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Renormalisation group study of the two-dimensional Hubbard model

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Abstract. The Hubbard model in two dimensions is studied using a recently proposed renormalisation group method for fermion systems. We find that there are no phase transitions in the model and that the ground state is ordered antiferromagnetically.

We also discuss the use of group theory in the renormalisation for large cells.

1. Introduction

A real space renormalisation group method appropriate for fermion systems was recently introduced (Vanderzande and Stella 1984). This method works both at finite and at zero temperatures. Furthermore, it correctly deals with Fermi statistics in all dimensions. So far, it has only been applied to the one-dimensional Hubbard model. Because the Jordan-Wigner transformation allows us to rewrite a fermion model in one dimension as a spin model, real fermion effects (due to anticommutation relations) only occur in higher dimensions. In the present paper, we therefore extend our study to the two-dimensional Hubbard model.

The Hubbard model was originally introduced (Hubbard 1963) to evaluate the effects of correlations on electrons in narrow energy bands. In later years, it has been increasingly studied as one of the simplest fermion systems in statistical mechanics.

The model is defined via its Hamiltonian

$$H-\mu N = t\sum_{\langle i,j\rangle}\sum_{\sigma}(c_{i\sigma}^{+}c_{j\sigma}+c_{j\sigma}^{+}c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i}\sum_{\sigma}n_{i\sigma} \tag{1}$$

where $c_{i\sigma}^{+}(c_{i\sigma})$ are creation (annihilation) operators for electrons with spin σ (which can be up ($\uparrow$) or down ($\downarrow$)) in the Wannier state centred at site i of a lattice, and $n_{i\sigma}=c_{i\sigma}^{+}c_{i\sigma}$. The parameter μ is the chemical potential, U measures the intra-atomic Coulomb repulsion and t is the hopping parameter between nearest-neighbour sites. We will only consider the half-filled band, which implies $\mu = U/2$. We can then rewrite the Hamiltonian (1) as

$$H-\mu N = t\sum_{\langle i,j\rangle}\sum_{\sigma}(c_{i\sigma}^{+}c_{j\sigma}+c_{j\sigma}^{+}c_{i\sigma})-\tfrac{1}{2}U\sum_{i}(n_{i\uparrow}-n_{i\downarrow})^{2}. \tag{2}$$

For the following, it is important to have a clear idea of the symmetries present in the model (2). The grand partition function of (2)

$$Z(t,U)=\mathrm{Tr}\exp[-\beta(H-\mu N)] \tag{3}$$

is invariant under a local phase change of the Wannier representation $c_{i\sigma}\rightarrow c_{i\sigma}\exp(\mathrm{i}\alpha_i)$.

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On a non-frustrated lattice, like the square one, we can choose $\alpha_i - \alpha_j = \pm\pi$ for every pair of nearest neighbours, and therefore we have

$$Z(t, U) = Z(-t, U). \tag{4}$$

If we combine the phase change described above with a particle-hole exchange

$$c_{i\sigma} \leftrightarrow c_{i\sigma}^{+} \exp(i\alpha_i), \qquad \sigma = \uparrow \text{ or } \downarrow, \tag{5}$$

we have a transformation which leaves the Hamiltonian (2) invariant. This symmetry is not present on a frustrated lattice, like the triangular one. In this case the possible critical behaviour of the model may be different from the one on a hypercubic lattice. This can be understood in another way: in the large-U limit, (2) becomes equivalent to an antiferromagnetic Heisenberg model (Richmond and Sewell 1968). It is therefore clear that the model behaves differently, depending on whether the lattice is frustrated or not.

In this paper, we study the Hubbard model on a square lattice. The properties of this model are little known. A Mermin-Wagner-like theorem shows that there is no magnetic ordering at finite temperature (Jedrzejewski and Verbeure 1981).

Some authors suggest that on hypercubic lattices, the ground state is insulating as soon as U is non-zero (Richmond 1969, Chaikin *et al* 1975). Mean-field-like calculations, on the other hand, indicate the presence of a transition in the ground state or at finite temperature (Caron and Pratt 1968, Wolff 1983), or indicate that the ground state is antiferromagnetically ordered (Oitmaa and Betts 1978). Of course, these mean-field results are rather doubtful. Recently, the two-dimensional Hubbard model has been studied using a Monte Carlo method (Hirsch 1983). The ground state was found to be antiferromagnetic, whereas at finite temperature the model was an insulating paramagnet. Neither in the ground state, nor at finite temperature do the Monte Carlo results suggest the presence of phase transitions. There is thus no clear idea of the critical behaviour of this model. It is therefore clear that an independent calculation of the properties of this model as presented in this paper is very useful.

2. The renormalisation group method

We study the two-dimensional Hubbard mdel using a real space renormalisation group method. In this method, we divide the lattice into cells of n_s sites. In our calculation $n_s = 5$, and the cells are cross-shaped (figure 1)†. The Hamiltonian is split into intracell parts $H_{0,\alpha}$ (α labels the cell) and intercell interactions $V_{\alpha,\beta}$ such that

$$H = H_0 + V \tag{6}$$

where

$$H_0 = \sum_{\alpha} H_{0,\alpha} \tag{7a}$$

and

$$V = \sum_{\langle \alpha,\beta \rangle} V_{\alpha\beta}. \tag{7b}$$

† On a square lattice, the simplest possible cell would be a square cell with $n_s = 4$. The spectrum of this cell does not however have the right symmetry properties. The ground state of the cell Hamiltonian would be a boson state. It can then be calculated that U', the renormalised Coulomb interaction, would become negative. Furthermore, experience (Hanke and Hirsch 1982) tells us that for fermion systems cells with an odd number of sites give better results.

The next step consists of the diagonalisation of $H_{0,\alpha}$. In principle, this requires the diagonalisation of a $4^5 \times 4^5 = 1024 \times 1024$ matrix. We will return to this problem later.

The energy eigenstates are divided into four groups, corresponding to cell states $|\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}\rangle$. The cell occupation numbers $\nu_{\alpha\uparrow}$ and $\nu_{\alpha\downarrow}$ can be either zero or plus one (e.g. the cell state $|+\rangle'$ has $\nu_{\alpha\uparrow} = 1$, $\nu_{\alpha\downarrow} = 0$; $|0\rangle'$ has $\nu_{\alpha\uparrow} = \nu_{\alpha\downarrow} = 0, \ldots$).

Within each group, the states are labelled with some extra index τ_α, so that the set of eigenstates of $H_{0,\alpha}$ can be denoted as

$$|\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha\rangle \qquad \nu_{\alpha\uparrow} = 0, 1, \qquad \nu_{\alpha\downarrow} = 0, 1, \qquad \tau_\alpha = 1, 4^{n_s-1} = 256.$$

A state of the whole lattice can then be written as

$$|\{\nu_{\alpha\uparrow}\}, \{\nu_{\alpha\downarrow}\}, \{\tau_\alpha\}\rangle \equiv \prod_\alpha{}^{\otimes} |\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha\rangle \tag{8a}$$

whereas a configuration of cell states will be denoted as

$$|\{\nu_{\alpha\uparrow}\}, \{\nu_{\alpha\downarrow}\}\rangle \equiv \prod_\alpha{}^{\otimes} |\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}\rangle. \tag{8b}$$

Because of the Fermi character, a convention has to be made concerning the ordering of the states in (8*a*) and (8*b*). This problem will also be discussed below.

We are now ready to set up our renormalisation transformation. This maps the Hamiltonian H onto a renormalised one, H', defined by

$$\langle\{\nu_{\alpha\uparrow}\}, \{\nu_{\alpha\downarrow}\}|\exp(-\beta' H')|\{\nu'_{\alpha\uparrow}\}, \{\nu'_{\alpha\downarrow}\}\rangle$$
$$= \mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\nu_{\alpha\uparrow}\}, \{\nu_{\alpha\downarrow}\}, \{\tau_\alpha\}|\exp(-\beta H)|\{\nu'_{\alpha\uparrow}\}, \{\nu'_{\alpha\downarrow}\}, \{\tau_\alpha\}\rangle. \tag{9}$$

This mapping preserves the free energy.

In almost all cases of interest, (9) cannot be worked out exactly. Therefore the exponentials in (9) are developed using the Feynman identity (Stella *et al* 1983)

$$\exp(-\beta H) = \exp(-\beta H_0)\, T_\lambda \left[\exp\left(-\int_0^\beta \mathrm{d}\lambda\, \exp(\lambda H_0)\, V \exp(-\lambda H_0)\right)\right] \tag{10}$$

with T_λ being a 'time ordering' operator with respect to the variable λ. Similarly, the exponential on the LHS of equation (9) is developed in powers of V', the intercell hopping. The Hamiltonian H'_0 describes the intracell Coulomb repulsion. In this way, H' can be determined order by order in V.

In this paper, we have performed our calculation to first order. It can be shown (Stella *et al* 1983) that the mapping defined by (9) and (10) has a meaningful ground state ($\beta \to \infty$) limit. Indeed, going to first order, one recovers in that limit a well known renormalisation transformation for quantum systems (Pfeuty *et al* 1982).

We now turn to the problem of the ordering in product states like (8*a*) and (8*b*). In a previous paper (Vanderzande and Stella 1984), we have shown that this ordering is in fact irrelevant as long as the division of the eigenstates of $H_{0,\alpha}$ into four groups obeys one rule: fermion states should be mapped onto fermion states, and boson states onto boson states. For example, a state with four electrons present, all of them with spin up, should be mapped either onto the cell state with no electrons present, or onto the cell state with two electrons, but not onto the state with one electron with spin up ($|+\rangle'$), as would be done in a majority-like rule of the type often used in magnetic spin problems. In this way, a correct description of the fermion character puts limits on the freedom inherent in the map (9).

We choose the following division of the eigenstates into four groups,

(i) states with zero, two or four (resp six, eight or ten) electrons present are mapped onto the $|0\rangle'$ (resp $|\pm\rangle'$) state,

(ii) fermion states (one, three, five, seven or nine electrons) for which $\Sigma_{i\in\alpha} s^z_{\alpha,i} > 0 (<0)$ are mapped onto the $|+\rangle'$ ($|-\rangle'$) state. ($s^z_{\alpha,i} = n_{\alpha i,\uparrow} - n_{\alpha i,\downarrow}$) (see also table 1). This division is possible because both $\Sigma_{i\in\alpha}\Sigma_\sigma n_{\alpha i,\sigma}$ and $\Sigma_{i\in\alpha} s^z_{\alpha i}$ commute with $H_{0,\alpha}$.

3. The τ_α labelling problem; use of group theory

The transformation (9) has a threefold freedom. Firstly, one can choose to work either with eigenstates of $H_{0,\alpha}$ as we do, or with other states $|\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha\rangle$. We will make further use of this freedom in this paper. Secondly, there is a freedom in the choice of the division of the eigenstates into four groups: we dealt with this in the preceding section. Finally, one has the freedom of giving the states within a group a label τ_α. Because (9) in first order (see equations (11) and (13) below) involves the calculation of matrix elements of V between states in different groups with the same τ_α, it is the relative τ_α labelling which is important.

In the choice of this labelling, symmetry principles can be very helpful. (Vanderzande and Stella 1984, Stella *et al* 1983). As in the case of the Hubbard model in $d = 1$, in order to preserve the basic symmetry (5), states in the $|0\rangle'$ ($\nu_{\alpha\uparrow} = \nu_{\alpha\downarrow} = 0$) and $|\pm\rangle'$ ($\nu_{\alpha\uparrow} = \nu_{\alpha\downarrow} = 1$) group which can be connected by applying the operation (5) on every site of the cell are given the same τ_α label. A similar correspondence is made between states in the $|+\rangle'$ group ($\nu_{\alpha\uparrow} = 1$, $\nu_{\alpha\downarrow} = 0$) and $|-\rangle'$ group ($\nu_{\alpha\uparrow} = 0$, $\nu_{\alpha\downarrow} = 1$) by applying spin-inversion symmetry $c_{i\sigma} \leftrightarrow c_{i-\sigma}$. This leaves us with the problem of combining the τ_α labels of states in e.g. the $|0\rangle'$ group with states in the $|+\rangle'$ group.

We have connected this problem with the problem of diagonalising $H_{0,\alpha}$. As stated previously $\Sigma_{i\in\alpha} s^z_{\alpha i}$ and $\Sigma_{i\in\alpha} n_{\alpha i,\sigma}$ commute with $H_{0,\alpha}$.

In table 1 we report the possible values that these quantum numbers take and the number of states with these values in the $|0\rangle'$ and $|+\rangle'$ groups, respectively.

If for a moment, we consider the simultaneous eigenstates of

$$N \equiv \sum_i \sum_\sigma n_{\alpha i,\sigma}$$

Table 1. Number of eigenstates of $H_{0,\alpha}$ with given $\Sigma_i \Sigma_\sigma n_{\alpha i,\sigma}$ and $\Sigma_i s^z_{\alpha i}$ in the groups with $\nu_{\alpha\uparrow} = \nu_{\alpha\downarrow} = 0$ ($|0\rangle'$ group) and $\nu_{\alpha\uparrow} = 1$, $\nu_{\alpha\downarrow} = 0$ ($|+\rangle'$ group). The crosses indicate states between which matrix elements of c_σ or c^+_σ operators can be non-zero.

	$\|0\rangle'$			$\|+\rangle'$	
$\Sigma_i \Sigma_\sigma n_{\alpha i,\sigma}$	$\Sigma_i s^z_{\alpha i}$			$\Sigma_i \Sigma_\sigma n_{\alpha i,\sigma}$	$\Sigma_i s^z_{\alpha i}$
0	0	1	5	5	1
2	2	10	+ 3	3	10
2	0	25	5	3	25
2	−2	10	7	3	10
4	4	5	1	1	5
4	2	50	+ 3	1	50
4	0	100	+ 5	1	100
4	−2	50	7	1	50
4	−4	5	9	1	5

and

$$S^z \equiv \sum_i s^z_{\alpha i}$$

we see that states which are in the same row of table 1 can be obtained from one another by interchanging $|0\rangle$ and $|+\rangle$ states and $|-\rangle$ and $|\pm\rangle$ states, at every site. For example, with this operation the state $|+++0-\rangle$ ($N=4$, $S^z=2$) becomes $|0\,0\,0+\pm\rangle$ ($N=3$, $S^z=1$). This operation is not a symmetry of H, except when $U=0$. For $U\neq 0$, it is however a symmetry between the classes of states in the same row of table 1. We will therefore give the eigenstates of $H_{0,\alpha}$ which are in the same row of table 1 the same set of τ_α labels. In this way, the τ_α label has still to be specified within the nine classes of states in table 1. Let us now write down the first-order term of the RHS of (10). It is, between cells α and β (figure 1):

$$\begin{aligned} t\sum_\sigma \sum_{\tau_\alpha}\sum_{\tau_\beta} [&\langle \nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha | c^+_{\alpha 2\sigma} | \nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha\rangle \langle \nu_{\beta\uparrow}, \nu_{\beta\downarrow}, \tau_\beta | c_{\beta 5\sigma} | \nu'_{\beta\uparrow}, \nu'_{\beta\downarrow}, \tau_\beta\rangle \\ &+ \langle \nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha | c^+_{\alpha 3\sigma} | \nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha\rangle \\ &\times \langle \nu_{\beta\uparrow}, \nu_{\beta\downarrow}, \tau_\beta | (c_{\beta 4\sigma} + c_{\beta 5\sigma}) | \nu'_{\beta\uparrow}, \nu'_{\beta\downarrow}, \tau_\beta\rangle + \text{CC}] \\ &\times \chi[\beta E_0(\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha) + \beta E_0(\nu_{\beta\uparrow}, \nu_{\beta\downarrow}, \tau_\beta), \beta E_0(\nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha) \\ &+ \beta E_0(\nu'_{\beta\uparrow}, \nu'_{\beta\downarrow}, \tau_\beta)]. \end{aligned} \tag{11}$$

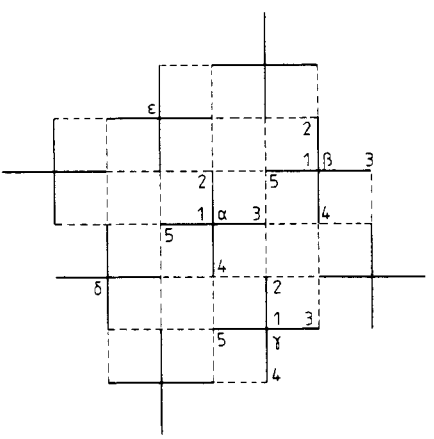

Figure 1. Division of the cubic lattice into cross-shaped cells.

(CC stands for complex conjugate; a phase factor coming from fermion anticommutations was not written down because it drops out with a similar factor of the RHS of equation (9) (Vanderzande and Stella 1984).) The function $\chi(x, y)$ is defined by

$$\begin{aligned} \chi(x,y) &= (e^x - e^y)/(x-y) && \text{if } x \neq y \\ &= e^x && \text{if } x = y. \end{aligned} \tag{12}$$

The matrix elements are non-zero only between states for which both N and S^z differ by one, i.e. only between states in the rows which are indicated by a cross in table 1. For the other states, the τ_α label is irrelevant (up to first order).

A problem arises when we write down the interaction between cells α and γ in figure 1, which is:

$$t\sum_{\sigma}\sum_{\tau_\alpha}\sum_{\tau_\gamma}[\langle \nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha|c^{+}_{\alpha 3\sigma}|\nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha\rangle\langle \nu_{\gamma\uparrow}, \nu_{\gamma\downarrow}, \tau_\gamma|c_{\gamma 2\sigma}|\nu'_{\gamma\uparrow}, \nu'_{\gamma\downarrow}, \tau_\gamma\rangle$$
$$+\langle \nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha|c_{\alpha 4\sigma}|\nu'_{a\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha\rangle$$
$$\times\langle \nu_{\gamma\uparrow}, \nu_{\gamma\downarrow}, \tau_\gamma|(c_{\gamma 2\sigma}+c_{\gamma 5\sigma})|\nu'_{\gamma\uparrow}, \nu'_{\gamma\downarrow}, \tau_\gamma\rangle+\mathrm{CC}]$$
$$\times\chi[\beta E_0(\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha)+\beta E_0(\nu_{\gamma\uparrow}, \nu_{\gamma\downarrow}, \tau_\gamma), \beta E_0(\nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha)$$
$$+\beta E_0(\nu'_{\gamma\uparrow}, \nu'_{\gamma\downarrow}, \tau_\gamma)]. \tag{13}$$

Can we be sure that (11) and (13) give the same t' (t, U)? In general, it is quite possible that the interaction t' will be anisotropic. In order to solve this question, together with the problem of the remaining τ_α labelling (and to simplify the diagonalisation of e.g. the 100×100 matrices, table 1), we consider the symmetry group C_{4v} of the cell. The character table of this group is, for convenience, represented in table 2. We use standard notation for the group elements and representations (see e.g. Landau and Lifschitz 1967).

Table 2. Character table of the point group c_{4v} (d is the dimension of the representation).

	E	C_2	C_4	σ_v	σ'_v	d
A_1	1	1	1	1	1	1
A_2	1	1	1	−1	−1	1
B_1	1	1	−1	1	−1	1
B_2	1	1	−1	−1	1	1
E	2	−2	0	0	0	2

We will take our eigenstates of $H_{0,\alpha}$ to also be eigenstates of $U(C_4)$, the representation matrix of the group element C_4. In this case, all matrix elements in (11) and (13) can be written in terms of matrix elements of the annihilation operator at site 2 of a cell; $c_{2\sigma}$. This gives a fourfold reduction in the number of matrix elements to be calculated. For example

$$\langle \nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha|c^{+}_{\alpha 3,\sigma}|\nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha\rangle$$
$$=\langle \nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha|U^{-1}(C_4)U(C_4)c^{+}_{\alpha 3,\sigma}U^{-1}(C_4)U(C_4)|\nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha\rangle$$
$$=\varepsilon_0(\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha; C_4)^{*}\varepsilon_0(\nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha; C_4)$$
$$\times\langle \nu'_{\alpha\uparrow}, \nu'_{\alpha\downarrow}, \tau_\alpha|c_{\alpha 2\sigma}|\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha\rangle^{*} \tag{14}$$

where we have defined for the group element g (which can be C_4, $C_2=C_4^2$, C_4^3)

$$U(g)|\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha\rangle=\varepsilon_0(\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha; g)|\nu_{\alpha\uparrow}, \nu_{\alpha\downarrow}, \tau_\alpha\rangle. \tag{15}$$

For eigenstates of $H_{0,\alpha}$ belonging to the one-dimensional representations of C_{4v}, ε_0 can be ±1, whereas for the E-representations it can also be $\pm i$. To fix our ideas, let us now consider the subset of states with $N=4$, $S^z=2$ in the $|0\rangle'$ group, and the subset with $N=3$, $S^z=1$ in the $|+\rangle'$ group. They both contain 50 elements (similar arguments to the ones below can be applied to the other subsets, indicated by a cross, in table 1). Using group theory, we can calculate how many of the common eigenstates of

Table 3. Division of the eigenstates with ($N=4$, $S^z=2$), ($N=3$, $S^z=1$) according to the representation of C_{4v}, the last two columns give the number of states transforming according to some representation.

	$\varepsilon_0(C_4)$	$\varepsilon_0(C_2)$	$N=4$, $S^z=2(\|0\rangle')$	$N=3$, $S^z=1(\|+\rangle')$
A_1	1	1	4	7
A_2	1	1	8	5
B_1	−1	1	5	8
B_2	−1	1	7	4
E	$+i$	−1	13	13
	$-i$	−1	13	13

$H_{0,\alpha}$ and $U(C_4)$ in this space belong to a certain representation: these numbers are given in table 3.

From this it is obvious to give e.g. the states of the $|0\rangle'$ set which transform according to A_1 the same τ_α label as the states in the $|+\rangle'$ set transforming according to B_2, to connect A_2 in $|0\rangle'$ with B_1 in $|+\rangle'$, etc. We have now greatly simplified our calculation. Firstly, the largest matrices to be diagonalised become 24×24 (complex) matrices, which can easily be diagonalised using standard algorithms (they are in the ($N=5$, $S^z=1$) and ($N=4$, $S^z=0$) groups, E representations). Furthermore, again using elementary group theory, we can derive selection rules for the matrix elements of $c_{2\sigma}$, the only matrix elements we still had to calculate (equation (14)).

These rules indicate that matrix elements between states of the A_1 and B_2, or between states of the A_2 and B_1 representations are zero. Because these states are connected by our τ_α correspondence (table 3), in the sum of equation (11) (or (13)) only matrix elements between states in the E representations survive, so that only for these states does the τ_α labelling have to be specified. We give the τ_α labelling in these spaces according to the energy of the state: increasing τ_α label for decreasing energy. Because of this τ_α labelling, and because of the selection rules, we only have to calculate 80 (instead of 256) matrix elements of $c_{2\sigma}$.

Finally, with this choice of the labelling we can show that t' calculated with (11) or (13) is the same, thus removing the anisotropy problem. If we calculate t' it turns out to be complex (because the eigenstates of $U(C_4)$ have complex coefficients). Due to the freedom in the choice of the phase of the Wannier states, we only have to consider the absolute value of t'. It is important to point out once again the considerable simplification which has occurred in the technical problem of calculating t' via (11) or (13), using group theoretical arguments. If we also take into account the total spin $(\Sigma_{i\in\alpha} S_i)^2$ which also commutes with $H_{0,\alpha}$, and the quantum number for Hubbard-like models introduced by Nowak (1981), further simplification could arise. However this is no longer necessary because the calculation has already become quite tractable. These techniques could also be applied to other models. It would be relatively easy to study e.g. the two-dimensional XY model using a square cell of nine spins.

4. Results and discussion

We calculated the flow generated by the map (9). The calculation (construction of the Hamiltonian, transformation to eigenstates of C_4, diagonalisation, calculation of matrix elements and flow) was completely done by computer.

One new type of interaction is generated by the map, when U and the temperature T are both different from zero. It is of the same type as in the one-dimensional case (Vanderzande and Stella 1984),

$$-D\sum_{\langle i,j\rangle}\sum_{\sigma}(c_{i\sigma}^{+}c_{j\sigma}+c_{j\sigma}^{+}c_{i\sigma})(1-n_{i-\sigma}-n_{j-\sigma})^{2}. \tag{16}$$

We took this interaction into account perturbatively.

As shown in Stella *et al* (1983), in the zero-temperature limit our renormalisation scheme coincides with the so-called block-spin method for quantum systems (Pfeuty *et al* 1982). In this scheme, only the states with lowest energy, in each of the four groups (corresponding to the effective cell states) are considered. In this model, and with the cell we choose, there is a selection rule for V between these states so that we obtain $t'(t, U, D)=0$, when $T=0$. The solution to this problem in the ground state renormalisation of Pfeuty *et al* (1982) is well known. One simply considers four low-lying states with non-zero matrix elements instead of the four with lowest energy. In the appendix we show how this procedure also can be obtained from a scheme like ours, in the zero-temperature limit. Here, we choose the lowest energy states in the E representation space (with $\varepsilon_0(C_4)=+i$) though our results seem rather insensitive to the specific choice made.

The flow in parameter space resulting from our calculation is shown schematically in figure 2 (projected on the plane $D=0$). We find only trivial fixed points. Except when $U/t=0$, the ground state always renormalises to $U/t=\infty$. In that limit the model is equivalent to an antiferromagnetic Heisenberg model, so that we can conclude that the ground state is always antiferromagnetic. There is no transition for finite U/t in the ground state. This is in contradiction with previous results which were obtained with a one-dimensional cell (Hirsch 1980). There are also indications (Dasgupta and Pfeuty 1981) that a calculation with a 3×3 cell would give a transition in the ground state. At this moment the reason for this discrepancy is not clear. On the other hand, the Monte Carlo calculations of Hirsch (1983) agree with our results, not only at zero temperature but also at finite temperatures, where neither of the two calculations show the presence of a transition. We have calculated the ground state energy, which is found to have the same qualitative behaviour as the Monte Carlo calculations.

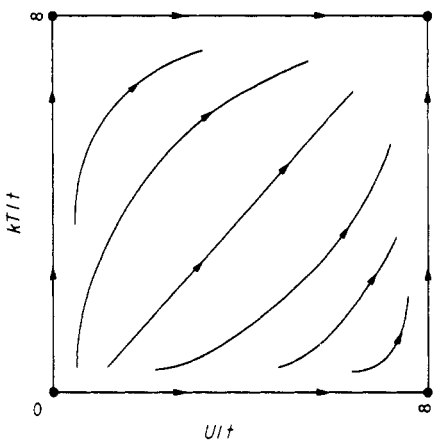

Figure 2. Renormalisation flow for the two-dimensional Hubbard model according to the present calculation (projection on the plane $D=0$).

However, the cell we have used is too small, or we should go to higher order in perturbation theory to determine accurate thermodynamic properties.

Summarising, in this paper, we have presented the first real space renormalisation study of a fermion model, in two dimensions and at arbitrary temperature. We have showed how group theory can considerably simplify the calculation. We have found that the Hubbard model in two dimensions, about which very few results are established, shows no magnetic nor metal-insulator phase transition. The ground state is antiferromagnetic. These results agree with Monte-Carlo calculations. The paper shows how Monte Carlo methods, which are more 'experimental', and renormalisation group techniques, which are more analytic, can complement each other in the study of complicated quantum systems. It is certainly possible that a combination of the two methods may be able to give insight into the three-dimensional Hubbard model. We hope that the techniques established in this paper will also be useful in dealing with other quantum spin or fermion models.

Acknowledgment

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Appendix

In a previous paper (Stella *et al* 1983) we showed how the block spin ground state renormalisation method (Pfeuty *et al* 1982) for quantum systems can be seen as the $T \to 0$ limit of a transformation like (9), using (10) up to first order.

In this way, one always finds that the ground state renormalised interaction is determined by the states with lowest energy belonging to a group of states, corresponding to an effective cell spin value. In the notation of the paper we have, for a fermion system, at $T = 0$

$$\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\}|V'|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\}\rangle = \langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{1\}|V|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\},\{1\}\rangle. \tag{A1}$$

Sometimes it can be useful, from the ground state point of view, to have other states as 'effective cell states at $T = 0$', and this is indeed done in several calculations. One example is when the RHS of (A1) would be zero. We can derive this procedure from (9) in the limit $T \to 0$, by introducing into (9) a unitary operator (Stella *et al* 1983), which in fact means nothing more than working with states $|\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{\tau_\alpha\}\rangle$ which are no longer eigenstates of $H_{0,\alpha}$.

In this way, we change (9) into

$$\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\}|\exp(-\beta' H')|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\}\rangle$$
$$= \mathrm{Tr}_{\{\tau_\alpha\}}\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{\tau_\alpha\}|U^{-1}\exp(-\beta H)U|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\},\{\tau_\alpha\}\rangle \tag{A2}$$

where

$$U = 1 + U_1 + U_2 + \ldots \tag{A3}$$

and U_i is of order V^i. Consequently,

$$U^+ = U^{-1} = 1 - U_1 + (U_1^2 - U_2) + \ldots. \tag{A4}$$

Suppose we want to have instead of (A1)

$$\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\}|V'|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\}\rangle=\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{\bar{\tau}_\alpha\}|V|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\},\{\bar{\tau}_\alpha\}\rangle \tag{A5}$$

where $\{\bar{\tau}_\alpha\}$ is a certain configuration of τ_αs, different from $\{1\}$. This can be obtained as a $T\to 0$ limit of (A2) by imposing

$$\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{1\}|U_1|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\},\{1\}\rangle$$
$$=\frac{\langle\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{\bar{\tau}_\alpha\}|V|\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\},\{\bar{\tau}_\alpha\}\rangle}{E_0(\{\nu_{\alpha\uparrow}\},\{\nu_{\alpha\downarrow}\},\{1\})-E_0(\{\nu'_{\alpha\uparrow}\},\{\nu'_{\alpha\downarrow}\},\{1\})} \tag{A6}$$

and all other matrix elements of U_1 equal to zero. It can easily be verified that this is a unitary transformation.

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