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The half-filled Hubbard model in the pair approximation of the cluster variation method

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Abstract. The half-filled Hubbard model is studied in the pair approximation of the cluster variation method (cvm). The use of the $SO(4)$ symmetry of the model makes it possible to give a complete analytical characterization of the ground state, by means of explicit expressions for the double occupancy and the nearest-neighbour correlation functions. The finite-temperature analysis is reduced to the numerical solution of only two coupled transcendental equations. The behaviour of local magnetic moment, specific heat and correlation functions is given for some typical cases in one and two dimensions. We obtain good qualitative agreement with exact and numerical results in one dimension. The results for finite temperatures show a rapid evolution, with increasing temperature, from a strongly antiferromagnetic behaviour to a disordered one; in the high-temperature region a maximum (which has been related to a 'gradual' metal-insulator transition) is found in the specific heat for very large values of the Coulomb repulsion.

1. Introduction

The Hubbard model [1, 2] is the simplest model of itinerant electrons which takes into account the interaction between electrons. It was originally proposed to describe the behaviour of d-electrons in transition metals, and it is expected to describe the metal-insulator (Mott) transition. In recent years, interest in this model has been greatly revived by the discovery of high- T_c superconductors, since these materials are generally good Mott insulators and, in the superconducting phase, exhibit strong antiferromagnetic correlations, just like the half-filled Hubbard model at low temperatures.

The model is defined by the following grand-canonical Hamiltonian:

$$H = U \sum_i n_{i+} n_{i-} - \mu \sum_{i\sigma} n_{i\sigma} - t \sum_{\langle ij \rangle, \sigma} a_{i\sigma}^\dagger a_{j\sigma} \quad (1)$$

where $U, t > 0$ and $a_{i\sigma}, a_{i\sigma}^\dagger$ and $n_{i\sigma}$ are, respectively, annihilation, creation and number operators for electrons at site i with spin $\sigma \in \{+, -\}$. The first term represents the Coulomb repulsion between electrons at the same site (all other interactions are neglected); the second term is the chemical potential, and the third one is the kinetic term, which describes hopping of the electrons between sites, with the sum restricted to non-oriented nearest-neighbour (NN) pairs.

The Hubbard model has been studied by many different techniques (for reviews see [3, 4] and references therein) but an exact solution is available only in one dimension [5, 6], while in two dimensions or more there are only a few exact results in very particular cases. For $U/t = 0$ the model describes a system of non-interacting, moving electrons and is exactly solvable in any dimension. On the other side, for $U/t = \infty$ (atomic limit) and at

half filling (i.e. $\langle n_i \rangle = \langle n_{i+} + n_{i-} \rangle = 1$) the ground state is that of an antiferromagnetic insulator [7], with exactly one electron per site. At half filling two other very important rigorous results hold:

- (i) the chemical potential is given by $\mu = U/2$ for any value of U/t and at any temperature [8], and
- (ii) Hamiltonian (1) has, for $\mu = U/2$, an $SO(4)$ symmetry [9].

In this paper we investigate the D -dimensional Hubbard model at half filling in the pair approximation of the cluster variation method (CVM). The CVM was originally introduced by Kikuchi [10] and its convergence in the thermodynamic limit has been demonstrated by Schlijper [11]. Recently the method has been given a very elegant formulation by An [12], in terms of Möbius inversion. The simplest level of approximation in the CVM is the site approximation, which is equivalent to the ordinary mean-field theory; then we have the pair approximation, which can be shown to be equivalent to the Bethe approximation.

The pair approximation of the CVM has already been applied to the Hubbard model in [13–16]. Unfortunately, in these references only the $U(1) \otimes U(1)$ Cartan subgroup of the $SO(4)$ symmetry group later studied by Yang and Zhang was used, and the authors had to deal with large sets of coupled transcendental equations, which they could solve only for relatively high temperatures ($kT/t > 1$, with k Boltzmann's constant and T absolute temperature). Furthermore, in [14–16] equivalence is assumed between sites belonging to the two interpenetrating sublattices which form a bipartite lattice.

In this paper we apply the pair approximation of the CVM to the Hubbard model on a bipartite lattice (that is, a lattice which is made of two interpenetrating sublattices, say A and B , in such a way that a site belonging to sublattice A has all its nearest neighbours in the B sublattice and vice versa: examples are the 1D chain, HC, SQ, SC and BCC lattices) by taking into account the full $SO(4)$ symmetry of the model. Furthermore, the equivalence between the two sublattices is not assumed, but it is derived from the thermodynamics of the model. The ground state is determined analytically, i.e. explicit expressions are derived for the double occupancy and the NN correlation functions at $T = 0$, for any number of dimensions and any value of the interaction U/t . For the finite temperature case, the problem is reduced to the numerical solution of two coupled transcendental equations. Such equations can be solved at any temperature and in the limit $T \rightarrow 0$ the ground-state solution is recovered.

The validity of the approximation is first checked by comparing the behaviour of the zero-temperature local magnetic moment versus U/t in $D = 1$ with the exact solution for the infinite chain reported by Hirsch [17], and then by comparing the same quantity at finite temperature for typical values of U/t with the numerical results for finite chains obtained by Shiba and Pincus [18]. Once the validity of the method has been established, we report on the numerical results at finite temperature for $D \geq 1$: correlation functions, hopping expectations and specific heat are given in some typical cases, and the antiferromagnetic behaviour of the system as well as the inhibition of certain hopping processes at low temperatures are discussed. Finally, it is noticed that a high-temperature maximum appears in the specific heat for very large values of the interaction, in agreement with previous studies where this maximum was related to a gradual metal–insulator transition.

The paper is organized as follows: in section 2 we construct the trial free energy according to the pair approximation of the CVM, taking into account the symmetry of the Hamiltonian. In section 3 the ground state is obtained and discussed, and the zero-temperature local magnetic moment is compared with the exact result for the infinite chain. In section 4 the analysis is extended to finite temperature and the behaviour of various physical quantities is given and discussed and, finally, in section 5 some conclusions are drawn.

2. Free energy

Following An's formulation [12], the CVM trial free energy for a bipartite lattice in the pair approximation can be written as

$$f = \frac{E}{N} + k_B T \left\{ \frac{1-z}{2} [\text{Tr}(\rho_A \ln \rho_A) + \text{Tr}(\rho_B \ln \rho_B)] + \frac{z}{2} \text{Tr}(\rho_p \ln \rho_p) \right\} \quad (2)$$

where E is the internal energy, N is the number of lattice sites, and ρ_A , ρ_B and ρ_p are the reduced density matrices (to be determined by minimizing f) for a site belonging to sublattice A , a site belonging to sublattice B and a pair of nearest neighbours, respectively.

Before taking the variation of f with respect to the reduced density matrices, let us determine which constraints for such density matrices can be derived from the symmetry group of the Hamiltonian. As shown in [9], Hamiltonian (1), with $\mu = U/2$ because of the half-filling condition, commutes with a $SO(4) = SU(2) \otimes SU(2)/\mathbb{Z}_2$ group, where one $SU(2)$ (referred to as the magnetic one) is generated by

$$J_z = \frac{1}{2} \sum_i (n_{i+} - n_{i-}) \quad J_+ = \sum_i a_{i+}^\dagger a_{i-} \quad J_- = \sum_i a_{i-}^\dagger a_{i+} \quad (3)$$

the other $SU(2)$ (called the pairing, or superconductive one), which is relevant only at half-filling, by

$$K_z = \frac{1}{2} \sum_i (n_{i+} + n_{i-} - 1) \quad K_+ = \sum_i e^{i\phi_i} a_{i+}^\dagger a_{i-}^\dagger \quad K_- = \sum_i e^{i\phi_i} a_{i-} a_{i+} \quad (4)$$

(the phase factor $e^{i\phi_i}$ is $+1$ for sites in sublattice A and -1 for sites in sublattice B) and \mathbb{Z}_2 interchanges the two $SU(2)$ symmetries. The presence or absence of this symmetry in the quantum state of the system characterizes the different phases: a disordered phase will be invariant under the whole $SO(4)$ symmetry group, while a phase with magnetic and/or superconductive order will be invariant under a reduced symmetry group, with both $SU(2)$ (or one) spontaneously broken down. Since in this paper we are concerned with the half-filled case, and it is conjectured that at half-filling the Hubbard model does not undergo any phase transition, we devote our attention to the disordered phase, thus assuming the whole $SO(4)$ symmetry (in view of the good agreement with exact results in one dimension, this assumption should be correct also at zero temperature). The possibility of a phase transition, associated with a spontaneous breaking of the magnetic $SU(2)$ symmetry group, will be examined in a forthcoming paper [19] for the extended Hubbard model at general filling.

In order to impose the commutation relations between the reduced density matrices and the $SO(4)$ generators defined above, we introduce in the site and pair reduced Fock spaces the customary basis of eigenstates of the number operators. In such a basis, requiring that the reduced density matrices commute with the Cartan operators J_z and K_z , ρ_A and ρ_B turn out to be diagonal, while for ρ_p one obtains the same block structure as in [16], with only 36 non-zero elements. By imposing furthermore the commutation with J_+ and K_+ (or, equivalently, with their hermitian conjugates J_- and K_-), one finds that ρ_γ ($\gamma = A, B$) has two distinct eigenvalues, say d_γ and $\frac{1}{2} - d_\gamma$, each with multiplicity 2, whereas ρ_p is a block diagonal matrix with

(i) two eigenvalues λ_1 and λ_2 , each with multiplicity 2;

(ii) four degenerate 2×2 blocks, which give rise to two eigenvalues λ_3 and λ_4 with multiplicity 4;

(iii) a 4×4 block with eigenvalues $\lambda_1, \lambda_2, \lambda_5$ and λ_6 .

Summarizing, we have six different eigenvalues, λ_1 and λ_2 with multiplicity $m_1 = m_2 = 3$, λ_3 and λ_4 with multiplicity $m_3 = m_4 = 4$, and λ_5 and λ_6 with multiplicity $m_5 = m_6 = 1$. Of these, only five are independent, because of the normalization condition $\text{Tr}(\rho_p) = 1$.

Recalling that the expectation value of an operator X is given by $\langle X \rangle = \text{Tr}(\rho X)$, one can compute, with some simple algebra, the expectation values of all the site and NN pair operators. The non-zero expectation values turn out to be (i and j nearest neighbours, $i \in A$ and $j \in B$)

$$\begin{aligned}
 \langle n_{i\sigma} \rangle &= \langle n_{j\sigma} \rangle = \frac{1}{2} & \langle n_{i+n_i-} \rangle &= d_A & \langle n_{j+n_j-} \rangle &= d_B \\
 c_p &\equiv \langle n_{i+n_j+} \rangle = \langle n_{i-n_j-} \rangle = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 \\
 c_a &\equiv \langle n_{i+n_j-} \rangle = \langle n_{j+n_i-} \rangle = \lambda_1 - \lambda_2 + \frac{1}{2}(1 - d_A - d_B) \\
 \langle n_{i+n_i-n_j+} \rangle &= \langle n_{i+n_i-n_j-} \rangle = \frac{1}{2}(d_A + c_p + c_a - \frac{1}{2}) \\
 \langle n_{j+n_j-n_i+} \rangle &= \langle n_{j+n_j-n_i-} \rangle = \frac{1}{2}(d_B + c_p + c_a - \frac{1}{2}) \\
 q &\equiv \langle n_{i+n_i-n_j+n_j-} \rangle = \lambda_1
 \end{aligned} \tag{5}$$

for the diagonal operators (notice that in this scheme the half-filling condition is derived from the symmetry and not imposed), and

$$\begin{aligned}
 p &\equiv \langle a_{i+}^\dagger a_{i-}^\dagger a_{j-} a_{j+} \rangle = \frac{1}{2} - c_p - c_a \\
 p' &\equiv \langle a_{i-}^\dagger a_{j+}^\dagger a_{i+} a_{j-} \rangle = c_a - c_p \\
 \frac{\tau_0}{2} &\equiv \langle a_{i\sigma}^\dagger a_{j\sigma} n_{i-\sigma} n_{j-\sigma} \rangle = \langle a_{i\sigma}^\dagger a_{j\sigma} (1 - n_{i-\sigma})(1 - n_{j-\sigma}) \rangle \\
 &= \frac{1}{2} \sqrt{(\lambda_3 - \lambda_4)^2 - \frac{1}{4}(d_A - d_B)^2} \\
 \frac{\tau_1}{2} &\equiv \langle a_{i\sigma}^\dagger a_{j\sigma} (1 - n_{i-\sigma}) n_{j-\sigma} \rangle = \langle a_{i\sigma}^\dagger a_{j\sigma} n_{i-\sigma} (1 - n_{j-\sigma}) \rangle \\
 &= \frac{1}{4} \sqrt{(\lambda_5 - \lambda_6)^2 - [2(d_A + d_B) - 1 - 3(\lambda_1 - \lambda_2)]^2}
 \end{aligned} \tag{6}$$

(together with the obvious Hermitian conjugates) for the non-diagonal operators.

The free energy per site, as a function of d_A, d_B and $\lambda_i, i = 1, \dots, 6$, is then

$$\begin{aligned}
 f &= \frac{U}{2}(d_A + d_B - 1) - 2zt \sqrt{(\lambda_3 - \lambda_4)^2 - \frac{1}{4}(d_A - d_B)^2} \\
 &\quad - zt \sqrt{(\lambda_5 - \lambda_6)^2 - [2(d_A + d_B) - 1 - 3(\lambda_1 - \lambda_2)]^2} \\
 &\quad + kT(1 - z) \sum_{\gamma=A,B} [d_\gamma \ln d_\gamma + (\frac{1}{2} - d_\gamma) \ln(\frac{1}{2} - d_\gamma)] \\
 &\quad + kT \frac{z}{2} \sum_{i=1}^6 (m_i \lambda_i \ln \lambda_i).
 \end{aligned} \tag{7}$$

3. The ground state

At $T = 0$, the free energy per site is but the internal energy, and is given by

$$f = \frac{U}{2} (d_A + d_B - 1) - 2zt \sqrt{(\lambda_3 - \lambda_4)^2 - \frac{1}{4}(d_A - d_B)^2} - zt \sqrt{(\lambda_5 - \lambda_6)^2 - [2(d_A + d_B) - 1 - 3(\lambda_1 - \lambda_2)]^2}. \quad (8)$$

The ground state can thus be obtained by minimizing f with respect to the d_ν and the λ_i . Since we are looking for an absolute minimum and our variables are subject to constraints (the eigenvalues of the density matrices, as well as the arguments of the square roots in (8) must be non-negative, and ρ_p must be properly normalized), we should search our minimum possibly at the domain boundary of the constrained variables, and not only in the interior.

Indeed, the minimum is found for

$$d_A = d_B \equiv d = \frac{1}{4} \left(1 - \frac{U}{\sqrt{U^2 + 16}} \right) \quad U = \frac{U}{zt} \quad (9)$$

$\lambda_5 = 1$ and $\lambda_i = 0, i \neq 5$.

The ground state is thus described by

$$\begin{aligned} d_A = d_B = d &= \frac{1}{4} \left(1 - \frac{U}{\sqrt{U^2 + 16}} \right) \\ c_a = \frac{1}{2} - d &= \frac{1}{4} \left(1 + \frac{U}{\sqrt{U^2 + 16}} \right) \\ \tau_1 = \sqrt{2d(1 - 2d)} &= \frac{2}{\sqrt{U^2 + 16}} \\ q = c_p = \tau_0 &= 0. \end{aligned} \quad (10)$$

The configuration of a pair of nearest neighbours in the ground state can be derived as the eigenvector of ρ_p corresponding to the eigenvalue $\lambda_5 = 1$. One obtains, up to a normalization constant,

$$|\Psi\rangle = \left[\frac{2}{\sqrt{U^2 + 16}} (a_{i+}^\dagger a_{i-}^\dagger + a_{j+}^\dagger a_{j-}^\dagger) + \frac{1}{2} \left(1 + \frac{U}{\sqrt{U^2 + 16}} \right) (a_{i+}^\dagger a_{j-}^\dagger + a_{j+}^\dagger a_{i-}^\dagger) \right] |0\rangle. \quad (11)$$

It is worth noticing that such a configuration is the superposition of an antiferromagnetic singlet pair (equivalent to that used by Anderson [20] in the construction of his RVB state) with a fraction of doubly occupied sites. The concentration of doubly occupied sites as well as the kinetic energy (the expectation value of the hopping term) vanish for large U and have their maximum for $U = 0$. The NN correlations are strictly antiferromagnetic (i.e., $c_p = 0$), as expected, and no phase transition is found in any number of dimensions. Some hopping processes, e.g. the hopping of an electron from a doubly occupied to a singly occupied site, or from a singly occupied to an empty site, turn out to be inhibited in the ground state.

In order to check the validity of our approximation, we compare the local magnetic moment at $T = 0$ versus U/t for the 1D chain ($z = 2$) with the exact result reported in [18]. The local magnetic moment S is proportional to the expectation value of the square of the magnetization

$$S = \frac{3}{4} \langle (n_{i+} - n_{i-})^2 \rangle \quad (12)$$

and is directly related to the double occupancy, since

$$S = \frac{3}{4}(1 - 2d) = \frac{3}{8} \left(1 + \frac{U}{\sqrt{U^2 + 16}} \right). \quad (13)$$

Equation (13) is exact both in the non-interacting case ($U = 0, S = \frac{3}{8}$) and in the atomic limit ($U = \infty, S = \frac{3}{4}$). Figure 1 shows the comparison between our results for $z = 2$ (solid line) and the exact solution for the 1D chain (circles). The agreement is within 10% for all values of U/t .

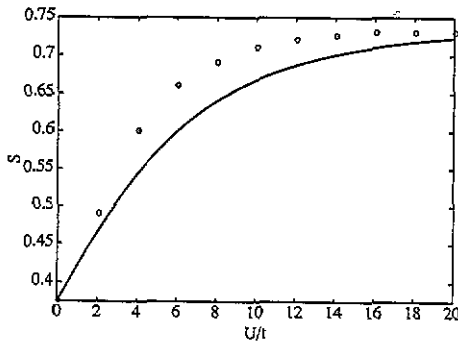


Figure 1. Local magnetic moment at $T = 0$. Our result (solid line) and result from [17] (circles).

4. Finite temperature

Since we have found $d_A = d_B = d$ in the ground state, and the entropy contribution favours this latter condition, one can expect this symmetry relation to hold even at finite temperature. Furthermore, a breaking of such symmetry at finite temperature would yield a re-entrant phase with staggered double occupancy, and there is no indication of such phases in the Hubbard model. Indeed, we have checked numerically that the minima of f always appear for $d_A = d_B = d$. We shall therefore assume from now on the latter relation.

In this way we obtain a free energy which is a function of six independent variables only: d and five of the λ_i . Instead of minimizing f directly, we introduce the following new set of independent variables:

$$\begin{aligned} \delta &= 4d - 1 \\ r_{n,n+1} &= m_n(\lambda_n - \lambda_{n+1}) & n = 1, 3, 5 \\ R_{n,n+1} &= m_n(\lambda_n + \lambda_{n+1}) & n = 1, 3 \end{aligned} \quad (14)$$

and we define $R_{56} = 1 - R_{12} - R_{34}$. After rewriting f , as given by (2), in terms of the above variables, the minimum- f requirement gives (assuming, with no loss of generality, $\lambda_3 > \lambda_4$)

$$\begin{aligned}
 0 &= \frac{\partial f}{\partial \delta} = \frac{U}{4} + zt \frac{\delta - r_{12}}{2\tau_1} + kT \frac{1-z}{2} \ln \frac{1+\delta}{1-\delta} \\
 0 &= \frac{\partial f}{\partial r_{12}} = -zt \frac{\delta - r_{12}}{2\tau_1} + kT \frac{z}{4} \ln \frac{R_{12} + r_{12}}{R_{12} - r_{12}} \\
 0 &= \frac{\partial f}{\partial r_{34}} = -\frac{z}{2}t + kT \frac{z}{4} \ln \frac{R_{34} + r_{34}}{R_{34} - r_{34}} \\
 0 &= \frac{\partial f}{\partial r_{56}} = -\frac{zt}{2\tau_1} r_{56} + kT \frac{z}{4} \ln \frac{R_{56} + r_{56}}{R_{56} - r_{56}} \\
 0 &= \frac{\partial f}{\partial R_{12}} = kT \frac{z}{4} \left(\ln \frac{R_{12}^2 - r_{12}^2}{36} - \ln \frac{R_{56}^2 - r_{56}^2}{4} \right) \\
 0 &= \frac{\partial f}{\partial R_{34}} = kT \frac{z}{4} \left(\ln \frac{R_{34}^2 - r_{34}^2}{64} - \ln \frac{R_{56}^2 - r_{56}^2}{4} \right).
 \end{aligned} \tag{15}$$

Upon defining $x = r_{12} - \delta$, and after some algebra, three of the above equations can be solved for r_{34} , R_{12} , R_{34} and δ (or r_{12}), leaving us with the following two coupled transcendental equations for x and r_{56} :

$$\begin{aligned}
 x &= \tanh \left[\frac{z}{2(z-1)} \beta \left(\frac{x}{\tau_1} - \frac{U}{2} \right) \right] - 6R \sinh \left(\beta \frac{x}{\tau_1} \right) \\
 r_{56} &= 2R \sinh \left(\beta \frac{r_{56}}{\tau_1} \right)
 \end{aligned} \tag{16}$$

where $\beta = (kT/t)^{-1}$, $\tau_1 = \frac{1}{2} \sqrt{r_{56}^2 - x^2}$ and

$$R = \left[6 \cosh \left(\beta \frac{x}{\tau_1} \right) + 8 \cosh \beta + 2 \cosh \left(\beta \frac{r_{56}}{\tau_1} \right) \right]^{-1}. \tag{17}$$

Once (16) has been solved, the remaining variables are given by the following relations:

$$\begin{aligned}
 r_{12} &= -6R \sinh \left(\beta \frac{x}{\tau_1} \right) \\
 R_{12} &= 6R \cosh \left(\beta \frac{x}{\tau_1} \right) \\
 r_{34} &= 8R \sinh \beta \\
 R_{34} &= 8R \cosh \beta.
 \end{aligned} \tag{18}$$

As a check for the whole procedure, we compare in figure 2 our results for the local magnetic moment for $z = 2$ and some typical values of U/t with the exact (numerical) results obtained by Shiba and Pincus [18] for a six-sites chain with periodic boundary

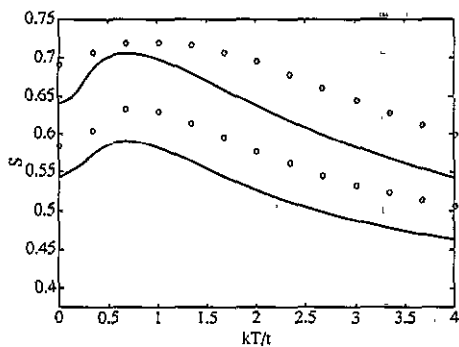


Figure 2. Local magnetic moment at finite temperature for $U/t = 8$ (upper curves) and $U/t = 4$ (lower curves). Solid lines are our results, circles are from [18].

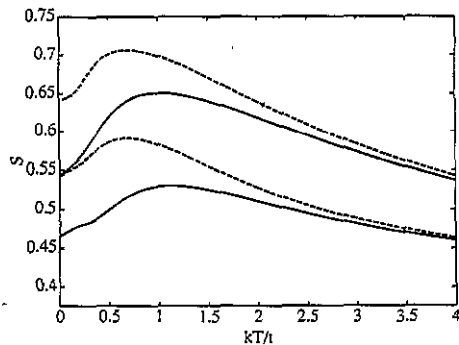


Figure 3. Local magnetic moment at finite temperature for $U/t = 8$ (upper curves) and $U/t = 4$ (lower curves). Dashed lines are for the linear chain and solid lines for the square lattice.

conditions. We find good qualitative agreement, and again differences are contained within 10%. It can be observed that the solution for low temperatures converges to the value predicted by the ground-state analysis. The results for the chain are compared with those for the square lattice ($z = 4$) in figure 3: our analysis shows, as expected from numerical simulation [17], that the local moment increases with increasing U/t and with decreasing dimensionality.

In figure 4 we report the correlation functions c_p (lower curves) and c_a (upper curves), in figure 5 the hopping contributions τ_0 (lower curves) and τ_1 (upper curves), in figure 6 the 'double hoppings' p (lower curves) and p' (upper curves) and in figure 7 the specific heat, for $U/t = 8$ (solid lines) and $U/t = 4$ (dashed lines) for a square lattice.

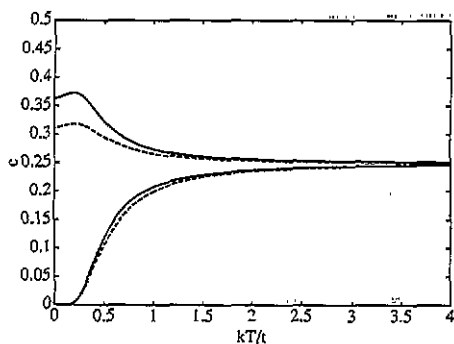


Figure 4. Correlation functions c_p (lower curves) and c_a (upper curves) on the square lattice for $U/t = 8$ (solid lines) and $U/t = 4$ (dashed lines).

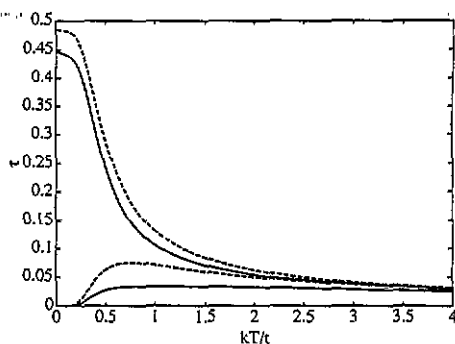


Figure 5. Hopping expectation values τ_0 (lower curves) and τ_1 (upper curves) on the square lattice for $U/t = 8$ (solid lines) and $U/t = 4$.

Of course there is no evidence of a true phase transition (the specific heat exhibits a maximum, but not a sharp peak), but we can clearly distinguish a low-temperature behaviour ($kT/t < 0.5$) from a high-temperature one ($kT/t > 1$). The low-temperature region is characterized by strong antiferromagnetic correlations and by a relatively large kinetic energy associated with the moving electrons, due almost entirely to double hoppings and to hopping processes from doubly occupied to empty sites and vice versa, while the

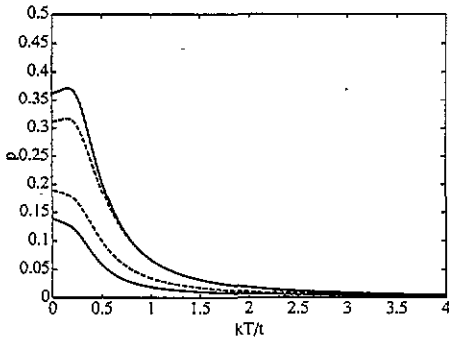


Figure 6. Double hoppings p (lower curves) and p' (upper curves) on the square lattice for $U/t = 8$ (solid lines) and $U/t = 4$ (dashed lines).

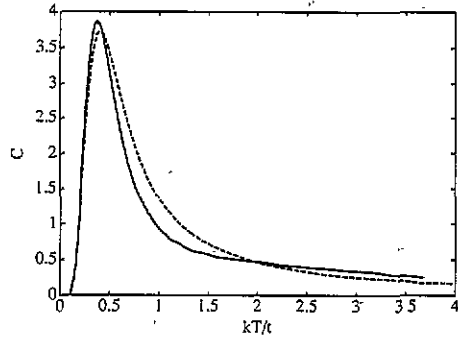


Figure 7. Specific heat on the square lattice for $U/t = 8$ (solid lines) and $U/t = 4$.

remaining processes are strongly inhibited because of the ground-state configuration. The high-temperature region, besides, looks like a true disordered phase, with almost equally distributed correlations ($c_p \approx c_a \approx \frac{1}{4}$) and low kinetic energy. Furthermore in this region, as already noticed in [16], for very large values of the interaction U/t a spread maximum appears in the specific heat, which was related by Ho and Barry to a 'gradual' metal-insulator transition.

5. Conclusions

We have investigated the half-filled Hubbard model in the pair approximation of the cluster variation method, making use of the full $SO(4)$ symmetry of the model. We have given an analytical description of the ground state, by means of the double occupancy and of the NN correlation functions and, for finite temperature, we have derived a pair of coupled transcendental equations. Numerical solution shows two different behaviours, connected by a smooth but rapid change in the values of the parameters. The low-temperature behaviour is strongly antiferromagnetic and exhibits the inhibition of certain hopping processes, while a large kinetic energy is associated with the others. In the high-temperature region we find a quite disordered behaviour, with a spread maximum, which was related to a metal-insulator transition, for very large values of the interaction. Good agreement is found with exact and numerical results in one dimension.

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