresses the proximity effect coming from the coupling to the superconducting plane which is otherwise effective for $y>y_c$. Therefore it is the competition between the AF order and the proximity effect that leads to the superconductor-insulator transition in the chain.

When m_c equals zero, the Hamiltonian for the system can be written as a 4×4 matrix.^{14,15} The gap symmetry induced by the proximity effect may be examined by looking at the anomalous Green's functions of the chain electrons, $F_c(\mathbf{k}, \omega)=\sum_i U_{3i}(\mathbf{k}, \omega)U_{4i}(\mathbf{k}, \omega)/[i\omega-E_i(\mathbf{k}, \omega)]$. U_{ij} are the elements of the matrix that diagonalizes the mean-field Hamiltonian and $E_i(\mathbf{k}, \omega)$ the quasiparticle energy at the i energy band (i runs from 1 to 4), which are defined following the notations of Refs. 14 and 15. Because $U_{3i}U_{4i}\propto \tilde{\Delta}_\mathbf{k}^p$ (Ref. 14) ($\tilde{\Delta}_\mathbf{k}^p$ is the superconducting gap in the plane with a $d_{x^2-y^2}$ symmetry), the induced gap of the chain fermions is also of $d_{x^2-y^2}$ symmetry.

Besides the superconductor-insulator transition observed at low frequencies, the experiment in Ref. 11 also shows that the chain optical conductivity has a high-frequency tail and exhibits a one-dimensional scaling feature consistent with a prediction of the Tomonaga-Luttinger liquid theory.²⁵ This

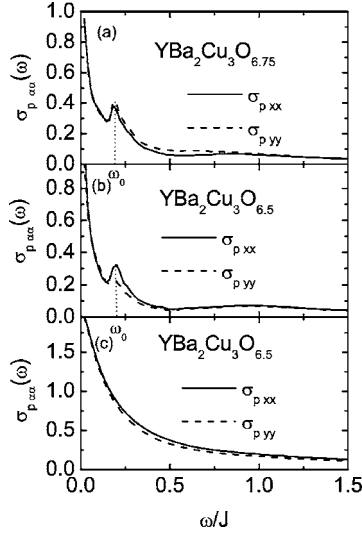


FIG. 3. The real parts of the in-plane optical conductivity as a function of frequency ω for different y . Panel (a) shows the spectra for $y=6.75$ sample in the superconducting state, panels (b) and (c) are the spectra for the ortho-II phase $y=6.5$ sample with the planar doping density $\delta_p=0.097$ in the superconducting state at $T=0.0005J$ and in the normal state at $T=T_c=0.033J$, respectively.

scaling behavior cannot be reproduced based on the perturbation calculation starting from the mean-field theory presented here, because the mean-field analysis fails for the one-dimensional problem. A more rigorous study beyond the mean-field level is needed for this analysis, such as the exact diagonalization for the one-dimensional t - J model.^{26,27} However, a coupled one-dimensional system will exhibit a quasi-two-dimensional behavior at low energies.²⁸ In this case which our analysis focuses on, the perturbation calculation from a mean-field theory provides us an efficient and at least qualitative way to study the effect of the coupling between the plane and chain, particularly for the low-energy behavior of the chain optical conductivity and the superconductor-insulator transition. In fact, besides the coupling between the plane and chain, there is also a coupling between chains. We expect that the effect of the latter might be similar to the former, namely it causes the one-dimensional conduction in the chain to exhibit a two-dimensional behaviors (or an anisotropic three-dimensional behaviors) at low energies, and leads to the situation which a perturbation calculation based on a mean-field theory may be applied. In addition, with the decrease of the oxygen content, the finite chain fragment length will decrease, so it will lead to the decrease of the hopping integral along the chain t_c . This effect is equivalent to the increase of the AF exchange integral in the chain J_c and consequently enhances the AF correlation, because it is the ratio of J_c/t_c that is related to the emergence of the AF order. Therefore our model has the similar effect on the transition with the picture of the finite chain fragment length. Finally we also note that our analysis is only applied to the case which the chain is hole doped, i.e., the oxygen content $y > y_m$. For the case of an electron-doped chain, the energy band structure of the chain electrons will change correspondingly and a different model is demanded for the CuO chain.

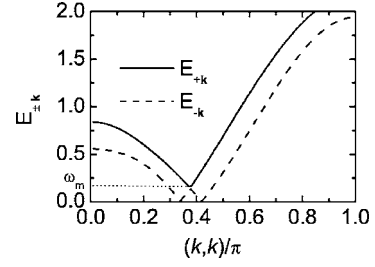


FIG. 4. The quasiparticle energy $E_{\pm k}$ vs the wave vector \mathbf{k} along the diagonal direction in $\text{YBa}_2\text{Cu}_3\text{O}_{6.75}$.

B. In-plane spectra

Now we study how the in-plane optical conductivity is influenced by the coupling to the chain. The real part of the in-plane optical conductivity $\sigma_1(\omega)$ is shown in Fig. 3 for the superconducting [Figs. 3(a) and 3(b)] and the normal state [Fig. 3(c)], respectively. In the superconducting state, a Drude-like peak at the dc limit and a MIR hump around $\omega \sim J$ is evident from Figs. 3(a) and 3(b), which reproduces what has been observed in the twinned samples.²⁹ These features are also consistent with previous theoretical calculations^{20,30,31} in which only the in-plane electrodynamics is considered. A different feature observed here is that an extra peak emerges between the Drude-like peak and the MIR hump. Moreover, this extra peak disappears completely in the normal state, as seen from Fig. 3(c). These results are consistent with the very recent experimental data.¹³ We also note that there is only a weak a - b anisotropy in the spectra around this peak. In the meantime, the in-plane spectra in the superconducting state are nearly isotropic both in the dc limit and in high frequencies. As a result, the plane-chain coupling does not cause an obvious in-plane anisotropy in the optical conductivity. Therefore we expect that the anisotropy observed in the experiments, which is obtained by subtracting the a -axis spectra from the b -axis spectra, is mainly contributed by the chain contribution.

Due to the coupling between the plane and chain, the energy band of the in-plane quasiparticle is split into two branches with frequencies $E_{\pm k}$.¹⁴ In the superconducting state, the low-energy optical response comes mainly from the charge excitations around the nodal direction due to the presence of the superconducting gap. In Fig. 4, we plot $E_{\pm k}$ with \mathbf{k} along the diagonal direction. Around the Fermi wave vector, there is a minimum $\omega_m \approx 0.18J$ in E_{+k} , and the band E_{-k} is below this minimum. When the excitation frequency is below ω_m , the optical response comes only from the E_{-k} band. When $\omega \geq \omega_m$, an additional scattering channel from the E_{+k} band contributes to the response and leads to a peak around ω_m . In the normal state, the excitations near the entire Fermi surface are available, so that the minimum in E_{+} varies at different wave vectors. As a result, the combined effect of these excitations causes no extra peak.

IV. SUMMARY

To summarize, starting from the slave-boson approach to the t - J model and considering the coupling between the

CuO₂ plane and CuO chain, we have elaborated that the competition of the plane-chain coupling and the antiferromagnetic order in the chain leads to the superconductor-insulator transition in the optical conductivity of the CuO chain. Specifically, the proximity superconductivity in the chain is induced by the plane-chain coupling while the insulating property is caused by the antiferromagnetic order. Meanwhile, we find an extra peak in the in-plane optical spectra at low frequencies in the superconducting state, which is between the Drude-like peak and mid-infrared component. This peak disappears in the normal state. These

results are well consistent with the recent optical conductivity measurements.

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