Superconducting, magnetic, and charge correlations
in the doped two-chain Hubbard model

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Abstract

We have studied the superconducting, magnetic and charge correlation functions and the spin excitation spectrum in the doped two chain Hubbard model by projector monte carlo and Lanczos diagonalization methods. The exponent of the interchain singlet superconducting correlation function, $\gamma$, is found to be close to $2.0$ as long as two distinct non-interacting bands cross the Fermi level. Magnetic and charge correlation functions decay more rapidly than or as fast as the interchain singlet superconducting correlation function along the chains. The superconducting correlation in the doped two chain Hubbard model is the most long range correlation studied here. Implications of the results for the possible universality class of the doped two chain Hubbard model are discussed.

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I. INTRODUCTION

In relation to possible superconductivity in the two dimensional Hubbard model \cite{1-5}, the two chain Hubbard model and/or the two chain t-J model, which may be realized in oxygen deficient Sr_{n-1}Cu_{n+1}O_2n \cite{6} have attracted much interest recently. Although superconductivity has not yet been observed in this material, it may be worthwhile to study these models because they may make it possible for us to understand dimensional crossover between one and two dimensions. Information obtained in them may be of help in understanding the two dimensional models. The two dimensional models are more difficult to study than the one dimensional models and the two chain models. Though direct studies of the two dimensional models \cite{1-5} are also very important, here we follow the argument in Refs. \cite{7-9} and study the doped two chain Hubbard model, which is defined by the following Hamiltonian:

\[
H = -t_\parallel \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.C.) + U \sum_i n_{i\uparrow}^c n_{i\downarrow}^c \\
- t_\parallel \sum_{\langle i,j \rangle, \sigma} (d_{i\sigma}^\dagger d_{j\sigma} + H.C.) + U \sum_i n_{i\uparrow}^d n_{i\downarrow}^d \\
- t_\perp \sum_{i \sigma} (c_{i\sigma}^\dagger d_{i\sigma} + H.C.).
\]

(1)

We take \( t_\parallel = 1.0 \) and adopt it as the unit of energy hereafter. Diagonalization studies of the doped two chain models suggest that the superconducting correlation function may be rather long range. \cite{7,10} The cluster size accessible by the Lanczos method is obviously too small compared with the superconducting correlation length in these models to make a convincing conclusion. The problem should be examined with more sophisticated methods in computational physics without any approximation and with sufficiently large system size.

The recently developed density-matrix real space numerical renormalization group method has been applied to study the long range superconducting correlation in the doped two chain Hubbard model. \cite{9} The authors concluded that there is an enhancement of the superconducting correlation function over the non-interacting case on up to as large as \( 32 \times 2 \) system sizes when \( t_\perp = 1.5, U = 8.0 \) at \( N_e/N_s = 0.875 \) filling, where \( N_e \) and \( N_s \) are the num-
ber of electrons and the number of sites, respectively. They also have found persistence of
the spin gap after doping with the same parameter values.

Though their method seems to be quite useful at least in some of one dimensional spin
systems, we take here a different approach to study some interesting phases of the doped two
chain Hubbard model. For most of this article we adopt the projector quantum monte carlo
method. While the method is quite useful to our model in the small-U region, the method
currently has difficulty in the large-U region due to the fermion sign problem. Our strategy
here is to derive reliable results in the small-U region, which still has not been explored as well
as to get some preliminary information in the large-U region. The similarity or dissimilarity
of the two regions should be of great interest. So long as each numerical method has both
pros and cons, the author believes that the problem should be approached with various
numerical techniques.

II. STATIC AND DYNAMIC CORRELATION FUNCTIONS

Here we study singlet superconducting \( < O_i O_j^\dagger > \), magnetic \( < S_i^z S_j^z > \) and charge
\( < n_i n_j > - < n >^2_{ave} \) correlation functions and dynamic spin correlation function \( S^{zz}(\vec{k}, \omega) \)
in the ground state of the doped two chain Hubbard model. We have employed the projector
monte carlo method to study the interchain singlet superconducting correlation function
\( < O_i O_j^\dagger > \), where

\[
O_j^\dagger = \frac{1}{\sqrt{2}}(c_{j\uparrow}^\dagger d_{j\downarrow}^\dagger - c_{j\downarrow}^\dagger d_{j\uparrow}^\dagger),
\]

(2)
magnetic \( < S_i^z S_j^z > \) and charge \( < n_i n_j > - < n >^2_{ave} \) correlation functions, where

\[
S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})
\]

(3)
and

\[
n_i = n_{i\uparrow} + n_{i\downarrow}
\]

(4)
and the Lanczos and the recursion methods to study \( S^{zz}(\vec{k}, \omega) \):
\[ S^{zz}(\vec{k}, \omega) = -\frac{1}{N\pi} \text{Im} G(\vec{k}, E_0 + \omega + i\eta), \] (5a)

\[ G(\vec{k}, x) = \langle \psi_0 | (S^z_{\vec{k}})^\dagger (x - H)^{-1} S^z_{\vec{k}} | \psi_0 \rangle. \] (5b)

We have adopted periodic boundary condition throughout this article. 36 \times 2 and 24 \times 2 lattices were used for projector monte carlo calculations. A 6 \times 2 lattice was used for Lanczos and recursion calculations. The projecting time \( \tau = 10.0 \) and \( \tau = 1.5 \) in units of \( t_\parallel \) were used for \( U = 2.0 \) and \( U = 6.0 \), respectively, in the projector monte carlo calculations. We have adopted the unrestricted Hartree-Fock (UHF) wavefunction as a trial function of the projector monte carlo calculation here. Details of these methods should be looked up in the previous papers and references cited therein. \[4,5\] The two chain Hubbard model with various parameter sets at 0.833 filling \( (N_e/N_s = 0.833) \) is studied here. The singlet superconducting correlation function in the non-interacting case is given by:

\[ \langle O_i O_j^\dagger \rangle_{U=0} = \frac{1}{8\pi^2 l^2 \gamma} [2 - \cos(2k_f(0)l) - \cos(2k_f(\pi)l)], \] (6)

where \( k_f(0) = \cos^{-1}(t_\perp + \mu)/2 \), \( k_f(\pi) = \cos^{-1}(t_\perp - \mu)/2 \) and \( \gamma = 2 \), when \( U = 0.0 \). The upper bound of \( \langle O_i O_j^\dagger \rangle \) in the non-interacting case is given by \( 0.05 R_{ij}^{-2} \), where \( l \) and \( R_{ij} \) are distance between the i-th and j-th sites.

First of all, we study long-range behaviors of some of static correlation functions in small-U region of the model. \( \langle O_i O_j^\dagger \rangle \) when \( t_\perp = 1.5, U = 2.0 \) and \( t_\perp = 2.5, U = 2.0 \) were calculated and they are plotted along with the upper bound of the non-interacting case in Fig.\[4\]. It should be noted that while two distinct bands cross the Fermi level when \( t_\perp = 0.5, U = 0.0 \) and \( t_\perp = 1.5, U = 0.0 \), one of them is raised in energy and does not cross the Fermi level when \( t_\perp = 2.5, U = 0.0 \). The correlation function with \( t_\perp = 2.5, U = 2.0 \) is strongly suppressed from the non-interacting one, which does not contradict the result obtained from the more general superconducting correlation function. \[4\] The suppression may originate from the separation of the bands. The correlation function with \( t_\perp = 1.5, U = 2.0 \) is somewhat enhanced or remains comparable to the non-interacting correlation function. This parameter region should be examined more carefully.
The superconducting correlation function $\langle O_iO_j^\dagger \rangle$ with $t_\perp = 1.5, U = 2.0$ was replotted along with the upper bound of the non-interacting case on a log-log scale in Fig. 3. The correlation function has inversion symmetry at the inversion center: $|i - j| = 17.5$. We show only the left hand side of the function. Though the correlation function itself is somewhat enhanced over the non-interacting one, the exponent of the correlation function $\gamma$ remains close to that of the non-interacting case: 2.0.

At this stage, we compare the long range behaviors of the interchain singlet superconducting, magnetic and charge correlation functions. We have calculated these correlation functions with $t_\perp = 1.5, U = 2.0$ in $24 \times 2$ lattice and plotted them in Fig. 3. As mentioned earlier, $\langle O_iO_j^\dagger \rangle$ scales as $0.05R_{ij}^{-2}$. The data points of the magnetic $\langle S_i^xS_j^z \rangle$ and charge $\langle n_in_j \rangle - \langle n \rangle^2_{\text{ave}}$ correlation functions are found between $\pm 0.05R_{ij}^{-2}$ and that means the magnetic and the charge correlation functions decay more rapidly than or as fast as the interchain singlet superconducting correlation function. The interchain singlet superconducting correlation function is the most long range correlation function among these three correlation functions. This is quite different from finite-U one dimensional Hubbard model.

The superconducting correlation function $\langle O_iO_j^\dagger \rangle$ with $t_\perp = 1.5, U = 6.0$ and $t_\perp = 0.5, U = 2.0$ were plotted along with the upper bound of the non-interacting case in Fig. 4. $\langle O_iO_j^\dagger \rangle$ for both the two parameter sets scale as $0.05R_{ij}^{-2}$ like $\langle O_iO_j^\dagger \rangle$ for $t_\perp = 1.5, U = 2.0$ does. The oscillatory part for $t_\perp = 1.5, U = 6.0$ is more enhanced than that for $t_\perp = 1.5, U = 2.0$. The oscillatory part with $t_\perp = 0.5, U = 2.0$ is largely reduced compared with that of $t_\perp = 1.5, U = 2.0$. The fermion sign problem in our present version of projector monte carlo method does not allow us to use larger projecting time than $\tau = 1.5$ when $t_\perp = 1.5, U = 6.0$ at 0.833 filling. The result with $U = 6.0$ should be taken preliminary. Whether or not the large-U region and small-U region can be classified into the same universality class (possibly with a spin gap) or not may be a subject of future interest.

We are not able to decide if the spin gap persists after doping or not from our data on the correlation function because of the size of the error bars and the oscillatory behavior.
The authors of Refs. [7,9,11] believe that the spin gap persists based on their numerical results. If the spin gap persists after doping, one of the possibilities is that our model is classified into the Luther-Emery (LE) liquid phase with exponential decay of the $2k_F$ magnetic correlation function. (see Table II of Ref. [12]) As the exponent of power-law decay of $\langle O_i O_j^\dagger \rangle$, $\gamma$, is estimated to be about 2, the exponent of $2k_F$ charge correlation function should be about 0.5 in the LE liquid phase. This leads to a conclusion that the $2k_F$ charge correlation is the most long-range. Clearly, our data with $U = 2.0$ (Fig. 3) is not consistent with this LE picture. Some other exotic possibilities consistent with the spin gap should be pursued. [11] In spite of slow convergence of $\ln b(2k_F, L/2)$ versus $\ln L$ in the Fig. 5 of the previous communication [4], we may not be able to exclude a possibility of the Tomonaga-Luttinger (TL) liquid phase in the small-U region, however.

The dynamic spin correlation function was calculated. The elementary spin excitation spectrum was obtained by tracing out $\omega$, giving the first peak of $S^{zz}(\vec{k}, \omega)$, where $\vec{k} = (k_\parallel, k_\perp)$ with $k_\parallel$ defined along the chains and $k_\perp$ defined vertical to the chains. It should be noted that the spectrum can be also obtained from the energy eigenvalues in subspaces with definite $\vec{k}$ values. Both the $k_\perp = 0$ and $k_\perp = \pi$ branches of the spectra are plotted in Figs. 3. Three different parameter sets; $t_\perp = 0.5, U = 2.0$, $t_\perp = 1.5, U = 2.0$ and $t_\perp = 1.5, U = 8.0$ have been used. The spectra at half-filling ($N_e/N_s = 1.0$) are shown in the insets. Spectra of the three parameter sets at half-filling are isomorphic to each other irrespective of values of the parameters in both the $k_\perp = 0$ and the $k_\perp = \pi$ channels. In the $k_\perp = 0$ channel, $k_\perp = \pi$ is no longer one of the lowest energy states unlike in the one dimensional half-filled Hubbard model. At 0.833 filling, spectra for $t_\perp = 1.5, U = 2.0$ and $t_\perp = 1.5, U = 8.0$ are isomorphic to each other in both the $k_\perp = 0$ and the $k_\perp = \pi$ channels. The spectrum for $t_\perp = 0.5, U = 2.0$ is quite different from them. The spin dynamics in the doped two chain Hubbard model changes with $t_\perp$. The change occurs between $t_\perp = 0.5$ and $t_\perp = 1.5$. We do not observe the change in the half-filled state. The reduction of the oscillatory part of $\langle O_i O_j^\dagger \rangle$ for $t_\perp = 0.5, U = 2.0$ may originate from the change in spin dynamics. The change has no effect on $\gamma$. In the non-interacting case, we have two separated bands when $t_\perp \neq 0$.  

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Both of the two bands are partially filled in both the two cases studied here; \( t_\perp = 0.5 \) and \( t_\perp = 1.5 \). It seems unlikely that the change in the spin dynamics is related with the number of partially filled bands. The Fermi wave vector of the second band (higher in energy) \( k_{F2} \) in the noninteracting case is \( \pi/3 \), which is closest to \( \pi/2 \) in this system size. The spin dynamics when \( t_\perp = 0.5 \) and \( U = 2.0 \) at 0.833 filling may be related with the phase with two gapless spin modes and one gapless charge mode found by using weak coupling renormalization group techniques (the C1S2 phase in the notation of the authors of Ref. [13]).

It should be noted that the smallest energy differences with the ground state are given at \((k_\parallel, k_\perp) = (0.17\pi, 0.0), (0.50\pi, 0.0), (0.67\pi, 0.0)\) and \((0.83\pi, 0.0)\) for \( t_\perp = 0.5, U = 2.0 \) and at \((0.17\pi, \pi), (0.50\pi, \pi), (0.67\pi, \pi)\) and \((0.83\pi, \pi)\) for \( t_\perp = 1.5, U = 2.0 \) and \( t_\perp = 1.5, U = 8.0 \), respectively. The smallest energy differences for these parameter sets are 0.08, 0.10 and 0.37, respectively. The possible spin gap for \( U = 2.0 \) is less clear than that with \( U = 8.0 \) in this small system size.

### III. CONCLUSIONS

We have calculated the interchain singlet superconducting, magnetic and charge correlation functions and the spin excitation spectrum in the doped two chain Hubbard model. The exponent of the interchain singlet superconducting correlation function, \( \gamma \), is found to be close to 2.0 as long as two distinct non-interacting bands cross the Fermi level. Our data is not consistent with the LE picture. Some other exotic possibilities consistent with the spin gap should be pursued. Of the three correlation functions, the interchain singlet superconducting, magnetic and charge correlation functions, the interchain singlet superconducting correlation function is the most long range correlation function in the doped two chain Hubbard model. This is quite different from finite-U one dimensional Hubbard model.

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There were some typographical errors in this reference. Equations (1a), (1b) and (8) should be read as

\[ C(0) = \sum_{\vec{\ell},\vec{\ell}'} \lambda_{\vec{\ell}}^\ast \lambda_{\vec{\ell}'} \gamma_{\vec{\ell},\vec{\ell}'} \]

\[ \gamma_{\vec{\ell},\vec{\ell}'} = \frac{1}{N} \sum_{ij} \langle c^\dagger_{i\downarrow} c^\dagger_{i+\vec{\ell} \uparrow} c_{j+\vec{\ell} \downarrow} c_{j\uparrow} \rangle \text{ and } \langle n^c_{0\uparrow} n^c_{r\downarrow} \rangle \propto \cos(2k_F r) r^{-(k_F r+1)} \text{, respectively.} \]

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FIGURES

FIG. 1. The superconducting correlation function $< O_i O_j^\dagger >$ at 0.833 filling on a $36 \times 2$ lattice is plotted versus $|i - j|$. Circles and squares are the data obtained with $t_\perp = 1.5, U = 2.0$ and $t_\perp = 2.5, U = 2.0$, respectively. The upper bound of $< O_i O_j^\dagger >_{U=0}$: $0.05R_{ij}^{-2}$ is plotted as well, where $R_{ij}$ is distance between sites in the rung.

FIG. 2. The superconducting correlation function $< O_i O_j^\dagger >$ at 0.833 filling on a $36 \times 2$ lattice is plotted versus $|i - j|$ on a log-log scale. Closed circles connected with real line are the data obtained with $t_\perp = 1.5, U = 2.0$. A dotted line is upper bound of $< O_i O_j^\dagger >_{U=0}$: $0.05|i - j|^{-2}$. The correlation function has inversion symmetry at the inversion center: $|i - j| = 17.5$. We show only the left half of the function.

FIG. 3. The superconducting $< O_i O_j^\dagger >$, magnetic $< S_i^z S_j^z >$ and charge $< n_i n_j > - < n >_{\text{ave}}^2$ correlation functions at 0.833 filling on a $24 \times 2$ lattice with $t_\perp = 1.5, U = 2.0$ are plotted versus $|i - j|$. Circles, squares and crosses are the superconducting, magnetic and charge correlation functions, respectively. The functions $\pm 0.05R_{ij}^{-2}$ are also plotted as guides.

FIG. 4. The superconducting correlation function $< O_i O_j^\dagger >$ at 0.833 filling on a $36 \times 2$ lattice is plotted versus $|i - j|$. Circles and squares are the data obtained with $t_\perp = 1.5, U = 6.0$ and $t_\perp = 0.5, U = 2.0$, respectively. The upper bound of $< O_i O_j^\dagger >_{U=0}$: $0.05R_{ij}^{-2}$ is plotted as well, where $R_{ij}$ is the distance between sites in the rung.

FIG. 5. The spin excitation spectrum of a $6 \times 2$ two chain Hubbard model at 0.833 filling. The $k_\perp = 0$ and $k_\perp = \pi$ channel are plotted in (a) and (b), respectively. Open squares, closed squares and closed circles are the spectra obtained with $t_\perp = 0.5, U = 2.0$, $t_\perp = 1.5, U = 2.0$, and $t_\perp = 1.5, U = 8.0$, respectively. The horizontal axis is the wavenumber in units of $\pi$. The corresponding spectra at half-filling ($N_e/N_s = 1.0$) are depicted in the insets.