Doping dependence of charge dynamics in electron-doped cuprates

Tianxing Ma, Huaiming Guo, and Shiping Feng

Department of Physics, Beijing Normal University, Beijing 100875, China

Within the $t$-$t'$-$J$ model, the doping dependence of charge dynamics in the electron-doped cuprates is studied. The conductivity spectrum shows an unusual pseudogap structure with a low-energy peak appearing at $\omega \sim 0$ and an rather sharp midinfrared peak appearing around $\omega \sim 0.3 | t |$, and the resistivity exhibits a crossover from the high temperature metallic-like to low temperature insulating-like behavior in the relatively low doped regime, and a metallic-like behavior in the relatively high doped regime, in qualitative agreement with experiments. Our results also show that the unusual pseudogap structure is intriguingly related to the strong antiferromagnetic correlation in the system.

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The parent compounds of cuprate superconductors are believed to belong to a class of materials known as Mott insulators with the antiferromagnetic (AF) long-range order (AFLRO), then superconductivity occurs by electron or hole doping\textsuperscript{1,2}. It has been found from experiments that only an approximate symmetry in the phase diagram exists about the zero doping line between the electron- and hole-doped cuprates\textsuperscript{3,4}, and the significantly different behavior of the electron- and hole-doped cuprates is observed\textsuperscript{5-6}, reflecting the electron-hole asymmetry. For the hole-doped cuprates\textsuperscript{1}, AFLRO disappears rapidly with doping, and is replaced by a disordered spin liquid phase with characteristics of incommensurate short AF correlations, then the systems become superconducting over a wide range of the hole doping concentration $\delta$, around the optimal $\delta \sim 0.15$. However, AFLRO survives until superconductivity appears over a narrow range of $\delta$ around the optimal $\delta \sim 0.15$ in the electron-doped cuprates, where the underdoped superconducting regime is absent, and the maximum achievable superconducting transition temperature is much lower than the hole-doped cuprates\textsuperscript{3,7}. Moreover, commensurate spin response in the superconducting state of the electron-doped cuprates is observed\textsuperscript{8}. Therefore the investigating similarities and differences of the hole- and electron-doped cuprates would be crucial to understanding physics of the high-$T_c$ superconductivity.

Among the striking features of the normal-state properties, the physical quantity which most evidently demonstrates the nonconventional property is the charge dynamics\textsuperscript{8-11}, which is manifested by the optical conductivity and resistivity. Although the resistivity shows a tendency to deviate from the linear behavior in temperature for the hole-doped cuprates\textsuperscript{9,11}, a pseudogap-like feature in the electron-doped cuprates has been observed in the optical conductivity\textsuperscript{10,11}. This pseudogap energy increases with decreasing doping\textsuperscript{11,12}. Moreover, a clear departure from the universal Wiedemann-Franz law for the typical Fermi-liquid behavior is observed\textsuperscript{13}, which shows that the anomalous charge transport of the electron-doped cuprates does not fit in the conventional Fermi-liquid theory. These unusual physical properties of the charge dynamics in the electron-doped cuprates offer the unique possibility of comparison with those in their hole-doped counterparts which can serve as a touchstone for theory. Wei\textsuperscript{14} have developed a fermion-spin theory based on the charge-spin separation to study the physical properties of the hole-doped cuprates, where the electron operator is decoupled as the gauge invariant dressed holon and spinon. Within this theory, we have discussed the doping dependence of the charge transport in the hole-doped cuprates\textsuperscript{14,15}, and the results are in agreement with experiments\textsuperscript{1}. It has been shown that the charge transport of the hole-doped cuprates is mainly governed by the scattering from the dressed holons due to the dressed spinon fluctuation\textsuperscript{14,15}. In this paper, we apply this successful approach to study the doping dependence of the charge dynamics in the electron-doped cuprates. Within the $t$-$t'$-$J$ model, we show that as in the hole-doped cuprates the unusual behavior of the charge dynamics in the electron-doped cuprates is intriguingly related to the AF correlations.

In the electron-doped cuprates, the characteristic feature is the presence of the two-dimensional CuO$_2$ plane\textsuperscript{4-6} as in the hole-doped case, and it seems evident that the unusual behaviors are dominated by this plane. It is believed that the essential physics of the electron-doped CuO$_2$ plane is contained in the $t$-$t'$-$J$ model on a square lattice\textsuperscript{2},

$$H = t \sum_{i\sigma} P C^\dagger_{i\sigma} C_{i+\hat{\eta}\sigma} P^\dagger - t' \sum_{i\sigma} P C^\dagger_{i\sigma} C_{i+\hat{\tau}\sigma} P^\dagger - \mu \sum_{i\sigma} P C^\dagger_{i\sigma} C_{i\sigma} P^\dagger + J \sum_{i\hat{\eta}\hat{\tau}} S_{i\hat{\eta}} \cdot S_{i+\hat{\tau}},$$

(1)

where $t < 0$ and $t' < 0$ in the electron-doped case, $\hat{\eta} = \pm \hat{x}, \pm \hat{y}$, $\hat{\tau} = \pm \hat{x} \pm \hat{y}$, $C^\dagger_{i\sigma}$ ($C_{i\sigma}$) is the electron creation (annihilation) operator, $S_i = C^\dagger_i \sigma C_i / 2$ is the spin operator with $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ as the Pauli matrices, $\mu$ is the chemical potential, and the projection operator $P$ removes zero occupancy, i.e., $\sum_{\sigma} C^\dagger_{i\sigma} C_{i\sigma} \geq 1$ . The importance of $t'$ term in Eq. (1) has been emphasized by many authors. It has been argued that although $t'$ term does not change spin configuration because of the same sublattice hoppings, it can stabilize the AF correlation in the electron-doped cuprates, and distinguishes between...
the hole- and electron-doped cases. For the hole-doped cuprates, a fermion-spin theory based on the charge-spin separation has been developed to incorporate a single occupancy local constraint. To apply this theory in the electron-doped cuprates, the \( t'-t' \)-model (1) can be rewritten in terms of a particle-hole transformation \( C_{\sigma} \rightarrow f_{\sigma}^{\dagger} \) as,

\[
H = -t \sum_{i \sigma} f_{i \sigma}^{\dagger} f_{i+\hat{\eta} \sigma} + t' \sum_{i \sigma} f_{i \sigma}^{\dagger} f_{i+\hat{\tau} \sigma} + \mu \sum_{i \sigma} f_{i \sigma}^{\dagger} f_{i \sigma} + J \sum_{i \eta} S_i \cdot S_{i+\hat{\eta}},
\]

supplemented by a local constraint \( f_{i \sigma}^{\dagger} f_{i \sigma} \leq 1 \) to remove double occupancy, where \( f_{i \sigma}^{\dagger} (f_{i \sigma}) \) is the hole creation (annihilation) operator, and \( S_i = f_{i}^{\dagger} \sigma f_{i} / 2 \) is the spin operator in the hole representation. Now we follow the charge-spin separation fermion-spin-14 theory, and decouple hole operators \( f_{i \uparrow} \) and \( f_{i \downarrow} \) as,

\[
f_{i \uparrow} = a_{i \uparrow}^{\dagger} S_{i}^{-}, \quad f_{i \downarrow} = a_{i \downarrow}^{\dagger} S_{i}^{+},
\]

where the spinful fermion operator \( a_{i \sigma} = e^{-i \psi_{\sigma} a_{i}} \) describes the charge degree of freedom together with some effects of the spin configuration rearrangements due to the presence of the doped electron itself (dressed fermion), while the spin operator \( S_i \) describes the spin degree of freedom (dressed spinon), then the no double occupancy local constraint, \( \sum_{\sigma} f_{i \sigma}^{\dagger} f_{i \sigma} = S_{i}^{+} a_{i \uparrow}^{\dagger} S_{i}^{-} + S_{i}^{-} a_{i \downarrow}^{\dagger} S_{i}^{+} = a_{i \uparrow}^{\dagger} S_{i}^{+} + a_{i \downarrow}^{\dagger} S_{i}^{-} = 1 - 2a_{i \sigma} \leq 1 \) is satisfied, and the double dressed fermion occupancy, \( a_{i \sigma} a_{i \sigma} a_{i \sigma} a_{i \sigma} = e^{i \psi_{\sigma} a_{i}} e^{i \psi_{\sigma} a_{i}} = 0 \) and \( a_{i \sigma} a_{i \sigma} a_{i \sigma} a_{i \sigma} = e^{-i \psi_{\sigma} a_{i}} e^{-i \psi_{\sigma} a_{i}} = 0 \), are ruled out automatically. These dressed fermion and spinon have been shown to be gauge invariant, and in this sense, they are real and can be interpreted as the physical excitations. We emphasize that this dressed fermion \( a_{i \sigma} \) is a spinless fermion \( a_{i} \) incorporated a spin cloud \( e^{-i \psi_{\sigma} a_{i}} \) (magnetic flux), and is a magnetic dressing. In other words, the gauge invariant dressed fermion carries some spin messages, i.e., it shares its nontrivial spinon environment. Although in common sense \( a_{i \sigma} \) is not a real spinful fermion, it behaves like a spinful fermion. In this charge-spin separation fermion-spin representation, the low-energy behavior of the \( t'-t' \)-model (2) can be expressed as,

\[
H = -t \sum_{i \eta} \left( a_{i+\hat{\eta}}^{\dagger} S_{i}^{-} a_{i+\hat{\eta}} S_{i}^{+} + a_{i \eta} S_{i}^{-} a_{i+\hat{\eta}}^{\dagger} S_{i+\hat{\eta}}^{+} \right) + t' \sum_{i \tau} \left( a_{i+\hat{\tau}}^{\dagger} S_{i}^{+} a_{i+\hat{\tau}} S_{i}^{-} + a_{i \tau} S_{i}^{+} a_{i+\hat{\tau}}^{\dagger} S_{i+\hat{\tau}}^{-} \right) - \mu \sum_{i \sigma} a_{i \sigma} a_{i \sigma} + J_{\text{eff}} \sum_{i \eta} S_{i} \cdot S_{i+\hat{\eta}},
\]

with \( J_{\text{eff}} = (1 - \delta) J \), and \( \delta = \langle a_{i \sigma} a_{i \sigma} \rangle = \langle a_{i \sigma} a_{i \sigma} \rangle \) is the electron doping concentration. At the half-filling, the \( t'-t' \)-model is reduced to the Heisenberg model with AFLRO. As we have mentioned above, the phase with this AFLRO is much more robust in the electron-doped cuprates and persists to much higher doping levels, therefore in this paper we only discuss the charge dynamics in the doped regime without AFLRO, i.e., \( \langle S_{\tau}^{z} \rangle = 0 \).

Since the local constraint has been treated properly within the charge-spin separation fermion-spin theory, this leads to disappearing of the extra gauge degree of freedom related to the local constraint, and then the charge fluctuation only couples to dressed fermions. In this case, the doping dependence of the charge dynamics of the hole-doped cuprates has been discussed. Following their discussions, the optical conductivity of electron-doped cuprates can be obtained as,

\[
\sigma(\omega) = \frac{1}{4} (Zc)^{2} \sum_{k \sigma} \frac{\gamma_{k}^{2}}{\omega_{F}^{2}} \sum_{q} A_{k}^{(a)}(k, \omega' + \omega) \times A_{k}^{(\bar{a})}(k, \omega') \frac{\mu_{p}(\omega' + \omega) - n_{F}(\omega')}{\omega'},
\]

where \( Z \) is the number of the nearest neighbor sites, \( \gamma_{k}^{2} = [(\chi_{l} t - 2\chi_{l} t \cos k_{p} s_{l})^{2} \sin^{2} k_{p} + (\chi_{l} t - 2\chi_{l} t \cos k_{p})^{2} \sin^{2} k_{p} s_{l}] / 4n_{F}(\omega) \) is the fermion distribution function, while the dressed fermion spectral function \( A_{k}^{(a)}(k, \omega) \) is obtained as \( A_{k}^{(a)}(k, \omega) = -2n_{F}(k, \omega) \), where the full dressed fermion Green’s function \( g_{k}^{(a)}(k, \omega) = g_{k}^{(a)}(1, \omega) - \Sigma^{(a)}(k, \omega) \) with the mean-field dressed fermion Green’s function \( g_{k}^{(a)}(1, \omega) = \omega - \xi_{k} \), and the second-order dressed fermion self-energy from the dressed spinon pair bubble.

\[
\Sigma^{(a)}(k, \omega) = \frac{1}{2} Z^{2} \sum_{n_{F}} \sum_{p} \gamma_{k}^{2}(k, p, q, \omega) \sum_{n_{F}} B_{q+p} B_{q} \times \left( F^{(a)}(k, p, q) + F^{(a)}(k, q, p) \right) \left( \omega + \omega_{q+p} - \omega_{q} - \xi_{k} \right) + \left( F^{(a)}(k, p, q) + F^{(a)}(k, q, p) \right) \left( \omega + \omega_{q+p} - \omega_{q} - \xi_{k} \right),
\]
the experimental result in Fig. 1 (inset). This conductivity spectrum shows (dash-dotted line) for parameters $t/J = -2.5$, $t'/t = 0.15$ at temperature $T = 0$ are shown in Fig. 1, where the charge $e$ has been set as the unit. For a comparison, the experimental result$^{11}$ of Nd$_{2-\delta}$Ce$_\delta$CuO$_4$ is also plotted in Fig. 1 (inset). This conductivity spectrum shows a pseudogap structure, where a low-energy peak appears at $\omega \sim 0$, which decays rapidly, and a rather sharp mid-infrared peak appears around $\omega \sim 0.3 | t |$, which is in contrast to the case for the hole-doped cuprates, where a broad distribution of the spectral weight of the mid-infrared band is observed$^{14,15}$. Since the spectral function (then full dressed fermion Green’s function) in the optical conductivity (5) is obtained by considering the second-order corrections due to the dressed spinon pair bubble, then our present results reflect that the AF spin correlation in the electron-doped case is stronger than that in the hole-doped case, and the pseudogap structure or very sharp midinfrared peak is closely related to the strong AF spin correlations. This is consistent with the results from numerical simulations$^{21}$, where the pseudogap structure in the electron-doped cuprates is very sensitive to not only $J$, but also $t'$. Although $t'$ does not change spin configuration, it can enhance the AF correlation in the electron-doped cuprates. With increasing the value of $t'/t$, the gap increases in energy$^{21}$. Moreover, the unusual midinfrared peak is electron doping dependent, and the component increases with increasing electron doping for $0.08 | t | < \omega < 0.5 | t |$, and is nearly independent of electron doping for $\omega > 0.5 | t |$. This reflects an increase in the mobile carrier density, and indicates that the spectral weight of the midinfrared sidepeak is taken from the Drude absorption, then the spectral weight from both low energy peak and midinfrared peak represent the actual free-carrier density. For a better understanding of the optical properties of the electron-doped cuprates, we have studied the conductivity at different temperatures, and the results at $\delta = 0.10$ for $t/J = -2.5$ and $t'/t = 0.15$ with $T = 0$ (solid line), $T = 0.1J$ (dashed line), and $T = 0.2J$ (dash-dotted line) are plotted in Fig.$^{2}$ 2 in comparison with the experimen-

\[
\frac{\alpha \chi_1^2}{2} + \alpha \lambda_1 \lambda_2 (C_3 + \epsilon \chi_2)/2, \quad A_5 = -3\alpha \lambda_1^2 \chi_2/(2Z) + \alpha \lambda_1 \lambda_2 (\chi_1^2 + \epsilon \chi_1/2 + C_5^2), \quad A_6 = \lambda_2^2 \chi_2/(4Z) - \alpha \chi_1^2/(2Z) + \epsilon^2 (\alpha \chi_1 + \epsilon \chi_1/2 - \alpha \chi_1^2/2) + \lambda_2^2 (\alpha C_2 + (1-\alpha)/(2Z) - \alpha \chi_1^2/2) - \alpha \lambda_1 \lambda_2 C_3, \quad \text{and the spinon correlation functions} \quad \chi_i^2 = \langle S_i^z S_{i+\eta}^z \rangle, \quad \chi_2 = \langle S_i^z S_{i+\eta}^z \rangle, \quad C_1 = (1/Z^2) \sum_q \eta_q \langle S_{i+q}^z S_{i+q+\eta}^z \rangle, \quad C_1^z = (1/Z^2) \sum_{q,\eta} \langle S_{i+q}^z S_{i+q+\eta}^z \rangle, \quad C_2 = (1/Z^2) \sum_{q,\eta} \langle S_{i+q}^z S_{i+q+\eta}^z \rangle, \quad C_3 = (1/Z) \sum_{\eta} \langle S_{i+q}^z S_{i+q+\eta}^z \rangle, \quad C_3^z = (1/Z) \sum_{r,\eta} \langle S_{i+q}^z S_{i+q+\eta}^z \rangle. \]

In order to satisfy the sum rule for the correlation function $\langle S_i^z S_{i+\eta}^z \rangle = 1/2$ in the absence of AFLRO, a decoupling parameter $\alpha$ has been introduced in the MF calculation, which can be regarded as the vertex correction$^{18,19}$. All these mean-field order parameters, decoupling parameter, and the chemical potential are determined self-consistently$^{18}$.

The optical conductivity measurement is a powerful probe for interacting electron systems$^{20}$, and can provide very detailed knowledges about the low-energy excitations as electrons are doped to Mott insulators. We have performed a numerical calculation for the optical conductivity in Eq. (5), and the results at electron doping $\delta = 0.10$ (solid line), $\delta = 0.12$ (dashed line), and $\delta = 0.15$ (dash-dotted line) for parameters $t/J = -2.5$ and $t'/t = 0.15$ at temperature $T = 0$ are shown in Fig. 1, where the charge $e$ has been set as the unit. For a comparison, the experimental result$^{11}$ of Nd$_{2-\delta}$Ce$_\delta$CuO$_4$ is also plotted in Fig. 1 (inset). This conductivity spectrum shows a pseudogap structure, where a low-energy peak appears at $\omega \sim 0$, which decays rapidly, and a rather sharp mid-infrared peak appears around $\omega \sim 0.3 | t |$, which is in contrast to the case for the hole-doped cuprates, where a broad distribution of the spectral weight of the mid-infrared band is observed$^{14,15}$. Since the spectral function (then full dressed fermion Green’s function) in the optical conductivity (5) is obtained by considering the second-order corrections due to the dressed spinon pair bubble, then our present results reflect that the AF spin correlation in the electron-doped case is stronger than that in the hole-doped case, and the pseudogap structure or very sharp midinfrared peak is closely related to the strong AF spin correlations. This is consistent with the results from numerical simulations$^{21}$, where the pseudogap structure in the electron-doped cuprates is very sensitive to not only $J$, but also $t'$. Although $t'$ does not change spin configuration, it can enhance the AF correlation in the electron-doped cuprates. With increasing the value of $t'/t$, the gap increases in energy$^{21}$. Moreover, the unusual midinfrared peak is electron doping dependent, and the component increases with increasing electron doping for $0.08 | t | < \omega < 0.5 | t |$, and is nearly independent of electron doping for $\omega > 0.5 | t |$. This reflects an increase in the mobile carrier density, and indicates that the spectral weight of the midinfrared sidepeak is taken from the Drude absorption, then the spectral weight from both low energy peak and midinfrared peak represent the actual free-carrier density. For a better understanding of the optical properties of the electron-doped cuprates, we have studied the conductivity at different temperatures, and the results at $\delta = 0.10$ for $t/J = -2.5$ and $t'/t = 0.15$ with $T = 0$ (solid line), $T = 0.1J$ (dashed line), and $T = 0.2J$ (dash-dotted line) are plotted in Fig. 2 in comparison with the experimen-

\[\text{FIG. 1. The conductivity of electron-doped cuprates at } \delta = 0.10 \text{ (solid line), } \delta = 0.12 \text{ (dashed line), and } \delta = 0.15 \text{ (dash-dotted line) for } t/J = -2.5 \text{ and } t'/t = 0.15 \text{ with } T = 0. \text{ Inset: the experimental result on Nd$_{2-\delta}$Ce$_\delta$CuO$_4$ taken from Ref.$^{11}$.}
\]

\[\text{FIG. 2. The conductivity of electron-doped cuprates at } \delta = 0.10 \text{ for } t/J = -2.5 \text{ and } t'/t = 0.15 \text{ with } T = 0 \text{ (solid line), } T = 0.1J \text{ (dashed line), and } T = 0.2J \text{ (dash-dotted line). Inset: the experimental result on Nd$_{2-\delta}$Ce$_\delta$CuO$_4$ taken from Ref.$^{11}$.}
\]
nal data\textsuperscript{11} taken from Nd$_{2-x}$Ce$_x$CuO$_4$ (inset). Our results show that the conductivity spectrum is temperature dependent for $\omega < 0.5 \mid t \mid$, and almost temperature independent for $\omega > 0.5 \mid t \mid$. The component in the low energy region increases with increasing temperatures, then there is a tendency towards the Drude-like behavior, while the unusual midinfrared peak is severely suppressed with increasing temperatures, and vanishes at high temperatures. This reflects that the spin correlation rapidly decreases with increasing temperature. These results are in qualitative agreement with experiments\textsuperscript{11} and the numerical simulations\textsuperscript{21}. As in the hole-doped cuprates, the charge transport is governed by the dressed fermion scattering, therefore $\delta$ dressed fermions are responsible for the optical conductivity, i.e., the optical conductivity in the electron-doped cuprates is carried by $\delta$ electrons. Since the strong electron correlation is common for both hole- and electron-doped cuprates, these similar behaviors observed from the optical conductivity are expected.

The quantity which is closely related to the conductivity is the resistivity, which can be obtained as $\rho(T) = 1/\lim_{\omega \rightarrow 0} \sigma(\omega)$. This resistivity has been calculated numerically, and the results for $t/J = -2.5$ and $t'/t = 0.15$ at $\delta = 0.09$ (solid line) and and $\delta = 0.15$ (dashed line) are plotted in Fig. 3, in comparison with the experimental data\textsuperscript{8} taken from Nd$_{2-x}$Ce$_x$CuO$_4$ (inset). It is shown obviously that the resistivity is characterized by a crossover from the high temperature metallic-like to low temperature insulating-like behavior in the relatively low doped regime, and a metallic-like behavior in the relatively high doped regime. But even in the relatively low doped regime, the resistivity exhibits the metallic-like behavior over a wide range of temperatures, which also is in qualitative agreement with experiments\textsuperscript{11,8}.

The physical interpretation to the above obtained results is very similar to these in the hole-doped case\textsuperscript{14,15}, since the $t$-$t'$-$J$ model in both hole- and electron-doped cuprates is characterized by a competition between the kinetic energy and magnetic energy, with the magnetic energy favors the magnetic order for spins, while the kinetic energy favors delocalization of electrons and tends to destroy the magnetic order. However, it needs more kinetic energy to drive the motion of charged carriers in the electron-doped case since the strong spin correlation. In the charge-spin separation fermion-spin theory, although both dressed fermions and spinons contribute to the charge dynamics, the dressed fermion scattering dominates the charge dynamics\textsuperscript{14,15}, where the dressed fermion scattering rate is obtained from the full dressed fermion Green’s function (then the dressed fermion self-energy and spectral function) by considering the dressed fermion-spinon interaction. In this case, the crossover from the high temperature metallic-like to low temperature insulating-like behaviors in the relatively low electron-doped regime, and the metallic-like behavior in the relatively high electron-doped regime in the resistivity is closely related to this competition between the kinetic energy and magnetic energy. In lower temperatures, the dressed fermion kinetic energy is much smaller than the magnetic energy in the relatively low electron-doped regime, then the magnetic fluctuation is strong enough to severely reduce the dressed fermion scattering and thus is responsible for the insulating-like behavior in the resistivity. With increasing temperatures, the dressed fermion kinetic energy is increased, while the dressed spinon magnetic energy is decreased. In the region where the dressed fermion kinetic energy is much larger than the dressed spinon magnetic energy at higher temperatures or relatively high electron-doped regime, the dressed fermion scattering would give rise to the metallic-like resistivity.

In summary, we have studied the doping dependence of the charge dynamics in the electron-doped cuprates within the $t$-$t'$-$J$ model. The optical conductivity spectrum shows an unusual pseudogap structure with a low-energy peak appearing at $\omega \sim 0$ and an rather sharp midinfrared peak appearing around $\omega \sim 0.3 \mid t \mid$, and the resistivity exhibits a crossover from the high temperature metal-like to low temperature insulating-like behavior in the relatively low electron-doped regime, and a metallic-like behavior in the relatively high electron-doped regime. Our results also show that the unusual pseudogap structure is intriguingly related to the strong AF correlation in the system.

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