Current-current correlations in the three-band model for two-leg CuO ladders: Density-matrix renormalization group study

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We study current-current correlations in the three-band Hubbard model for two-leg CuO ladders using the density-matrix renormalization group method. We find that these correlations decrease exponentially with distance for low doping but as a power law for higher doping. Their pattern is compatible with the circulating current (CC) phase which Varma has proposed to explain the pseudogaped metallic phase in underdoped high-temperature superconductors. However, for model parameters leading to a realistic ground state in the undoped ladder, the current fluctuations decay faster than the *d*-wavelike pairing correlations in the hole-doped state, at least up to a doping of 10%. Thus we conclude that no phase with CC order or dominant CC fluctuations occur in the three-band model of two-leg CuO ladders at low doping.

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Since the discovery of the high-temperature superconducting copper oxide compounds, the anomalous behavior of the contiguous "pseudogap" phase has been considered a key to understanding the superconductivity mechanism in these materials. However, the nature of the pseudogap transition and its order parameter remained a puzzle. Early μSR experiments[1] on $YBa_2Cu_3O_{6+x}$ crystals showed evidences for the onset of spontaneous static magnetic fields near what was called the pseudogap crossover temperature $T^*(x)$. In addition, different photocurrents for left- and right-circularly polarized photons in angle-resolved photoemission spectroscopy[2] were reported for $Bi_2Sr_2CaCu_20_{8+\delta}$. Now recent polarized neutron scattering[3] and Kerr effect[4] measurements on $YBa_2Cu_3O_{6+x}$ provide new evidence that there is a pseudogap phase associated with a novel magnetic transition. The neutron-scattering experiments observe a phase characterized by a magnetic order which does not break translational symmetry and the polar Kerr studies find the phase transition at $T^*(x)$ which breaks time-reversal symmetry. There is at present no agreement regarding a theory which encompasses all of these observations.

Theoretically, ground states, in which circulating currents (CC) form spontaneously and thus break the time-reversal symmetry, have been found in several models[5] but in the more realistic *t-J* model the current-current correlations decrease exponentially fast on a two-leg ladder.[6] However, Varma has argued[7] that the minimal model for a CC state is a doped three-band Hubbard-type model with one Cu *d* orbital, one O p_x orbital, and one O p_y orbital per unit cells. Using a mean-field approach he has found that a CC ground state is possible in this model if the Cu-O hopping integral t_{pd} is of the same order of magnitude as the nearest-neighbor Coulomb interaction V_{pd} between the Cu and the O orbitals and larger than the energy difference Δ_{pd} between these orbitals. This CC state, which breaks time-reversal symmetry but not translational symmetry, is consistent with the neutron-scattering experiments but further additions[8] to the model are required to obtain results compatible with the orientation of the moments and the Kerr rotation results. Moreover, since the interaction between particles is strong, the mean-field approach cannot reliably determine if a CC phase really exists in the three-band model.

Several studies of this model have been carried out to check Varma's theory using methods for strongly correlated systems. Power-law current-current correlations have been observed in CuO chains.[9] A related "staggered flux" phase but no CC phase has been found in the weak- and strong-coupling phase diagram of undoped two-leg ladders.[10] Recently, a phase with dominant orbital current fluctuations has been reported in the weak-coupling phase diagram of doped two-leg ladders.[11] Also, a stabilization of orbital currents by apical oxygen atoms has been suggested.[12] However, exact diagonalizations of small square clusters[13] show no evidence for CC patterns in the ground state. Thus, the existence of a CC order or dominant CC fluctuations in the three-band model is still an open question.

In this paper we supplement our previous studies of the three-band model for two-leg CuO ladders[14,15] by an analysis of the current-current correlation functions in doped systems for various parameters Δ_{pd} and V_{pd}. The hole Hamiltonian for this model is given by

$$\begin{aligned} H = & -t_{pd}\sum_{\langle ij\rangle\sigma}(d^\dagger_{i\sigma}p_{j\sigma}+p^\dagger_{j\sigma}d_{i\sigma}) - t_{pp}\sum_{\langle ij\rangle\sigma}(p^\dagger_{i\sigma}p_{j\sigma}+p^\dagger_{j\sigma}p_{i\sigma}) \\ & + U_d\sum_i d^\dagger_{i\uparrow}d_{i\uparrow}d^\dagger_{i\downarrow}d_{i\downarrow} + U_p\sum_i p^\dagger_{i\uparrow}p_{i\uparrow}p^\dagger_{i\downarrow}p_{i\downarrow} \\ & + V_{pd}\sum_{\langle ij\rangle\sigma\sigma'} p^\dagger_{i\sigma}p_{i\sigma}d^\dagger_{j\sigma'}d_{j\sigma'} + \Delta_{pd}\sum_{i\sigma} p^\dagger_{i\sigma}p_{i\sigma}, \end{aligned} \tag{1}$$

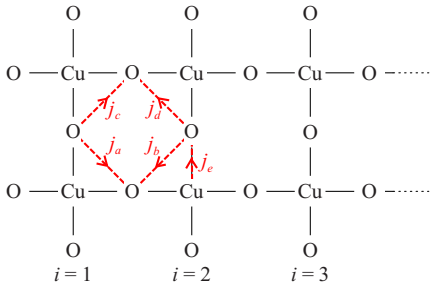

FIG. 1. (Color online) Schematic lattice structure of a two-leg CuO ladder. $j_r(r=a,b,c,d,e)$ denote various local-current operators considered in this work. i is the rung index.

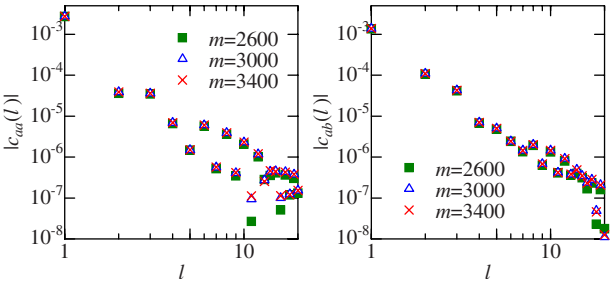

FIG. 2. (Color online) Log-log plot of the correlation functions $|c_{aa}(l)|$ and $|c_{ab}(l)|$ versus l at $\Delta_{pd}=3$, $V_{pd}=1$, and $y=0.9$ for several values of m.

where the operators $d^{\dagger}_{i\sigma}$ and $p^{\dagger}_{i\sigma}$ create holes with spin σ in the Cu d orbitals and the O p orbitals, respectively. The geometry of the two-leg CuO ladder is illustrated in Fig. 1, where the rung and leg O sites represent p_y and p_x orbitals, respectively. The first and fifth sums are over all nearest-neighbor Cu-O pairs while the second sum is over all nearest-neighbor p_x-p_y pairs on O sites. The index i runs over all Cu sites in the third term and over all O sites in the fourth and sixth sums. t_{pd} is the hopping integral between nearest-neighbor Cu and O sites (solid lines in Fig. 1) and t_{pp} is the hopping integral between nearest-neighbor p_x-p_y pairs on O sites. We have chosen the phases of the orbitals such that the signs of the hopping matrix elements are constant. With the minus sign convention of Eq. (1) one has $t_{pd}>0$ and $t_{pp}\geq 0$. U_d and U_p are the on-site Coulomb energies for Cu and O sites, respectively. We will work in units where $t_{pd}=1$ and use the typical values $t_{pp}=0.5$, $U_d=8$, and $U_p=3$, throughout.[16] In this model an undoped CuO ladder corresponds to a density of one hole per Cu site. The hole concentration per Cu atom is $x=1+y$ with the doping rate $y=N/(2L)$, where N is the number of doped holes ($N>0$, $y>0$) or doped electrons ($N<0, y<0$) in a ladder with $L\times 2$ Cu atoms.

In this work correlation functions are calculated numerically using the density-matrix renormalization group (DMRG) method.[17,18] As in Ref. 13 we define current-current correlations

$$c_{rs}(i_1,i_2)=\langle j_r(i_1)j_s(i_2)\rangle \tag{2}$$

of various local currents j_r between nearest-neighbor O sites or nearest-neighbor Cu-O pairs which are illustrated in Fig. 1. We have used up to $m=3400$ density-matrix eigenstates to build the DMRG basis and the maximum truncation error, i.e., the discarded weight, is 1×10^{-6}. The DMRG ground-state energy is estimated to be accurate to parts in $10^{-2}t_{pd}$ or better for ladders with open-boundary conditions and up to 40×2 Cu sites [corresponding to a total of 282 sites (Cu or O)]. In order to check the accuracy of our calculations, the DMRG results of $c_{aa}(l)$ and $c_{ab}(l)$ are plotted in Fig. 2 as a function of the distance $l=|i_2-i_1|$ for $\Delta_{pd}=3$, $V_{pd}=1$, and $y=0.9$. We can see that the correlation functions are well converged at $m\geq 3000$.

We have not found any long-range-ordered current patterns for any set of the model parameters that we have investigated. Current-current correlations always decay faster than $1/l$ as a function of distance $l=|i_2-i_1|$ in the present two-leg ladder system. Despite the absence of long-range order we can search for patterns in the sign of the correlation functions c_{rs}. Close to the ladder ends these signs fluctuate as widely as in small square clusters.[13] In the middle of long enough ladders, however, the sign of a given function c_{rs} does not change with the distance $l=|i_2-i_1|$. In that case, the relative phases of the current-current correlations for various directions are compatible with the translationally invariant CC pattern θ_I proposed by Varma.[7] This differs from the weak-coupling renormalization group (RG) result[11] in which the current-current correlations are expected to have a $Q=2k_F$ oscillation. We observe a dominant $Q=0$ term and a weaker $Q\approx 2k_F$ contribution in the correlation function but our data set is restricted to short distances (≤ 20 unit cells). It is possible that the $Q\approx 2k_F$ oscillation could dominate at truly long distances. We conclude that two-leg CuO ladders have CC-like current fluctuations.

The various correlation functions c_{rs} show a qualitatively similar dependence on the interaction parameters and the hole concentration. Therefore, we will discuss only $c_1=c_{aa}$ hereafter. As open boundary conditions are used, the correlation functions $c_1(l)=c_{aa}(i_1,i_2)$ have been calculated using distances $l=|i_1-i_2|$ taken about the midpoint of the ladders (i.e., the integer part of $\frac{i_1+i_2}{2}$ equals $L/2$). We only show results for $l\lesssim L/2=20$ which have been obtained in ladders with 40×2 Cu atoms, so that edge effects are small.

We first investigate the evolution of the current-current correlations upon doping. Some results for $c_1(l)$ versus l are shown in Fig. 3 for various hole concentrations x. Although there are substantial differences between hole-doped and electron-doped two-leg ladders in the three-band model,[14] we have found that the current-current correlations are qualitatively similar in both cases. In systems doped with two holes or two electrons these correlations decay exponentially with distance (see the inset of Fig. 3). This behavior can be seen for all interaction parameters that we have used. In ladders doped with at least four electrons or holes ($|y|\geq 5\%$), however, we have found that current-current correlation functions exhibit an approximate power-law decay $l^{-\nu}$ with $1<\nu\leq 2$ for $l\gtrsim 3$. The overall magnitude of the correlation function $|c_1(l)|$ is larger for six or eight doped particles than for four doped particles We therefore conclude that current-current fluctuations are enhanced upon doping in agreement with the weak-coupling RG results.[11]

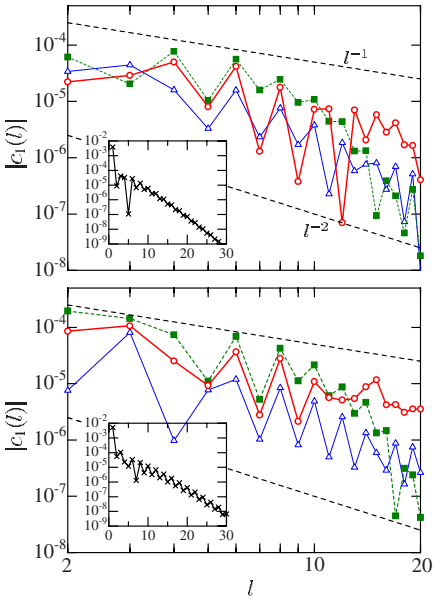

FIG. 3. (Color online) Log-log plot of the correlation function $|c_1(l)|$ versus l for an electron-doped (top panel) and a hole-doped (bottom panel) ladder with $\Delta_{pd}=3$ and $V_{pd}=0$. Triangles, squares, and circles correspond to four, six, and eight doped particles ($|y|=5,7.5,10\%$), respectively. Lines are guides for the eyes. The dashed lines have slope −1 and −2. Inset: semilog plot of $|c_1(l)|$ for a ladder doped with two particles ($|y|=2.5\%$).

We next turn to the effect of the Coulomb interaction V_{pd} between nearest-neighbor Cu and O sites. Figure 4 shows the current-current correlation function $|c_1(l)|$ versus l for $V_{pd}=0,1,2$. (A recent *ab initio* calculation[19] suggests that $V_{pd}\sim 1-1.5$ is appropriate for cuprates.) The doping is $|y|=10\%$ (eight doped electrons or holes) which is close to the optimal doping in high-temperature superconducting cuprates. We see that the results are similar for hole and electron doping and do not substantially change as a function of V_{pd}. Although the overall amplitude of $|c_1(l)|$ is slightly reduced by increasing V_{pd}, its order of magnitude does not change from $V_{pd}=0$ to 2.

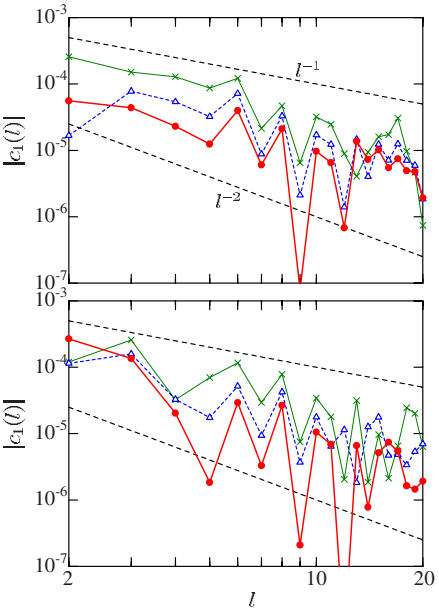

FIG. 4. (Color online) Correlation function $|c_1(l)|$ versus l for an electron-doped (top panel) and a hole-doped (bottom panel) ladder ($|y|=10\%$) with $\Delta_{pd}=2$. Crosses, triangles, and circles correspond to $V_{pd}=0$, 1, and 2, respectively. Lines are guides for the eyes. Dashed lines have slope −1 and −2.

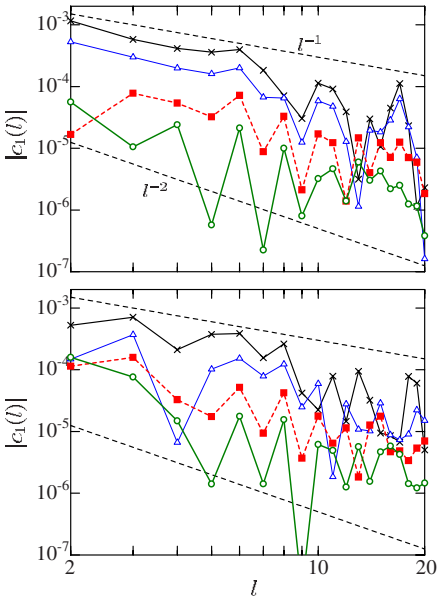

FIG. 5. (Color online) Correlation function $|c_1(l)|$ versus l for an electron-doped (top) and a hole-doped (bottom) ladder ($|y|=10\%$) with $V_{pd}=1$. Crosses, triangles, squares, and circles correspond to $\Delta_{pd}=0$, 1, 2, and 3, respectively. Lines are guides for the eyes. Dashed lines have slope −1 and −2.

The current-current correlation depends more significantly on the energy difference Δ_{pd} than on the Coulomb repulsion V_{pd}. In Fig. 5, we show $|c_1(l)|$ versus l for several values of Δ_{pd}. While it has been generally accepted[16] that $\Delta_{pd}=2-3$, Varma has proposed[7] that the CC patterns are stabilized only when $\Delta_{pd}\lesssim\mathcal{O}(t_{pd})$. We have indeed found that the amplitude of the current-current correlations decreases with increasing Δ_{pd}. For $\Delta_{pd}=3$, $|c_1(l)|$ is an order of magnitude smaller than for $\Delta_{pd}=0$.

Our data show that the overall amplitude of current fluctuations (for $l\leq 20$) increases with doping, decreases markedly with increasing $\Delta_{pd}\leq 3$ but is little affected by V_{pd}. However, to understand the long-range behavior of power-law correlations, it is necessary to investigate the variations of their exponent ν. We have estimated ν by fitting our numerical data for the correlation function $|c_1(l\geq 2)|$ to a function $Al^{-\nu}$, where both A and ν are fit parameters. As an illustration Fig. 6(a) shows two such fits: The first one corresponds to a rapid decay ($\nu\approx 2$) of the current-current correlations while the second one yields one of the smallest exponent, $\nu\approx 1.2$, that we have found. As we use data for short distances $l\leq 20$ only and the correlation functions oscillate widely, the fitted values of ν are not quantitatively accurate. Nevertheless, we think that the variations of the fitted exponent ν give a qualitative indication of the variations in the long-range behavior of the corresponding corre-

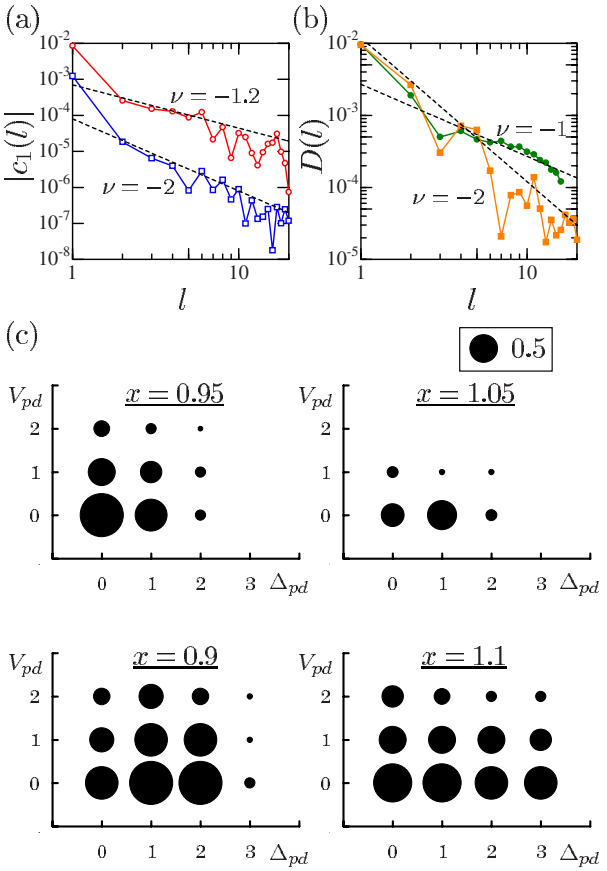

FIG. 6. (Color online) Correlation function (a) $|c_1(l)|$ for $(\Delta_{pd}, V_{pd}, x)=(2,0,0.9)$ (circle) and (3,2,0.95) (square) and (b) $D(l)$ for $(\Delta_{pd}, V_{pd}, x)=(3,0,0.95)$ (circle) and (1,1,0.9) (square). The dashed lines are the fitted functions $Al^{-\nu}$. (c) Fitted values of ν in the parameter space (Δ_{pd}, V_{pd}) for various hole concentrations x. The radius of the solid circles is proportional to $2-\nu$.

lation functions. For comparison, in Fig. 6(b) we show the Cu rung-rung pair field correlation function

$$D(l) = \langle \Delta_{i+l} \Delta_i^\dagger \rangle \tag{3}$$

with

$$\Delta_i^\dagger = d_{i1\uparrow}^\dagger d_{i2\downarrow}^\dagger - d_{i1\downarrow}^\dagger d_{i2\uparrow}^\dagger. \tag{4}$$

Here, $d_{i\lambda s}^\dagger$ creates an electron of spin s on the ith rung and the $\lambda=1$ or 2 leg of the ladder.

Figure 6(c) shows the fitted values of $2-\nu$ for the current-current correlations $c_1(l)$ in the parameter space (Δ_{pd}, V_{pd}) for several hole concentrations. (We use the deviation of the exponent from its value in a Fermi sea, $2-\nu$, as a measure of the strength of current-current correlations.) Two clear trends can be observed both for electron and hole dopings: the current fluctuations decrease faster for low doping $|y|=5\%$ than for high doping $|y|=10\%$ and ν increases with the nearest-neighbor coupling V_{pd}. This suppression of the current correlations by V_{pd} appears to be consistent with the phase diagram found in the weak-coupling RG analysis.[11] The dependence of ν on the energy difference Δ_{pd} is irregular but a large value $\Delta_{pd} \geq 3$ results in a rapid decay of current-current correlation functions. The smallest exponent $\nu \approx 1.2$ is found around $\Delta_{pd}=1-2$ for electron doping. For hole doping, however, the smallest exponent $\nu \approx 1.3$ is found for $\Delta_{pd}=0-1$.

In our previous work[14] we studied the pairing correlations in the three-band model for two-leg CuO ladders. We found that electron- and hole-doped systems exhibit d-wavelike power-law pairing correlations. Therefore, the three-band model at low doping ($|y| \lesssim 2.5\%$) and the t-J model have similar properties: power-law pairing correlations and exponentially decaying current fluctuations.[6] At high enough doping, however, both pairing and current power-law fluctuations seem to coexist in the three-band model. Comparing fitted exponents for the current and pairing correlation functions in hole-doped ladders ($5 \leq y \leq 10\%$), we find that pairing correlations always dominate (i.e., decay significantly slower) with an exponent close to 1 for $\Delta_{pd} \geq 2$ while current correlations dominate only in a small region of parameter space ($\Delta_{pd} \leq 2$, $V_{pd} \leq 1$) at the highest doping rate investigated ($y=10\%$), where pairing correlations decay as l^{-2} [see Fig. 6(b)]. Thus in the hole-doped three-band model on two-leg ladders, there is a region of enhanced and apparently dominant current fluctuations in agreement with the weak-coupling RG analysis.[11]

For these parameters, however, we showed in our previous study[14] that the undoped ladder has only very small charge and spin gaps (which probably vanish in the limit of infinitely long ladders). Moreover, local spin moments are not formed on the Cu sites as holes are not localized on those sites at any doping and thus there is no tendency toward (short-range) antiferromagnetic order between the Cu sites. Therefore, in the regime of the three-band model, where dominating current fluctuations are found in two-leg ladders, the undoped system is a paramagnetic metal or small-gap insulator. In the regime of the three-band model where undoped ladders are "antiferromagnetic" insulators (see Ref. 14) current fluctuations are not enhanced ($\nu \approx 2$) or decay faster than pairing correlations for hole doping $y \leq 10\%$. We conclude that no phase with CC order or dominating CC fluctuations occurs in the three-band model on an underdoped two-leg ladder with realistic parameters for cuprate compounds.

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