

Stripes in a three-chain Hubbard ladder: A comparison of density-matrix renormalization group and constrained-path Monte Carlo results

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Using both the density-matrix renormalization group method and the constrained-path quantum Monte Carlo method, we studied the ground-state energies and the spin and hole densities of a 12×3 Hubbard model with open boundary conditions and six holes doped away from half-filling. Results obtained with these two methods agree well in the small and intermediate U regimes. For $U/t \geq 6$ we find a ground-state with charge inhomogeneities consistent with stripes.

One lesson learned from the search for an electronic model of high temperature superconductivity is that computing the low lying states of even simple many-electron models is difficult. The difficulty in fact has prevented definitive statements about the superconducting nature of the ground state of the one and three-band Hubbard models and the t - J model in two dimensions. Recently, two methods for computing ground-state properties of many-body systems were developed that in a number of respects represent significant advances over previous methods. These are the density-matrix renormalization group (DMRG) and the constrained-path Monte Carlo (CPMC) methods.

The DMRG method¹ is a variational procedure which produces reliable estimates of the ground-state energy as well as an exact upper bound on this energy. It can also be used to compute various kinds of correlation functions. The DMRG method is extremely accurate for low-dimensional many-body systems with short-range interactions. Unfortunately, it has trouble dealing with periodic boundary conditions, and in two dimensions its computational effort increases very quickly (probably exponentially) with the width of the system, although only linearly with the length. The largest DMRG calculations for a two-dimensional doped system have been for 28×8 t - J lattices.² However, these calculations were not nearly as accurate as previous DMRG calculations on narrower ladder systems.

The CPMC method³ also produces very accurate estimates of the ground-state energy and correlation functions. It is a quantum Monte Carlo method that projects the ground state from a trial state $|\Psi_T\rangle$ by means of a branched random walk. It prevents the Fermion sign problem from occurring by eliminating any random walker whose state $|\phi\rangle$ develops a negative overlap $\langle \Psi_T | \phi \rangle$ with the trial state. This constraint converts the procedure, which is otherwise exact within statistical errors, into an approximate method, but it can treat relatively large systems sizes (e.g., 16×16 lattices), and unlike the DMRG method, without any limitations arising from dimensionality or boundary conditions.

While the existence of striped states was predicted nearly a decade ago by the Hartree-Fock⁴ method, confirmation of stripe formation with more reliable numerical techniques was lacking. Recently, however, there has been a surge of interest in stripes because of their apparent experimental observation not only in the superconducting cuprates⁵ but also in nonsuperconducting nickelates. A stripe is simply a domain wall ordering of holes and spins. Spins in the regions between the walls are antiferromagnetically ordered and across a wall are correlated with a π phase shift. The wall, at most a few lattice spacings wide, is a hole rich region. Very recently, White and Scalapino^{2,6,7} used the DMRG method in several studies of the existence and structure of striped states in the two-dimensional t - J model and in t - J ladders of several widths. They found that stripes form under a wide variety of circumstances. Since the t - J model is a strong-coupling *approximation* to the Hubbard model, it is natural to ask if numerical methods can find stripes in the latter model and if these states also appear in the weak coupling limit. It is known that within the Hartree-Fock approximation for the Hubbard model stripes exist when the Coulomb interaction U/t exceeds a critical value which is approximately 3.

In this paper we report on a numerical study of striped states in a three-chain Hubbard model, based on both the CPMC and DMRG methods. The two methods complement each other. In this system the DMRG method is most effective for large U , while the CPMC method is most effective for small U . We find the two methods agreeing pleasingly well in both the small and intermediate U regimes. We do not find stripes at small U ; at $U/t \sim 6$ stripes appear and the Hubbard model results seemingly map nicely onto previous DMRG t - J model results.

We used the Hubbard model

$$H = -t \sum_{(i,j),\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

defined on a *rectangular* lattice with *open* boundary conditions. Open boundary conditions are used to break the trans-

lational invariance of the system, allowing striped patterns to appear as local density variations. If periodic boundary conditions are used, for example, in the CPMC simulations, charge-charge and spin-spin correlation functions show little, if any, indications of stripes. Open boundary conditions also make the DMRG method more accurate. We report results on a 12×3 three-chain ladder, doped six holes away from half-filling, as a function of U/t . This system was selected based on t - J results showing pronounced charge inhomogeneities, which are interpreted as indicating the presence of two pronounced three-hole transverse stripes.⁷ However, it is not our goal to study the nature of the stripelike oscillations in detail, only to test for their presence as a function of U , and to compare the ability of the two numerical techniques to obtain them.

For different values of U , we computed the ground-state energy and ground state expectation values of the rung spin density

$$S(i) = \sum_j (-1)^{j-1} \langle s_j^z(i) \rangle \quad (2)$$

and the rung hole density

$$R(i) = \sum_{j\sigma} \langle 1 - n_{j\sigma}(i) \rangle. \quad (3)$$

Here i labels the rung, and j is the chain index. We remark that in all of our results $\sum R(i) = N_h = 6$.

The CPMC method uses a trial wave function $|\Psi_T\rangle$ for three purposes: as a starting point, as an importance function, and as a constraining function. The first use influences the Monte Carlo dynamics; the second, the statistical error of the results; and the third, the systematic error. In the simulations reported here, we used two types of trial functions. One is the wave function of the noninteracting ($U=0$) problem, the free-electron (FE) solution. This single Slater determinant state does not exhibit a striped pattern. The second is the unrestricted Hartree-Fock (UHF) solution. This single Slater determinant shows a striped pattern provided U/t is approximately 3 or larger. We note that for $U/t=3$ the value of the overlap $\langle \text{UHF} | \text{FE} \rangle$ is small (~ 0.1) and becomes even smaller ($\sim 10^{-5}$) as U/t is increased to 8.

In our ‘‘quick and dirty’’ method of obtaining the UHF solution, each $\langle n_{i\sigma} \rangle$ was obtained independently without imposing the point group symmetry of the rectangle. Accordingly the UHF wave function did not precisely display the symmetries of the rectangle, with the mirror symmetry, $y \leftrightarrow -y$, being noticeably absent. If we used multiple Slater determinants for $|\Psi_T\rangle$ that restored the broken mirror symmetry, either as a two determinant trial function with the UHF solution and its mirror symmetric solution or as a four determinant solution obtained by applying the four group operations of the rectangle to the UHF solution, we would find the expectation value of the energy and the rung densities virtually unchanged. The main difference is the symmetrized UHF state has $\langle s_j^z(i) \rangle = 0$; the unsymmetrized state does not. In the results reported below we used the single Slater determinant UHF state as our constraining and initial wave functions.

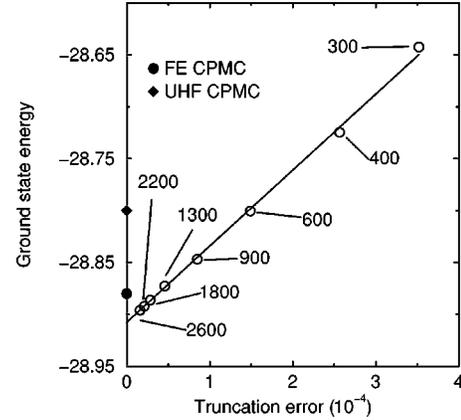


FIG. 1. The DMRG ground-state energy for $U/t=6$ as a function of the truncation error parametrized by m , the number of density matrix eigenstates.

We remark that we used the UHF solution for $U/t=3$ even though the simulation was for a Hubbard model with a larger U . The smaller U starting point, a point at which a striped state in the UHF wave function has become easily noticeable, produced expectation values with less variance than results obtained by starting with the UHF solution for the value of U in the simulation. The smaller U starting point also tended to produce less localized stripes. The Hartree-Fock solution for the larger values of U has a more spatially restricted domain wall, eventually becoming one rung of lattice sites. When we put the FE wave function as $|\Psi_T\rangle$, the final result for any U does not have stripes, and when we put UHF wave functions as $|\Psi_T\rangle$, it does for $U/t \geq 5$. The CPMC simulations generally used 500 random walkers (on the average). We estimate that the systematic error due to the Trotter approximation was within the statistical error.

Unlike the Monte Carlo method the DMRG method does not have a statistical error which is reduced by increasing the length of simulations. Instead it has a truncation error which is reduced by keeping larger numbers m of density matrix eigenstates (for more details see Ref. 1). Varying m allows one to compute physical quantities for different truncation errors and thus to obtain error estimates on these quantities. In Fig. 1, for $U/t=6$, we show the DMRG ground-state energy as a function of the truncation error parametrized by m . For large m the energy $E(P_m)$ decreases almost linearly with the truncation error P_m . Thus, we can extrapolate to the limit $P_m \rightarrow 0$ to estimate the ground-state energy $E(P_m=0)$ more accurately. Usually the slight deviation from linearity in the function $E(P_m)$ has a positive second derivative, so extrapolated values usually increase slightly when the accuracy is increased. Thus our results for $E(P_m \rightarrow 0)$ are likely to be slightly lower than the exact results. Based on observation of the dependence of the rung densities on m , we estimate that the errors in the rung densities are generally no more than 1%.

As for the CPMC method, the starting wave function used by the DMRG method can be varied. This starting wave function is simply the DMRG approximation to the ground state at the end of the warmup sweep, before the finite system sweeps begin. After these initial sweeps the initial wave function has no effect. However, it may be that there are a few ‘‘metastable’’ low energy states, in which case, with a

TABLE I. Ground-state energies. For the CPMC results, FE and UHF refer to results obtained when either the free-electron or unrestricted Hartree-Fock wave function was chosen for both the initial and constraining wave functions. The numbers in parenthesis are the estimated statistical error. For the DMRG results the variational energy is the one obtained for the maximum number of states kept. This number is shown in parenthesis. The extrapolated values are the results obtained by the analysis illustrated in Fig. 1. The number in parenthesis is an estimate of the error.

U/t	CPMC		DMRG	
	FE	UHF	Var. bound (m)	Extrapolation
1	-45.4171 (4)	-45.4161 (4)	-45.3985 (2200)	-45.419 (4)
2	-40.581 (2)	-40.560 (2)	-40.5436 (1600)	-40.590 (9)
3	-36.622 (1)	-36.566 (7)	-36.6056 (1600)	-36.627 (4)
4	-33.438 (2)	-33.364 (7)	-33.4259 (2200)	-33.448 (6)
5	-30.911 (2)	-30.807 (7)	-30.8927 (1600)	-30.915 (8)
6	-28.873 (4)	-28.807 (6)	-28.8962 (2600)	-28.907 (4)
7	-27.211 (5)	-27.133 (6)	-27.2537 (1200)	-27.31 (1)
8	-25.93 (3)	-25.94 (8)	-25.9502 (1200)	-25.997 (9)
12			-22.5688 (800)	-22.63 (1)
16			-20.7596 (800)	-20.81 (1)

poor initial wave function, the DMRG method can become stuck for a significant number of sweeps. If m is increased enough, the method will always find the correct ground state, but the calculation may not always be practical. Thus it is often wise, particularly in 2D systems, to try several different initial wave functions.² Usually we generate distinct initial wave functions by varying the quantum numbers of the target state as the system is built up from scratch. This crude approach is usually sufficient to avoid getting stuck in metastable states. For the system studied here, it was feasible to increase m enough to tunnel out of metastable ground states, which allowed a check on whether we had tried enough initial wave functions.

Our main results for the energies are reported in Table I. Two sets of CPMC results are given. The labels FE and UHF indicate the choice of $|\Psi_T\rangle$. For U/t less than about 8, the FE CPMC energies lie lower than the UHF CPMC energies, suggesting, but not proving, the CPMC state associated with the FE trial state is the one most representative of the ground state. This state does not show a static striped state. For $U/t=6$ and 7 the difference in the FE and UHF CPMC energies is of the order of 10^{-2} which is likely to be the size of the systematic error. This picture gets modified somewhat when the DMRG results are considered.

Two sets of DMRG results are also presented in Table I: the lowest variational bounds obtained (with the largest number of states m used to reach this bound also given) and the extrapolated ground-state energies $E(P_m=0)$. For $U/t < 6$ DMRG bounds lie above the FE CPMC results and the extrapolated DMRG energies agree with the FE CPMC energies within error estimations. This demonstrates the accuracy of both methods in the weak coupling regime.

For $U/t < 6$ neither the CPMC nor DMRG ground states clearly show a static striped state. This is consistent with weak coupling renormalization group calculations which do not show any indication of stripes in three-chain Hubbard ladders.⁸ However, the UHF CPMC results and some results for metastable DMRG ground states do suggest that low-lying states with stripes exist for relatively small U .

Results are significantly different for $U/t \geq 6$. DMRG

variational bounds are now lower than the CPMC energies, although differences remain small. Moreover, DMRG ground states clearly show striped hole patterns in this regime. Therefore, these results suggest that stripes appear in the ground state of the three-chain Hubbard model around $U/t=6$. However, for $U/t \leq 8$ both the FE CPMC results and DMRG metastable state results show that there are states without stripes very close to the ground state. For larger U/t (≥ 12) DMRG calculations converge very easily to a ground state with stripes and show little indication of low-lying states without stripes. CPMC simulations were not attempted for these larger values of U . In Figs. 2 and 3, we show the striped spin and holes densities for the $U/t=8$ case, along with UHF results for $U/t=$ and 8. We note the striking similarity of the CPMC and the DMRG results with each other and with the $U/t=3$ UHF results, even though the UHF state has a much higher energy. (The UHF energies for $U/t=3$ and 8 are -33.3009 and -19.1907 .) From Fig. 2, we identify two domain walls to be at rung positions 3 and 4 and at

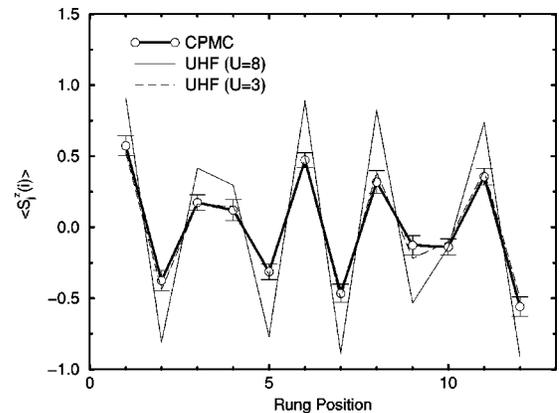


FIG. 2. For $U/t=8$, the expectation values of the z component of the rung spin as a function of rung position along the middle chain. The solid line is the CPMC result using the $U/t=3$ UHF wave function as the initial and constraining state. Also shown are the UHF results for $U/t=3$ and 8. The DMRG predicts a zero expectation value.

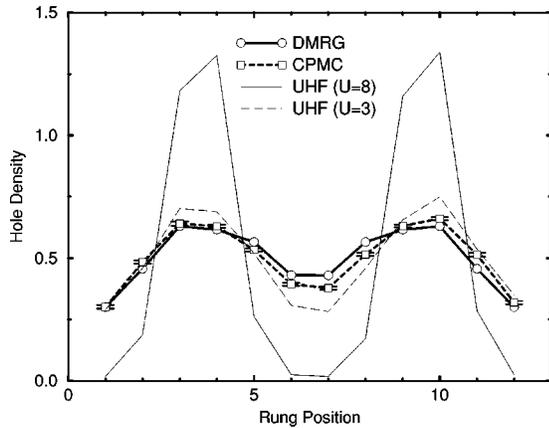


FIG. 3. For $U/t=8$, the expectation values of the rung hole density as a function of rung position. The solid line is the CPMC result using the $U/t=3$ UHF wave function as the initial and constraining state. The dotted line is the DMRG results. Also shown are the UHF results for $U/t=3$ and 8.

9 and 10. In each case the spins on either side of the wall are ferromagnetically aligned but shifted by a phase π from what they would be if there were complete antiferromagnetic order. Antiferromagnetic order exists between the walls. We remark the two-rung domain wall width is similar to that found by White and Scalapino for the t - J model.

The qualitative conclusions of this work are that (1) the same characteristic features, indicating a striped state that were found in the three-chain t - J model,⁷ are also found in the Hubbard model at strong to intermediate interaction U and (2) these features seem to disappear at weaker coupling. This suggests that stripes are a strictly strong-coupling phenomenon.

Furthermore, it is remarkable how closely two quite different numerical methods agree on a very subtle issue. As used here, these methods come at the problem with different strengths and hence mutually calibrate each other. However, it is crucial to point out that great care must be used in applying the methods to avoid coming to erroneous conclusions. In particular, the CPMC method does not show stripes

even at large U when the FE trial function is used. This underscores the importance of using trial wave functions appropriate to the parameter range of the model, particularly when the nature of the ground state is unknown.

In closing we remark that for periodic boundary conditions and square lattices, the CPMC method does not find stripes either in the spin and hole densities or in spin-spin and hole-hole correlation functions. (We did not use the DMRG method with periodic boundary conditions.) We note that under these conditions it is probably very difficult to see stripes in correlation functions for small to intermediate values of U/t . In these regimes the density of virtual holes (associated with the formation of doubly occupied sites) can be comparable to the density of holes introduced by doping. These uncorrelated virtual holes are likely to hide hole correlations associated with a stripe. As U increases this problem becomes less severe because the density of doubly occupied sites decreases. An additional complication is that with periodic boundary conditions, any type of striped state, whether it is purely dynamic, or static (in the thermodynamic limit), would appear in the ground state as a uniform superposition of striped patterns at different positions and orientations. Such a superposition, and the associated near degeneracy of the ground state, could be very difficult to deal with numerically. In the present calculations, for large U , a static striped pattern results from the open boundary conditions breaking translational symmetry. In physical systems, various lattice defects break this symmetry. The main point is that the low-lying striped states seen with these boundary conditions are present in the Hubbard model for strong to intermediate values of U , but are not seen at small U .

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