Charge transport in underdoped bilayer cuprates

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Within the $t$-$J$ model, we study the charge transport in underdoped bilayer cuprates by considering the bilayer interaction. Although the bilayer interaction leads to the band splitting in the electronic structure, the qualitative behavior of the charge transport is the same as in the case of single layer cuprates. The conductivity spectrum shows a low-energy peak and the unusual midinfrared band. This midinfrared band is suppressed severely with increasing temperatures, while the resistivity in the heavily underdoped regime is characterized by a crossover from the high temperature metallic-like to the low temperature insulating-like behaviors, which are consistent with the experiments.

74.20.Mn, 74.25.Fy, 74.72.-h

It has become clear in the past ten years that cuprate superconductors are among the most complex systems studied in condensed matter physics$^{1,2}$. 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 cuprate superconductors, and (2) extreme sensitivity of the properties to the compositions (stoichiometry) which control the carrier density in the CuO$_2$ plane, and therefore the regimes have been classified into the underdoped, optimally doped, and overdoped, respectively$^{1,2}$. In the underdoped and optimally doped regimes, the experimental results$^3$ show that the ratio of the c-axis and in-plane resistivities $R = \rho_c(T)/\rho_a(T)$ ranges from $R \sim 100$ to $R > 10^5$, which reflects that the charged carriers are tightly confined to the CuO$_2$ planes. This large magnitude of the resistivity anisotropy also leads to the general notion that the physics of doped cuprates is almost entirely two-dimensional, and can be well described by a single CuO$_2$ plane$^4$. However, this picture seems to be incompatible with the fact that the superconducting transition temperature $T_c$ is closely related to the number of CuO$_2$ planes per unit cell, with single layer compounds of a family generically having lower $T_c$ than bilayer or trilayer compounds$^2$. Additionally, there are some subtle differences of the magnetic behaviors between doped single layer and bilayer cuprates. By virtue of systematic studies using NMR and $\mu$SR techniques, particularly the inelastic neutron scattering, only incommensurate neutron scattering peaks for the single layer lanthanum cuprate are observed in the underdoped regime$^5$, however, both low-energy incommensurate neutron scattering peaks and high-energy commensurate $[\pi,\pi]$ resonance for the bilayer yttrium cuprate in the normal state are detected$^6$. These experimental results highlight the importance of some sort of coupling between the CuO$_2$ planes within a unit cell. It is believed that all these experiments produce interesting data that introduce the important constraints on the microscopic models and theories.

The charge transport of doped single layer cuprates has been addressed from several theoretical viewpoints$^{7,8}$. Based on the charge-spin separation, an attractive proposal is spinons and holons as basic low-energy excitations, serving as the starting point for the gauge-theory approach$^7$. It has been shown$^7$ within the $t$-$J$ model that above the Bose-Einstein temperature, the boson inverse lifetime due to scattering by the gauge field is of order $T$, which suppresses the condensation temperature and leads to a linear $T$ resistivity. On the other hand, the spin-fermion model near the antiferromagnetic instability has been developed to study the normal-state properties of doped cuprates$^8$. This spin-fermion model describes low-energy fermions interacting with their own collective spin fluctuations. Within this approach$^8$, the anomalous transport of doped single layer cuprates has been studied extensively$^9$, and the results are consistent with the experiments.

As regards an intracell hopping, the band splitting in doped bilayer cuprates was shown by the band calculation$^9$, and clearly observed$^{10,11}$ recently by the angle-resolved-photoemission spectroscopy in the doped bilayer cuprate Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ above $T_c$. This bilayer band splitting is due to a nonvanishing intracell coupling. Moreover, the magnitude of the bilayer splitting is constant over a large range of dopings$^{11}$. Considering these
highly unusual normal state properties in the underdoped regime\textsuperscript{1,2,5,6}, a natural question is what is the effect of the intracell coupling on the normal state properties of doped bilayer cuprates. This is a challenge issue since the mechanism for the superconductivity in doped cuprates has been widely recognized to be closely related with the anisotropic normal-state properties\textsuperscript{12}. Based on the \textit{t-J} model, the charge transport and spin response of doped single layer cuprates in the underdoped regime have been discussed\textsuperscript{13-15} within the fermion-spin theory\textsuperscript{16}, and the obtained results are consistent with experiments\textsuperscript{17}. In this paper, we apply this successful approach to study the intracell coupling on the normal state properties of underdoped bilayer cuprates. This is a challenge issue since the single occupancy local constraint has been treated properly within the fermion-spin theory, this leads to disappearing of the extra gauge degree of freedom related with this local constraint under the charge-spin separation\textsuperscript{16}. In this case, the charge fluctuation couples only to holons\textsuperscript{13,14}. However, the strong correlation between holons and spinons is still included self-consistently through the spinon’s order parameters entering the hole’s propagator, therefore both holons and spinons are responsible for the charge transport. In this case, the conductivity can be expressed as $\sigma_\parallel (\omega) = -\text{Im} \Pi_\parallel (h_\omega) / \omega$, with $\Pi_\parallel (h_\omega)$ is the holon current-current correlation function, and is defined as $\Pi_\parallel(-\tau + \tau') = \langle T_\tau \hat{j}^{(h)}(\tau) \hat{j}^{(h)}(\tau') \rangle$, where $\tau$ and $\tau'$ are the imaginary times, and $T_\tau$ is the $\tau$ order operator. Within the Hamiltonian (2), the current density of holons is obtained by the time derivation of the polarization operator using Heisenberg’s equation of motion as,

$$j^{(h)}(\omega) = 2\chi e t \sum_{a\bar{\eta}} \hat{\eta} h^{\dagger}_{a \bar{\eta}} h_{a \bar{\eta}},$$

where $R_{1i}, (R_{2i})$ is lattice site of the CuO$_2$ plane 1 (plane 2). $\chi = \langle S^{+}_{a \bar{\eta}} S^{-}_{a \bar{\eta}} \rangle$ and $\chi_\perp = \langle S^{\perp}_{a \bar{\eta}} S^{\perp}_{a \bar{\eta}} \rangle$ are the spinon correlation functions, and $e$ is the electronic charge, which is set as the unit hereafter. The holon current-current correlation function can be calculated in terms of the holon Green’s function $g(k, \omega)$ as in the single layer case\textsuperscript{13,14}. However, in the bilayer system, because there are two coupled CuO$_2$ planes, then the energy spectrum has two branches. In this case, the holon Green’s function can be expressed as a matrix $g(i - j, \tau - \tau') = g_L(i - j, \tau - \tau') + \sigma g_T(i - j, \tau - \tau')$, with the longitudinal and transverse parts are defined as $g_L(i - j, \tau - \tau') = \langle T_{\tau} h_{a \bar{\eta}}(\tau) h_{a \bar{\eta}}^{\dagger}(\tau') \rangle$ and $g_T(i - j, \tau - \tau') = \langle T_{\tau} h_{a \bar{\eta}}(\tau) h_{a \bar{\eta}}^{\dagger}(\tau') \rangle (a \neq a')$, respectively. Following discussions of the single layer case\textsuperscript{13,14}, we obtain the conductivity of doped bilayer cuprates as $\sigma(\omega) = \sigma^{(L)}(\omega) + \sigma^{(T)}(\omega)$, with the longitudinal and transverse parts are given by,

$$\sigma^{(L)}(\omega) = \frac{1}{N} \sum_{k} [(2 \chi_\parallel s_k^2) + (2 \chi_\perp t_{\perp}^2)] \times \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A_L^{(h)}(k, \omega' + \omega) A_L^{(h)}(k, \omega'),$$

where $A_L^{(h)}(k, \omega') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega'} A_L^{(h)}(k, \omega' + \omega).$
the fermion distribution function. The longitudi-
the plane,

\[ \Sigma_L(k, \omega) = \frac{1}{N^2} \sum_{\nu} \sum_{\nu'} \Xi_{\nu\nu'\nu}(k, p, q, \omega), \]  

\[ \Sigma_T(k, \omega) = \frac{1}{N^2} \sum_{\nu} \sum_{\nu'} (-1)^{\nu+\nu'+1+1} \times \Xi_{\nu\nu'\nu}(k, p, q, \omega), \]

respectively, with \( \Xi_{\nu\nu'\nu}(k, p, q, \omega) \) is given by,

\[
F_{\nu'\nu'\nu}(k, p, q, \omega) = (Z) \left[ \gamma_{q+p+k} + \gamma_{q-k} + t_{\perp} \left[ (-1)^{\nu+\nu'} + (-1)^{\nu'+\nu''} \right] \right] \times \left( \frac{F_{\nu'\nu'\nu}^{(3)}(k, p, q)}{\omega - \omega_{q+p} + \omega_{q'} - \xi_{p+k}} + \frac{F_{\nu'\nu'\nu}^{(3)}(k, p, q)}{\omega + \omega_{q+p} + \omega_{q'} - \xi_{p+k}} \right)
\] 

\[
F_{\nu'\nu'\nu}^{(3)}(k, p, q) = n_F(\omega_{q+p}) - n_F(\omega_{q'+p}) + n_B(\omega_{q+p}) \] 

\[ F_{\nu'\nu'\nu}^{(4)}(k, p, q) = \left[ 1 + n_B(\omega_{q+p}) \right] \left[ 1 + n_B(\omega_{q'+p}) \right] - n_B(\omega_{q+p}) \left[ 1 + n_B(\omega_{q'+p}) \right]. \]

where \( n_B(\omega_{k}^{(\nu)}) \) is the boson distribution function, the MF holon excitation \( \xi_{\nu\nu}(k) = 2\pi L_{\nu\nu} \epsilon_{\nu\nu}(k) = 2\pi L_{\nu\nu} \epsilon_{\nu\nu}(k) \), the MF spinon excitation \( (\omega_{q+p})^2 = \omega_{q+p}^2 + \Delta_{k}^2(1)^{\nu+1} \), with \( \Delta_{k}^2 = A_1 \gamma_{k} + A_2 \gamma_{k} + A_3, A_2 = X_k \gamma_{k} + X_2 \), and

\[ A_1 = \alpha \chi^2(\epsilon_{\nu\nu}/Z + \epsilon_{\nu\nu}^2), \] 

\[ A_2 = \epsilon^2 \left( \frac{1 - Z}{Z} \right) \alpha (\chi_{\nu\nu}/Z + \chi_{\nu\nu}^2)/Z \] 

\[ - \alpha (\chi_{\nu\nu}/Z + \chi_{\nu\nu}^2)/Z \] 

\[ + \alpha \lambda \rho \epsilon_{\nu\nu}/Z + \rho \epsilon_{\nu\nu}^2 + 1/4, \] 

\[ X_1 = \alpha \lambda \rho \epsilon_{\nu\nu}/Z + \rho \epsilon_{\nu\nu}^2 + 1/4, \] 

\[ X_2 = -\alpha \lambda \rho \epsilon_{\nu\nu}/Z + \rho \epsilon_{\nu\nu}^2 + 1/4. \] 

The frequency- and temperature-dependent conductivity is a powerful probe for systems of interacting electrons, and provides very detailed information of the excitations, which interacts with carriers in the normal-state and might play an important role in the superconductivity. In Fig. 1, we present the results of the conductivity \( \sigma(\omega) \) at doping \( \delta = 0.05 \) (solid line), \( \delta = 0.06 \) (dashed line), and \( \delta = 0.07 \) (dotted line) for parameters \( t/J = 2.5, t_{\perp}/t = 0.25, J_{\perp}/J = 0.25 \) with temperature \( T = 0 \) in comparison with the experimental data taken on the underdoped YBa2Cu3O6−x (YBCO) (inset). The conductivity of bilayer cuprates in the underdoped regime shows a sharp low-energy peak at \( \omega < 0.5t \) and the unusual midinfrared band appearing inside the charge-transfer gap of the undoped system. After an analysis, we found that this low-energy peak decays fastly as \( \sigma(\omega) \sim 1/\omega \) (non-Drude fall-off) with increasing energies. Moreover, the weight of the midinfrared peak is doping dependent, and the peak position is shifted to low energy.
with increasing dopings. For a better understanding of the optical properties of doped bilayer cuprates, we have studied conductivity at different temperatures, and the results at doping $\delta = 0.06$ for $t/J = 2.5$, $t_{\perp}/t = 0.25$, and $J_{\perp}/J = 0.25$ in $T = 0$ (solid line), $T = 0.3J$ (dashed line), and $T = 0.5J$ (dotted line) are plotted in Fig. 2 in comparison with the experimental data\textsuperscript{19} taken on the underdoped YBCO (inset). It is shown that $\sigma(\omega)$ is temperature dependent, and the charge-transfer gap is severely suppressed with increasing temperatures, and vanishes at higher temperature ($T > 0.4J$). Our results are in qualitative agreement with the experiments\textsuperscript{19}. In comparison with the results from Refs.\textsuperscript{13,14}, it is shown that the present conductivity also is qualitatively consistent with these in the single layer case. In the above calculations, we also find that the conductivity $\sigma(\omega)$ is essentially determined by its longitudinal part $\sigma^{(L)}(\omega)$, this is why in the present doped bilayer cuprates the conductivity spectrum appears to reflect the single layer nature of the electronic state\textsuperscript{1,2,13,14}. This is also why the in-plane charge dynamics is rather universal within whole doped cuprates\textsuperscript{1,2}.

Now we turn to discuss the resistivity, which is closely related to the conductivity, and can be obtained as $\rho(T) = 1/\lim_{\omega \to 0} \sigma(\omega)$. This resistivity has been calculated, and the results at doping $\delta = 0.05$ (solid line), $\delta = 0.06$ (dashed line), and $\delta = 0.07$ (dotted line) for $t/J = 2.5$, $t_{\perp}/t = 0.25$, and $J_{\perp}/J = 0.25$ are plotted in Fig. 3 in comparison with the experimental results\textsuperscript{20} taken on the underdoped YBCO (inset). These results show that in the heavily underdoped regime, although the temperature-dependent resistivity is characterized by a crossover from the high temperature metallic-like to the low temperature insulating-like behaviors, the nearly temperature liner dependence in the resistivity dominates over a wide temperature range, in agreement with the experimental results\textsuperscript{20}. In comparison with the results from Refs.\textsuperscript{13,14}, it is shown that the present resistivity also is qualitatively consistent with these in the single layer case. We emphasize that since the order parameters, decoupling parameter $\alpha$, and the chemical potential $\mu$ have been determined self-consistently, then these theoretical results were obtained without any adjustable parameters. Furthermore, it is found in the above discussions that the present results are insensitive to the reasonable values of $t/J$, $t_{\perp}/t$, and $J_{\perp}/J$ as in the single layer case\textsuperscript{13,14}.

An explanation for the metal-to-insulating crossover in the resistivity in the heavily underdoped regime can be found from the competition between the kinetic energy and magnetic energy in the system. Since cuprate superconducting materials are doped Mott insulators, obtained by chemically adding charge carriers to a strongly correlated antiferromagnetic insulating state, therefore doped cuprates are characterized by the competition between the kinetic energy ($t$) and magnetic energy ($J$).
The magnetic energy $J$ favors the magnetic order for spins, while the kinetic energy $t$ favors delocalization of holes and tends to destroy the magnetic order. In the present fermion-spin theory, although both holons and spinons contribute to the charge transport, the scattering of holons dominates the charge transport\(^\text{13}\), where the charged holon scattering rate is obtained from the full holon Green’s function (then the holon self-energy (5) and holon spectral function) by considering the holon-spinon interaction, therefore in the heavily underdoped regime the observed crossover from the high temperature metallic-like to the low temperature insulating-like behaviors in the resistivity is closely related with this competition. In lower temperatures, the holon kinetic energy is much smaller than the magnetic energy, in this case the magnetic fluctuation is strong enough to severely reduce the charged holon scattering and thus is responsible for the insulating-like behavior in the resistivity. With increasing temperatures, the holon kinetic energy is increased, while the spinon magnetic energy is decreased. In the region where the holon kinetic energy is much larger than the spinon magnetic energy at higher temperatures, the charged holon scattering would give rise to the temperature linear resistivity.

In summary, we have studied the charge transport in the underdoped bilayer cuprates by considering the bilayer interaction. It is shown that although the bilayer interaction leads to the band splitting in the electronic structure, the qualitative behavior of the charge transport is the same as in the single layer case. The conductivity spectrum shows a low-energy peak and the anomalous midinfrared band. This midinfrared band is suppressed severely with increasing temperatures, while the resistivity exhibits a crossover from the high temperature metallic-like to the low temperature insulating-like behaviors. Our results also show that the mechanism that cause this unusual charge transport in the underdoped cuprates is closely related to the background antiferromagnetic correlations.

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