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Renormalization group recursion without proliferation of terms in the one-band Hubbard model

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Abstract. The real space renormalization group block method is analysed We deduce the conditions for avoiding the proliferation of couplings in a fermion system like the one-band Hubbard model We also extend the method for two and three dimensions

1. Introduction

Several years ago real space renormalization group (RSRG) methods were extensively applied to quantum lattice systems [1-7]. There are three main kinds of recursions techniques: (i) the Niemejer-van Leeuwen method (see [2] for a critical analysis), (ii) the Migdal-Kadanoff approach [3]; (iii) the block method [1].

We are interested here in the study of fermion systems on a lattice in any dimension of physical interest, $d = 1, 2, 3$. The Niemejer-van Leeuwen recursion has a great amount of arbitrariness in the choice of renormalization transformation and is hardly generalizable to the fermion systems. The Migdal-Kadanoff method fails in describing the ground state of the system, and produces proliferation of couplings for the fermion systems even in one dimension [4]. The last one, the block technique, was originally introduced similarly to a variational approach to φ^4 theory in a lattice [1] This paper is devoted to this technique.

The first systems analysed by mean of the block method were spin systems, afterwards the technique was generalized to fermion systems in one dimension [5-7]. This approach gives reasonable results mainly for the Ising model in a transverse field and the Hubbard Hamiltonian, both in one dimension and at $T = 0$, but fails in describing $T \neq 0$ systems and it is difficult to generalize it to higher dimensions. Here we give a brief outline of the RSRG block method applied to the Hubbard model and deduce the conditions under which the renormalized Hamiltonian has the same form as the original one. By using these conditions we are able to define a well-behaved renormalization flux and keep constant the dimension of the parameter space, i.e no spurious interactions will be created. We then extend the method to $d = 2, 3$.

2. The block method

The Hubbard Hamiltonian is

$$H = H_t + H_u + H_\mu = -\sum_{\langle ij\rangle,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \tag{1}$$

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where t_{ij} is the nearest-neighbour hopping term, U is the local repulsive interaction and μ is the chemical potential. Let us assume that we know how to solve the Hamiltonian (1) for a block α of size s^d where d is the dimension of the system, and to obtain all the eigenvectors $|\varphi_{i\alpha}\rangle$ for this block.

We could try to rewrite (1) on this basis:

$$H = \sum_{\psi,\psi'} |\psi\rangle\langle\psi|H|\psi'\rangle\langle\psi'| \tag{2}$$

where $|\psi\rangle = \Pi_\alpha |\varphi_{i\alpha}\rangle$.

There are, however, too many states, and our task is to project out a part of $|\psi\rangle$s, both to diminish the degrees of freedom of the system and to obtain recurrence relations between H and the projected part that we shall call H'. To get this recurrence we keep four of the eigenvectors of each block, $|\varphi_{0\alpha}\rangle$, and eliminate the rest. We define in this way a new Hamiltonian representing a system whose size has changed by a factor s†,

$$H' = P_0 H P_0 \tag{3}$$

where $P_0 = \Sigma_{\psi_0} |\psi_0\rangle\langle\psi_0|$ and $|\psi_0\rangle = \Pi_\alpha |\varphi_{0\alpha}\rangle$.

These are the traditional 'recipes' for the RSRG method. The problems appear when we try to write (3) in a way analogous to (1). We will find terms of the type H'_u and H'_μ, but the hopping term H'_t will not be, in general, equivalent to H_t.

3. Choosing the basis $|\varphi_{0\alpha}\rangle$

In order to label the $|\varphi_{0\alpha}\rangle$s we shall use the total number of electrons $N_{e,\alpha} = \Sigma_{i\in \text{Block},\sigma} n_{i,\sigma}$, the projection of total spin $S_{z,\alpha} = \frac{1}{2}\Sigma_{i\in\text{Block}}(n_{i,\uparrow} - n_{i,\downarrow})$ and the spatial symmetry Γ_i. Here the Γ_is denote the irreducible representations of the point group under which H is invariant. We shall use two other symmetries if necessary, the total spin S^2 and the quasi-spin Casimir operator $Z^- Z^+$‡, where

$$Z^+ = \sum_i \nu_i c^+_{i\downarrow} c^+_{i\uparrow}. \tag{4a}$$

We assume here a bipartite AB-type lattice, then we have $\nu_i = 1$ for the A sites and $\nu_i = -1$ for the B sites. It is amusing to observe that we can write Z^+ into the block as

$$Z^+_\alpha = \sum_k d^+_{k,\downarrow} d^+_{\pi-k,\uparrow} \tag{4b}$$

where $k = (k_x, k_y)$, $\pi \to (\pi, \pi)$, for example in the two-dimensional case; and the $d_{k,\sigma}$ operators diagonalize the H_t term in the block. We can see then how to construct invariants of any band term in a lattice if it has an energy spectrum so that $\varepsilon(k) + \varepsilon(G+k) = 0$, which is a property of the AB-type lattices. The Z^+, Z^- and $Z_3 = \frac{1}{2}(N_e - N_s)$, where N_s is the number of sites, obey the commutations relations of quasi-spin operators, and they can be seen as a generalization of the seniority§ to the lattice case. We obtain for the Z-operators the following general relations:

$$[H, Z^+] = (U - 2\mu)Z^+ \qquad [N_e, Z^\pm] = \pm 2Z^\pm \qquad [S^\pm, Z^+] = 0 \tag{5}$$

† Equation (3) is in fact the first-order term of the 'exact' $H' = P_0 PHPP_0 = P_0[H_0 + V + V(1-P_0)V/(E - H_0) + \ ]P_0$ where V is the hopping interblocks. See [5] for a more detailed analysis.

‡ Novak and Zhang [8] rediscovered this symmetry.

§ By definition the seniority is the number of unpaired particles on a site. The generalization to a solid leads to a slightly different picture because $Z^-|\psi\rangle = 0$, for example, does not imply necessarily that there are not paired particles in a many-body state $|\psi\rangle$ (in the one-band Hubbard model paired particles means a double-occupied site). See [9] and references therein.

where $S^+ = \Sigma_i c_{i\uparrow}^+ c_{i\downarrow}$. The spectrum of $Z^- Z^+$ was obtained by Nowak [9]. For a fixed S_z and $N_e \leqslant N_s$ the eigenvalues of $Z^- Z^+$ are

$$\theta_k = (k+1)(N_s - N_e + k) \qquad k = 0, 1, \ldots, [\tfrac{1}{2}N_e - |S_z|].$$

We restrict our analysis to a fixed-filling N_0, and then we choose the two following states in each block:

$$\begin{aligned} &|N_e = N_0 - 1,\ S = S_1,\ S_z = S_{z_1},\ \Gamma_1,\ E_1\rangle_\alpha \equiv |0'\rangle_\alpha \\ &|N_e = N_0,\ S_z = S_{z_1} - \tfrac{1}{2},\ \theta_k, \Gamma_2,\ E_2\rangle_\alpha \equiv |\downarrow'\rangle_\alpha = c_{\alpha\downarrow}'^+ |0'\rangle_\alpha \end{aligned} \tag{6a}$$

where the total spin S_1, quasi-spin θ_k (seniority), and the spatial symmetries are not yet fixed. The energies E_1, E_2, will be the lower energies of $H_u + H_t$ compatible to the last choice of the symmetries. It seems natural to define two other states as

$$\begin{aligned} &Z_\alpha^+ |0'\rangle_\alpha = |\downarrow\uparrow'\rangle_\alpha = c_{\alpha\downarrow}'^+ c_{\alpha\uparrow}'^+ |0'\rangle_\alpha \\ &S_\alpha^+ |\downarrow'\rangle_\alpha = |\uparrow'\rangle_\alpha = c_{\alpha\uparrow}'^+ |0'\rangle_\alpha \end{aligned} \tag{6b}$$

in order to obtain a formal analogy to the one-electron states.

4. Renormalizing parameters

Let us rewrite (1) as

$$H = \sum_\alpha H_{0\alpha} + \sum_{\alpha\beta} V_{\alpha\beta} = H_0 + V$$

here H_0 is the intrablock Hamiltonian and $V_{\alpha\beta}$ is the hopping term between nearest-neighbour blocks α and β (see figure 1 for an example). What we want is to establish a correspondence like

$$P_0 H_0 P_0 \to H_u' + H_\mu' + K' \tag{7a}$$

$$P_0 V P_0 \to H_t'. \tag{7b}$$

For the (7a) part it is straightforward to get

$$P_0 H_0 P_0 = U' \sum_\alpha n_{\alpha\downarrow}' n_{\alpha\uparrow}' - \mu' \sum_{\alpha\sigma} n_{\alpha\sigma}' + \sum_\alpha K_\alpha' \tag{8}$$

where

$$U' = 2(E_1 - E_2) + U \qquad \mu' = E_1 - E_2 + \mu \qquad K_\alpha' = E_1 - (N_0 - 1)\mu.$$

The kinetic term, $P_0 V P_0$, does not transform so clearly. First it is interesting to write the $c_{i\sigma}$ operators in a more appealing way,

$$c_{i\sigma} = |0\rangle_{ii}\langle\sigma| + \mathrm{sgn}(-\sigma)|\sigma\rangle_{ii}\langle\downarrow\uparrow| = c_{i\sigma}(1 - n_{i-\sigma}) + c_{i\sigma} n_{i-\sigma} \tag{9}$$

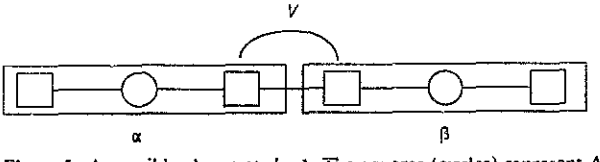

Figure 1. A possible choice at $d = 1$. The squares (circles) represent A (B) sites. V is the hopping between nearest-neighbours blocks α and β.

and then assuming a natural definition of the operators on the border of the block in the subspace spanned by the $|0'\rangle_\alpha$, $|\downarrow'\rangle_\alpha$, ...

$$c_{i\sigma}(\alpha) = r_{i\alpha,\alpha} c'_{\alpha\sigma}(1 - n'_{\alpha-\sigma}) + v_{i_\alpha\,\sigma} c'_{\alpha\sigma} n'_{\alpha-\sigma}. \tag{10}$$

Where the $r_{i_\alpha,\sigma}$ and $v_{i_\alpha,\sigma}$ are real numbers,

$$\begin{aligned} r_{i_\alpha\,\sigma} &= {}_\alpha\langle 0'|c_{i\sigma}(\alpha)|\sigma'\rangle_\alpha = r^*_{i_\alpha,\sigma} \\ v_{i_\alpha\,\sigma} &= \mathrm{sgn}(-\sigma)\ {}_\alpha\langle -\sigma'|c_{i\sigma}(\alpha)|\downarrow\uparrow'\rangle_\alpha = v^*_{i_\alpha\,\sigma} \end{aligned} \tag{11}$$

the other matrix elements vanish

We can then write (7*b*) more explicitly by using (10)

$$\begin{aligned} P_0 V P_0 = \sum_{\sigma,i_\alpha,i_\beta,(\alpha,\beta)} & [(r_{i_\alpha\,\sigma} r_{i_\beta,\sigma} - r_{i_\alpha,\sigma} v_{i_\beta\,\sigma} - v_{i_\alpha\,\sigma} r_{i_\beta\,\sigma} + v_{i_\alpha\,\sigma} v_{i_\beta\,\sigma}) n'_{\sigma,-\sigma} n'_{\beta\ \sigma} \\ & + (v_{i_\alpha\,\sigma} r_{i_\beta\,\sigma} - r_{i_\alpha\,\sigma} r_{i_\beta\,\sigma}) n'_{\alpha\,-\sigma} + (r_{i_\alpha\,\sigma} v_{i_\beta\,\sigma} - r_{i_\alpha,\sigma} r_{i_\beta\,\sigma}) n'_{\beta\,-\sigma} + r_{i_\alpha\,\sigma} r_{i_\beta\,\sigma}] c'^{+}_{\alpha\sigma} c'_{\beta\sigma} \end{aligned} \tag{12}$$

It is clear that the three parentheses in the rhs of (12) must cancel to get a hopping part without spurious terms We now try to obtain the $r_{i_\alpha\,\sigma}$ and $v_{i_\alpha,\sigma}$ factors in our model First it is useful to write some commutators,

$$[Z^+, c_{i\downarrow}] = -\nu_i c^+_{i\uparrow} \tag{13a}$$

$$[Z^+, c_{i\uparrow}] = \nu_i c^+_{i\downarrow} \tag{13b}$$

$$[S^+, c_{i\uparrow}] = -c_{i\downarrow} \tag{13c}$$

$$[S^+, c^+_{i\downarrow}] = c^+_{i\uparrow} \tag{13d}$$

which can be easily specified for a block. We calculate the matrix element of (13*a*) (bearing in mind that we treat the operators in the block) between $|0'\rangle_\alpha$ and $|\uparrow'\rangle_\alpha$, using the definitions (6) we obtain

$${}_\alpha\langle\uparrow'|c_{i\downarrow}|\downarrow\uparrow'\rangle_\alpha = {}_\alpha\langle\uparrow'|Z^+_\alpha c_{i\downarrow}|0'\rangle_\alpha + \nu_{i_\alpha\,\alpha}\langle\uparrow'|c^+_{i\uparrow}|0'\rangle_\alpha \tag{14a}$$

We repeat the process with (13*b*), (13*c*) and (13*d*)

$${}_\alpha\langle\downarrow'|c_{i\uparrow}|\downarrow\uparrow'\rangle_\alpha = {}_\alpha\langle\downarrow'|Z^-_\alpha c_{i\uparrow}|0'\rangle_\alpha - \nu_{i_\alpha\,\alpha}\langle\downarrow'|c^+_{i\downarrow}|0'\rangle_\alpha \tag{14b}$$

$${}_\alpha\langle 0'|c_{i\downarrow}|\downarrow'\rangle_\alpha = -{}_\alpha\langle 0'|S^+_\alpha c_{i\uparrow}|0'\rangle_\alpha + {}_\alpha\langle 0'|c_{i\uparrow}|\uparrow'\rangle_\alpha \tag{14c}$$

$${}_\alpha\langle\downarrow'|c_{i\downarrow}|0'\rangle_\alpha = {}_\alpha\langle\uparrow'|c^-_{i\downarrow}S^-_\alpha|0'\rangle_\alpha + {}_\alpha\langle\uparrow'|c^+_{i\uparrow}|0'\rangle_\alpha. \tag{14d}$$

It should be noted that for a single site we have ${}_i\langle 0|c_{i\downarrow}|\downarrow\rangle_i = {}_i\langle 0|c_{i\uparrow}|\uparrow\rangle_i = -{}_i\langle\downarrow|c_{i\uparrow}|\downarrow\uparrow\rangle_i$ and so on In order to obtain an almost fermionic behaviour we now require $|0'\rangle_\alpha$, $|\sigma'\rangle_\alpha$, $|\downarrow\uparrow'\rangle_\alpha$ to satisfy

$$Z^-_\alpha|\sigma'\rangle_\alpha = 0 \tag{15a}$$

$$S^-_\alpha(|0'\rangle_\alpha, |\downarrow\uparrow'\rangle_\alpha) = 0 \tag{15b}$$

Equation (15*a*) implies the choice of $\theta_k = \theta_{k=0} = N_s - N_e$, and for (15*b*) we have to choose $S = 0$, that is, N_0 must be odd† The expression (12) may now be simplified

† It is easy to see that if $[Z^-Z^+, Z^-] = 2Z^-Z_3 \Rightarrow Z^-|\lambda, \theta_k\rangle \propto |\lambda, \theta'_k\rangle$ where $\theta'_k = \theta_k + N_e - N_s$ If we restrain the study to the case $N_s \geq N_e$ then $\theta_k \geq 0$ If we choose $\theta_{k=0} = N_s - N_e$ then $\theta'_k = 0$. This is only possible for $N_e = N_s$ but $N'_e = N_e - 2$ and by hypothesis was $N_e \leq N_s$, therefore $N'_e \leq N_e - 2$ It is impossible then to arrive to zero eigenvalue for θ'_k so $Z^-|\sigma'\rangle_\alpha$ must cancel For the spin case it is obvious that (15*b*) implies $s = 0$.

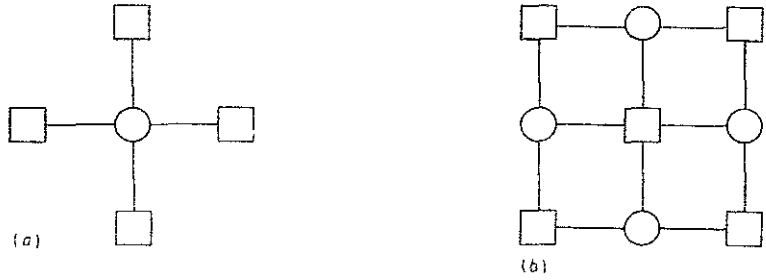

Figure 2 The two suitable block choices in a square lattice (*a*) There are only A-sites on the border and we obtain a one-dimensional-like behaviour (*b*) In this case we find two types of sites on the border

if we put $r_{i_\alpha\sigma} = \lambda_{i_\alpha}$, $v_{i_\alpha\sigma} = \nu_{i_\alpha}\lambda_{i_\alpha}$.

$$P_0VP_0 = \sum_{\sigma i_\alpha i_\beta,(\alpha\beta)} \lambda_{i_\alpha}\lambda_{i_\beta}[(1-\nu_{i_\beta}-\nu_{i_\alpha}+\nu_{i_\alpha}\nu_{i_\beta})n'_{\alpha-\sigma}n'_{\beta-\sigma} + (\nu_{i_\alpha}-1)n'_{\alpha-\sigma} + (\nu_{i_\beta}-1)n'_{\beta,-\sigma}+1]c'^{+}_{\alpha\sigma}c'_{\beta\sigma} \tag{16}$$

From (16) it is easier to analyse the different cases.

5. One-dimensional case

We can make two different choices for the blocks, with an even or odd number of sites. For each of these blocks we have one site on the border. In the odd case the border sites in the same block (see figure 1) are always of the same type, i.e. A-sites, so we can put $\nu_{i_\alpha} = \nu_{i_\beta} = 1$, and the resulting renormalized hopping is like the original one. In the even case there are two different types of site on the border, and we obtain

$$P_0VP_0 = \sum_{(\alpha\beta),\sigma} (-2n'_{\beta-\sigma}+1)c'^{+}_{\alpha\sigma}c'_{\beta\sigma} \tag{17}$$

6. Two-dimensional case

There are two possible choices of blocks (see figure 2) to prevent proliferation terms. In the five-site blocks (figure 2(*a*)) all the border sites are of the same type, i.e. A-sites. We therefore obtain the same behaviour as in the one-dimensional case. The block of nine sites (figure 2(*b*)) has, however, two types of sites on the border, but it is not difficult to eliminate the hopping between the B-sites if we choose a suitable spatial symmetry for the $|\sigma'\rangle_\alpha$s, so that

$$_\alpha\langle 0'|c_{i\sigma}(B)|\sigma'\rangle_\alpha = 0. \tag{18}$$

The Hamiltonian (1) is invariant under C_{2v} [10] and if we use the A_2 irreducible representation for the $|\sigma'\rangle_\alpha$s and A_1 for the $|0'\rangle_\alpha$, $|{\downarrow\uparrow}'\rangle_\alpha$ we obtain (18)

7. Three-dimensional case

Now, it is not possible to have several sizes of blocks as in one dimension, or to draw two different shapes as in two dimensions. If we want to preserve the number of

Hamiltonian parameters in the H' and at the same time to pave completely a cubic lattice, we have only one possible block choice: a cube of $3^3 = 27$ sites. H is invariant in three dimensions under the D_{2h} group, and as in the two-dimensional case it is possible to choose the completely symmetric irreducible representation of D_{2h} for the $|0'\rangle_\alpha$, $|\downarrow\uparrow'\rangle_\alpha$ and the antisymmetric representation under plane reflexions for the $|\sigma'\rangle_\alpha$s to obtain condition (18).

8. Conclusion

We have analysed the RSRG block method in the one-band Hubbard model. We have found the conditions under which the process is exact. The expression is exact here, makes no reference to an analytical or numerical result but, instead, there is a formal analogy between the original Hamiltonian and the renormalized one. We have shown how to apply the method to $d = 1, 2, 3$ systems. Particularly in the one-dimensional case we have solved exactly the question of parity of the number of sites in each block [5–7].

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