Quantum Renormalization Group

for

1 Dimensional Fermion Systems :

a Modified Scheme

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Abstract

Inspired by the superblock method of White, we introduce a simple modification of the standard Renormalization Group (RG) technique for the study of quantum lattice systems. Our method which takes into account the effect of Boundary Conditions (BC), may be regarded as a simple way for obtaining first estimates of many properties of quantum lattice systems. By applying this method to the 1-dimensional free and interacting fermion system, we obtain the ground state energy with much higher accuracy than the standard RG. We also calculate the density-density correlation function in the free-fermion case which shows good agreement with the exact result.

PACS : 71.10.Fd, 71.10.Pm, 05.30.Fk

Keywords : Quantum renormalization group, Fermion systems.

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1 Introduction

In spite of the enormous recent interest in correlated fermion systems, it still remains a challenging task to solve the interacting many fermion problem. Due to the difficulty of obtaining exact solutions, one often looks for a reasonably good approximation scheme for solving such problems. However each approximation scheme has its own limits and drawbacks. Mean-field methods neglect the effects of fluctuations to a great extent; the perturbative methods, on the other hand, do not work over the whole range of the parameter space. Among the other methods a real space renormalization group (RG) technique [1-7], often referred to as the block RG, seems to be promising in this respect. This relatively simple method includes some effects of fluctuations and also works over the whole regime of the parameter space. But the approximation involved in this scheme affects sometimes seriously the renormalization of the parameters (especially the off-diagonal ones like the single particle hopping amplitude). This, in turn, restricts the reliability of the numerical results produced by this method.

As far as the calculation of ground state energy is concerned, the main difficulty of the method is the fact that by fixing a particular Boundary Conditions (BC) on a block one may lose a number of states which contribute to the ground state of the whole lattice. This point is clearly highlighted in 1D Tight Binding model in which the standard RG fails for some type of BCs [8,9,10]. It must be noticed that this difficulty is not removed by increasing the size of blocks.

In 1992 White [11] succeeded in greatly improving the efficiency of the RG method by inventing the Density Matrix Renormalization Group (DMRG) scheme. In this approach, one embeds each block into a larger (super) block and considers the block as a quantum
system in interaction with a reservoir (the rest of the superblock). The block can then be described by a reduced density matrix, whose eigenkets with the highest eigenvalues are used to construct the embedding operator \( (T) \) (see [12] and references therein), which is the mathematical artifact which reduces the dimension of the Hilbert space in each step of RG. Although DMRG gives very accurate results compared with previous simple RG schemes, its practical implementation is much more difficult and time consuming.

Regarding the fermion systems an improved scheme to the standard RG was also proposed for free-fermion systems [13] which converges to the exact results of the ground state energy faster than the standard RG, but was not applied to interacting systems.

In this paper we apply a modification of the standard RG scheme to a one dimensional interacting fermion system and obtain the ground state of the system with much higher accuracy compared with the standard RG [14]. For free-fermion model, our prescription yields much closer results to the exact values compared with those obtained from the standard RG and those obtained in Ref.[13], we also obtain the density-density correlation function, which is in a rather good agreement with the exact one.

Our method, although does not yield as much accuracy as in DMRG, is much simpler practically, so that one can easily implement it on a personal computer. The required time is less than one second for a Pentium machine. The results are compared in table-1, table-2 and Fig.3.
2 The Model

We will consider the following 1D Hamiltonian, for spinless fermions

\[ H = t \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + G \sum_i (n_in_{i+1}) - \mu \sum_i n_i, \]

(1)

where \( c_i^\dagger \) and \( c_i \) are the usual creation and annihilation fermion operators on the \( i \)-th site and \( n_i = c_i^\dagger c_i \) is the fermion number operator. When \( G = 0 \) (free fermion case), \( t \) represents the hopping parameter and \( \mu \) is the site energy while \( G \) is a positive electron-electron repulsion between electrons on neighbouring sites. We will consider the electron-hole symmetric case where there is an average of \( \frac{1}{2} \) electron per sites (half-filled case). In this case the Fermi energy \( \mu \) is conveniently taken equal to \( G \) and, adding a constant, the Hamiltonian is rewritten as follows

\[ H = t \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + G \sum_i (n_i - \frac{1}{2})(n_{i+1} - \frac{1}{2}). \]

(2)

It is clear that the two terms in (2) play opposite roles. We can distinguish two different regimes : (i) when \( \frac{G}{2t} < 1 \) the system is conducting and \( < n_i > = \frac{1}{2} \) on each site and (ii) when \( \frac{G}{2t} > 1 \) the system organizes itself in two sub-lattices \( A \) and \( B \) such that \( < n_i > \approx 0, i \in A \) and \( < n_i > \approx 1, i \in B \).

Our aim is to calculate the ground state energy of this fermionic system in the conducting regime using a modified RG prescription. In section (3) we apply the method to free-fermions \( (G = 0) \) and in section (4) we will consider the interacting case \( (G \neq 0) \).
3 Modified RG for Free-Fermions

In the free-fermion case the Hamiltonian will reduce to the following simple form

\[ H = t \sum_i (c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) , \]  

(3)

where the hopping parameter \( t \) is the only one that will be renormalized.

The decomposition of the lattice into isolated blocks and superblocks with an odd number of sites per each block is shown in Fig.1. In this case the size of blocks \( n_B \) and superblocks \( n_{SB} \) are taken to be 3 and 5 respectively for simplicity. Therefore the block Hamiltonian \( h^B \) and the superblock Hamiltonian \( h^{SB} \) are

\[ h^B = t(c_3^\dagger c_3 + c_4^\dagger c_4 + c_5^\dagger c_5) , \]  

(4)

\[ h^{SB} = t(c_2^\dagger c_2 + c_1^\dagger c_1) + h^B + t(c_5^\dagger c_5 + c_4^\dagger c_4) . \]  

(5)

We express our prescription in the following steps:

**step-1)** The superblock Hamiltonian \( h^{SB} \) is diagonalized exactly. The doubly degenerate ground state is in the subspaces of particle number \( \nu = 2 \) and 3,

\[ h^{SB}|\nu = 2(3)\rangle_{SB} = \varepsilon^{SB}_o(t)|\nu = 2(3)\rangle_{SB} , \]  

(6)

where

\[ \varepsilon^{SB}_o(t) = (-2.73246)t , \]

is the ground state energy of the 5 sites superblock. Note that the structure of the low lying levels of the superblock depends strongly on the parity of \( n_{SB} \). For \( n_{SB} \) even, the ground state is a singlet corresponding to the ground state of the subspace \( \nu = \frac{n_{SB}}{2} \), while for \( n_{SB} \)
odd the ground state is a doublet corresponding to the electron-hole degenerate ground state of the two subspaces $\nu = \frac{n_{SB} + 1}{2}$. Here it is essential to restrict ourselves to the case $n_{SB}$ odd, if we want, by keeping only two levels that the Hamiltonian conserves its initial form.

**step-2** In this step in view of the half-filled property of the system we project the degenerate ground state of the superblock ($|\nu = 2(3)\rangle_{SB}$) onto the $\nu = 1$ and 2 subspaces of the block Hilbert space respectively. *It is this step which effectively smoothes out the sharp effect of the boundary conditions by immersing the block into a superblock, i.e. the projected state is not restricted by any particular boundary conditions of an isolated block (open, periodic,...), as compared with the standard RG, but takes into account to some extent the quantum fluctuation of the rest of the lattice.* Moreover by emphasizing the half-filled property, our RG prescription leads to a form-invariant Hamiltonian. The resulting normalized state of this projection is named $|\nu = 1(2)\rangle_B$.

**step-3** The embedding operator is now constructed in the following form

$$ T_I = (|\nu = 1\rangle_B\langle 0|) + (|\nu = 2\rangle_B\langle 1|) , $$

(7)

where $|0\rangle$ and $|1\rangle$ are the renamed base kets of the effective Hamiltonian Hilbert space.

Having the form of the embedding operator, one can calculate the projection of any operator onto the effective Hilbert space [12], (labelling the sites in the block 1, 2, 3 from left to right) we will have

$$ T_I^\dagger c_{ji} T_I = \lambda c_I' \quad j = 1, 3 , $$

$$ T_I^\dagger c_{ji}^\dagger T_I = \lambda c_I'^\dagger \quad j = 1, 3 , $$

(8)
where \( c_{I}^{'} \) and \( c_{J}^{'} \) act as fermion operators in the new Hilbert space, and

\[
\lambda^2 = 0.47999 ,
\]

(a similar equation for \( j = 2 \) can be obtained, but this is not required here).

Using Fig.2 and the labelling mentioned above for sites in each block, one writes the interaction between blocks in the following form

\[
h_{I,J}^{BB} = t(c_{3I}^{\dagger}c_{1J} + c_{1J}^{\dagger}c_{3I}) .
\]

(9)

Then the effective Hamiltonian between the new sites is

\[
h_{I,J}^{eff} = T_{J}^{\dagger}T_{I}^{\dagger}h_{I,J}^{BB}T_{I}T_{J} ,
\]

(10)

where I and J are two neighbouring blocks, while \( T_{I} \) and \( T_{J} \) are their corresponding embedding operators. This leads to

\[
h_{I,J}^{eff} = t'(c_{I}^{\dagger}c_{J}^{'} + c_{J}^{\dagger}c_{I}^{'}),
\]

(11)

where

\[
t' = \lambda^2 t ,
\]

(12)

and \( c_{I(J)}^{'} \) and \( c_{I(J)}^{\dagger} \) are fermion operators for the new sites. This equation determines the renormalization of the coupling constant.

**step-4)** The crudest estimate for the ground state energy is just the sum of ground state energies of all the blocks or superblocks. Thus,

\[
\left( \frac{E}{N} \right)^{(0)} = \frac{1}{5} \xi^{SB}_{o}(t) ,
\]

(13)
or

\[
\left( \frac{E}{N} \right)^{(0)} = \frac{1}{3} \varepsilon_o^B (t) ,
\]

where \( \left( \frac{E}{N} \right)^{(0)} \) is the ground state energy per site of the whole system in the zeroth order approximation. Eq. (14) in fact defines \( \varepsilon_o^B \) as

\[
\varepsilon_o^B = \frac{3}{5} \varepsilon_o^{SB} .
\]

However this estimate clearly neglects the contribution to the energy from interaction between blocks. To take this missing contribution into account, we add to \( \left( \frac{E}{N} \right)^{(0)} \) the ground state energy of the new lattice, and obtain

\[
\left( \frac{E}{N} \right)^{(1)} = \frac{1}{3} \varepsilon_o^B (t) + \frac{1}{9} \varepsilon_o^B (t') .
\]

Iterating this procedure we finally obtain

\[
\frac{E}{N} = \sum_{n=0}^{\infty} \frac{1}{3^{n+1}} \varepsilon_o^B (t^{(n)}) ,
\]

or

\[
\frac{E}{N} = \sum_{n=0}^{\infty} \frac{1}{3^{n+1}} \left( \frac{3}{5} \varepsilon_o^{SB} (t^{(n)}) \right) ,
\]

where \( t^{(0)} = t \) and \( t^{(n)} \) is the renormalized coupling constant after \( n \) steps of RG. In fact, the above argument describes the physical interpretation of the formal limiting process defined in [12] in which the ground state energy is obtained as

\[
E = \lim_{n \to \infty} T^{+n} H T^n .
\]

However in the standard RG the term \( \varepsilon_o^B (t) \) is the result of diagonalization of \( h^B \), i.e.,

\[
T^+ h^B T = \varepsilon_o^B ,
\]

whereas in our method \( \varepsilon_o^B \) is just another expression for \( \frac{n_0}{n_{SB}} \varepsilon_o^{SB} \) where \( \varepsilon_o^{SB} \)
is the eigenvalue of $h^{SB}$. The results for the ground state energy per site, obtained by this modified RG method are collected in table-1. The results are compared both with the exact results and with those obtained from the standard RG [14]. It is seen that our modified RG scheme yields closer results to the exact one than the standard RG method.

We would like to comment on the non-variational nature of our results. This is caused by our crude estimate for the ground state energy of each block in terms of that of the superblock ($e_o^B = \frac{3}{5} e_o^{SB}$). However one should note that this behaviour is not unusual in RG treatment of lattice systems. For example in standard RG at second order perturbation of free-fermion model [2] and isotropic Heisenberg model [16], one obtains non-variational results. We have also obtained the ground state energy in this case for other $\frac{n_B}{n_{SB}}$ ratios, namely for the ratios $\frac{5}{7}$, $\frac{7}{9}$, $\frac{9}{11}$ and $\frac{11}{13}$; the results are collected in table-1. Note that our results in these cases are above the exact values of ground state energy. This indicates that the non-variational result in the $\frac{3}{5}$ case is due to the very small block and superblock sizes. Therefore we expect that when the sizes of block and superblock are not very small, our method must indeed reproduces the variational results. Our data in table-1 show more accuracy compared with the standard RG results for any values of the block size. These data also show that the result converges to the exact one by increasing the $\frac{n_B}{n_{SB}}$ ratios.

To have a better insight about the effective Hamiltonian obtained by this modified RG, one can look at the nature of the constructed wavefunction. In this respect we compute the density-density correlation function ($\langle n_i n_{i+r} \rangle$) in terms of the distance $r$. In order to do so by our RG prescription with a block size of $n_B = 3$, we consider a chain of length $3^N$ and let $N$ go to infinity. In this calculation the ground state of the whole system $|0\rangle$
is replaced by $T|0\rangle$ where $|0\rangle$ is the ground state of the effective Hilbert space. Then we compute $g(r) = \langle n_in_{i+r} \rangle$ for any value of $r$. Our results are plotted in Fig.3 and compared with the exact results [17]. Our results show a very good qualitative agreement with the exact results while the differences in the small $r$ is due to the finite size effect of the exact results as mentioned in ref [17]. Although this good agreement is not specifically due to our prescription and it can be obtained from other different schemes [2][3][4], this shows that the nature of the constructed wavefunction does not change in our scheme and the obtained effective Hamiltonian is a good approximate one.

4 Interacting Fermion system

The system under consideration is an interacting fermion system with the Hamiltonian defined in (2). Our RG prescription in this case is the same as in the free-fermion case. With $n_B = 3$ and $n_{SB} = 5$ the block and superblock Hamiltonians are (see Fig.1)

$$h_B = t(c_2^\dagger c_3 + c_3^\dagger c_2 + c_3^\dagger c_4 + c_4^\dagger c_3) + G(n_2 - \frac{1}{2})(n_3 - \frac{1}{2}) + G(n_3 - \frac{1}{2})(n_4 - \frac{1}{2}) , \quad (19)$$

$$h^{SB} = t(c_1^\dagger c_2 + c_2^\dagger c_1) + G(n_1 - \frac{1}{2})(n_2 - \frac{1}{2}) + h^B + t(c_4^\dagger c_5 + c_5^\dagger c_4) + G(n_4 - \frac{1}{2})(n_5 - \frac{1}{2}) , \quad (20)$$

Following the first three steps of our RG prescription we arrive at the effective operators

$$T_i^\dagger c_j T_i = \eta c_i^\prime \quad j = 1, 3 , \quad (21)$$

where $\eta$ is calculated to be

$$\eta = \frac{2\alpha \beta}{2\alpha^2 + \beta^2} . \quad (22)$$
Here

\[
\alpha = \varepsilon^4 + (1 - g^2)\varepsilon^2 + g\varepsilon - 2 ,
\]

\[
\beta = 2(\varepsilon - g)(2\varepsilon^2 + g\varepsilon - 2) ,
\]

\[
\varepsilon = \frac{1}{t}\varepsilon^o_{SB}(t, G) , \quad g = \frac{G}{2t} ,
\]

and as before \(\varepsilon^o_{SB}(t, G)\) is the ground state energy of \(h^{SB}\) which is some function of \(t\) and \(G\).

Following Fig.2 the interaction between blocks I and J is

\[
h^{BB}_{I,J} = t(c_1^{\dagger}c_1 + c_3^{\dagger}c_3 + G(n_3 - \frac{1}{2})(n_1 - \frac{1}{2})) .
\]  

(24)

Then the interaction between the new sites is given by

\[
h^{eff}_{I,J} = T_J^\dagger T_I^\dagger h^{BB}_{I,J} T_I T_J ,
\]

(25)

where \(T_I\) and \(T_J\) are the embedding operators of blocks I and J. In this way we arrive at

\[
h^{eff}_{I,J} = t'(c_1^{\dagger}c_1 + c_3^{\dagger}c_3 + G'(n_1 - \frac{1}{2})(n_1 - \frac{1}{2})) ,
\]

(26)

where \(t'\) and \(G'\) are the renormalized coupling constants given by

\[
t' = \eta^2 t ,
\]

\[
G' = \gamma^2 G ,
\]

(27)

and

\[
\gamma = \frac{\beta^2}{2\alpha^2 + \beta^2} .
\]

(28)

After performing step-4 in the preceding section the ground state energy of interacting fermion system will be obtained which is given in table-2. These data clearly show that
the modified RG method yields much better results than the standard RG method. The non-variational nature of these results is due to the same reason which was described in the free-fermion case. Moreover, these results will be variational, if one takes larger $n_B$ and $n_{SB}$.

5 Conclusions

In this letter we have introduced a version of RG scheme and applied it to the free and interacting fermion systems. In this modified scheme, we can take care of the effect of boundary conditions in a simple way. We have calculated the ground state energy of the free and interacting fermion model for different values of the block size. All of these results show more accuracy than the standard RG and one can see the convergence of these results to the exact ones. In the free case we have also calculated the density-density correlation function whose good agreement with the exact results verifies that the renormalized Hamiltonian is a good approximate Hamiltonian for the low energy spectrum of the original one. Using the renormalization of any operator, one can also compute the correlation function for any value of $g (= \frac{G}{2t})$ in the interacting case. This method can also be applied to spin systems [18]. One may hope that for a first estimate of many properties of these systems, our method or its improvements (or adaptation for other lattice systems) would give quite good results. In those cases where application of the more sophisticated DMRG method seems to be hopeless, like the two dimensional Heisenberg Anti-ferromagnet, we hope our method to give good approximate results. Work in this direction is in progress.
6 Acknowledgement

A. L. would like to thank M. R. Rahimi-Tabar for useful discussions, A. Shojaie for his useful comments on numerical computations, N. Heydari, A. Mostafazadeh for careful study of the manuscript and Mrs. M. Shafaati for her help in editing the manuscript.
References

[1] K. G. Wilson, Rev. Mod. Phys. 47 (1975) 773.

[2] P. Pfeuty, R. Jullien and K. L. Penson in : Real-Space Renormalization , eds.T. W. Burkhardt and J. M. J. van Leeuwen (Springer, Berlin, 1982) ch.5.

[3] J. E. Hirsch, Phys. Rev. B 22 (1980) 5259.

[4] C. Dasgupta and P. Pfeuty, J. Phys. C 14 (1981) 717.

[5] B. Bhattacharyya and S. Sil, Phys. Lett. A 180 (1993) 299; J. Phys. Cond. Matt. 7 (1995) 6663; B. Bhattacharyya and G. K. Roy, J. Phys. Cond. Matt. 7 (1995) 5537.

[6] J. Perez-Conde and P. Pfeuty, Phys. Rev. B 47 (1993) 856.

[7] J. Yi, L. Zhang and G. S. Canright, Phys. Rev. B 49 (1994) 15920.

[8] S. R. White and R. M. Noak, Phys. Rev. Lett. 68 (1992) 3487.

[9] M. A. Martin-Delgado and G. Sierra, Phys. Lett. B364 (1995) 41.

[10] M. A. Martin-Delgado, J. Rodriguez-Laguna and G. Sierra, Nucl. Phys. B473 (1996) 685.

[11] S. R. White, Phys. Rev. Lett. 69 (1992) 2863; S. R. White, Phys. Rev. B48 (1993) 10345.

[12] M. A. Martin-Delgado and G. Sierra, Int. J. Mod. Phys. A11 (1996) 3145, J. Gonzalez, M. A. Martin-Delgado, G. Sierra, A. H. Vozmediano in : Quantum Electron Liquids and
High-$T_c$ Superconductivity, Lecture Notes in Physics, Monographs. Vol 38 (Springer, Berlin, 1995) ch.11.

[13] B. Bhattacharyya and S. Sil, Phys. Lett. A 210 (1996) 129.

[14] G. Spronken, R. Jullien and M. Avignon, Phys. Rev. B 24 (1981) 5356.

[15] H. Bethe, Z. Physik 71 (1931) 205; R. Orbach, phys. Rev. 112 (1958) 309.

[16] M. A. Martin-Delgado, Proceedings of the El Escorial Summer School 1996 on Strongly Correlated Magnetic and Superconducting Systems; cond-mat/9610196.

[17] U. Busch and K. A. Penson, Phys. Rev. B36 (1987) 9271.

[18] V. Karimipour and A. Langari, ”A Modified Quantum Renormalization Group for the $xxz$ Spin Chain”, IPM-96-167; cond-mat/9611057.
**Figure Captions:**

**Fig.1)** Block and Super Block for the lattice chain.

**Fig.2)** The decomposition of the lattice into isolated blocks and the consideration of neglected bonds as the effective interactions in the new Hilbert space.

**Fig.3)** Density-density correlation function $g(r)$ versus separation $r = j - i$ between sites $i$ and $j$ for free-fermion chain.
Tables

Table-1.Ground state energy per site of standard RG, exact results and modified RG for an infinite free-fermion chain for different values of block size.

| Type of SB and B | Exact result ($-\frac{2}{\pi}$) | Standard RG | Modified RG | TSB = 5, nB = 3 |
|------------------|-------------------------------|-------------|-------------|----------------|
| $n_B = 3$        | $-0.63662$                   | $-0.565686$ | $-0.65058$  | $n_B = 3$      |
|                  |                               |             |             | $n_B = 5$      |
| $n_B = 5$         | $-0.5854$                   | $-0.62256$  |             | $n_B = 7$      |
| $n_B = 7$         | $-0.5966$                   | $-0.6193$   |             | $n_B = 9$      |
| $n_B = 9$         | $-0.6038$                   | $-0.6196$   |             | $n_B = 11$     |
| $n_B = 11$        | $-0.6088$                   | $-0.6206$   |             | $n_B = 13$     |

Table-2.Ground state energy per site of standard RG, exact results and modified RG for an infinite interacting fermion chain.

| $g (= \frac{G}{2\pi})$ | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 |
|-------------------------|-----|-----|-----|-----|-----|-----|
| $\left( \frac{E}{tN} \right)_{standard \, RG}$ | $-0.565686$ | $-0.584168$ | $-0.603266$ | $-0.623008$ | $-0.643424$ | $-0.664549$ |
| $\left( \frac{E}{tN} \right)_{exact}$ | $-0.636620$ | $-0.657384$ | $-0.679129$ | $-0.701826$ | $-0.725454$ | $-0.750000$ |
| $\left( \frac{E}{tN} \right)_{modified \, RG}$ | $-0.650583$ | $-0.671674$ | $-0.692069$ | $-0.714005$ | $-0.736275$ | $-0.758952$ |
Figure 1

Figure 2
