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Infinite-U Hubbard model in the large-spin regime: exact diagonalization study

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Abstract. The infinite-U Hubbard model on finite two-dimensional square lattices is investigated by the use of exact numerical diagonalization. Configurations with one spin flip away from the ferromagnetic state and up to three holes are studied for lattice sizes ranging from 4×4 to 12×12. For all these situations, the state with one spin flip is found to be more stable than the Nagaoka ferromagnetic state. The crystal momentum of the ground state in this spin sector depends on the system size. Systematic comparison with the Gutzwiller wavefunction shows that it reproduces qualitatively the crystal momentum dependence of the energy, but not the exact correlation between the spin flip and the holes.

1. Introduction

Much attention has been devoted recently to the problem of strongly interacting fermions on a lattice [1, 2]. The use of standard perturbation methods is difficult here owing to the absence of an obvious small expansion parameter. In this situation, numerical techniques provide useful information on the properties of such strongly interacting models [3]. More specifically, we present in this paper an exact diagonalization study of the Hubbard model in the infinite-interaction limit. In this limit, there is no energy scale, and the problem reduces to pure geometry via the non-double-occupancy constraint. The only parameter in the model is then the concentration of mobile vacancies. In the limit of a small electron concentration, the effect of hard-core repulsion is expected to be small and a singlet ground state is obtained [4]. In the opposite limit, where only one vacancy is present, it has been shown rigorously [5] that the ground state has the maximal total spin value on any bipartite lattice. The behaviour of the total spin in the ground state as a function of the hole density is still an unsettled question. Recent numerical diagonalizations have shown that on a finite system this quantity has a non-monotonic variation as the number of holes is increased [6]. This illustrates the importance of finite size effects in this limit. The origin of this sensitivity to the exact number of holes or boundary conditions comes from the very large number of low-lying states, in the presence of a small number of holes.

At finite hole densities, the instability of the Nagaoka ferromagnetic state has been recently investigated by variational calculations [7, 8]. They indicate that a finite critical concentration is required in order to destabilize the fully polarized state. In [8] a twisted

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static spin background has been considered whereas in [7] the Gutzwiller wavefunction with one spin flip is used.

In this paper, we shall restrict ourselves to the spin sector corresponding to a single spin flip away from the ferromagnetic state. This allows us to reach a larger lattice size than for the sector which contains the absolute ground state. For two holes, diagonalizations were performed for a lattice as large as 12×12 while, for three holes, the larger size was 7×7. First, a brief description of the method is presented. We then present our results for two holes and three holes. Comparison between exact diagonalization and the Gutzwiller wavefunction is detailed. We conclude by discussing the effect of a small nearest-neighbour antiferromagnetic exchange interaction on the ground-state quantum numbers.

2. Method

In this paper, we shall study the $U = \infty$ Hubbard model on a two-dimensional periodic square lattice. The Hamiltonian is

$$H = -t \sum_{ij\sigma} (1 - n_{i-\sigma}) c^{+}_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}). \tag{1}$$

Here t is the hopping matrix element chosen to be equal to unity. The sum runs over nearest-neighbour sites and spin indices. In equation (1) the constraint of non-double occupancy is enforced by projectors. In what follows, a systematic comparison between exact diagonalization and results for the Gutzwiller wavefunction will be presented. For one spin flip and n up spins, the Gutzwiller wavefunction is given by [9]

$$|\psi_0\rangle = P_G c^{+}_{p\downarrow} c^{+}_{k_1\uparrow} \ldots c^{+}_{k_n\uparrow} |0\rangle \tag{2}$$

where $P_G = \Pi_i (1 - n_{i\uparrow} n_{i\downarrow})$ removes the doubly occupied sites. In the case of one spin flip, P_G can be rewritten as

$$P_G = 1 - \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{3}$$

Using (2) and (3), the average kinetic energy is given by [7, 10]

$$\langle E \rangle = \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} = \frac{N_h}{N_h + 1} \sum_{i=1}^{n} \varepsilon(k_i) + \frac{2}{N_s(N_h + 1)} \sum_{\alpha = x,y} [C_\alpha^2 + S_\alpha^2 - (N_h + 1)^2] \cos p_\alpha. \tag{4}$$

Here $N_h = N_s - (n + 1)$ is the number of holes, N_s being the total number of lattice sites ($N_s = L^2$, where L is the linear size of the system). The free-particle energies are denoted by $\varepsilon(k) = -2(\cos k_x + \cos k_y)$. Furthermore,

$$C_\alpha = \sum_{j=1}^{N_h} \cos k_j^\alpha \qquad S_\alpha = \sum_{j=1}^{N_h} \sin k_j^\alpha. \tag{5}$$

In equation (5), the sum is over unoccupied states. This wavefunction is an eigenstate

Table 1. Lowest eigenenergy as a function of total momentum for $L = 8$ and two holes. The reciprocal space of the square lattice is displayed in the domain $0 \leqslant k_y \leqslant k_x \leqslant \pi$. Because of discrete symmetries of the lattice, all the eigenvalues are represented in this domain. The lower part of the table shows the results for Gutzwiller wavefunctions, without subtracting possible ferromagnetic components. If such corrections are required, the resulting values are shown as footnotes.

		Exact		
				−7.41542
			−7.41930	−7.41918
		−7.42535	−7.42666	−7.42798
	−7.41825	−7.42918	−7.43515	−7.43642
−7.41722	−7.41273	−7.43191	−7.43867	−7.43982
		Gutzwiller		
				−7.25199
			−7.24336	−7.25199
		−7.23621	−7.24231	−7.25199
	−7.21895[b]	−7.22758	−7.24231	−7.25199
−7.201693[a]	−7.21032	−7.21895	−7.24231	−7.25199

[a] −7.373448.
[b] −7.386605.

of the total spin operator only if p is equal to one of the occupied states $k_1, \ldots, k_n$ for the up spins. Otherwise, it is possible to obtain a state with a total spin corresponding to its maximal value reduced by unity. This is done by projecting out the ferromagnetic component in the original Gutzwiller wavefunction. The kinetic energy becomes

$$\langle E' \rangle = \langle E \rangle + \{N_s/[N_s - (N_h + 1)]N_h\}(\langle E \rangle - E_F). \tag{6}$$

In this equation, $\langle E \rangle$ is the average kinetic energy of the original Gutzwiller wavefunction given by (4), and E_F is the energy of the ferromagnetic component:

$$E_f = \varepsilon(p) + \sum_{i=1}^{n} \varepsilon(k_i). \tag{7}$$

It is convenient to use a representation of these wavefunctions as a function of hole and down-spin coordinates, denoted by $(x_1, \ldots, x_{N_h})$ and y, respectively. For the original Gutzwiller wavefunction, we have [11]:

$$\psi_0(x_1, \ldots, x_{N_h}, y) = \exp(\mathrm{i}py)\, \Phi^* \begin{pmatrix} p, k_1, \ldots, k_{N_h} \\ y, x_1, \ldots, x_{N_h} \end{pmatrix}. \tag{8}$$

Φ is the Slater determinant constructed from p and the unoccupied states $k_1, k_2, \ldots, k_n$. In the case where p is one of $k_1, \ldots, k_{N_h}$, after subtraction of the ferromagnetic component, the wavefunction becomes

$$\psi'(x_1, \ldots, x_{N_h}, y) = \psi_0(x_1, \ldots, x_{N_h}, y) - \frac{N_s}{N_s - N_h} \Phi^* \begin{pmatrix} k_1, \ldots, k_{N_h} \\ x_1, \ldots, x_{N_h} \end{pmatrix}. \tag{9}$$

These real-space wavefunctions have been used to calculate numerically various correlation functions involving the spin flip and holes.

Table 2. As for table 1 but for $L = 9$ and two holes.

		Exact		
				−7.55060
			−7.54468	−7.54750
		−7.53485	−7.53919	−7.54191
	−7.52447	−7.52909	−7.53289	−7.53491
−7.50193	−7.52169	−7.52813	−7.53291	−7.53496
		Gutzwiller		
				−7.53294
			−7.52934	−7.53114
		−7.52022	−7.52478	−7.52658
	−7.50984	−7.51503	−7.51959	−7.52139
−7.50306[a]	−7.50645	−7.51164	−7.51620	−7.51800

[a] 7.495549.

Table 3. As for table 1 but for $L = 10$ and two holes.

		Exact			
					−7.61078
				−7.61261	−7.61209
			−7.61785	−7.61598	−7.61550
		−7.62227	−7.62131	−7.62022	−7.61964
	−7.61980	−7.62364	−7.62468	−7.62369	−7.62230
−7.61817	−7.61596	−7.62451	−7.62606	−7.62502	−7.62425
		Gutzwiller			
					−7.50502
				−7.50229	−7.50502
			−7.49895	−7.50229	−7.50502
		−7.49386	−7.49641	−7.50229	−7.50502
	−7.48756[b]	−7.49071	−7.49513	−7.50229	−7.50502
−7.48247[a]	−7.48502	−7.48817	−7.49513	−7.50229	−7.50502

[a] −7.600292.
[b] −7.605336.

The diagonalizations were performed on a four-processor IBM 3090. We used the Lanczos [12] method to tri-diagonalize the Hamiltonian matrix. The parallelization of this algorithm is not difficult [13, 14]. The final diagonalization is achieved by direct resolution, refined by several power method steps. To find eigenvectors with a given total momentum and a given spin, we ran the Lanczos method starting from random state with these values of momentum and spin [14]. It turned out that the round-off error does not project the iteration out of this subspace, and the lowest eigenstate of a 1.462032×1.462032 matrix is found in less than 100 iterations.

3. Results

We now turn to the description of our numerical results. For two holes, they are summarized in tables 1–4, for energies as a function of total momentum and for various lattice sizes. The results for average distances are detailed in table 5.

Table 4. As for table 1 but for $L = 12$ and two holes.

			Exact			
						−7.72378
−7.73183						−7.73203
			Gutzwiller			
						−7.64984
					−7.648892	−7.64984
				−7.647032	−7.648892	−7.64984
			−7.645215	−7.647032	−7.648892	−7.64984
		−7.642734	−7.643975	−7.647032	−7.648892	−7.64984
	−7.640253[b]	−7.641494	−7.642734	−7.647032	−7.648892	−7.64984
−7.638437[a]	−7.639345	−7.640586	−7.642734	−7.647032	−7.648892	−7.64984

[a] −7.723210.
[b] −7.726455.

Table 5. Distances d_{exact} between the down spin and the closest hole for various lattice sizes ($L = 8, 9, 10, 12$). For comparison, d_0 is the average distance between two points on a periodic square lattice. d_1 is obtained by taking the same correlations between the two holes as in the exact ground state but with assuming that the down spin is uniformly distributed. d_{Gutz} is the result for the usual Gutzwiller wavefunction, whereas d'_{Gutz} is obtained by subtracting the ferromagnetic component from the Gutzwiller wavefunction.

	$L = 8$	$L = 9$	$L = 10$	$L = 12$[a]
d_0	4.0635	4.5	5.0505	6.0419
d_1	2.9931	3.3495	3.7191	4.6266
d_{exact}	2.9486	3.5419	3.7657	4.7510
d_{Gutz}	2.8114	3.4076	3.4852	4.1635
d'_{Gutz}	3.0159	3.4076	3.7662	4.5205

[a] $K = (0, 0), (0, \pi), (\pi, \pi)$ only.

First it is worth stressing that the state with one spin flip and two holes has a lower energy than the Nagaoka ferromagnetic state for two holes. This is consistent with previous analyses [6, 10]. However, the value of the total momentum turns out to be sensitive to the parity of L and to the actual size for a given number of holes. By contrast, Fang *et al* [10] claim that the ground state is achieved for $k = (0, \pi)$ or $(\pi, 0)$ for two holes and even L. We have recovered their results with a relative accuracy of 10^{-4} for the values of k and L that they have investigated. However, they do not seem to have included the values of k corresponding to the actual ground state. For instance, for $L = 10$, we find that $k = (0, 3\pi/5)$.

For odd L, the ground state is fourfold degenerate, corresponding to the values of k which are the closest to (π, π) in reciprocal space. The dispersion of $E(k)$ is also larger for $L = 9$ than $L = 8$ and $L = 10$ which suggests that it is the case for odd L versus even L. The origin of such different behaviours when the parity of L changes is the presence of frustration in the hopping motion of the holes. That is, the ground state of one hole in a ferromagnetic background is fourfold degenerate when L is odd.

Table 6. As for table 1 but for $L = 5$ and three holes.

	Exact	
		−9.60913
	−9.89698	−9.77652
−10.00694	−9.94828	−9.81117
	Gutzwiller	
		−9.52932
	−9.77653	−9.65292
−9.92932	−9.85292	−9.72932

We have compared these exact results with the Gutzwiller wavefunction. For $L = 9$, the Gutzwiller wavefunction reproduces exactly the ordering of energies as a function of total momentum k. For $L = 8$, 10 and 12 the energy of the Gutzwiller wavefunction is minimal at $k = (\pi, (2\pi/L)m)$, with an arbitrary value of the integer m. Then the ordering of energies is rather poorly reproduced by the Gutzwiller wavefunction which exhibits many degeneracies. We note that the relative energy difference from the exact ground state is less than 2%.

In order to get a more detailed comparison, we calculate density correlation functions between the down spin and holes. The results are featured in table 5. The main result of this study is that the average distance between the down spin and the closest hole is quite similar to the case of a uniformly distributed down spin. This strongly suggests that there is no actual bound state between the down spin and a hole, in spite of the fact that the ferromagnetic state is unstable towards one spin flip. As already mentioned [15], for a finite number of holes, the energy of the actual ground state is bounded below by the energy E_b of hard-core bosons and above by the energy E_f of spinless fermions. For instance, for $L = 10$, $E_b = -7.9530 \leqslant E = -7.6261 \leqslant E_f = -7.6180$. When the system size goes to infinity, $E_f - E_b$ vanishes and the ferromagnetic state is degenerate with the actual ground state. The behaviour of the down-spin–hole correlation function is consistent with this absence of binding.

The average distance between the down spin and the closest hole is found to be reduced in the Gutzwiller wavefunction. Furthermore, the relative error for the distance between the down spin and hole is 4.6% for $L = 8$ and 7.5% for $L = 10$.

It is interesting to note that, when a ferromagnetic component is removed, this distance increases significantly. An example is provided for $L = 12$. For the original Gutzwiller wavefunction, the energy is lower for $k = (\pi, (\pi/6)m)$, m integer, and the mean distance is 4.1635. By contrast, if an exact spin eigenstate is enforced, $k = (\pi/6, \pi/6)$ and the mean distance becomes 4.5205. We note that the later state has a lower energy, and that the mean distance in that case is closer to the exact value equal to 4.7510. This increase in the average distance first seems paradoxical, since removing the ferromagnetic component suppresses the node in the wavefunction when the down spin coincides with a hole. However, these two wavefunctions are constructed from a different set of single-particle states, and the exchange-induced repulsion is larger for $k = (\pi/6, \pi/6)$ than for $k = (\pi, (\pi/6)m)$. This turns out to be the dominant effect.

The results for three holes and $L = 5, 6, 7$ are summarized in tables 6–8. As for the two-hole cases the exact energies as a function of the crystal momentum are shown, as well as the energies for the Gutzwiller trial wavefunctions.

Table 7. As for table 1 but for $L = 6$ and three holes.

	Exact		
			−9.85869
		−10.03525	−10.02090
	−10.12758	−10.08289	−10.08892
−10.18392	−10.15391	−10.11027	−10.11764
	Gutzwiller		
			−9.63194
		−9.72222	−9.68056
	−9.84028	−9.81944	−9.77778
−9.86806	−9.88889	−9.86806	−9.82639

Table 8. As for table 1 but for $L = 7$ and three holes.

	Exact		
			−10.78191
		−10.84773	−10.82573
	−10.88577	−10.86330	−10.83647
−10.90300	−10.89385	−10.86878	−10.84015
	Gutzwiller		
			−10.75624
		−10.79795	−10.77709
	−10.8499	−10.82395	−10.80310
−10.87310	−10.86152	−10.83552	−10.81467

For odd linear size L, the Gutzwiller trial wavefunction is a very good approximation of the exact energy. For $L = 7$ the relative energy difference between the Gutzwiller wavefunction and the exact ground state is less than 0.3%. We note that the hierarchy of energies versus total momentum is also correct. In the Gutzwiller wavefunction, the four unoccupied states are the four states closest to (π, π). Their contribution to the total momentum is vanishing, and the total momentum is determined only by the momentum p of the magnon. The lowest energy is reached for $k = (0, 0)$, while the highest energy corresponds to the value of k which is the closest to (π, π). The bandwidth is equal to $(16/N_s)[1 + \cos(\pi/L)] \sin^2(\pi/L)$. This value is much larger than for the two-hole case, as can be expected [5]. For even L the situation is not so simple since there are several degenerate non-interacting Fermi seas to construct the Gutzwiller wavefunction. The wavefunction is also less accurate (2% for $L = 6$) and the hierarchy of the different subspace is not exactly reproduced, by contrast with the case of odd L. As for the case of two holes, the presence of frustration for odd values of L seems to improve the Gutzwiller wavefunction as an approximation of the ground state.

4. Discussion

Our results for finite lattices with two or three holes confirm that the ferromagnetic state is unstable against one spin flip. However, the total spin of the global ground state could

not be determined by this method. Study of the correlations between the holes and spin flip suggests that this instability is not related to the formation of a bound state. As was shown in [6], this instability depends on the choice of boundary conditions for the wavefunction of the holes [15]. As a result this mechanism is effective only for a finite number of holes. So the instability observed here appears to be a finite-size effect, consistent with a macroscopic magnetization in the thermodynamic limit, at small hole concentrations. Detailed comparison with the Gutzwiller wavefunction shows that it provides rather good estimates for the energy (around 1% accuracy). Furthermore, the ordering of $E(k)$ as a function of k is very well reproduced for frustrated lattices (L odd). However, correlations between holes and spin flip are not accurately described by this *ansatz*.

This suggests going beyond the usual Gutzwiller wavefunction in order to study the instability of the ferromagnetic state at finite hole densities. One way suggested to write the Gutzwiller wavefunction is

$$|\psi_0\rangle = \sum_{k'} S^-_{p-k'} c^+_{k'\uparrow} \prod_{i=1}^{n} c^+_{k_i\uparrow} |0\rangle.$$

A first possible generalization was studied in [7], which can be written as

$$|\psi\rangle = \sum_{k,k'} \Phi(k) S^-_{p-k'+k} c^+_{k'\uparrow} c_{k\uparrow} \prod_{i=1}^{n+1} c^+_{k_i\uparrow} |0\rangle.$$

$|\psi\rangle$ is a Gutzwiller-projected spin-wave type of excitation of the ferromagnetic Fermi sea. We are at present investigating the class of wavefunctions defined by

$$|\psi\rangle = \sum_{k,k'} \Phi(k,k') S^-_{p-k'+k} c^+_{k'\uparrow} c_{k\uparrow} \prod_{i=1}^{n+1} c^+_{k_i\uparrow} |0\rangle$$

by numerically solving the Schrödinger equation for $\Phi(k,k')$. Correlations between holes and magnons should be better described in this enlarged trial space.

Another question of interest is the influence of a nearest-neighbour antiferromagnetic coupling between spins. The so-called $t-J$ model has been widely studied in connection with the oxide superconductors [16]. We performed similar exact diagonalizations for non-zero J. Figure 1 shows the evolution of ground-state energies as a function of J for one down spin and two holes, for different values of k. This graph shows that many level crossings occur at small values of J. Such a behaviour suggests that the infinite-U ground state is not adiabatically related to the ground state at finite J. As a result, we observe that the spin flips which may be stabilized at $U=\infty$ are dramatically different from the antiferromagnetic state. Results for $U=\infty$ may not be extrapolated to the large-U Hubbard model. However, as the simplest strongly correlated model, the infinite-U limit still deserves further investigation.

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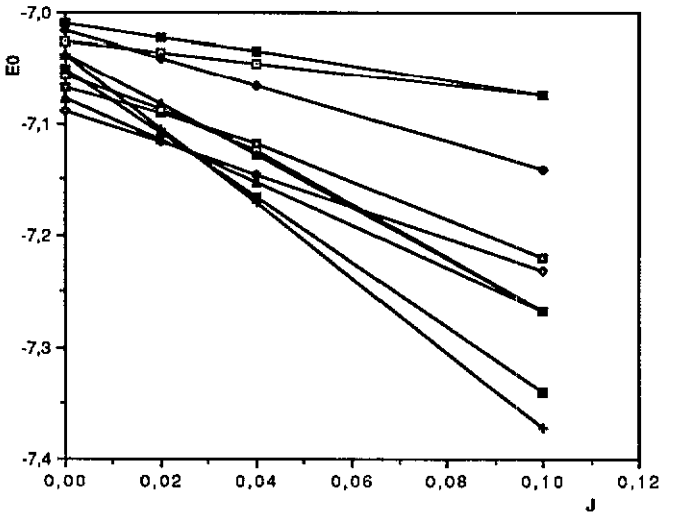

Figure 1. Ground-state energy for different values of k as a function of the antiferromagnetic coupling constant J: -□-, $(0, 0)$; -●-, $(0, \pi/3)$; -■- $(0, 2\pi/3)$; -◇-, $(0, \pi)$; -◆-, $(\pi/3, \pi/3)$; -□-, $(\pi/3, 2\pi/3)$; -▲-, $(\pi/3, \pi)$; -△-, $(2\pi/3, 2\pi/3)$; -■-, $(2\pi/3, \pi)$; -+-, (π, π).

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