Ground-state properties of the Hubbard model by Lanczos diagonalizations

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(Received 4 April 2000)

We investigate the Hubbard model on a two-dimensional cluster of 18 sites using Lanczos algorithm for different strengths of Coulomb repulsion in the low doping region. Energies and correlation functions are given for half-filling and two holes. In the strong coupling regime we compare our results with the t-J model. We confirm the tendency of holes to repel, although a significant value of the $d_{x^2-y^2}$-wave superconductive order parameter is measured. These data represent a benchmark for future quantum simulations.

The discovery of high-temperature superconductors has certainly stimulated considerable progress in the numerical methods for strongly correlated electron systems. An outstanding, yet unsolved, problem is if, despite the complexity of the real materials, it is possible to capture the basic low energy physics by simple models of interacting electrons. Indeed, after more than a decade of investigations, it is not clear what is the minimal model capable to describe their complex properties, and several proposals are still being debated. The simplest model describing interacting electrons in a two-dimensional lattice is the Hubbard model:[1]

$$\mathcal{H}=-t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma}+U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}, \qquad (1)$$

where $\langle\ \rangle$ stands for nearest neighbors, $c_{i,\sigma}$ ($c^{\dagger}_{i,\sigma}$) destroys (creates) an electron with spin σ at site i, and $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$.

The most interesting region is near half-filling at intermediate and large coupling, where correlations play a relevant role in renormalizing bare particle properties. In the strong coupling limit, i.e., $U\gg t$, projecting out the subspace with double occupancies, the Hubbard model can be mapped onto the so-called t-J model[2]

$$\mathcal{H}_{tJ}=J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{1}{4}n_i n_j\right)-t\sum_{\langle i,j\rangle,\sigma}\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}_{j,\sigma}, \qquad (2)$$

where $\tilde{c}^{\dagger}_{i,\sigma}=c^{\dagger}_{i,\sigma}(1-n_{i,\bar{\sigma}})$, $n_i=\Sigma_\sigma n_{i,\sigma}$ is the electron density on site i, $\mathbf{S}_i=\Sigma_{\sigma,\sigma'}\tilde{c}^{\dagger}_{i,\sigma}\boldsymbol{\tau}_{\sigma,\sigma'}\tilde{c}_{i,\sigma'}$ is the spin operator, being $\boldsymbol{\tau}_{\sigma,\sigma'}$ Pauli matrices. The antiferromagnetic coupling is related to Hubbard U by $J=4t^2/U$. In the following we set $t=1$.

No reliable analytical treatment of the Hubbard model at intermediate or strong coupling is available yet, while quantum Monte-Carlo simulations suffer from the Fermi sign problem and cannot reach the accuracy usually achieved in bosonic systems. On the other hand, Lanczos diagonalizations are hindered by the exponential growth of the Hilbert space dimensions and a systematic study of the two dimensional Hubbard model has been performed only for the 4 $\times$4 lattice.[3–5] By contrast, due to the smaller Hilbert space, several data on the t-J model are available in the literature for bigger lattices.[6–8]

Unfortunately, in the 4×4 cluster at low doping, the noninteracting (i.e., $U=0$) model is affected by a huge degeneracy, only barely lifted by the interaction. In such a circumstance, size effects are expected to be severe and calculations on small lattices cannot be considered representative of the thermodynamic limit. Instead, it is known that finite size effects for nondegenerate closed shell fillings are very well behaved. For instance, in one dimension,[9] it is possible to obtain accurate critical indices with a finite size scaling using only closed shell filling on small clusters. In the two-dimensional case, though it is not possible to perform an analogous finite size scaling by the Lanczos method, it is natural to expect reasonably well behaved finite size effects close to a nondegenerate filling. Therefore, it would be extremely useful to have precise Lanczos data for several physical quantities in a square cluster with the low doping region close to a nondegenerate filling. The most satisfactory geometry is probably the 45° tilted squares with $L=l\sqrt{2}\times l\sqrt{2}$ sites which possess the full spatial symmetries of the infinite lattice and, at the same time, have a nondegenerate ground state at $U=0$ and half-filling for l odd. The $3\sqrt{2}\times3\sqrt{2}$ sites, in this respect, is the nontrivial lattice, satisfying the above requirements, where exact diagonalization can still be afforded.

In this paper, we report extensive results for the Hubbard Hamiltonian (1) using the Lanczos technique on the $L=18$ site cluster. In the strong coupling limit, our data are compared with diagonalizations of the t-J model (2). Periodic boundary conditions are imposed in both systems. The model is studied in separate subspaces labeled by quantum numbers identifying the spatial symmetry: momentum $\mathbf{k}$ and, when defined, angular momentum (s, p, or d). We concentrate on the two cases of half-filling ($N=18$ electrons) and two holes ($N=16$) for several strengths of the local Coulomb repulsion U. The z component of the total spin is set equal to zero, thereby imposing no restriction on the total spin subspace. At half-filling, the Hilbert space dimension D_H is 16 421 304 in the one-dimensional representation of the full spatial symmetry group of the 18 site cluster. The largest calculation we

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TABLE I. Ground state energies for $N=18$ (first column) and $N=16$ (second column) as a function of U for the Hubbard model. At half-filling, the wave function has $\mathbf{k}=(0,0)$ and s-wave symmetry, for $N=16$ it has $\mathbf{k}=(0,0)$ and $d_{x^2-y^2}$ symmetry. The energy of the t-J model for $N=16$ is reported in the third column, the wave function has $\mathbf{k}=(0,0)$ and $d_{x^2-y^2}$ symmetry, the value of J is related to U by $J=4t^2/U$. The double occupancies $\langle D\rangle$ for $N=16$ in the Hubbard model are reported in the last column.

U	$E_{N=18}$	$E_{N=16}$	$E^{tJ}_{N=16}$	$\langle D\rangle$
0	−32.00000	−30.00000		0.194444
4	−17.25239	−19.28248		0.106440
6	−12.68227	−16.09451		0.072198
8	−9.869535	−13.96011		0.048118
10	−8.072161	−12.52076	−11.86277	0.033076
12	−6.827395	−11.50999	−10.86623	0.023796
16	−5.212890	−10.20242	−9.641987	0.013830
20	−4.211077	−9.400274	−8.921199	0.008966
40	−2.137196	−7.780419	−7.521899	0.002240

present here has $D_H=42\,982\,720$ and occurs for two holes at finite momentum. Use has been made of the factorization property of the kinetic matrix elements on the two spin projections in order to speed up the calculation.

According to a theorem by Lieb,[10] the ground state at half-filling $|\Psi_{0h}\rangle$ is unique and has $\mathbf{S}=0$ for every $U>0$. In a closed shell case, this theorem implies that the ground state is characterized by the same quantum numbers of the $U=0$ limit, i.e., s-wave symmetry and vanishing momentum for all U's. In Table I we report the values of the energy in this sector as a function of U. We remark that in a previous work on the same lattice,[11] only the energies at half-filling were presented. Moreover, we found that for large values of U these results are slightly overestimated, probably due to a lack of accuracy in the convergence criterion of the Lanczos algorithm.

For two holes, at $U=0$ and $S^z=0$, the ground state $|\Psi_{2h}\rangle$ is 16 times degenerate: 10 singlets and 6 triplets. First order perturbation theory in U partially lifts this degeneracy leaving as ground states a singlet with $\mathbf{k}=(0,0)$ and $d_{x^2-y^2}$ symmetry, a pair of triplets with $\mathbf{k}=(0,0)$ and p-wave symmetry, and four triplets with $\mathbf{k}=(\pm 2\pi/3,\pm 2\pi/3)$, odd in the $x\leftrightarrow y$ interchange. We checked that already at $U=1$ the d-wave singlet is the unique ground state. Therefore, we believe that the lowest energy state remains in this symmetry subspace even at larger U.[12] In Table II we show the energies of the three previously mentioned states at $U=1$ and $U=4$.

In the second and third columns of Table I, we report the ground state energies of two holes in the Hubbard and t-J model, respectively. Although they get closer for increasing U, at $U=40$ there is still a sizable difference, to be ascribed to the presence of three-site terms in the strong coupling limit of the Hubbard Hamiltonian.[2] In the last column of Table I we report the value of the double occupancies for $N=16$:

$$\langle D\rangle=\langle\Psi_{2h}|D|\Psi_{2h}\rangle, \tag{3}$$

where

$$D=\frac{1}{L}\sum_i n_{i,\uparrow}n_{i,\downarrow}. \tag{4}$$

Some interesting physics associated to the Hubbard model can be extracted from the static correlation functions. The charge fluctuations are related to the density-density correlations and may provide a clue about the possible occurrence of phase separation or charge ordering (stripe phases) in the model. We computed the density-density correlation functions

TABLE II. Energies for two holes in the symmetry subspaces mentioned in the text at $U=1$ and $U=4$. The quantum numbers identify the momentum of the state. The label stands for singlet (S) or triplet (T).

U	$(0,0)_S$	$(0,0)_T$	$\left(\pm\frac{2\pi}{3},\pm\frac{2\pi}{3}\right)_T$
1	−26.71409	−26.69543	−26.69349
4	−19.28248	−19.09544	−19.08215

TABLE III. Ground state values for the density-density correlation function $\langle N_R\rangle$ for $N=16$ electrons in the Hubbard model.

U	$R=1$	$R=\sqrt{2}$	$R=2$	$R=\sqrt{5}$	$R=3$
0	0.705248	0.777776	0.791666	0.765432	0.783950
4	0.737746	0.782798	0.783718	0.779566	0.785146
6	0.750564	0.784146	0.783728	0.782556	0.784968
8	0.760044	0.784976	0.784060	0.783958	0.784946
10	0.766380	0.785298	0.784318	0.784550	0.784996
12	0.770518	0.785342	0.784494	0.784814	0.785080
16	0.775182	0.785170	0.784714	0.785032	0.785282
20	0.777530	0.784958	0.784858	0.785136	0.785484
40	0.780776	0.784370	0.785204	0.785338	0.786096

TABLE IV. Ground state values for the hole-hole correlation function $\langle H_R\rangle$ for $N=16$ electrons for the Hubbard and the t-J model. The results for two hard core bosons (HCB) are also shown.

U	$R=1$	$R=\sqrt{2}$	$R=2$	$R=\sqrt{5}$	$R=3$
0	0.069173	0.090278	0.093750	0.085820	0.091449
4	0.031289	0.044764	0.044117	0.042808	0.044834
6	0.021030	0.030680	0.029681	0.029331	0.030262
8	0.014901	0.021978	0.020921	0.020949	0.021368
10	0.011435	0.016978	0.016029	0.016202	0.016433
12	0.009404	0.014027	0.013260	0.013489	0.013675
16	0.007271	0.010919	0.010545	0.010798	0.011040
20	0.006219	0.009387	0.009351	0.009590	0.009941
40	0.004646	0.007115	0.007965	0.008096	0.008854
HCB	0.004178	0.006368	0.007521	0.007639	0.008287
J					
0.4	0.006076	0.008704	0.005066	0.006776	0.004625
0.25	0.005015	0.007534	0.006308	0.007297	0.006495
0.2	0.004703	0.007146	0.006711	0.007428	0.007160
0.1	0.004185	0.006466	0.007411	0.007627	0.008357

TABLE V. Ground state values for the spin-spin correlation function $\langle S_R \rangle$ for $N=16$ electrons for the Hubbard and the t-J model.

U	$R=1$	$R=\sqrt{2}$	$R=2$	$R=\sqrt{5}$	$R=3$
0	−0.075231	0.000000	−0.010417	−0.009258	0.004630
4	−0.126253	0.020716	−0.013366	−0.013378	0.022120
6	−0.151878	0.032860	−0.010998	−0.016710	0.028539
8	−0.170436	0.041484	−0.008676	−0.019063	0.032266
10	−0.181257	0.045817	−0.008014	−0.019633	0.035292
12	−0.186952	0.047362	−0.008722	−0.019021	0.038352
16	−0.190945	0.046825	−0.011872	−0.016560	0.044284
20	−0.190963	0.044725	−0.015409	−0.013983	0.049314
40	−0.181974	0.034168	−0.027390	−0.006100	0.061881
J					
0.4	−0.222067	0.072946	0.026787	−0.044076	−0.001026
0.25	−0.207861	0.058035	0.003334	−0.027552	0.029508
0.2	−0.201502	0.051814	−0.005781	−0.021352	0.040615
0.1	−0.182838	0.035070	−0.026016	−0.008154	0.061084

$$\langle N_R \rangle = \langle \Psi_{2h} | N_R | \Psi_{2h} \rangle, \tag{5}$$

and the hole-hole correlations

$$\langle H_R \rangle = \langle \Psi_{2h} | H_R | \Psi_{2h} \rangle, \tag{6}$$

being

$$N_R = n_i n_j, \tag{7}$$

$$H_R = h_i h_j, \tag{8}$$

with $|i-j|=R$ and $h_i=(1-n_{i,\uparrow})(1-n_{i,\downarrow})$ is the hole density operator.

We report in Table III the values of Eq. (5) for the Hubbard model at different values of U and in Table IV the values of Eq. (6) for the Hubbard and t-J model. In both cases, the hole correlations are small but the overall behavior of the two models is rather different and gets similar only in the strong coupling regime. In the Hubbard model, the hole-hole correlations are always repulsive for all the interactions U and not very much structured. As the Coulomb potential is increased, holes repel each other more and more and Eq. (6) is strongly renormalized with respect to the noninteracting case. In agreement with previous calculations,[4] we confirm that no sign of charge ordering is present also in the 18 site cluster and the behavior of hole correlations is qualitatively similar to the hard core boson result, also shown in Table IV. Conversely, the t-J model shows some sign of attraction between holes which might indeed lead to some sort of charge ordering in larger systems. Only at small J, hole repulsion prevails and the charge correlations become quite close to the hard core boson result. It would be interesting to analyze the issue of charge ordering in the t-J model on larger sizes, necessarily by use of other numerical methods.

Another important quantity is the spin-spin correlation function

$$\langle S_R \rangle = \langle \Psi_{2h} | S_R | \Psi_{2h} \rangle, \tag{9}$$

being

$$S_R = \mathbf{S}_i \cdot \mathbf{S}_j. \tag{10}$$

In Table V we show the values of Eq. (9) for the Hubbard and the t-J model at different couplings and two holes. It is possible to appreciate the strong similarity between the two cases which becomes quantitative for $U \geqslant 16$: spin correlations do not distinguish between the two models.

One of the most interesting open questions in the physics of strongly correlated electron systems is to understand if it is possible to have a superconducting ground state in models with only repulsive forces. Clearly, we cannot address such a delicate issue by diagonalization on a small lattice. However, it is still interesting to see the trend of the superconductive order parameter as the coupling increases. Usually, the quantity which is measured in numerical calculations is the square of the order parameter,

$$\tilde{P}_d = \langle \Psi_{2h} | \tilde{\Delta}_d \tilde{\Delta}_d^\dagger | \Psi_{2h} \rangle, \tag{11}$$

where

$$\tilde{\Delta}_d^\dagger = \frac{1}{\sqrt{4L}} \sum_{i,j} \phi_{i,j} \tilde{c}_{i,\uparrow}^\dagger \tilde{c}_{j,\downarrow}^\dagger, \tag{12}$$

TABLE VI. Ground state values for $d_{x^2-y^2}$ superconducting order parameter (13) for the Hubbard and the t-J model. The values of Eq. (11) are also reported.

U	$\tilde{Z}_d$	$\tilde{Z}_d^{tJ}$	$\tilde{P}_d$	$\tilde{P}_d^{tJ}$
0	0.2117		0.1671	
4	0.1945		0.1077	
6	0.2112		0.0878	
8	0.2096		0.0737	
10	0.2004	0.2569	0.0639	0.0771
12	0.1915	0.2317	0.0570	0.0649
16	0.1763	0.1982	0.0478	0.0505
20	0.1642	0.1768	0.0419	0.0424
40	0.1303	0.1300	0.0291	0.0276

with $\phi_{i,j}=+1$ if $j=i\pm x$, $\phi_{i,j}=-1$ if $j=i\pm y$, and $\phi_{i,j}=0$ elsewhere. We believe that a more appropriate choice is to concentrate on the corresponding weight Z which is less affected by high energy processes. In the 18 site cluster we calculate the quantity:

$$\tilde{Z}_d=\langle\Psi_{0h}|\tilde{\Delta}_d^\dagger|\Psi_{2h}\rangle. \tag{13}$$

$\tilde{Z}_d$ is just the overlap between $|\Psi_{0h}\rangle$ and $\tilde{\Delta}_d^\dagger|\Psi_{2h}\rangle$. Indeed, due to the different quantum numbers of $|\Psi_{0h}\rangle$ and $|\Psi_{2h}\rangle$, an operator $\Theta_d^\dagger$ exists with $d_{x^2-y^2}$ symmetry that makes the overlap between $|\Psi_{0h}\rangle$ and $\Theta_d^\dagger|\Psi_{2h}\rangle$ sizable. The occurrence of superconductivity is related to the fact that such an operator is in fact *local*: acting only at short range. In our case we limit $\tilde{\Delta}_d$ to nearest neighbor sites. In Table VI we report the values of Eqs. (11) and (13) in the Hubbard and t-J model for different values of U and J. Again, the agreement between the two models is remarkable, suggesting that, for this range of couplings, the pairing properties in the two systems are indeed quite similar. However, $\tilde{Z}_d$ decreases with U (for $U>8$) suggesting that a strong Coulomb repulsion does not favor nearest neighbor pairing, probably due to the drastic reduction of nearest neighbor hole correlations (see Table IV) as U increases.

In conclusion, we performed Lanczos diagonalizations of the Hubbard model on the 18 site cluster at low doping. The results strongly support the picture that no charge ordering is present in this region of the phase diagram. A remarkable difference between the Hubbard and t-J models emerges in hole correlations which appear to be much more structured in the t-J case. Some signal of superconductivity can be found in both the Hubbard and t-J models, which in fact show quite similar behavior. These results, besides giving useful hints on the short range properties of the Hubbard model at intermediate and strong coupling, do provide a valuable benchmark for testing future numerical simulation algorithms.

We are greatly indebted to S. Cozzini for technical help on SGI-Origin 2000. One of us (A.P.) acknowledges the warm hospitality at SISSA.

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