The $U = \infty$ Hubbard model with few holes: Monte Carlo studies near half filling at nonzero temperatures.

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Abstract

We present an efficient Monte Carlo method to study the properties of the infinitely repulsive Hubbard model with few holes at finite nonzero temperatures. Using this method, magnetic and specific heat results are presented for a $10 \times 10$ lattice with two holes. Our results show that the magnetization increases with decreasing temperature for such a finite system.

I. INTRODUCTION

The magnetic behaviour of the Hubbard model in the $U = \infty$ limit is an old problem. For this case a well-known exact theorem is due to Nagaoka (1966) and Thouless (1965). It provides explicit, but highly idealized conditions under which ferromagnetism is stable in the Hubbard model. It proves that for infinitely large repulsive Hubbard $U$ the macroscopic degeneracy of the ground state at half filling (when the number of electrons $N$ is exactly equal with the number of lattice sites, hereafter denoted by $N_\Lambda$) is lifted by a single hole, i.e., when $N = N_\Lambda - 1$. In this case the saturated ferromagnetic ground state is stable for any value of the hopping amplitude $t$ on square, simple cubic and bcc lattices, and for $t < 0$ on triangle, fcc and hcp lattices. A very elegant and fully general proof was given
for this result by Tasaki (1989) based on the Perron–Frobenius theorem. For the Nagaoka mechanism to work, the lattice needs to contain loops along which the hole can move. Once the hole moves, the maximal overlap between the initial and the final state clearly occurs in a ferromagnetic configuration. The problems are that Nagaoka’s proof does not even extend to two holes, that a single hole is thermodynamically irrelevant, and that the limit of \( U = \infty \) is highly unrealistic. Moreover, several theoretical results state the instability of Nagaoka’s ferromagnetism for two holes, see e.g. Doucot and Wen (1989), Sütő (1991 a), Tóth (1991).

In a recent published paper (Gurin and Gulácsi, 2000) a formalism was presented which helps to deduce the partition function and some physical quantities of the system based on a loop summation (i.e. path integral on lattice) technique. The presented formulas have the advantage that the trace over the spin degrees of freedom has been taken exactly into account. Resembling technique was used by Sütő (1991 b) to analyze the magnetic behaviour of the system in thermodynamic limit. However, his result is valid in thermodynamic limit, only in the case \( N_h / N_\Lambda \to 0 \) where \( N_h = N_\Lambda - N \) and not for finite hole concentration and \( T \to 0 \). In this paper we investigate the behaviour of a small system with finite hole concentration, using Monte Carlo method at \( T \neq 0 \). Starting from the aim to enhance the study of magnetic properties in the presence of a small hole concentration even at finite nonzero temperatures, the procedure is described in detail. The studied system is a \( 10 \times 10 \) lattice with periodic boundary conditions containing two holes. The results show an increase of the magnetisation with the decrease of the temperature.

The remaining part of the paper is organized as follows: in Sec. II. we describe the representation of the Hilbert space in which the calculation is done, Sec.III. presents the partition function and the analyzed physical quantities, and Sec. IV. contains the Monte Carlo results obtained, together with a discussion of the deduced results.

II. REPRESENTATION OF THE HILBERT SPACE

Our Hamiltonian describes the one-band Hubbard model in \( U = \infty \) limit:
\[
\hat{H}_\infty = \sum_{i,j} t_{ij} \hat{H}_{\infty}^{ij} = \sum_{i,j} t_{ij} \hat{P} \left( \sum_{\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \right) \hat{P},
\]
where \( t_{ij} = -t \) are hopping matrix elements for nearest neighbour sites (otherwise \( t_{ij} = 0 \)).

The operators \( \hat{c}_{i,\sigma}^\dagger \) (\( \hat{c}_{i,\sigma} \)) creates (annihilates) an electron with spin \( \sigma \) at lattice site \( i \), and \( \hat{n}_i = \sum_{\sigma} \hat{n}_{i,\sigma} \) represents the particle number operator. The double occupancy is projected out by \( \hat{P} = \sum_{i} (1 - \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}) \).

In our study we need operations with permutations therefore we fix below some notations concerning them. We treat a permutation \( \mathcal{P} \) of degree \( n \) as a bijective function of the set of the first \( n \) natural numbers into themselves. The product of the permutations is the standard function composition: \( (\mathcal{P} \ Q)(i) = \mathcal{P}(\mathcal{Q}(i)) \). The symmetric group of degree \( n \) formed by all the permutations of degree \( n \) is denoted by \( S_n \). The complex Hilbert space generated by the elements of \( S_n \) as an abstract orthonormalized basis endowed by the product defined by the convolution is called the group algebra of the symmetric group. The parity of a permutation is \( |\mathcal{P}| \).

We study the one band \( U = \infty \) Hubbard model. In such a tight-binding description the electrons can live only on lattice sites in two orthogonal states with spin up and down. Due to the kinetic energy term, an electron hops from one site to another (while its spin state remains unchanged), changing however the locations of the empty and occupied sites. Hereafter, fixed positions of the occupied sites we call charge configuration which does not give account of the electronic spin states, only their places. Iterating the effect of the hopping term on a state several times, hopping around the lattice, the electrons produce different charge configurations, particularly they can produce the original configuration again as well. However, the spin up and spin down electrons are commingled, therefore the spin configuration can be different than in the original state. In our description a spin configuration is given by the position of sites occupied by spin up and separately spin down electrons, respectively. In this way, fixing the charge configuration and the third component of the total spin \( S_z \), the spin configuration can be described by an ordered set of the up and down spin states: \( (\sigma_i)_{i=1}^N \) in which \( \sigma_i \in \{\uparrow, \downarrow\} \) indicates the spin state of the electron situated
in the \textit{i-th occupied} lattice site. Certainly, at first, the occupied sites have to be labelled from 1 to \(N\). In this way, every spin configuration can be obtained by a permutation from 
\[ (\sigma^0(i))_{i=1}^{N} = (\uparrow, \uparrow, \ldots, \uparrow, \downarrow, \downarrow, \ldots, \downarrow), \]
where \(\sigma^0(i) = \uparrow\) if \(i = 1, \ldots, N_\uparrow = N/2 + S^z\) and \(\sigma^0(i) = \downarrow\) if \(i = N_\uparrow + 1, \ldots, N\).

Based on the above mentioned observations, the Hilbert space of the system and a basis of it can be expressed in terms of permutations. The charge configuration can be described by a function \(R : \{1, \ldots, N_\Lambda\} \rightarrow \{1, \ldots, N_\Lambda\}\) for which \(R(1), \ldots, R(N)\) are the occupied lattice sites (taken into account an arbitrary but fixed numbering of sites), and \(R(N+1), \ldots, R(N_\Lambda)\) are the positions of holes. Actually \(R \in S_{N_\Lambda}\), but hereafter we denote the charge configuration by \(\hat{R}\) for which we require that \(\hat{R}(1), \ldots, \hat{R}(N)\) have to be increasingly ordered. Moreover, we do not distinguish permutations which differ only in the order of the positions of the holes \(\hat{R}(N+1), \ldots, \hat{R}(N_\Lambda)\), everyone is denoted by \(\hat{R}\), and the further definitions and expressions do not depend on this undetermination. The Hilbert space generated by all the different charge configurations as an orthonormalized basis is denoted by \(\mathcal{H}_c\).

To label the occupied sites from 1 to \(N\) we use the function \(\hat{R}^{-1}\). After it, a spin configuration \((\sigma_i)_{i=1}^{N}\) can be described by a permutation \(P \in S_N\) which rearrange the basic order in \((\sigma^0(i))_{i=1}^{N}\) in such a way that \(\sigma^0(P(i)) = \sigma_i\). This means that in a state described by a charge configuration \(\tilde{R}\) and a spin configuration \(P\), the electron situated in the lattice site \(i\) is in the spin state \(\sigma^0(P\hat{R}^{-1}(i))\). More precisely, there is no unique connection between the spin configurations and permutations. A permutation uniquely determines a spin configuration, but the reverse is not true. Let \(Q \in S_N\) be a permutation which rearranges the elements of the subset \((\sigma^0)^{-1}(\uparrow) = \{1, \ldots, N_\uparrow\}\), and rearranges the elements of \((\sigma^0)^{-1}(\downarrow) = \{N_\uparrow + 1, \ldots, N\}\), but does not interchange the elements of these two subsets. It is clear for arbitrary permutation \(P\), that \(P\) and \(QP\) describe the same spin configuration, because \(\sigma^0(P(i)) = \sigma^0(QP(i))\) for all \(i\). Mathematically this means the following. The above defined permutations \(Q\) form a subgroup \(K_{S^z} \subset S_N\), and a right coset \(\hat{P} := \{QP : Q \in K_{S^z}\}\) is in one-to-one correspondence with a spin configuration.
Moreover, the Hilbert space generated by these right cosets as an orthonormalized basis, is isomorphic with a right ideal of the group algebra, which will be denoted by $\mathcal{H}_s^{S^z}$. On this line, an arbitrary state with given $S^z$, can be written as $\varphi_c \otimes \varphi_s^{S^z}$ where $\varphi_c \in \mathcal{H}_c$ and $\varphi_s^{S^z} \in \mathcal{H}_s^{S^z}$. Furthermore, $\{|\tilde{R}\rangle\}$ is a basis of $\mathcal{H}_c$, and $\{|\bar{P}\rangle\}$ is a basis of $\mathcal{H}_s^{S^z}$, respectively. The explicit expression of the above defined basis with the usual creation operators is

$$|\tilde{R}\rangle \otimes |\bar{P}\rangle = \prod_{i=1}^{N} c_{\tilde{R}(i),\sigma(\bar{P}(i))} |0\rangle,$$

where $\bar{P}$ is an arbitrary permutation of the right coset $\bar{P}$. Now it can be seen that the requirement that $\tilde{R}(1),...,\tilde{R}(N)$ have to be increasingly ordered is needed to fix the order of the creation operators in Eq.(2). Let $C$ a permutation which rearranges the first $N$ numbers and leaves unchanged the last $N_h$ ones. Using $\mathcal{R}' = \tilde{R} C$ instead of $\tilde{R}$ in Eq.(2), we get the same operators but in different order, supposing that it is also $\mathcal{R}'$ which is used to label the occupied sites from 1 to $N$. This rearrange of the creation operators involves a sign $(-1)^{|C|}$. To avoid this sign ambiguity, we use $\tilde{R}$ in Eq.(2), for which the order of the operators is well determined due to the requirement for the order of $\tilde{R}(1),...,\tilde{R}(N)$.

III. PARTITION FUNCTION AND PHYSICAL QUANTITIES

Now we study the changing of a state vector from Eq.(2) during the motion of the particles. Let’s study the hopping of particles step-by-step. Suppose, that the starting point is $\tilde{R} \otimes \bar{P}$ and in the first step an electron hops from site $i_1$ to site $j_1$, in the next step an other electron (or the same) from $i_2$ to $j_2$ and so on. The path in the charge configuration space $\gamma = (\tilde{R}, \tilde{R}_1, \ldots, \tilde{R}_{l-1}, \tilde{R}_l)$ is uniquely determined by the sequence of nearest neighbour pairs $(i_1, j_1), \ldots, (i_l, j_l)$. In the $n$th step a hole and an electron interchange their positions. This can be described by the transposition $\mathcal{P}^{i_n,j_n}$. Now we suppose, that after $l$ steps the system gets back to the original charge configuration. However the positions of holes are the same as in the original situation, the moving rearranged the electrons. The electron situated originally at site $i$ moved to site $j$. The new situation can be described by a
permutation $\mathcal{R}_\gamma \tilde{\mathcal{R}}$ where $\mathcal{R}_\gamma = \mathcal{P}^i_{j_1} \ldots \mathcal{P}^i_{j_l} \in S_{N_A}$ which takes $i$ to $j$ for all $i$ which label occupied sites and permutes somehow the labels of empty sites. Because the spin state of the electron remains unchanged during the hopping, the electron situated after the motion in site $j = \mathcal{R}_\gamma(i)$ is in the spin state $\sigma'_j = \sigma_i = \sigma_0(\mathcal{P} \tilde{\mathcal{R}}^{-1}(i)) = \sigma_0(\mathcal{P} \tilde{\mathcal{R}}^{-1} \mathcal{R}_\gamma(j))$. The charge configuration is the same as the starting $\tilde{\mathcal{R}}$ therefore to recognize the final spin state $\mathcal{P}'$ we have to write the final spin state of the electron situated in site $j$ as $\sigma_0(\bar{\mathcal{P}} \tilde{\mathcal{R}}^{-1}(j))$. As a consequence, we have $\bar{\mathcal{P}}' = \bar{\mathcal{P}} \tilde{\mathcal{R}}^{-1} \mathcal{R}_\gamma \tilde{\mathcal{R}} = \bar{\mathcal{P}} \mathcal{P}_\gamma^{-1}$ where $\mathcal{P}_\gamma = \tilde{\mathcal{R}}^{-1} \mathcal{R}_\gamma^{-1} \tilde{\mathcal{R}}$ is an element of $S_{N_A}$ but it rearranges the first $N$ numbers among themself and leaves unchanged the last $N_h$ ones, therefore it can be considered as an element of $S_N$. Furthermore the final charge configuration is again $\tilde{\mathcal{R}} = (\mathcal{R}_\gamma \mathcal{R}) \mathcal{P}_\gamma$ instead of $\mathcal{R}_\gamma \tilde{\mathcal{R}}$ therefore we have to take into account a sign $(-1)^{|P_\gamma|}$ — as we mentioned at the end of the previous Section — to write the final state as $\tilde{\mathcal{R}} \otimes (-1)^{|P_\gamma|} \bar{\mathcal{P}} \mathcal{P}_\gamma^{-1}$.

The mapping $\mathcal{P} \to (-1)^{|P_\gamma|} \mathcal{P} \mathcal{P}_\gamma^{-1}$ is defined on the basis of $\mathcal{H}_s^{S^z}$. The influence caused by a hopping of holes along a loop $\gamma$ is described by a linear operator which is the linear extension of the mapping $\mathcal{P} \to (-1)^{|P_\gamma|} \mathcal{P} \mathcal{P}_\gamma^{-1}$ to the whole $\mathcal{H}_s^{S^z}$. It is actually a linear representation of the symmetric group $S_N$ on $\mathcal{H}_s^{S^z}$ (Gurin and Gulácsi, 2000) hereafter denoted by $Ts^z[\mathcal{P}_\gamma]$.

Based on the above considerations, we can give expressions for the partition function as follows

$$Z = \text{Tr} \, e^{-\frac{\hat{H}_{\mathcal{Z}}}{kT}} = \sum_{S} \text{Tr}_{\mathcal{H}_s^{S^z}} e^{-\frac{\hat{H}_{\mathcal{Z}}}{kT}},$$

and the expectational value of the square of the total spin

$$\langle \hat{S}^2 \rangle = \frac{1}{Z} \text{Tr}(\hat{S}^2 \, e^{-\frac{\hat{H}_{\mathcal{Z}}}{kT}}) = \frac{1}{Z} \sum_{S} 3 (S^z)^2 \text{Tr}_{\mathcal{H}_s^{S^z}} e^{-\frac{\hat{H}_{\mathcal{Z}}}{kT}}$$

in which the sum over the spin degrees of freedom is expressed analitically in terms of the characters of the symmetric group. From the above expressions it can be seen that what we need for calculations is in fact

$$\text{Tr}_{\mathcal{H}_s^{S^z}} e^{-\frac{\hat{H}_{\mathcal{Z}}}{kT}} = \sum_{l=0}^{\infty} \frac{1}{l!} \left( \frac{t}{kT} \right)^l \sum_{\mathcal{R}} \sum_{\mathcal{P}} \sum_{\gamma \in \Omega_R(l)} \langle \mathcal{P} \mid T^{S^z}[\mathcal{P}_\gamma] \mid \bar{\mathcal{P}} \rangle$$
\[
\sum_{l=0}^{\infty} \frac{1}{l!} \left( \frac{t}{kT} \right)^l \sum_{\mathcal{R}} \sum_{\gamma \in \Omega_{\mathcal{R}}(l)} \chi^{S^z}(\mathcal{P}_\gamma).
\]

(5)

where \( \Omega_{\mathcal{R}}(l) \) denotes the set of the \( l \)-length loops (closed paths) with starting point \( \mathcal{R} \) in the space of charge configurations, and \( \chi^{S^z} \) is the character of the representation \( T^{S^z} \).

Every character is constant on an arbitrary conjugate class \( C \). Therefore, the above sum over \( \Omega_{\mathcal{R}}(l) \) has \( N(C) \) identical members, where \( N(C) \) represents the number of the loops with length \( l \) and starting point \( \mathcal{R} \) for which \( \mathcal{P}_\gamma \in C \). Now we use (see Gurin and Gulácsi, 2000)

\[
\sum_{s^z=-N/2}^{N/2} \chi^{S^z}(C) = (-1)^{|C|} 2\sum_{i=1}^{N} C_i,
\]

(6)

furthermore

\[
\sum_{s^z=-N/2}^{N/2} (S^z)^2 \chi^{S^z}(C) = (-1)^{|C|} 2\sum_{i=1}^{N} C_i \left( \frac{1}{4} \sum_{i=1}^{N} i^2 C_i \right).
\]

(7)

Here \( |C| \) is the parity of permutations from the conjugate class \( C \) and \( (C_1, C_2, \ldots, C_N) \) describes their cycle structure, i.e. these permutations contain \( C_i \) cycles with length \( i \).

Finally, inserting Eqs. (5, 6, 7) into Eqs. (3, 4) we obtain

\[
Z = \sum_{l=0}^{\infty} \frac{1}{l!} \left( \frac{t}{kT} \right)^l \sum_{\mathcal{R}} \sum_{C \subseteq S_N} N^{(C)}_{\mathcal{R}}(l) (-1)^{|C|} \left( \frac{1}{4} \sum_{i=1}^{N} i^2 C_i \right),
\]

(8)

and

\[
\langle \hat{S}^2 \rangle = \frac{3}{4Z} \sum_{l=0}^{\infty} \frac{1}{l!} \left( \frac{t}{kT} \right)^l \sum_{\mathcal{R}} \sum_{C \subseteq S_N} N^{(C)}_{\mathcal{R}}(l) (-1)^{|C|} \left( \frac{1}{4} \sum_{i=1}^{N} i^2 C_i \right).
\]

(9)

To determine the coefficients \( N^{(C)}_{\mathcal{R}}(l) \) we should follow the following procedure. Starting from a charge configuration \( \mathcal{R} \), holes moves \( l \) steps in such a way that finally the system goes back to the original hole configuration (this is a loop with length \( l \)). In this process, an arbitrary hole can be moved in every step, the order of the steps being relevant. A step means that we interchange a hole with an electron from its neighbourhood. Counting the number of \( l \)-loops for which the cycle structure of the permutation of electrons after the \( l \)th step is \( C \), we get the number \( N^{(C)}_{\mathcal{R}}(l) \).
IV. MONTE CARLO RESULTS AND DISCUSSIONS

The coefficients $N^{(C)}_{R}(l)$ can be determined by Monte Carlo method. By random sampling we can obtain the percentage of loops with a given length for which $P_{\gamma} \in C$. The Eqs.(8) and (9) have the advantage that the trace over the spin degrees of freedom has been taken already. Hence we need only to sample the loops (i.e. “world lines”) of holes instead of the loops of the electrons. This is advantageous since due to the presence of different possible electron spin configurations, the electron loops have $2^N$ times more starting points than the hole loops.

We studied by this method a 2D $10 \times 10$ lattice with periodic boundary conditions in the presence of two holes. We took into account every possible starting hole (charge) configuration. Because of the periodic boundary conditions, translational, rotational and reflection symmetries of the lattice, there are 20 essentially different charge configurations instead of $\binom{100}{2}$. Because of the fact that the contributions of the $2^{98}$ different spin configurations corresponding to a fixed charge configuration are taken into account analytically by Eqs.(8,9), we have taken into account every possible starting point of loops. Furthermore, starting from a charge configuration, we took into consideration every path up to the length $l = 14$. Thus, we counted exactly every loop up to $l \leq 14$, therefore the coefficients of our high temperature expansion are exact up to 14th order in $\beta / |t|$. Then, we continued every path with random directions up to $l = 100$.

The results can be seen in the Fig. 1. The continuous lines show the result of the high temperature expansion with exact coefficients up to 14th order. Taking into account further coefficients determined by Monte Carlo method up to 50th order we get the short-dash lines, and up to 100th order we get the long-dash lines. The expectation value of the square of the total spin goes to $3N / 4 = 73.5$ (and not to zero) as $T$ goes to infinity. It is understandable, because at very high temperature the likelihood of every possible states become equally $1 / Z$. (The spectrum of the Hamiltonian is bounded.) Therefore, the expectation value of an arbitrary quantity goes to its simple algebraic average over the all
states. This gives the result mentioned above for \( \langle \hat{S}^2 \rangle \). This means in fact paramagnetic behaviour, because a smaller total spin value has greater thermodynamic weight, i.e. the dimension of the eigensubspace of \( \hat{S}^2 \) is greater, therefore the \( S = 0 \) subspace is the greatest one, so this is the most probable value of the spin. Because of this reason, the total spin (but not \( \langle \hat{S}^2 \rangle \)) per particle is proportional to \( 1 / \sqrt{N} \) which goes to zero in thermodynamical limit.

Because of the inaccuracy and the complete neglect of the higher order coefficients in our expressions, the numerical error increases as the temperature decreases. Therefore we do not plot the \( T \to 0 \) temperature region in Fig. 1. Nevertheless, in the presented region the results are correct since the higher order terms do not improve the lower order contributions in this domain. At these temperatures however, due to the Monte Carlo method itself, small numerical errors are present of about 1%.

The obtained results show that the spontaneous magnetization increases as the temperature decreases. This tendency becomes stronger when we use more accurate approximation. At the same temperature range when \( \langle \hat{S}^2 \rangle \) starts to increase, the specific heat has a maximum. However this peak in the specific heat seems to be significant — in higher order approximations the curves have to break down as well since the specific heat has to go to zero in \( T \to 0 \) limit, — but the increase in \( \langle \hat{S}^2 \rangle \) is small, nevertheless very fast.

Related to the two and few hole cases in the literature it has been published (Doucot and Wen 1989, Sütő 1991 a, Tóth 1991) that the ground state cannot have maximal spin. This statement is based on variational calculations. There exists trial state with spin \( S = S_{\text{max}} - 1 \) which have lower energy than the fully polarized state with spin \( S_{\text{max}} \). However, up to now nobody can construct variational state with spin \( S \leq S_{\text{max}} - 2 \) which would have lower energy, thus these results do not exclude the ferromagnetic behaviour, only the highest spin value. Simultaneously our results suggest that the very low spin values can be exclude as well, and the ground state is not a singlet. As a conclusion we may state that the system behave at low temperature as a not fully saturated ferromagnet. This is consistent with
exact diagonalization results for small clusters (Arrachea 2000).

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FIGURES

FIG. 1. (a): square of the total spin and (b): specific heat as the function of the temperature measured in $|t|$ units. The continuous (lower) lines show the result of a 14th order high temperature expansion, the short-dash lines (in the middle) show the result of an 50th order high temperature expansion, the long-dash (upper) lines of a 100th order expansion based on coefficients determined by Monte carlo method.
