DMRG Investigation of Stripe Formation in Doped Hubbard Ladders

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Summary. Using a parallelized density matrix renormalization group (DMRG) code we demonstrate the potential of the DMRG method by calculating ground-state properties of two-dimensional Hubbard models. For 7×6, 11×6 and 14×6 Hubbard ladders with doped holes and cylindrical boundary conditions (BC), open in x-direction and periodic in the 6-leg y-direction, we comment on recent conjectures about the appearance of stripe-like features in the hole and spin densities. In addition we present results for the half-filled 4×4 system with periodic BC, advance to the 6×6 case and pinpoint the limits of the current approach.

1 Introduction

Density matrix renormalization group (DMRG) techniques have recently become an interesting alternative to exact diagonalization (ED) and quantum Monte Carlo methods for the investigation of ground-state but also dynamical properties of strongly correlated electron systems.

In this report we want to focus on recent efforts in the analysis of the ground-state characteristics of finite two-dimensional (2D) Hubbard systems,

$$H_{\mathrm{HM}} = -t \sum_{\langle ij \rangle, \sigma} \left[c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{H.c.} \right] + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \quad , \tag{1}$$

with varying system sizes and boundary conditions (BC). Here t denotes the transfer amplitude between neighbouring sites $\langle ij \rangle$, U is the on-site Coulomb interaction, and the $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) describe the creation (annihilation) of an electron with spin-projection σ at Wannier site i, where $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. Especially we address the problem of stripe formation in the 2D Hubbard ladder models with cylindrical, i.e. partly periodic BC, which recently has been intensively debated in the context of quasi-2D high-T_{c} cuprates. It is important to note that DMRG has as yet not managed to yield sufficiently accurate results for such cases, as opposed to the 1D case, where periodic

BC are not that problematic. We will show that although it is still difficult to get bulletproof DMRG results in two dimensions with periodic BC, it is nevertheless possible to make substantial progress in the controversial discussion about stripe formation.

The outline of the paper is the following: Section 2 briefly refers the basics of the DMRG algorithm and our method of parallelization. Without a parallel code one is quickly confronted with unmanageable runtimes. The numerical results obtained for Hubbard ladder and periodic 2D Hubbard models are presented in Sect. 3.1 and Sect. 3.2, respectively. In Sect. 4 we will give both a short summary and an outlook.

2 Algorithm and parallelization

The workings of the DMRG algorithm have been thoroughly documented elsewhere [1, 2, 3] and shall not be repeated here. A C++ package developed by White and Jeckelmann that implements the DMRG algorithm for several important physical setups has served as a starting point for parallelization. Profiling has revealed that in many cases the central superblock diagonalization via a Davidson algorithm is the dominant operation [4]. Essentially by parallelizing this component and linking

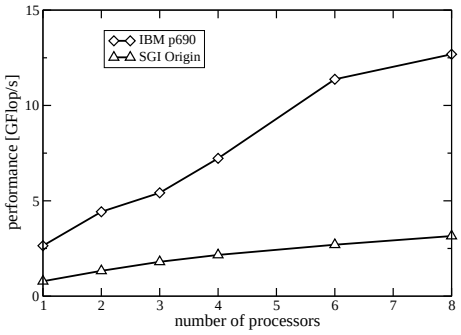

Fig. 1. Absolute performance in GFlop/s of a standard benchmark (described in [4]) on SGI Origin and IBM p690 systems.

with appropriate linear algebra libraries we could turn this application into a shared-memory code that runs effectively on most current supercomputer architectures [4, 5].

Fig. 1 shows the scalability of absolute performance with processor count for a standard test case (4×4 half-filled Hubbard model with periodic BC) using a 500 MHz SGI Origin and a 1.3 GHz IBM p690 system. Clearly the accuracy of observables like the ground-state energy depends on the number m of density matrix states kept. In these calculations we used $m = 2000$ target states. From the data it is obvious that parallel DMRG can reach a substantial fraction of peak performance and that modern shared memory nodes (SMP) nodes like the IBM p690 are the ideal target architecture. Right now the most efficient mode of operation can be achieved with four to eight CPUs per run.

3 Numerical results

3.1 Hole-doped 6-leg Hubbard ladders

There is a controversial discussion [6, 7, 8, 9, 10, and references therein] about whether the ground state of interacting doped lattice models in two dimensions like the t-J and the Hubbard Model forms stripes when subjected to particular, e.g. cylindrical boundary conditions.

Recently, White and Scalapino [10] published DMRG results for a 6-leg Hubbard ladder with cylindrical boundary conditions (7×6 sites, open BC in x- and periodic BC in y-direction) and doped with four holes. They conclude from their data that there is stripe formation in the ground state for $U \geq 8$ and that the stripe is broadened for smaller U and also for very large U (above 20). Here and in what follows all energies are measured in units of t.

In a first step we reproduce their results and try to establish improved numerical validity. The goal is to examine stripe formation in larger systems as well and pinpoint the influence of boundaries.

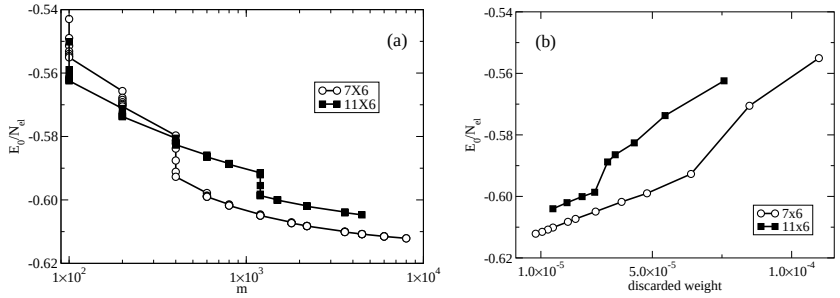

Fig. 2. Ground-state energy per electron in dependence on m (a) and as a function of the discarded weight (b) for a Hubbard ladder at $U = 12$, where cylindrical BC, i.e. open BC in x-direction and periodic BC in y-direction, were used. Circles ($m \leq 8000$) and squares ($m \leq 3600$) give the results for 7×6 and 11×6 systems, respectively.

The paper [10] comments only briefly on the exact DMRG algorithm used ("one-site method"). We therefore started with the usual strategy of using two intermediate sites and reflection symmetry. Fig. 2 (a) shows ground-state energy versus $m \leq 8000$ for $U = 12$. One significant difference compared to the data by White and Scalapino is the fact that the transition to the "striped" state happens already at very small $m \approx 600$, as opposed to $m \approx 1200$ in the paper. This could be due to differences in the algorithm (warmup), though. Regarding computational resources, to achieve the $m = 3600$ results with the same quality as in [10] our parallel DMRG code required roughly 6 hours on eight CPUs of an IBM p690 node. For the full $m = 8000$ run the walltime was about one week. Please note that although the ground-state energy suggests convergence (see Fig. 2 (a)), the discarded weight (Fig. 2 (b)) shows that there is still some room for improvement.

The "transition point" is marked by a qualitative change in the hole density (Fig. 3 (a)). At lower values of the Hubbard interaction, e.g., $U = 3$ Fig. 3 (b), though the density peak is significantly less pronounced, quite in agreement with [10].

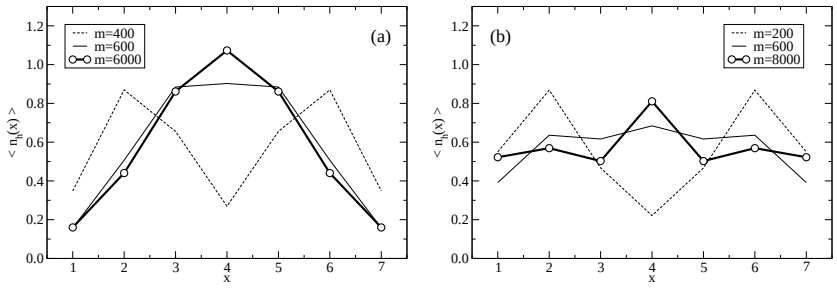

Fig. 3. Hole density in x-direction for the 7×6 Hubbard ladder for $U = 12$ (a) and $U = 3$ (b) at different m. The y-direction was summed over.

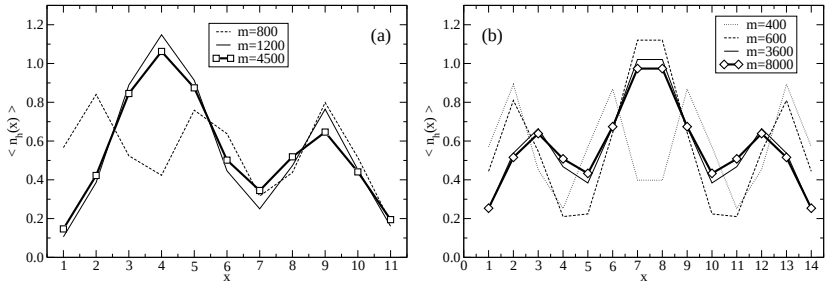

Fig. 4. Hole density in x-direction for the 11×6 (a) and 14×6 (b) Hubbard ladders ($U = 12$) with 6 and 8 holes, respectively. Reflection symmetry was not used for the 11×6 system but employed for the 14×6 system.

Interestingly, increasing m even further after the stripe has formed does not enhance but slightly flatten the peak for $m > 800$ (not shown in Fig. 3 (a)). If the stripe is really the ground state, it would thus not make sense to use $m \gg 1000$, at least with our algorithm. It is worth noting that although the hole density does not change significantly between $m = 800$ and $m = 8000$, we still get a lower ground-state energy than White and Scalapino [10].

An open question is whether stripe formation in the 7×6 system might be forced by the rather small lattice size in x-direction (in combination with open BC in this direction). In order to investigate this issue we performed DMRG calculations on the somewhat larger 11×6 and 14×6 ladders with 6 and 8 holes, respectively (see Figs. 4 (a) and (b)). Severe convergence problems have prevented us from using reflection symmetry with the 11×6 ladder at $U = 12$, but not for the 14×6 ladder.

For the 11×6 ladder the transition to a stripe-like state occurs at $m \approx 1000$. However, the resulting hole distribution shows two peaks of different heights. Obviously, four of the six holes are concentrated in one peak and the remaining two in the other one. Looking at the two-dimensional hole density distribution (Fig. 5, left panel) and also at the discarded weights (Fig. 2 (b)) it becomes clear that the algorithm has not really converged yet: the density fluctuates in the periodic (y-) direction, so a larger m and/or more sweeps are in order. Another important observ-

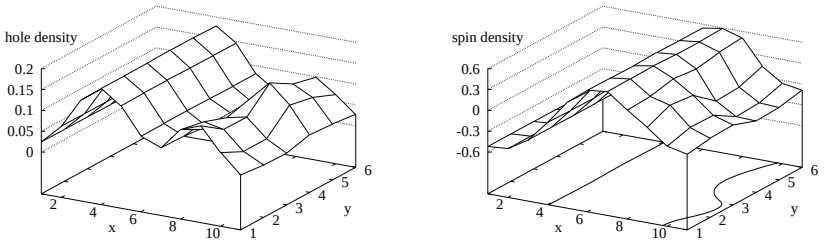

Fig. 5. Spatial distribution of the hole density (left panel) and the spin density $S_z(x,y)(-1)^{x+y}$ (right panel) for the 11×6 Hubbard ladder with 6 holes at $U = 12$. The lines in the bottom canvas mark zero-crossings.

able for stripe formation is the spin density distribution. There should be a phase shift of π in the spin density across the stripe. Despite the non-convergence of the 11×6 run at $U = 12$ this particular feature can be identified from Fig. 5 (right panel) showing the staggered spin density $S_z(x,y)(-1)^{x+y}$ and its zero-crossing contours. Two phase shifts are clearly visible (one along each stripe).

For the 14×6 Hubbard ladder with 8 holes, from Fig. 4 (b), we have seen that the transition to a striped state occurs already at very low $m \approx 600$. There are three "stripes" with two, four and two holes, respectively. Due to the fact that reflection symmetry was used, the formation of an asymmetric ground state like in the 11×6 case was ruled out from the beginning. The hole and spin densities for this system reveal, however, that the two smaller stripes have obviously not formed completely, even at $m = 8000$ (cf. Fig. 6). We therefore conclude that it can be numerically unfavorable to use reflection symmetry with Hubbard ladders, at least in some cases.

As a consequence we have repeated our analysis of the 14×6 case without using reflection symmetry. A comparison of ground-state energy versus m for symmetric and non-symmetric calculations is shown in Fig. 7 (a) and reveals that a non-symmetric calculation leads to lower energies at large m. The inappropriateness of reflection symmetry for the 14×6 system is also emphasized by the discarded weight (see Fig. 7 (b)).

In Fig. 8 we show the hole density (summed over the y-direction) for the 14×6 Hubbard ladder (8 holes) with and without using reflection symmetry. The transition to the striped state occurs at $m \approx 600$ in the former case and $m \approx 1500$ in the latter case. For the "true" ground-state solution (i.e. the one being lowest in energy) the

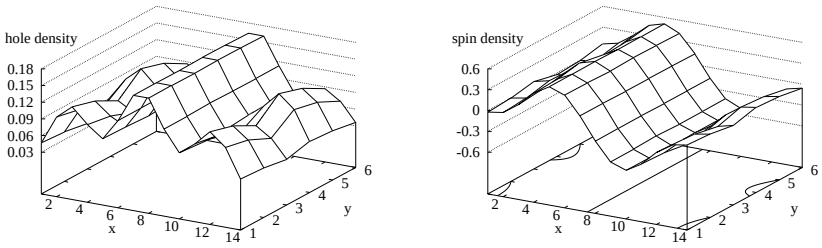

Fig. 6. Hole density (left) and spin density (right) for the 14×6 Hubbard ladder with 8 holes at $U = 12$ (reflection symmetry was used).

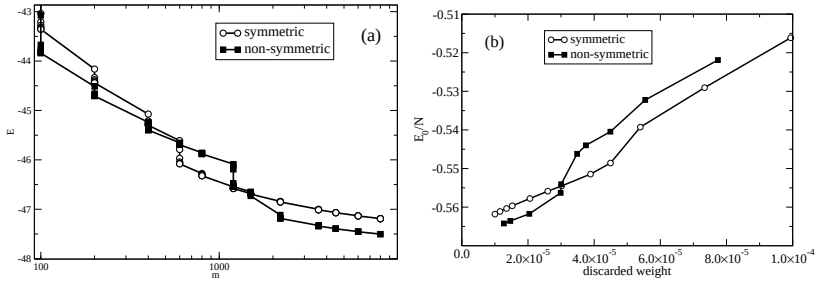

Fig. 7. Comparison of convergence of ground-state energy as a function of m for the 14×6 Hubbard ladder with and without using reflection symmetry (panel (a)). Ground-state energy per site vs. discarded weight for the 14×6 Hubbard ladder with and without using reflection symmetry (panel (b)).

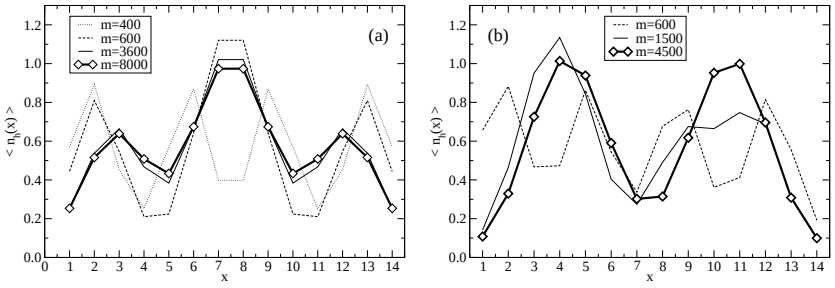

Fig. 8. Hole density in x-direction for the 14×6 Hubbard ladder at $U = 12$ with 8 holes. Reflection symmetry was employed in (a) but not used in (b).

hole and spin densities show clearly that there are two stripes with four holes each (cf. Fig. 9).

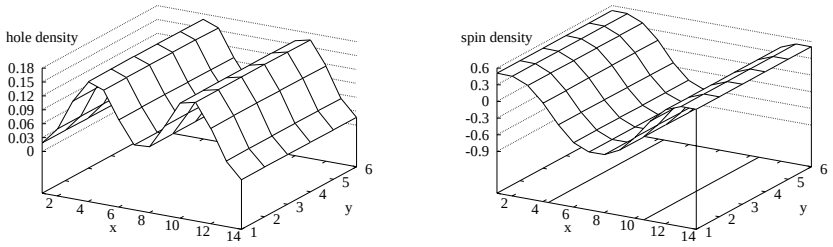

Fig. 9. Hole density (left) and spin density (right) for the 14×6 Hubbard ladder at $U = 12$ (8 holes, no reflection symmetry).

3.2 2D half-filled Hubbard model with periodic BC

In order to put the capabilities of parallel DMRG into some context we finally present results for ground-state properties of 2D 4×4 and 6×6 Hubbard systems with $U = 4$, subjected to periodic BC. Today the 4×4 system can be easily treated by DMRG even with up to $m = 10^4$ target states, and the agreement with an ED calculation of the ground-state energy is remarkable (see Fig. 10). Note that this calculation has very moderate resource requirements of about 6 GBytes of memory and 100 CPU hours on a 500 MHz MIPS processor. The 6×6 system, however,

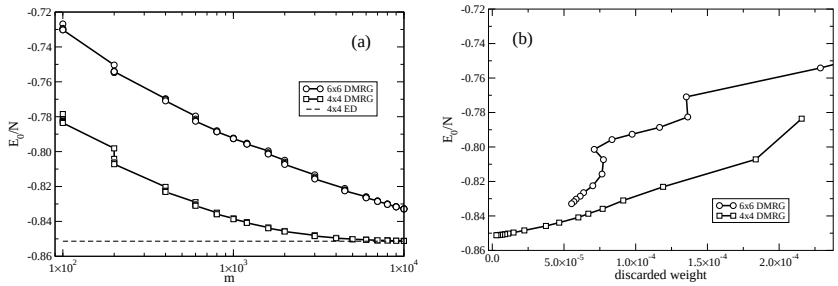

Fig. 10. Ground-state energy per site in dependence on m for the 4×4 and 6×6 Hubbard model with periodic BC. Different sweeps with same m have identical abscissas. For reference, the ED result for the 4×4 system is included.

requires significantly more resources. Figure 10 indicates that even using $m = 10^4$ target states DMRG has definitely not converged in that case (supported by Monte Carlo calculations we expect that the ground-state energy of the 6×6 Hubbard

system should be lower than for the 4×4 system [11]), but the memory requirement is already about 30 GBytes. On eight Itanium 2 CPUs the calculation took roughly 10 days. As a rough estimate one would expect to establish convergence similar to the 4×4 case at about $m = 10^5$, which is beyond reach right now.

4 Conclusion

In summary, we have shown that parallel DMRG on powerful shared memory nodes can push the largest manageable system size for ground-state calculations of 2D Hubbard systems to new heights, even for periodic boundary conditions. Although convergence of the ground state for the periodic 6×6 lattice is still beyond reach, we were able to derive reliable results concerning stripe structures for 7×6, 11×6 and 14×6 doped Hubbard ladders. Corresponding data for the 21×6 and 28×6 systems will be obtained on a IBM p690 in near future. However, due to the fact that solid convergence of DMRG calculations is hard to establish, further work will comprise a very careful analysis of stripe signatures, most notably including a finite-size scaling.

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