The Doped Two Chain Hubbard Model

R.M. Noack and S.R. White

Department of Physics University of California Irvine, CA 92717

D.J. Scalapino

Department of Physics University of California Santa Barbara, CA 93106

(September 14, 1994)

Abstract

The properties of the two–chain Hubbard Model doped away from half–filling are investigated. The charge gap is found to vanish, but a finite spin gap exists over a range of interchain hopping strength $t_\perp$. In this range, there are modified $d_{x^2-y^2}$–like pairing correlations whose strength is correlated with the size of the spin gap. It is found that the pair field correlations are enhanced by the onsite Coulomb interaction $U$.

PACS Numbers: 74.20Hi, 75.10Lp, 71.10+x
Studies of two chain $t$–$J$ and Hubbard models provide insight into the development of pairing correlations in strongly coupled electron systems which can exhibit a spin–gap phase. For example, Lanczos calculations for a $t$–$J$ model by Dagotto et al. [1] suggested that antiferromagnetic $S = 1/2$ coupled chains such as $(\text{VO})_2\text{P}_2\text{O}_7$ [2] should have a spin gap and that if this system could be doped, it would have enhanced superconducting or charge–density–wave correlations in the ground state. Rice and coworkers [3,4] discussed $\text{Sr}_2\text{Cu}_4\text{O}_6$, which consists of layers containing weakly coupled CuO ladders [5], and based upon their analysis of a $t$–$J$ model suggested that if this system were lightly doped, the spin gap phase would persist and a ground state with dominant superconducting correlations could be realized.

Various approaches to the two–chain Hubbard model have also been reported [6–11]. Renormalization group calculations [8–11] find evidence for a variety of phases. However, a number of these phases correspond to renormalization flows to strong coupling, making it important to have the guidance provided by independent numerical calculations. Previous density matrix numerical renormalization group calculations [12] suggested that the two chain Hubbard model has a spin gap at half–filling, provided the onsite Coulomb interaction $U$ and the interchain hopping $t_\perp$ are finite. For $U = 8t$ and $t_\perp = t$, with $t$ the one electron hopping along a chain, a spin gap was also found for band fillings of $\langle n \rangle = 0.875$ and $\langle n \rangle = 0.75$ electrons per site. In addition, for the doped case, the equal time pair field correlations were observed to decay as a power law, but with an exponent similar to that of the noninteracting ($U = 0$) system. Here we extend these two–chain Hubbard calculations to explore the dependence of the doped state on the strength of the interchain hopping $t_\perp$. We find that the charge gap vanishes in the doped state, but that a spin gap exists over a range of $t_\perp$. Furthermore, the decay of the pair field correlations depends on $t_\perp$, with the strongest correlations appearing when the spin gap is a maximum.

The two chain Hubbard model has a Hamiltonian

$$H = -t \sum_{i,\lambda,\sigma}(c_{i,\lambda,\sigma}^\dagger c_{i+1,\lambda,\sigma} + c_{i+1,\lambda,\sigma}^\dagger c_{i,\lambda,\sigma}) - t_\perp \sum_{i,\sigma}(c_{i,1\sigma}^\dagger c_{i,2\sigma} + c_{i,2\sigma}^\dagger c_{i,1\sigma}) + U \sum_{i,\lambda} n_{i,\lambda\uparrow} n_{i,\lambda\downarrow}. \quad (1)$$
Here $c_{i,j,\sigma}^+$ creates an electron of spin $\sigma$ on rung $j$ and chain $\lambda$, with $\lambda = 1$ or 2. The one-electron hopping along a chain is $t$, the hopping between chains is $t_\perp$, and the onsite Coulomb interaction is $U$. We will measure energies in units of $t$.

The calculations were carried out using the density matrix renormalization group (DMRG) \cite{14}. This technique allows the calculation of ground state energies and correlation functions in a controlled way. The details of the techniques used for two Hubbard chains are described in Ref. \cite{15}. We studied lattices with open boundary conditions of various sizes up to $2 \times 40$ sites, keeping up to 500 states per block. The discarded weight of the density matrix (the truncation error) ranged from $3.7 \times 10^{-5}$ to less than $10^{-8}$. We estimate that the maximum errors on the quantities shown in this paper are at most a few percent, and typically are of the order of the plotting symbol size or less.

The charge and spin gaps are defined in terms of the ground state energy $E_0(N_\uparrow, N_\downarrow)$ for $N_\uparrow$ spin–up and $N_\downarrow$ spin–down electrons. The charge gap is given by

$$\Delta_C = \frac{[E_0(N-1, N-1) + E_0(N+1, N+1) - 2E_0(N, N)]}{2}, \quad (2)$$

while the spin gap is

$$\Delta_S = E_0(N+1, N-1) - E_0(N, N). \quad (3)$$

These quantities are shown in Fig. 1, calculated for Hubbard ladders of different lengths $L$. In Fig. 1(a) we show $\Delta_C$ for $U = 8$, $t_\perp = 1$, and several different band fillings. At half–filling, $\Delta_C$ scales to a large finite value $\Delta_C(L = \infty) \approx 4.5$, whereas in the doped case, with $\langle n \rangle$ slightly less than 1, we find that the charge gap vanishes in the thermodynamic limit.

For the spin gap, shown Fig. 1(b), the finite size scaling must be done carefully in order to determine the behavior because the finite size effects are relatively large and have a different character in different regimes. We fit the data using a least squares fit to polynomials in $L^{-1}$. At half–filling, we use a third order polynomial to fit six system sizes. At $\langle n \rangle = 0.875$, fewer sizes are available with the correct filling, so we fit to a second order polynomial. The polynomial fits are shown as the lines in 1(b). At half–filling, $\Delta_S(\infty) \approx 0.12$ and is clearly
nonvanishing. The system is an insulator with short–range antiferromagnetic correlations. For the doped system, there are three distinct regimes for which we show representative curves with different finite size behavior. For small $t_\perp$, illustrated by the $t_\perp = 0.5$ curve, the finite size effects are large with a large linear coefficient. In the thermodynamic limit, the spin gap becomes small. For a smaller $t_\perp$ of 0.3, we find $\Delta_S(32) \approx 3 \times 10^{-3}$. Therefore, we believe that $\Delta_S(\infty)$ vanishes for $t_\perp < 0.5$. For intermediate $t_\perp$, shown for $t_\perp = 1.0$, the coefficient of the quadratic term is large and positive and the spin gap scales to a finite value. For large $t_\perp$, shown for $t_\perp = 2.0$, the finite size effects are smaller, the scaling is linear in $1/L$ and $\Delta_S(\infty)$ vanishes.

We plot the spin gap extrapolated to the thermodynamic limit as a function of $t_\perp$ in Fig. 2. It appears that in the doped system, a finite value of $t_\perp$ is required to produce an interchain rung exchange $J_\perp \sim 4t_\perp^2/U$ which is sufficient to create a spin gap. This differs from the half–filled case where our earlier work suggests that a spin gap opens for all $t_\perp > 0$ \cite{12,16}. For $t_\perp > 1.7$, as shown in Fig. 2, the spin gap is suppressed. In a weak coupling picture, a two chain model leads to bonding and antibonding bands split by the coupling $t_\perp$. For $U = 0$, the antibonding band is completely unoccupied at $\langle n \rangle = 0.875$ when $t_\perp > 1.85$, suggesting that the transition at $t_\perp \approx 1.7$ is related to the band splitting. In the spin gap phase, the spin–spin correlations are short–range, incommensurate, and antiferromagnetic in nature. They give rise to a Lorentzian peak in the magnetic structure factor \cite{12}.

In order to further characterize the spin gap region, we have calculated the equal–time rung–rung pair field correlation function $\langle \Delta_i \Delta_j^\dagger \rangle$. Here

$$\Delta_j^\dagger = (c_{j,1\uparrow}^\dagger c_{j,2\downarrow}^\dagger - c_{j,1\downarrow}^\dagger c_{j,2\uparrow}^\dagger)$$

(4)

creates a spin singlet pair across the $j$th rung and $\Delta_i$ destroys a singlet pair on the $i$th rung. For comparison with the spin gap, Fig. 2 also shows the pair field correlation function $\langle \Delta_i \Delta_j^\dagger \rangle$ averaged over separations $8 \leq |i - j| \leq 12$. It is clear that the size of the spin gap and the pair field are correlated.

Figure 3(a) shows a log–log plot of $\langle \Delta_i \Delta_j^\dagger \rangle$ versus $|i - j|$ with $\langle n \rangle = 0.875$, $U = 8$ and
$t_\perp = 1.5$ for various length chains. As discussed earlier, the calculational procedure which we have implemented has open end boundary conditions. The correlation functions shown in Fig. 3(a) are obtained by averaging over a number of $i$ and $j$ for a given $|i - j|$. We have found that this procedure removes most of the finite size effects due to the open boundary conditions. One can see that the boundary effects are small in Fig. 3(a) by the overlap of the numerical results for chains of different lengths. Only when $|i - j|$ is large enough that both $i$ and $j$ are within a few lattice spacings of the boundaries do significant differences appear. The dashed curve corresponds to the $|i - j|^{-2}$ decay of the non–interacting pair field correlations and one sees that for $t_\perp = 1.5$, the pair field correlations of the interacting system are enhanced over the $U = 0$ system. In Fig. 3(b), we show $\langle \Delta_i \Delta_j^\dagger \rangle$ versus $|i - j|$ calculated on a $2 \times 32$ system for $\langle n \rangle = 0.875$, $U = 8$, and various values of $t_\perp$. For small values of $t_\perp$, the pair field correlations decay rapidly. As $t_\perp$ increases, the pair field correlations are enhanced until $t_\perp \approx 1.7$, after which they are suppressed by further increasing $t_\perp$.

It is also possible to determine the internal structure of a pair. We have calculated the pair wave function obtained from the off–diagonal ground state expectation value

$$\Psi(i, j) = \frac{N}{N-2} \langle \psi_0 | (c_j^\dagger c_i^\downarrow - c_j^\downarrow c_i^\uparrow) | \psi_0 \rangle_N. \quad (5)$$

Here $(c_j^\dagger c_i^\downarrow - c_j^\downarrow c_i^\uparrow)$ removes a singlet pair with one electron on the $i$th site and one on the $j$th site. Near the center of the ladder, $\Psi(i + \hat{x}, i) = 0.1$ and $\Psi(i + \hat{y}, i) = -0.08$ for $U = 8$, $t_\perp = 1.5$, and $\langle n \rangle = 0.875$. In the cuprate chain systems, $t_\perp$ and $t$ have the same sign so that the relative negative sign of $\Psi(i + \hat{x}, i)$ and $\Psi(i + \hat{y}, i)$ is physically relevant and corresponds to a modified $d_{x^2-y^2}$–like state as previously discussed. The small amplitude for removing a pair from a rung, 0.1, reflects the spatial extent of the relative, internal coordinate of the pair wave function and the fact that the $c_{i,\lambda\sigma}^\dagger$ operators are bare quasi–particle operators. When one takes out a factor of $(0.1)^2$ associated with this overlap of $\Delta_i$ and $\Delta_j^\dagger$ with the internal pair wave function, it is clear that there are significant pair-field–pair-field center of mass correlations present in the doped system for $t_\perp = 1.5$.

Recently, we described an intuitive picture for the spin–liquid state of two coupled chains
based on a resonating valence bond (RVB) variational ansatz. This picture is also useful for describing the apparent destruction of the spin–liquid state for both small and large $t_\perp$. In the latter region, the bonding and antibonding orbitals on a single rung separate to the extent that a state with two holons on a rung becomes higher in energy than two widely separated excitations each consisting of a hole in the bonding orbital of a rung. These quasiparticle excitations are described in RVB language as a bound holon-spinon pair, and were first observed by Tsunetsugu, et. al. The RVB picture suggests that the spin–liquid state is not really destroyed in this regime, only hidden by the spin degrees of freedom of the quasiparticles. This picture is quite compatible with the weak–coupling, band–separation picture mentioned above.

In contrast, a band picture is not useful for small $t_\perp$. In this regime, there is little difference in energy between the “staggered” and “resonant” valence bond configurations, and the average separation between two holons in a pair $\xi_h$ becomes substantial. When $\xi_h$ becomes comparable to $1/\delta$, where the doping $\delta = 1 - \langle n \rangle$, the pairs overlap, and the holons become essentially free. Since they are topological excitations residing on a single site, the free holons destroy the confinement mechanism responsible for the spin-liquid state. In this regime the system may resemble a doped system with an odd number of chains, where confinement never takes place.

It is interesting to compare our results with several renormalization group calculations, which have also suggested the relevance of $t_\perp$ and the possibility of interchain pairing. Based upon a weak coupling renormalization group analysis, Fabrizio et al. have suggested a possible $U$–$t_\perp$ phase diagram for the two chain Hubbard model. In the small $t_\perp$ region, they conjecture that there may be several phases in which pairing correlations are dominant. In one of these phases, called “SC1” in Ref., these pairing correlations have the same modified $d_{x^2-y^2}$ character we find. However, contrary to our results, they find a divergent spin–spin correlation function for $\mathbf{q} = (2k_F,0)$ rather than a spin gap state. Furthermore, they find this behavior for arbitrarily small values of $t_\perp$ and for generic, non-commensurate fillings. This differs from our findings that the pairing is associated with a
spin gap state and requires a finite value of $t_\perp > 0.5$. Furthermore, we find that a doping of $\langle n \rangle$ near 1 is required for significant pairing.

Recently, Khveshchenko and Rice \cite{11} have carried out a renormalization group analysis near half-filling where umklapp processes become relevant. They argue that in the lightly doped system, the presence of the interchain hopping $t_\perp$ is sufficient to generate an antiferromagnetic exchange $J_\perp$ leading to a spin gap, and that this state supports a modified $d_{x^2-y^2}$–like pairing. This scenario is certainly closer to what we find, except, as shown in Fig. 2, we find that a finite value of $t_\perp$ is required to produce a spin gap.

The authors thank N. Bulut, M.P.A. Fisher, W. Hanke, M. Imada, T.M. Rice, R.T. Scalettar, and H. Tsunetsugu for useful discussions. R.M.N. and S.R.W. acknowledge support from the Office of Naval Research under grant No. N00014-91-J-1143 and D.J.S. acknowledges support from the Department of Energy under grant DE–FG03–85ER45197 and the Program on Correlated Electrons at the Center for Materials Science at Los Alamos National Laboratory. The numerical calculations reported in this paper were performed at the San Diego Supercomputer Center.
REFERENCES

[1] E. Dagotto, J. Riera, and D.J. Scalapino, Phys. Rev. B 45, 5744 (1992).

[2] D.C. Johnston et al., Phys. Rev. B 35, 219 (1987).

[3] T.M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. 23, 445 (1993).

[4] H. Tsunetsugu, M. Troyer, and T.M. Rice, Phys. Rev. B 49, 16078 (1994).

[5] Z. Hiroi, M. Azuma, M. Takano, and Y. Bando, J. Solid State Chem., 95, 230 (1991).

[6] R.M. Noack, R.T. Scalettar, N. Bulut, and D.J. Scalapino (unpublished).

[7] K. Yamaji and Y. Shimo, Physica C 222, 349 (1994).

[8] H.J. Schulz, Int. J. Mod. Phys. B 5, 57 (1991).

[9] A.M. Finkel’stein and A.I. Larkin, Phys. Rev. B 47, 10461 (1993).

[10] M. Fabrizio, A. Parola, and E. Tosatti, Phys. Rev. B 46, 3159 (1992); M. Fabrizio, Phys. Rev. B 48, 15838 (1993).

[11] D.V. Khveshchenko, and T.M. Rice, Phys. Rev. B 50, 252 (1994); D.V. Khveshchenko, Phys. Rev. B 50, 380 (1994).

[12] R.M. Noack, S.R. White, and D.J. Scalapino, Phys. Rev. Lett. 73, 882 (1994).

[13] K. Yamaji, T. Yanagisawa, and Y. Shimo, preprint, and Ref. [7] have carried out exact diagonalization for 10 electrons on a $2 \times 6$ cluster and found that the near neighbor and next near neighbor singlet rung–rung pair field correlations for $U = 5$ are enhanced for $0.93 \leq t_{\perp} \leq 1.74$.

[14] S.R. White, Phys. Rev. Lett. 69, 2863 (1992), Phys. Rev. B 48, 10345 (1993).

[15] R.M. Noack, S.R. White and D.J. Scalapino, to appear in Computer Simulations in Condensed Matter Physics VII, Eds. D.P. Landau, K.K. Mon, and H.B. Schüttler (Spinger Verlag, Heidelberg, Berlin, 1994).
[16] S.R. White, R.M. Noack, and D.J. Scalapino, Phys. Rev. Lett. 73, 886 (1994).

[17] S.A. Kivelson, D.S. Rokhsar, and J.P. Sethna, Phys. Rev. B 35, 8865 (1987); S. Liang, B. Douçot, and P.W. Anderson, Phys. Rev. Lett. 61, 365 (1988).
FIGURES

FIG. 1. (a) The charge gap $\Delta_C$ versus the inverse chain length $L^{-1}$ for $t_\perp = 1$, $U = 8$ and various fillings. The inset shows an enlarged view for $\langle n \rangle = 0.875$. (b) The spin gap $\Delta_S$ versus $L^{-1}$ for $t_\perp = 1.0$ at $\langle n \rangle = 1.0$ and a number of $t_\perp$ values for $\langle n \rangle = 0.875$. The lines are least squares fits to polynomials in $L^{-1}$.

FIG. 2. The spin gap $\Delta_S$ versus $t_\perp$ for $U = 8$ and $\langle n \rangle = 0.875$ calculated from the $L \rightarrow \infty$ extrapolations of Fig. 1(b). The open circles show the magnitude of the pair field correlation function $\langle \Delta_i \Delta_j^\dagger \rangle$ averaged over separations $8 \leq |i - j| \leq 12$ versus $t_\perp$ for the same parameters on a $2 \times 32$ lattice.

FIG. 3. (a) The equal time rung–rung pair field correlation function $\langle \Delta_i \Delta_j^\dagger \rangle$ versus $|i - j|$ plotted on a log-log scale for $t_\perp = 1.5$ and for ladders of length $L = 16$, $L = 24$, and $L = 32$. The dashed line corresponds to the $|i - j|^{-2}$ decay of the non-interacting pair field correlations. (b) The equal time pair field correlation function $\langle \Delta_i \Delta_j^\dagger \rangle$ versus $|i - j|$ for various values of $t_\perp$. 
Fig. 1(a)
Fig. 1(b)
Fig. 2
\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3a}
\caption{Fig. 3(a)}
\end{figure}
Fig. 3(b)