Correlations in a two–chain Hubbard model

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Abstract

Equal time spin–spin and pair field correlation functions are calculated for a two-chain Hubbard model using a density–matrix numerical renormalization group approach. At half–filling, the antiferromagnetic and pair field correlations both decay exponentially with the pair field having a much shorter correlation length. This is consistent with a gapped spin-liquid ground state. Below half–filling, the antiferromagnetic correlations become incommensurate and the spin gap persists. The pair field correlations appear to follow a power law decay which is similar to their non-interacting $U = 0$ behavior.

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Materials such as (VO)$_2$P$_2$O$_7$ \cite{1} and Sr$_2$Cu$_4$O$_6$ \cite{2,3} contain weakly coupled arrays of metal-oxide-metal ladders. In the nominal insulating state, the metal ions have spin one-half and the oxygens mediate an antiferromagnetic superexchange coupling. Calculations for a two-chain antiferromagnetic model with an exchange interaction $J$ along each chain and $J'$ across each rung have shown that the insulating state can have a spin gap \cite{4–7}. A $t$–$J$, $t'$–$J'$ model was introduced to describe the hopping of holes in the doped system. Lanczos calculations for this model with $J' > t'$ found enhanced pairing correlations on a $2 \times 8$ ladder doped near one-quarter filling \cite{4}. A mean-field analysis of this model using a Gutzwiller renormalization of the matrix elements \cite{8} found a spin gap in the insulating state which initially increases with doping. In addition, the doped system near half-filling was found to have a mean-field superconducting order parameter with a modified d–wave structure.

Another representation of coupled chains is provided by the two-chain Hubbard model \cite{9}. Here we report results obtained for the ground-state magnetic and pairing correlations of the two–chain Hubbard model using a density–matrix numerical renormalization group approach \cite{10} to study lattices of up to $2 \times 32$ sites. We find that at half-filling, the dominant correlations are antiferromagnetic, but that these decay exponentially because of a spin gap, which we calculate directly. The singlet pair field correlations also decay exponentially but with a short correlation length of the order of the lattice spacing. The ground state at half-filling is thus a spin liquid. As the system is doped away from half-filling, the antiferromagnetic correlations show an incommensurate structure and a peak develops in the magnetic structure factor at a wave vector proportional to the filling. The spin gap decreases as the system is doped, but persists down to an occupation of 0.75 electrons per site or less. The singlet pair field correlations are enhanced and exhibit a power–law decay, but the form of the decay is approximately $\ell^{-2}$, where $\ell$ is the separation distance. This is the same power-law dependence as for the noninteracting, $U = 0$, system.

We picture the two–chain Hubbard model as a ladder standing along the $y$–axis with its rungs along the $x$–axis so that
\[ H = -t_y \sum_{i,\lambda \sigma} (c_{i,\lambda \sigma}^\dagger c_{i+1,\lambda \sigma} + c_{i+1,\lambda \sigma}^\dagger c_{i,\lambda \sigma}) - t_x \sum_{i,\sigma} (c_{i,1\sigma}^\dagger c_{i,2\sigma} + c_{i,2\sigma}^\dagger c_{i,1\sigma}) + U \sum_{i,\lambda} n_{i,\lambda \uparrow} n_{i,\lambda \downarrow}. \]  

Here \( c_{i,\lambda \sigma}^\dagger \) creates an electron of spin \( \sigma \) at rung \( j \) and side \( \lambda = 1 \) (left) or 2 (right), the hopping along a chain is \( t_y \), the hopping between chains on a rung is \( t_x \), and \( U \) is the on-site Coulomb repulsion.

The density matrix formulation of the renormalization group \[10\] provides a controlled approximation for the calculation of ground–state energies and correlation functions. We have used the finite–system method with open boundaries and have studied \( 2 \times 16, 2 \times 24, \) and \( 2 \times 32 \) lattices, keeping up to 400 states per block. Details of the calculations will be published elsewhere. The discarded density matrix weight (truncation error) varies from \( 5.5 \times 10^{-5} \) to less than \( 10^{-9} \) for the \( 2 \times 32 \) results shown here. In addition, we have examined the convergence of measured quantities as a function of the number of states kept and ascertained that the symmetries of the Hamiltonian are preserved. The maximum errors in the quantities shown here are at most a few percent, and in most cases are much smaller. Since the method works best with chains that have open boundaries at the ends, all results here have open boundaries.

We have calculated the equal–time spin and pair field correlation functions \( S_{\lambda \lambda'}(i, j) = \langle M_{i,\lambda}^z M_{j,\lambda'}^z \rangle, \ D_{xx}(i, j) = \langle \Delta_{xi} \Delta_{xj}^\dagger \rangle, \) and \( D_{yx}(i, j) = \langle \Delta_{yi} \Delta_{xj}^\dagger \rangle \) with

\[
M_{i,\lambda}^z = n_{i,\lambda \uparrow} - n_{i,\lambda \downarrow}, \\
\Delta_{xi}^\dagger = c_{i,1\uparrow}^\dagger c_{i,2\downarrow}^\dagger - c_{i,1\downarrow}^\dagger c_{i,2\uparrow}^\dagger, \\
\Delta_{yi}^\dagger = c_{i+1,2\downarrow}^\dagger c_{i,2\uparrow}^\dagger - c_{i,1\uparrow}^\dagger c_{i+1,2\downarrow}^\dagger. 
\]

Here \( S_{11}(i, j) \) and \( S_{12}(i, j) \) measure the spin–spin correlations along a chain and between the chains respectively, and \( D_{xx}(i, j) \) measures the singlet pair field correlations in which a singlet pair is added at rung \( j \) and removed at rung \( i \). In addition, \( D_{yx}(i, j) \) measures the pair field correlations in which a singlet pair is added to rung \( j \) and removed from the right–hand chain between rungs \( i \) and \( i + 1 \). The relative phase of the pair wave function across the \( i \)th rung to along one chain from \( i \) to \( i + 1 \) is given by comparing the phase of \( D_{xx}(i, j) \) to \( D_{yx}(i, j) \). This turns out to be negative, corresponding to the mean field result
obtained in Ref. [8]. However, the non-interacting $U = 0$ result at a filling $\langle n \rangle = 0.875$ is also negative.

Because of the open boundaries at the ends, the system is not translationally invariant. Therefore, the correlation functions are dependent on both $i$ and $j$, whereas in the thermodynamic limit or with periodic boundary conditions, they are a function of only $|i - j|$. We have found that the spin correlations at all fillings and the pairing correlations at half-filling are not strongly dependent on the placement of $i$ and $j$, so we choose them to be as symmetric about the center of the lattice as possible, in order to minimize end effects. The pair correlations away from half-filling have strong variation with lattice placement, so in order to minimize these effects, we average over a number of $i$ and $j$ for a given $|i - j|$. We will then discuss the correlation functions as functions of $\ell \equiv |i - j|$ with these procedures implicit. As we shall see, there will be discernible boundary effects, but the lattices are long enough that one can still extract the general behavior. We also discuss the average filling, defined as $\langle n \rangle = 1/N \sum_{i, \lambda \sigma} n_{i, \lambda \sigma}$ where $N$ is the number of lattice sites.

In order to understand the nature of the spin–spin correlations we have calculated the magnetic structure factor $S(q_x, q_y)$ by taking the fourier transform of $S_{\lambda \lambda'}(i, j)$. Since there are two chains, $q_x$ can take on only the values 0 and $\pi$. For the purposes of the fourier transform, we take $S_{\lambda \lambda'}(\ell) = 0$ for $\ell$ larger than the lattice size. This introduces only a small error since the $S_{\lambda \lambda'}(\ell)$ decays exponentially with $\ell$, and has decayed by a factor of at least 50 at the maximum lattice separation. The correlation function $S(\pi, q_y)$ is shown for four different fillings, $\langle n \rangle = 1$, $\langle n \rangle = 0.9875$, $\langle n \rangle = 0.875$, and $\langle n \rangle = 0.75$ in Fig. 1. These fillings correspond to doping the half-filled system with 0, 2, 8, and 16 holes. At $\langle n \rangle = 1$, there is a single strong peak at $q_y = \pi$. As the system is doped away from half-filling, the peak at $q_y = \pi$ is strongly suppressed and $S(\pi, q_y)$ peaks at $q_y = \langle n \rangle \pi$. The residual peak at $q_y = \pi$ is present only for even numbers of hole pairs. Therefore, we believe that it is a finite size effect and will vanish in the thermodynamic limit. Since the correlations are strongly antiferromagnetic across the chain, $S(0, q_y)$ (not shown) is small, flat and does not change much with the filling.
At half–filling, \( \langle n \rangle = 1 \), the magnetic structure factor shown in Fig. 1 has a Lorentzian line shape corresponding to an exponential decay of the spin–spin correlations. This is illustrated in Fig. 2, in which the logarithm of \( S_{11}(\ell) \) is plotted versus \( \ell \) for various values of \( U \). The oscillatory deviations from linear behavior at large separation are due to the effects of the open end boundary conditions. From the slopes of the straight line segments, we have determined the correlation length \( \xi \) and this is plotted versus \( U/t_y \) in the inset of Fig. 2. As \( U/t_y \) increases, \( \xi \) decreases, saturating at a value of order 3 lattice spacings for \( t_x = t_y \). The interchain spin–spin correlations \( S_{12}(\ell) \) decay with the same correlation length as \( S_{11}(\ell) \). At half–filling, the pair field correlations also decay exponentially, but with a correlation length of order the lattice spacing or smaller. Thus the pair field correlations are negligible at half–filling.

We have also carried out calculations for \( U = 8t_y \) at a cross–chain hopping \( t_x = 0.5t_y \) and \( 1.2t_y \). The correlation length decreases with increasing \( t_x \), ranging from 10.4 lattice spacings at \( t_x = 0.5t_y \), to 4.3 lattice spacings at \( t_x = t_y \) and 2.9 lattice spacings at \( t_x = 1.2t_y \). We expect the correlation length to diverge as \( t_x \to 0 \) because on a single chain there is no spin gap and the spin–spin correlation function decays as a power law. The largest spin gap and thus the smallest correlation length should occur in the large \( t_x/t_y \) limit, in which the system can be described as decoupled spin singlets on the rungs of the ladder.

In order to calculate the spin gap directly, one can calculate the energy difference between the lowest \( S_z = 0 \) state and the lowest \( S_z = 1 \) state. For the \( 2 \times 32 \) system, the energy gap at half–filling is given by \( \Delta_{\text{spin}} = E(32, 32) - E(33, 31) \) where \( E(N_\uparrow, N_\downarrow) \) is the ground state energy of the system with \( N_\uparrow \) up electrons and \( N_\downarrow \) down electrons. The spin gap as a function of \( U \) at half–filling for \( t_x = t_y \) is shown in the main plot in Fig. 3 for a \( 2 \times 32 \) lattice. We have examined the spin gap as a function of lattice size in order to confirm that the gap is present in the thermodynamic limit. For \( U = 8t_y \), \( \Delta_{\text{spin}} = 0.151t_y \) on a \( 2 \times 16 \) lattice and \( \Delta_{\text{spin}} = 0.132t_y \) on a \( 2 \times 32 \) lattice. At \( U = 0 \), the spin gap vanishes because there are a set of degenerate, half-occupied states on the Fermi surface. The gap peaks at approximately \( U = 8t_y \) then decreases with increasing \( U \). The gap decreases for large \( U \) because it varies...
as $J = 4t_y^2/U$ in the large $U$ limit. In this same limit, the correlation length saturates since it varies as the spin wave velocity divided by the gap. The inset plot shows the spin gap as a function of filling for $U = 8t_y$. The gap decreases fairly rapidly with filling, but is still present at $\langle n \rangle = 0.75$.

When the Hubbard ladder is doped away from half–filling, ($\langle n \rangle = 0.875$) one sees from Fig. 2 that the antiferromagnetic correlations develop an incommensurate peak. The pairing correlation functions $D_{xx}(\ell)$ and $D_{yx}(\ell)$ are shown in Fig. 4 for $t_x = t_y$ and $U = 8t_y$ at fillings of $\langle n \rangle = 1$ and $\langle n \rangle = 0.875$. At $\langle n \rangle = 1$, the pairing correlations decay quite strongly compared to those at $\langle n \rangle = 0.875$. The relative sign of $D_{xx}(\ell)$ and $D_{yx}(\ell)$ is negative at both fillings, consistent with a modified $d$-wave structure. In order to determine the strength of the pairing correlations, one must consider their $\ell$–dependence at large distances. For a one–dimensional system, we expect that any pairing correlation will at best decay as a power of $\ell$ and can in some cases decay exponentially, as we have seen for the half-filled system. For two chains, one can compare with the the non-interacting $U = 0$ ladder, for which

$$D_{xx}(\ell) = (1/2\pi\ell)^2 [2 - \cos(2k_f(0)\ell) - \cos(2k_f(\pi)\ell)].$$

(3)

Here $k_f(0) = \cos^{-1}(t_x + \mu)/2$ and $k_f(\pi) = \cos^{-1}(t_x - \mu)/2$ are the Fermi wave vectors corresponding to the bonding and antibonding bands of the two coupled chains with $\mu$ the chemical potential. In order to examine the decay of the pair correlations, we have made the log-log plot of $D_{xx}(\ell)$ shown in Fig. 5. We compare the $U = 8t_y$ results with the infinite system $U = 0$ results given by Eq. (3). Our results for the interacting $2 \times 16$ and $2 \times 24$ lattices are consistent with Fig. 5 and thus while end effects are present, it appears that the equal time pair field correlations of the interacting system decay approximately as $\ell^{-2}$.

In summary, we have found that the Hubbard model on two chains exhibits spin–liquid behavior at half–filling. Both spin–spin and pairing correlations decay exponentially with the pairing correlations having a much shorter correlation length. There is a spin gap which increases as the interaction $U$ is turned on, peaks, and then becomes smaller. When the system is doped away from half–filling, the spin gap decreases with filling but persists down
to at least $\langle n \rangle = 0.75$. The spin–spin correlations become incommensurate and the $d$–wave–like pair field correlation are enhanced. The pair field correlations appear to decay as a power law with exponent close to $-2$, similarly to those in the non-interacting $U = 0$ system.

We have recently received a preprint by Tsunetsugu et al. [12] in which the spin gap and binding energy for two holes is calculated for the $t$–$J$ model on two chains via Lanczos diagonalization.

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FIGURES

FIG. 1. The fourier transform $S(\pi, q_y)$ of the spin–spin correlation function $S_{\lambda \lambda'}(\ell)$. Here $t_x = t_y$ and $U = 8t_y$ and the calculations were made on a $2 \times 32$ lattice.

FIG. 2. A semilog plot of the spin–spin correlation function for $\langle n \rangle = 1$ as a function of $U/t_y$ for $t_x = t_y$ on a $2 \times 32$ lattice showing the exponential decay of these correlation functions. The inset shows the correlation length in units of the lattice spacing taken from the slopes of the lines.

FIG. 3. The spin gap $\Delta_{\text{spin}}$ as a function of $U/t_y$ for $t_x = t_y$ calculated on a $2 \times 32$ lattice at $\langle n \rangle = 1.0$. The inset shows $\Delta_{\text{spin}}$ plotted as a function of filling $\langle n \rangle$ for $U/t_y = 8$.

FIG. 4. The pair field correlation functions $D_{xx}(\ell) = \langle \Delta_{xi} \Delta_{xj}^\dagger \rangle$ and $D_{yx}(\ell) = \langle \Delta_{yi} \Delta_{xj}^\dagger \rangle$ versus $\ell \equiv |i - j|$ for $\langle n \rangle = 1.0$ and $\langle n \rangle = 0.875$. Here $t_x = t_y$ and $U = 8t_y$ on a $2 \times 32$ lattice.

FIG. 5. Log-log plot of $D_{xx}(\ell) = \langle \Delta_{xi} \Delta_{xj}^\dagger \rangle$ versus $l \equiv |i - j|$ at $\langle n \rangle = 0.875$. The $U = 0$ results are taken from Eq. (3) and the dashed line has slope $-2$. 

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Fig. 1
\[ \langle n \rangle = 1.0 \]

\[ \left| \langle M_{i,1}^z, M_{j,1}^z \rangle \right| \]

- \( U = 4t_y \)
- \( U = 8t_y \)
- \( U = 12t_y \)
- \( U = 16t_y \)

\[ |i-j| \]

\[ U/t_y \]

**Fig. 2**
Fig. 3
Fig. 4
Fig. 5