

Analytic Formulations of the Density Matrix Renormalization Group*

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Abstract

We present two new analytic formulations of the Density Matrix Renormalization Group Method. In these formulations we combine the block renormalization group (BRG) procedure with Variational and Fokker-Planck methods. The BRG method is used to reduce the lattice size while the latter are used to construct approximate target states to compute the block density matrix. We apply our DMRG methods to the Ising Model in a transverse field (ITF model) and compute several of its critical properties which are then compared with the old BRG results.

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1 Introduction

The Density Matrix Renormalization Group Method (DMRG) introduced by White [1] has arguably become the most powerful numerical tool to retrieve the essential features of interacting quantum Hamiltonians in 1D such as spin systems [1], [2] and fermion systems [3]. This method is a real-space renormalization group (RG) method which is specially well suited when dealing with zero temperature properties of many-body systems, a situation where the Quantum MonteCarlo methods happen to be particularly badly behaved as far as fermionic systems are concerned [4].

The origin of the density matrix RG method relies on the special treatment carried out by White and Noack [5] on the 1D tight-binding model, the lattice version of a single particle in a box. It was Wilson the first to point out the relevance of this simple model in understanding the sometimes bad numerical performance of the standard Block Renormalization Group (BRG) method. In reference [5] the authors proposed a method called Combination of Boundary Conditions (CBC) which performs extremely well as compared to the exact known solution of the model. Recently, we have clarified the role played by the boundary conditions in the real-space renormalization group method [6] by constructing a new analytical BRG-method which is able to give the exact ground state of the model and the correct $1/N^2$ -law for the energy of the first excited state in the large N (size)-limit.

The problem with the CBC method is the difficulty when trying to generalize it to interacting models. In [5] yet another method was presented called the Superblock Method which is the precursor of the density matrix RG method. The DMRG method is able to treat many-body problems as for example the 1D Heisenberg model of spin $S = 1$ [1], [2] which happens to be a non-integrable model.

In this paper we present two novel versions of the DMRG method based upon the Perturbative-Variational and Fokker-Planck approaches to quantum lattice Hamiltonians recently introduced in references [7] and [8] respectively. We arrived at these new methods by searching for an analytical formulation of the density matrix RG method. As it happens, the usual implementations of the DMRG method are intrinsically numerical for they rely on Wilson's procedure of enlarging the system size in his RG-treatment of the Kondo problem [9]. We find interesting to address the problem of constructing analytical extensions of the DMRG method for several reasons. Firstly, it is known that standard block RG methods proved to be useful when dealing with qualitative features of some important models such as the ITF model [10], Lattice Gauge Model [11], Heisenberg model [12], Hubbard model [13], etc. and we want to see how the DMRG method performs when compared to those analytical BRG treatments. To this purpose, we have applied our Variational and Fokker-Planck DMRG methods to the Ising model in a tranverse field (ITF model). There are more interesting models, but the ITF model is simple enough for a first application of these methods. As a matter of fact, it was Drell and the SLAC group [10] who started to apply the standard Block Renormalization Group method to study QCD and they used the ITF model as a test model. Later on in the 80's this BRG method has been also applied to the study of strongly correlated systems and its implications in High- T_c Superconductivity. Secondly, the DMRG method as it stands is also intrinsically one-dimensional and it is an open problem to find feasible numerical schemes to work with higher dimensional systems. As it happens, our Variational and Fokker-Planck DMRG methods are generalizable to dimension higher than one and we might consider them as a first attempt to solving this important extension of the DMRG method.

This paper is organized as follows. In Sect.2 we present a brief introduction to the Block Renormalization Group methods based upon the concept of the intertwiner operator T . This allow us to make a unified formulation of both the standard BRG methods and the new Density Matrix RG method according to our analytic formulation. In Sect.3 the Block RG-method is applied to the ITF model following the formulation of Sect.2 and several critical exponents are computed. In Sect.4 we present our new DMRG methods and apply them to compute the intertwiner operator and critical exponents for the ITF model. The results are compared with the old BRG results and we find that the density matrix methods perform better. Sect.5 is devoted to conclusions and prospectives.

2 Block Renormalization Group Methods (BRG): Brief Review

In this section the block renormalization group method is revisited and we present a new and unified reformulation of it based on the idea of the *intertwiner operator* T to be discussed below. This formulation will allow us to introduce the new Variational and Fokker-Planck DMRG methods on equal footing as the standard BRG method. For a more extensive account on this method we refer to [14] and chapter 11 of reference [15] and references therein.

The block RG-method is a real-space RG-method introduced and developed by the SLAC group [10]. Let us recall that Wilson developed his numerical real-space renormalization group procedure to solve the Kondo problem [9]. It was clear from the beginning that one could not hope to achieve the accuracy Wilson obtained for the Kondo problem when dealing with more complicated many-body quantum Hamiltonians as the ones mentioned in the introduction. The *key difference* is that in the Kondo model there exists a *recursion relation* for Hamiltonians at each step of the RG-elimination of degrees of freedom. Schematically,

$$H_{N+1} = H_N + \text{hopping boundary term} \quad (2.1)$$

$$H_{N+1} = R(H_N) \quad (2.2)$$

The existence of such recursion relation facilitates enormously the work, but as it happens it is specific of *impurity problems*.

From the numerical point of view, the Block Renormalization Group procedure proved to be not fully reliable in the past particularly in comparison with other numerical approaches, such as the Quantum MonteCarlo method which were being developed at the same time. This was one of the reasons why the BRG methods remained undeveloped during the '80's until the beginning of the '90's when they are making a comeback as one of the most powerful numerical tools when dealing with zero temperature properties of many-body systems.

Let us first summarize the main features of the real-space RG. The problem that one faces generically is that of diagonalizing a quantum lattice Hamiltonian H , i.e.,

$$H|\psi\rangle = E|\psi\rangle \quad (2.3)$$

where $|\psi\rangle$ is a state in the Hilbert space \mathcal{H} . If the lattice has N sites and there are k possible states per site then the dimension of \mathcal{H} is simply

$$\dim\mathcal{H} = k^N \quad (2.4)$$

As a matter of illustration we cite the following examples: $k = 4$ (Hubbard model), $k = 3$ (t-J model), $k = 2$ (Heisenberg model) etc.

When N is large enough the eigenvalue problem (2.3) is out of the capability of any human or computer means unless the model turns out to be integrable which only happens in some instances in $d = 1$.

These facts open the door to a variety of approximate methods among which the RG-approach, specially when combined with other techniques (e.g. numerical, variational etc.), is one of the most relevant. The main idea of the RG-method is the mode elimination or thinning of the degrees of freedom followed by an iteration which reduces the number of variables step by step until a more manageable situation is reached. These intuitive ideas give rise to a well defined mathematical description of the RG-approach to the low lying spectrum of quantum lattice hamiltonians.

To carry out the RG-program it will be useful to introduce the following objects:

- \mathcal{H} : Hilbert space of the original problem.

- \mathcal{H}' : Hilbert space of the effective degrees of freedom.
- H : Hamiltonian acting in \mathcal{H} .
- H' : Hamiltonian acting in \mathcal{H}' (effective Hamiltonian).
- T : embedding operator : $\mathcal{H}' \longrightarrow \mathcal{H}$
- T^\dagger :truncation operator : $\mathcal{H} \longrightarrow \mathcal{H}'$

The problem now is to relate H , H' and T . The criterium to accomplish this task is that H and H' have in common their low lying spectrum. An exact implementation of this is given by the following equation:

$$HT = TH' \quad (2.5)$$

which imply that if $\Psi'_{E'}$ is an eigenstate of H' then $T\Psi'_{E'}$ is an eigenstate of H with the same eigenvalue (unless it belongs to the kernel of T : $T\Psi'_{E'} = 0$), indeed,

$$HT\Psi'_{E'} = TH'\Psi'_{E'} = E'\Psi'_{E'} \quad (2.6)$$

To avoid the possibility that $T\Psi' = 0$ with $\Psi' \neq 0$, we shall impose on T the condition,

$$T^\dagger T = 1_{\mathcal{H}'} \quad (2.7)$$

such that

$$\Psi = T\Psi' \Rightarrow \Psi' = T^\dagger\Psi \quad (2.8)$$

Condition (2.7) thus establishes a one to one relation between \mathcal{H}' and $\text{Im}(T)$ in \mathcal{H} . Observe that Eq. (2.5) is nothing but the commutativity of the following diagram:

$$\begin{array}{ccc} \mathcal{H}' & \xrightarrow{T} & \mathcal{H} \\ H' \downarrow & & \downarrow H \\ \mathcal{H}' & \xrightarrow{T} & \mathcal{H} \end{array}$$

Eqs. (2.5) and (2.7) characterize what may be called exact renormalization group method (ERG) in the sense that the whole spectrum of H' is mapped onto a part (usually the bottom part) of the spectrum of H . In practical cases though the exact solution of Eqs. (2.5) and (2.7) is not possible so that one has to resort to approximations (see later on). Considering Eqs. (2.5) and (2.7) we can set up the effective Hamiltonian H' as:

$$H' = T^\dagger HT \quad (2.9)$$

This equation does not imply that the eigenvectors of H' are mapped onto eigenvectors of H . Notice that Eq.(2.9) together with (2.7) does not imply Eq. (2.5). This happens because the converse of Eq.(2.7), namely $TT^\dagger \neq 1_{\mathcal{H}}$ is not true, since otherwise this equation together with (2.7) would imply that the Hilbert spaces \mathcal{H} and \mathcal{H}' are isomorphic while on the other hand the truncation inherent to the RG method assumes that $\dim \mathcal{H}' \ll \dim \mathcal{H}$.

What Eq.(2.9) really implies is that the mean energy of H' for the states Ψ' of \mathcal{H}' coincides with the mean energy of H for those states of \mathcal{H} obtained through the embedding T , namely,

$$\langle \Psi' | H' | \Psi' \rangle = \langle T\Psi' | H | T\Psi' \rangle \quad (2.10)$$

In other words $T\Psi'$ is used as a variational state for the eigenstates of the Hamiltonian H . In particular T should be chosen in such a way that the states truncated in \mathcal{H} , which go down to \mathcal{H}' , are the ones expected to contribute the most to the ground state of H . Thus Eq. (2.9) is the basis of the so called variational renormalization group method (VRG)¹. As a matter of fact, the VRG method was the first one to be proposed. The ERG came afterwards as a perturbative extension of the former (see later on).

More generally, any operator \mathcal{O} acting in \mathcal{H} can be “pushed down” or renormalized to a new operator \mathcal{O}' which acts in \mathcal{H}' defined by the formula,

$$\mathcal{O}' = T^\dagger \mathcal{O} T \quad (2.11)$$

Notice that Eq.(2.9) is a particular case of this equation if choose O to be the Hamiltonian H .

In so far we have not made use of the all important concept of the block, but a practical implementation of the VRG or ERG methods does require it. The central role played by this concept makes all the real-space RG-methods to be block methods.

Once we have established the main features of the RG-program, there is quite freedom to implement specifically these fundamentals. We may classify this freedom in two aspects:

- The choice of how to reduce the size of the lattice.
- The choice of how many states to be retained in the truncation procedure.

We shall address the first aspect now. There are mainly two procedures to reduce the size of the lattice:

- by dividing the lattice into blocks with n_s sites each. This is the blocking method introduced by Kadanoff to treat spin lattice systems.
- by retrieving site by site of the lattice at each step of the RG-program. This is the procedure used by Wilson in his RG-treatment of the Kondo problem. This method is clearly more suitable when the lattice is one-dimensional.

We shall be dealing with the Kadanoff block methods mainly because they are well suited to perform analytical computations and because they are conceptually easy to be extended to higher dimensions. On the contrary, the DMRG method introduced by White [1] works with the Wilsonian numerical RG-procedure what makes it intrinsically one-dimensional and difficult to be generalized to more dimensions. Thus why we shall formulate our Variational and Fokker-Planck DMRG procedures as block renormalization methods in section 4.

Block RG-methods have recently received also renewed attention in one-dimensional problems in connection to what is called a *quantum group* symmetry [16]. Based upon this symmetry we have constructed a new BRG-method that we call q -RG which among other features it is able to predict the exact line of critical XXZ models in the Anisotropic Heisenberg model, unlike the standard BRG-method.

To exemplify the standard BRG-method we shall study a 1d-lattice Hamiltonian, the Ising model in a transverse field (ITF model). The main ideas are also valid in higher dimensions although computations are more involved. Hence we shall be dealing with a one-dimensional lattice, usually a periodic chain. In every site of the chain there are k degrees of freedom, hence:

$$\mathcal{H} = \mathcal{C}^k \otimes \dots \otimes \mathcal{C}^k := \otimes^N \mathcal{C}^k \quad (2.12)$$

We shall consider Hamiltonians H containing operators which involve only a single-site part H_S or two-nearest-neighbour-site part H_{SS} and will be symbolically depicted as in Fig.1, in such a way that,

¹The word variational here is used with a different meaning as in the introduction of this paper where it refers to the variational choice of the target state in the DMRG method to be discussed in section 4.

$$H = H_S + H_{SS} \quad (2.13)$$

As a matter of illustration, let us give one example of this decomposition in the ITF model which will turn out to be very useful in putting many key ideas to the test.

3 Block RG-Approach to the Ising Model in a Transverse Field (ITF)

The Ising Model in a Transverse Field is originally a one-dimensional quantum lattice system with quantum critical properties equal to the well-known thermal critical properties of the classical 2D-Ising Model. The lattice Hamiltonian of the ITF model is:

$$H_N(\Gamma, J) = -\Gamma \sum_{j=1}^N \sigma_j^x - J \sum_{j=1}^N \sigma_j^z \sigma_{j+1}^z \quad (3.14)$$

where σ_j^x and σ_j^z are the standard Pauli matrices acting at the j -th site of the chain.

The Hilbert space of states and the intrablock and interblock Hamiltonians for this model are, respectively:

$$\mathcal{H} = \otimes_1^N \mathcal{C}^2 \quad (3.15)$$

$$H_S = -\Gamma \sum_{j=1}^N \sigma_j^x \quad (3.16)$$

$$H_{SS} = -J \sum_{j=1}^N \sigma_j^z \sigma_{j+1}^z \quad (3.17)$$

The first step of the BRG method consists in assembling the set of lattice points into disconnected blocks of n_B sites each, as in Fig.2.

In this fashion there are a total of $N' = N/n_B$ blocks in the whole chain. This partition of the lattice into blocks induces a decomposition of the Hamiltonian (2.13) into an intrablock Hamiltonian H_B and a interblock Hamiltonian H_{BB} as illustrated in Fig.3.

Observe that the block Hamiltonian H_B is a sum of commuting Hamiltonians each acting on every block. The diagonalization of H_B can thus be achieved for small n_B either analytically or numerically. The content of Fig. 3 can be written as

$$H = H_B + \lambda H_{BB} \quad (3.18)$$

where λ is a coupling constant which is already present in H or else it can be introduced as a parameter characterizing the interblock coupling and in this latter case one can set it to one at the end of the discussion.

Eq. (3.18) suggests that we should search for solutions of the intertwiner equation (2.5) in the form of a perturbative expansion in the interblock coupling constant parameter λ , namely,

$$T = T_0 + \lambda T_1 + \lambda^2 T_2 + \dots \quad (3.19)$$

$$H' = H'_0 + \lambda H'_1 + \lambda^2 H'_2 + \dots \quad (3.20)$$

To zeroth order in λ Eq. (2.5) becomes

$$H_B T_0 = T_0 H'_0 \quad (3.21)$$

Since H_B is a sum of disconnected block Hamiltonians $h_{j'}^{(B)}$, $j' = 1, \dots, N'$ implicitly defined through the relation

$$H_B = \sum_{j'=1}^{N'} h_{j'}^{(B)} \quad (3.22)$$

one can search for a solution of T_0 in a factorized form

$$T_0 = \prod_{j'=1}^{N'} T_{0,j'} \quad (3.23)$$

and an effective Hamiltonian H'_0 which acts only at the site j' of the new chain,

$$H'_0 = \sum_{j'=1}^{N'} h_{j'}^{(s')} = H'_{s'} \quad (3.24)$$

Observe that $H'_{s'}$ is nothing but a site-Hamiltonian for the new chain. Eq. (3.21) becomes for each block:

$$h_{j'}^{(B)} T_{0,j'} = T_{0,j'} h_{j'}^{(s')} \quad (3.25)$$

The diagonalization of $h_{j'}^{(B)}$ for $j' = 1, \dots, N'$ will allow us to write

$$h_{j'}^{(B)} = \sum_{i=1}^{k'} |i\rangle_{j'} \epsilon_i {}_{j'}\langle i| + \sum_{\alpha=1}^{k^{n_s}-k'} |\alpha\rangle_{j'} \epsilon_{\alpha} {}_{j'}\langle \alpha| \quad (3.26)$$

where $|i\rangle_{j'}$ for $j = 1, \dots, k'$ are the k' -lowest energy states of $h_{j'}^{(B)}$. Moreover, we suppose that $h_{j'}^{(B)}$ is the same Hamiltonian for each block so that ϵ_i does not depend on the block.

The truncated Hamiltonian $h_{j'}^{(s)}$ and the intertwiner operator $T_{0,j'}$ are then given by:

$$h_{j'}^{(s')} = \sum_{i=1}^{k'} |i\rangle'_{j'} \epsilon_i {}_{j'}\langle i|' \quad (3.27)$$

$$T_{0,j'} = \sum_{i=1}^{k'} |i\rangle'_{j'} {}_{j'}\langle i|' \quad (3.28)$$

Later on we shall show examples of these relations.

To obtain the first order correction to the Hamiltonian H'_1 we must consider Eq. (2.5) to first order in λ :

$$H_{BB}T_0 + H_B T_1 = T_0 H'_1 + T_1 H'_0 \quad (3.29)$$

Multiplying the left hand side by T_0^\dagger and using $T_0^\dagger T_0 = 1$ along with $H_B T_0 = T_0 H'_0$ we readily obtain:

$$T_0^\dagger H_{BB} T_0 + H'_0 T_0^\dagger T_1 = H'_1 + T_0^\dagger T_1 H'_0 \quad (3.30)$$

We would like to kill the term proportional to $T_0^\dagger T_1$. For this purpose Eq. (2.7) which implies $T_0^\dagger T_1 + T_1 T_0^\dagger = 1$ is not very useful. A resolution of this problem can be accomplished if instead of the operator T one uses another operator \tilde{T} satisfying the defining equations:

$$H\tilde{T} = \tilde{T}H' \quad (3.31)$$

$$T_0^\dagger \tilde{T} = 1_{\mathcal{H}'} \quad (3.32)$$

Then $\tilde{T}_0 = T_0$ and $T_0^\dagger \tilde{T}_1 = 0$ in which case Eq. (3.30) simply becomes:

$$H'_1 = T_0^\dagger H_{BB} T_0 = H'_{s's'} \quad (3.33)$$

We can summarize these results saying that up to first order in λ , the effective Hamiltonian H' can be obtained using simply the zeroth order intertwiner operator T_0 (see Fig.4):

$$H'_{(\text{up to order } \lambda)} = H'_{s'} + H'_{s's'} = T_0^\dagger (H_B + \lambda H_{BB}) T_0 \quad (3.34)$$

This is precisely the prescription of Drell et al. [10].

The second order correction to H' can be obtained again from Eqs. (3.31)-(3.32) and is given by

$$H'_2 = T_0^\dagger H_{BB} \tilde{T}_1 \quad (3.35)$$

There is a close parallelism between the perturbative solution of Eqs. (2.5) or (3.31)- (3.32) and the perturbation theory of the Schrodinger equation for a Hamiltonian of the form $H_0 + \lambda H_1$. As a matter of fact, the normalization condition (3.32) for operators is equivalent to the standard normalization for wavefunctions $\langle \Psi_0 | \Psi(\lambda) \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$ that is adopted to avoid normalization complications. In what follows we shall mainly concentrate on the first order solution Eq. (3.34).

The final outcome of this analysis is that the effective Hamiltonian H' has a similar structure to the one we started with, H . The operators involved in $H'_{s'}$ and $H'_{s's'}$ may by all means differ from those of H_s and H_{ss} , but in some cases the only difference shows up as a change in the coupling constants. This is known as the renormalization of the bare coupling constants. When this is the case, one may easily iterate the RG-transformation and study the RG-flows.

Let us summarize the RG-prescription we have introduced so far in Table 1.

We have denoted this prescription by BRG1(n_s, k') where n_s and k' have been defined earlier and 1 denotes that we are working to first order in perturbation theory.

For the ITF model we shall consider blocks of two sites ($n_s = 2$) and truncation to two states ($k' = 2$). The block Hamiltonian has two sites and has the form,

$$h^{(B)} = -\Gamma(\sigma_1^x + \sigma_2^x) - J\sigma_1^z \sigma_2^z \quad (\Gamma, J > 0) \quad (3.36)$$

The eigenstates of this block Hamiltonian (3.36) are given in increasing order of energies by,

$$|G\rangle = \frac{1}{\sqrt{1+a^2}}(|00\rangle + a|11\rangle) \quad E = -\sqrt{J^2 + 4\Gamma^2} \quad (3.37)$$

$$|E\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \quad E = -J \quad (3.38)$$

$$|E'\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \quad E = J \quad (3.39)$$

$$|E''\rangle = \frac{1}{\sqrt{1+a^2}}(-a|01\rangle + |10\rangle) \quad E = \sqrt{J^2 + 4\Gamma^2} \quad (3.40)$$

$|0\rangle$ and $|1\rangle$ are the eigenstates of σ^x ,

$$\sigma^x |0\rangle = |0\rangle, \quad \sigma^x |1\rangle = -|1\rangle \quad (3.41)$$

and $a = a(g)$ is the following function of the ratio $J/2\Gamma := g$,

$$a(g) = \frac{-1 + \sqrt{1 + g^2}}{g} \quad (3.42)$$

which in turn satisfies

$$a(0) = 0, \quad a(\infty) = 1 \quad (3.43)$$

The intertwiner operator within each block has the form

$$T_0(a) = |G\rangle \langle 0|' + |E\rangle \langle 1|' \quad (3.44)$$

where $|0\rangle'$ and $|1\rangle'$ form a basis of states at each point of the new chain. The effective Hamiltonian H' up to order J can be computed from Eq. (3.34).

Thus to get \mathcal{H}' we have to study the renormalization of the various operators entering in its definition. Using (3.44) and (3.37)-(3.40) one obtains after some elementary algebra:

$$T^\dagger \sigma_j^x T = \frac{1 - a^2}{2(1 + a^2)} (1 + \sigma_{j'}^x) \quad (3.45)$$

$$T^\dagger \sigma_j^z T = \frac{1 + a}{\sqrt{2(1 + a^2)}} \sigma_{j'}^z \quad (3.46)$$

$$T^\dagger \sigma_{2j-1}^z \sigma_{2j}^z T = \frac{(1 + a)^2}{2(1 + a^2)} 1 + \frac{(1 - a)^2}{2(1 + a^2)} \sigma_{j'}^x \quad (3.47)$$

$$T^\dagger \sigma_{2j}^z \sigma_{2j+1}^z T = \frac{(1 + a)^2}{2(1 + a^2)} \sigma_{j'}^z \sigma_{j'+1}^z \quad (3.48)$$

The range of the indexes run as follows:

$$j = 2j' - 1 + p \quad (3.49)$$

$$j = 1, \dots, N \quad (3.50)$$

$$j' = 1, \dots, N/2 \quad p = 0, 1 \quad (3.51)$$

Applying Eqs. (3.45)-(3.48) to the ITF Hamiltonian, one gets

$$T^\dagger H_N(\Gamma, J) T = \Delta E + H_{N/2}(\Gamma', J') \quad (3.52)$$

where

$$\Delta E = -\frac{N}{2} \left[\Gamma \frac{1 - a^2}{(1 + a^2)} + \frac{J(1 + a)^2}{2(1 + a^2)} \right] \quad (3.53)$$

$$\Gamma' = \Gamma \frac{1 - a^2}{(1 + a^2)} - J \frac{(1 + a)^2}{2(1 + a^2)} \quad (3.54)$$

$$J' = J \frac{(1 + a)^2}{2(1 + a^2)} \quad (3.55)$$

The derivation of Eqs. (3.45)-(3.48) and (3.52)-(3.55) does not make use of Eq. (3.42) and hence have a more general validity. In other words, we can use the function $a(g)$ as a variational function in order to construct better ground states in the spirit of the VRG.

Eq. (3.42) is one of the numerous choices we can make. We shall consider later on other examples. Schematically we can set up the following relationship,

$$\text{RG-Prescription with } n_s = 2, k' = 2 \iff \begin{cases} a(g) \geq 0 \\ a(0) = 0, \quad a(\infty) = 1 \end{cases} \quad (3.56)$$

The physical properties of $H_N(\Gamma, J)$ depend only upon the ratio $g = J/2\Gamma$. If $0 \leq g \leq 1/2$ one is in a disordered region characterized by a unique ground state with unbroken symmetry ($\langle \sigma^z \rangle = 0$). If $g > 1/2$ the Z_2 symmetry associated to the operator $Q = \prod_j \sigma_j^z$, which commutes with H_N for N even, is broken. This is the ordered phase which has two degenerate ground states corresponding to $\langle \sigma^z \rangle = \pm m \neq 0$.

At $g = g_c = 1/2$ the system is critical and belongs to the same universality class as the 2D-classical Ising model. The critical exponents can be defined in terms of the behaviour of the “quantum observables” as functions of $g_c - g$.

Most of the critical exponents can be computed from the properties of the RG-transformation. In the case of the ITF model the RG-transformation can be obtained from Eq.(3.53)-(3.55):

$$g' := \frac{J'}{2\Gamma'} := R(g) = \frac{1}{2} \frac{g(1+a(g))^2}{1-a(g)^2 - g(1-a(g))^2} \quad (3.57)$$

For any function $a(g)$ satisfying Eq. (3.56), this transformation has 3 fixed points $g_* = 0, g_c, \infty$. The fixed points $g_* = 0$ and ∞ are attractive and correspond to the disordered and ordered phases respectively. The fixed point at g_c is repulsive and correspond to the critical point of the ITF Hamiltonian. The value of the function $a(g)$ at $g = g_c$ is a function only of g_c and does not depend on the particular prescription chosen, that is, it is a *universal function* :

$$g_c = R(g_c) \Rightarrow a(g_c) = \frac{2\sqrt{1-2g_c} + 2g_c - 1}{3 + 2g_c} \quad (3.58)$$

This equation implies in particular that whatever prescription is chosen, assuming that a is real, the critical value obtained from Eqs.(3.53)-(3.55) will always be less than the exact value $1/2$.

$$g_c \leq g_c^{\text{exact}} = 1/2 \quad (3.59)$$

To get the value of g_c for a given prescription one has simply to find the intersection of the function $a(g)$ and the function,

$$f(g) = \begin{cases} \frac{2\sqrt{1-2g}+2g-1}{3+2g} & 0 \leq g \leq 1/2 \\ 0 & g \geq 1/2 \end{cases} \quad (3.60)$$

as is shown in Fig.7.

The analysis of the RG-equations usually has to be done numerically. However, there is a great deal of information that can be retrieved without completely solving the RG-equations if we know whether the successive coupling constants $g_n \rightarrow g_{n+1} = R(g_n)$ increase or decrease during the iteration procedure. To this end it is convenient to introduce the the familiar beta function $\beta(g)$ of quantum field theory which in this context is [10],

$$\beta(g) := R(g) - g \quad (3.61)$$

In Fig.8 we have plotted the beta function for the ITF model we are analyzing. A fixed point of the transformation occurs at values of g which reproduce themselves under the RG-iteration, i.e., they are the zeroes of the beta function:

$$\beta(g_c) = 0 \quad (3.62)$$

There are 3 fixed points for besides the two zeroes at $g = 0$ and 0.39 , $g = \infty$ is also a fixed point for it cannot be reduced by further iterations.

There is additional qualitative information which can be extracted from the shape of the beta function $\beta(g)$. In particular, the sign of $\beta(g)$ is responsible for the stability character of the fixed point. When $\beta(g) < 0$ (> 0) this means that g decreases (increases) after one iteration and the resulting g' lies to the left (right) of the g we started with.

The outcome of this RG-analysis can be summarized by saying that the fixed points $g_* = 0, \infty$ are *stable fixed points* while $g_c = 0.39$ is an *unstable fixed point*.

Given the RG-transformation Eq. (3.57) we can compute several critical exponents and compare them with the exact results in order to check the accuracy of the method.

Correlation Length Exponent ν . It gives the behaviour of the correlation length in the vicinity of g_c

$$\xi \sim (g - g_c)^{-\nu} \quad (3.63)$$

Under the RG-transformation (3.57) $\xi \rightarrow \xi' = \xi/2$ which leads immediately to an expression for ν in terms of the derivative of $R(g)$ evaluated at the critical point,

$$\frac{1}{\nu} = \frac{\ln R'(g_c)}{\ln 2} \quad (3.64)$$

From Eq. (3.57) we can evaluate $R'(g_c)$ as a function of $a_c = a(g_c)$ and $a'_c = \frac{da}{dg}|_c$,

$$\lambda_T := R'(g_c) = 1 + 2g_c \left(\frac{1 - a_c}{1 + a_c} \right)^2 + 4 \frac{a'_c g_c \sqrt{1 - 2g_c}}{(1 + a_c)^2} \quad (3.65)$$

In Table 2 we show the value of ν obtained for different choices of the function $a(g)$.

Dynamical Exponent z . At the critical point where $g' = g$ holds, the Hamiltonian changes by an overall factor which in turn defines the dynamical exponent z

$$H_c \longrightarrow H'_c = \frac{1}{2^z} H_c \quad (3.66)$$

In order to get z we notice that

$$\frac{1}{2^z} = \left(\frac{J'}{J} \right)_c = \left(\frac{\Gamma'}{\Gamma} \right)_c \quad (3.67)$$

Hence

$$z = \frac{\ln(\frac{J'}{J})}{\ln 2} = 1 + \frac{\ln [(1 + a_c^2)/(1 + a_c)^2]}{\ln 2} \quad (3.68)$$

It follows from Eq. (3.68) and the positivity property of a_c (3.56) that z is always less than the exact value,

$$z \leq z^{exact} = 1 \quad (3.69)$$

Magnetic Exponent β . This critical exponent is defined through the spontaneous magnetization M_z in the ordered phase,

$$M = \langle \sigma_j^z \rangle \quad (3.70)$$

Above a_c but close to the critical point we will have

$$M \sim (g - g_c)^\beta \quad (3.71)$$

Gap Exponent s . Using scaling arguments satisfied by the BRG method, the gap G behaves like

$$G \sim (g - g_c)^s \quad (3.72)$$

with

$$s = \nu z \quad (3.73)$$

Equation (3.46) relates the magnetization M and the one obtained after the RG-transformation

$$M = \frac{1+a}{\sqrt{2(1+a^2)}} M' \quad (3.74)$$

Combining Eqs.(3.74), (3.71) and $g' = R(g)$ we arrive at,

$$\frac{M'}{M} = [R'(g_c)]^\beta = 2^{\beta/\nu} = \frac{1+a_c}{\sqrt{2(1+a_c^2)}} \quad (3.75)$$

Using Eq.(3.68) we are able to relate the critical exponents β , ν and z through the following scaling relation,

$$\beta = \frac{1}{2} z \nu \quad (3.76)$$

This relation is valid for any choice of the function $a(g)$ and therefore it is characteristic of using a block containing two sites. Observe that the exact exponents of the ITF model never satisfy this scaling relation (3.76). This shows the limitation of the block method when using a two-site block.

4 Density Matrix RG Method: Analytic Formulation

The Density Matrix RG-method (DMRG) is an improved version of the real-space renormalization group methods introduced by White [1] as a further elaboration of the ideas concerning the Combination of Boundary Conditions method [5].

The fundamental difficulty of the BRG method lies in choosing the eigenstates of the block Hamiltonian H_B to be the states kept. Since H_B contains no connections to the rest of the lattice its eigenstates have inappropriate features at the block ends. The CBC method of White and Noack is a first attempt to solving this intrinsic problem. The rationale of this method was that quantum fluctuations in the rest of the system effectively apply a variety of boundary conditions to the block. The CBC method proved to be very effective for the simple single-particle problem studied by White and Noack, but it happens to be ill-suited to interacting systems. The importance of the CBC method relies more on the lessons we can learn from it rather than the specific technicalities pertaining the simple case where it is applied successfully. There are two main ideas in order to proceed towards density matrix RG-method, namely:

- The block is not isolated.
- The eigenstates retained are not eigenstates of a unique block Hamiltonian H_B .

The DMRG method is in a sense an evolution of the CBC method in which we “let the system” to choose the best boundary conditions. White suggests that for a system which is *strongly coupled* to the outside “universe” (the rest of the lattice), it is much more appropriate to use *eigenstates of the block density matrix* to describe the system (block), rather than the eigenstates of the system’s Hamiltonian H_B . White’s proposal can be stated by saying:

- Choose to keep the n_B most probable eigenstates of the block density matrix.

It is possible to show that keeping the most probable eigenstates of the density matrix gives the most accurate representation of the state of the system as a whole [1]. This is the basis of the Density Matrix Renormalization Group (DMRG) method.

For the sake of completeness we present a brief introduction to the DMRG method. A superblock is called to a large block which contains several smaller blocks, one of which is the block to be used in the blocking procedure of the BRG method. Let us suppose that we have diagonalized a superblock and thereby obtained one particular state $|\psi\rangle$ which is called the *target state* and probably will be the ground state. Let $\{|i\rangle, i = 1, \dots, l\}$ be a complete set of states of the the block B which we call “the system”. Let also $\{|j\rangle, j = 1, \dots, J\}$ be a complete set of states of the superblock which we call “the universe” (see Fig.5). Now we proceed to decompose the target state $|\psi\rangle$ into its system- and universe-parts according to the following equation,

$$|\psi\rangle = \sum_{i,j} \psi_{ij} |i\rangle |j\rangle \quad (4.77)$$

Next we want to devise a procedure to produce a set of states of the system denoted by

$$|u^\alpha\rangle, \quad \alpha = 1, \dots, n_B \quad \text{with} \quad |u^\alpha\rangle = \sum_i u_i^\alpha |i\rangle \quad (4.78)$$

which are optimal for representing the target state $|\psi\rangle$ in a sense to be specified below. The number of states kept is such that $n_B < l$ so that $|\psi\rangle$ is represented approximately, that is,

$$|\psi\rangle \approx |\tilde{\psi}\rangle := \sum_{\alpha,j} a_{\alpha,j} |u^\alpha\rangle |j\rangle \quad (4.79)$$

where $a_{\alpha,j}$ are components to be determined by demanding that the following distance to be a minimum:

$$\mathcal{D} := ||\psi\rangle - |\tilde{\psi}\rangle|^2 \quad (4.80)$$

This minimization problem requires to vary over all $a_{\alpha,j}$ and u^α subject to the condition,

$$\langle u^\alpha | u^{\alpha'} \rangle = \delta_{\alpha\alpha'} \quad (4.81)$$

White has proved that the solution to this minimization problem is given by the *optimal states* u^α being eigenvectors of the reduced density matrix of the system as part of the universe whose eigenvalues are the n_B largest in magnitude [1].

The reduced density matrix for the system depends on the state of the universe which in this case is a pure state $|\psi\rangle$. Therefore, the density matrix for the system is given by,

$$\rho_{ii'} = \sum_j \psi_{ij} \psi_{i'j} \quad (4.82)$$

To summarize, *when the entire lattice is assumed to be in a pure state, the optimal states to be kept are then n_B most significant states of the reduced density matrix of the block, say B .*

Next step in putting density matrix RG ideas at work is to devise an efficient algorithm based upon these developments. A density matrix algorithm is defined mainly by two features, the same as the standard BRG algorithm is, namely, according to the form of the superblock and the manner in which the block are enlarged, e.g., doubling the block $B' = B B$ (Kadanoff) or adding a single site $B' = B + \text{site}$ (Wilson in Kondo).

As far as computer power is concerned, generally is more efficient to enlarge the block by adding a *single site* rather than doubling the block. The reason for this is that the diagonalization of a superblock composed of say p identical blocks is difficult for a many-particle interacting system for the dimension of the Hilbert space of states goes like n_B^p , assuming that n_B states are kept per block.

This has led White to propose a variety of density matrix algorithms for both finite and infinite size systems which rely on Wilson's method for enlarging the system. Thus, they are intrinsically one-dimensional methods.

In this paper we are presenting two new DMRG methods (Variational and Fokker-Planck) which are based on the blocking procedure of reducing the system size as the standard Block Renormalization Group method of the previous section. This makes them potentially well-suited to address higher dimensional systems.

Moreover, the DMRG algorithms introduced by White are intrinsically numerical for they are based upon Wilson's procedure of enlarging the system size. On the contrary, the BRG study of the ITF model carried out in the previous section was done in an analytical fashion mainly because it is a blocking procedure. We shall present hereby a new treatment of the ITF model along the lines of the density matrix RG method which is *analytical*.

To this purpose, we have incorporated the block method in the DMRG algorithm. In addition, we shall incorporate another ingredient for the algorithm to become analytical: we shall choose the target state (ground state) using a variational method or a Fokker-Planck method, and then compare the results obtained in these two fashions with the standard BRG results of the previous section.

The way to combine the above tools is as follows. We first set up a variational ground state for the *whole chain* whose energy is determined by solving the corresponding minimization equations. Next we use this state to construct a block density matrix ρ for a block having two sites in the philosophy of the BRG method. This ρ turns out to be (see below) a 4×4 matrix whose two largest eigenvalues denoted by $|A\rangle$ and $|B\rangle$ are kept to construct the intertwiner operator T_0 as in sections 2 and 3. Once we make contact with the blocking method, the iteration procedure goes over and over. The important point now is that we can keep the DMRG study at an analytical level.

It is worth noticing that we are introducing two new features in this fashion. In the original DMRG method of White the target state selected comprises just a few sites of the chain while now we are using the whole chain. On the contrary, in doing so we have to resort to variational or Fokker-Planck methods to handle the problem, while in the numerical DMRG the target state selected is exact for the particular size of the superblock chosen.

4.1 Variational DMRG.

In reference [7] a new method based on the combination of perturbative and variational techniques was presented to study quantum lattice Hamiltonians. The general ideas of this method are illustrated in the example of the Ising model in an transverse field. The method relies on the choice of an exponential ansatz $\psi(\lambda) \exp[U(\lambda)]\psi_0$, which is a sort of generalized lattice version of a Jastrow wave function. Perturbative and variational techniques are used to get successive approximations of the operator $U(\lambda)$. Perturbation theory is used to set up a variational method which in turn produces nonperturbative results. This method allows one to associate to the original quantum-mechanical problem a statistical-mechanical system defined in the same spatial dimension. In some instances these

statistical-mechanical systems turn out to be integrable, which allows one to obtain exact upper bounds to the energy. We shall briefly review this method hereby but for a detailed account we refer to [7].

Let us suppose that we are given a hamiltonian of the form $H(\lambda) = H_0 + \lambda H_1$, where H_0 has a nondegenerate ground state ψ_0 and λ is a coupling constant. In reference [7] it was proposed to construct the ground state $\psi(\lambda)$ of $H(\lambda)$ as

$$\psi(\lambda) = \exp\left(\sum_{n=1}^{\infty} \lambda^n U_n\right) \psi_0 \quad (4.83)$$

Solving perturbation theory in λ to order ν implies the knowledge of the collection of operators $\{U_n\}_{n=1,\dots,\nu}$. Each operator U_n consist in fact of a sum of “irreducible” operators V_I ,

$$U_n = \sum_I p_{n,I} V_I \quad (4.84)$$

Hence inserting (4.84) into (4.83) and interchanging the order of the sums one arrives to a “dual” description of the ground state

$$\psi(\lambda) = \exp\left(\sum_I \alpha_I(\lambda) V_I\right) \psi_0 \quad (4.85)$$

where $\alpha_I(\lambda) = \sum_n \lambda^n p_{n,I}$.

This expression suggests an alternative approximation to the ground state $\psi(\lambda)$ which consists in choosing only a class of irreducible operators V_I whose weights α_I are determined variationally. This was precisely the approach applied in [7] to the Ising model in a transverse field.

According to the perturbative-variational (PV) method [7] we must first determine the form of the set operators $\{U_n\}$ by inserting the exponential ansatz (4.83) in the Schrodinger equation for H . Then these operators serve us to construct variational wave functions by inserting them back in the exponential ansatz. The perturbative equations that determine the U_n for the lowest order in perturbation theory obey the equations,

$$\text{order } \lambda: \quad ([H_0, U_1] + H_1)\psi_0 = E^{(1)}\psi_0 \quad (4.86)$$

$$\text{order } \lambda^2: \quad ([H_0, U_2] + [H_1, U_1] + 1/2([H_0, U_1], U_1))\psi_0 = E^{(2)}\psi_0 \quad (4.87)$$

where $E^{(1)}$ and $E^{(2)}$ are the perturbative energies to first and second order.

A solution of equations (4.86) and (4.87) in the case where $H_0 = -\sum_j \sigma_j^x$ and $H_1 = -\sum_j \sigma_j^z \sigma_{j+1}^z$ is the following,

$$U_1 = \frac{1}{4} \sum_j \sigma_j^z \sigma_{j+1}^z \quad (4.88)$$

$$U_2 = \frac{1}{16} \left\{ \sum_j \sigma_j^z \sigma_{j+2}^z + \sum_j \sigma_j^z (\sigma_{j+1}^z + \sigma_{j-1}^z) \right\} \quad (4.89)$$

In the following we shall make use of the simplest exponential ansatz based on the U_1 operator only.

Now let us start searching for the block density matrix using the variational method. Recall that the density matrix in Eq. (4.82) can be rewritten as a scalar product of two block states $|\psi\rangle_B$ and $|\psi'\rangle_{B'}$ given by their defining system-universe decomposition of the previous section:

$$|\psi\rangle_B = \sum_{i \in B} \sum_{j \in B^c} \psi_{ij} |i\rangle |j\rangle \quad (4.90)$$

$$|\psi'\rangle_{B'} = \sum_{i' \in B'} \sum_{j' \in B'^c} \psi_{i'j'} |i'\rangle |j'\rangle \quad (4.91)$$

where i, i' are system-indexes, j, j' are universe-indexes, B, B' are system-blocks and B^c, B'^c are universe-blocks. The density matrix ρ is given by the scalar product of these two block states:

$$\rho =_B \langle \psi | \psi' \rangle_{B'} \quad (4.92)$$

for upon substitution of Eqs. (4.90), (4.91) we arrive at

$$\begin{aligned} \rho &= \sum_{ij} \sum_{i'j'} \langle i | \langle j | \psi_{ij} \psi_{i'j'} | i' \rangle | j' \rangle \\ &= \sum_{i'i} |i'\rangle \langle i | \rho_{ii'} \end{aligned} \quad (4.93)$$

with $\rho_{ii'}$ as in Eq.(4.82).

Now let us consider the following variational state ansatz for the ground state $|\psi_0\rangle_{1,2,3,\dots,N}$ of the ITF model in a lattice with N sites:

$$|\psi_0\rangle_{1,2,3,\dots,N} = \exp\left(\frac{\alpha}{2} \sum_{j=1}^N \sigma_j^z \sigma_{j+1}^z\right) |0\rangle_{1,2,3,\dots,N} \quad (4.94)$$

where α is a variational parameter which is determined by minimizing the vacuum expectation value of the ITF Hamiltonian in this state, thereby making the parameter to become a function $\alpha = \alpha(J/2\Gamma)$ of the coupling constant of the model; and $|0\rangle_{1,2,3,\dots,N} = |0\rangle_1 \otimes \dots \otimes |0\rangle_N$ with $|0\rangle$ being the ground state of the σ^x matrix. This exponential-variational ansatz constitutes part of a method called Perturbative-Variational method (PV) developed in [7] for spin systems and in [18] for fermionic systems. The PV method is essentially a cluster method which combines perturbative and variational techniques. Using Eq. (4.92) we construct the block density matrix out of this target state for a block containing 2 sites as:

$$\rho^{PV} = \frac{1}{Z_N(\alpha)} {}_{1,2} \langle \psi_0 | \psi_0 \rangle_{1',2'} \quad (4.95)$$

where $Z_N(\alpha)$ is a normalization factor being the norm of the state which can be interpreted as the partition function of a certain associated statistical model [7]. As a matter of fact, in the large N limit, it turns out to be simply:

$$Z_N(\alpha) = \langle \psi_0 | \psi_0 \rangle = (\cosh \alpha)^N, \quad N \gg 1 \quad (4.96)$$

Inserting the ansatz (4.94) into (4.95) we can express the density matrix in a more appealing form, namely,

$$\rho^{PV} = \frac{1}{Z_N(\alpha)} {}_{1,2} \langle 0 | \exp \frac{\alpha}{2} (\sigma_1^z \sigma_2^z + \sigma_1^z \sigma_2^z) Z_{N-2}^{(0)}(\alpha, h, h') | 0 \rangle_{1',2'} \quad (4.97)$$

where we have defined the following quantities,

$$Z_{N-2}^{(0)}(\alpha, h, h') := {}_{3,\dots,N} \langle 0 | \exp(\alpha \sum_{j=3}^{N-3} \sigma_j^z \sigma_{j+1}^z + h \sigma_3^z + h' \sigma_N^z) | 0 \rangle_{3,\dots,N} \quad (4.98)$$

$$h := \frac{\alpha}{2} (\sigma_2^z + \sigma_2^z) \quad (4.99)$$

$$h' := \frac{\alpha}{2}(\sigma_1^z + \sigma'_1{}^z) \quad (4.100)$$

For the time being, it is convenient to shift $N - 2 \rightarrow N$ in order to make expressions easier (at the end we shall come back to the correct value).

It is possible to recast $Z_{N-2}^{(0)}(\alpha, h, h')$ into the following form,

$$\begin{aligned} Z_N^{(0)}(\alpha, h, h') &=_{1, \dots, N} \langle 0 | \exp(\alpha \sum_{j=1}^{N-1} \sigma_j^z \sigma_{j+1}^z + h \sigma_1^z + h' \sigma_N^z) | 0 \rangle_{1, \dots, N} \\ &= \frac{1}{2^N} \sum_{\{\sigma_1, \dots, \sigma_N\}} \exp(\alpha \sum_{j=1}^{N-1} \sigma_j \sigma_{j+1} + h \sigma_1 + h' \sigma_N) \end{aligned} \quad (4.101)$$

Now we can recognize this equation as the partition function for the Ising model on an open chain of N sites subject to an external magnetic field applied only at the ends of the chain. This partition function can be worked out exactly using standard transfer matrix calculations yielding the result:

$$\begin{aligned} Z_N^{(0)} &= \frac{1}{2^N} \{ [\cosh(h + h') + \cosh(h - h')] (2 \cosh \alpha)^{N-1} \\ &\quad + [\cosh(h + h') - \cosh(h - h')] (2 \sinh \alpha)^{N-1} \} \end{aligned} \quad (4.102)$$

In the $N \rightarrow \infty$ limit in which we are interested in, it further simplifies to:

$$Z_{N \rightarrow \infty}^{(0)} = \frac{1}{2} (\cosh \alpha)^{N-1} [\cosh(h + h') + \cosh(h - h')] \quad (4.103)$$

Inserting now Eq.(4.103) in Eq.(4.97) we arrive at the following expression for the PV block density matrix:

$$\begin{aligned} \rho^{PV} &= \frac{1}{2(\cosh \alpha)^3} {}_{1,2} \langle 0 | \exp \frac{\alpha}{2} (\sigma_1^z \sigma_2 + \sigma'_1{}^z \sigma'_2{}^z) \\ &\quad \times [\cosh \frac{\alpha}{2} (\sigma_1^z + \sigma_2^z + \sigma'_1{}^z + \sigma'_2{}^z) + \cosh \frac{\alpha}{2} (\sigma_1^z - \sigma_2^z + \sigma'_1{}^z - \sigma'_2{}^z)] | 0 \rangle_{1',2'} \end{aligned} \quad (4.104)$$

This is a nice result. Observe that the piece ${}_{1,2} \langle 0 | \exp \frac{\alpha}{2} (\sigma_1^z \sigma_2) \exp(\sigma'_1{}^z \sigma'_2{}^z) | 0 \rangle_{1',2'}$ corresponds to a density matrix of a pure state $\rho = |\phi\rangle_{1',2'} {}_{1,2} \langle \phi|$ is the projection of the target state ψ_0 onto the block $(1, 2)$. The extra terms in Eq.(4.104) are the novel features that the DMRG(PV) method brings about.

To proceed further and give ρ^{PV} a simple matricial form, it is convenient to change basis from eigenstates $|0\rangle, |1\rangle$ of σ^x to eigenstates $|+\rangle, |-\rangle$ of σ^z . The notation is,

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (4.105)$$

$$|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (4.106)$$

In the new basis $\{|+\rangle, |-\rangle\}$ the components of ρ^{PV} are:

$$\begin{aligned} \rho_{\sigma'_1 \sigma'_2 \sigma_1 \sigma_2}^{PV} &= \frac{1}{8(\cosh \alpha)^3} \exp \frac{\alpha}{2} (\sigma_1 \sigma_2 + \sigma'_1 \sigma'_2) \\ &\quad \times [\cosh \frac{\alpha}{2} (\sigma_1 + \sigma_2 + \sigma'_1 + \sigma'_2) + \cosh \frac{\alpha}{2} (\sigma_1 - \sigma_2 + \sigma'_1 - \sigma'_2)] \end{aligned} \quad (4.107)$$

Now ρ^{PV} takes the following matricial form in the basis $\{++, --, +-, -+\}$:

$$\rho^{PV} = \frac{1}{4(\cosh \alpha)^3} \begin{pmatrix} e^\alpha (\cosh \alpha)^2 & e^\alpha & \cosh \alpha & \cosh \alpha \\ e^\alpha & e^\alpha (\cosh \alpha)^2 & \cosh \alpha & \cosh \alpha \\ \cosh \alpha & \cosh \alpha & e^{-\alpha} (\cosh \alpha)^2 & e^{-\alpha} \\ \cosh \alpha & \cosh \alpha & e^{-\alpha} & e^{-\alpha} (\cosh \alpha)^2 \end{pmatrix} \quad (4.108)$$

We can readily check that ρ^{PV} is normalized:

$$\text{tr} \rho^{PV} = 1 \quad (4.109)$$

Next step in the DMRG algorithm is to diagonalize the density matrix (4.108) and truncate to the largest ones; in this case the truncation is to two states to be denoted by $|A\rangle$ and $|B\rangle$ and will play the parallel role of the states $|G\rangle$ and $|E\rangle$ for the block Hamiltonian H_B of Section 3.

We do not need to make a “blind” diagonalization of this 4×4 matrix for we may take advantage of what we have learnt in Section 3 about the eigenstates of the H_B in the ITF model. Then, the largest eigenvector say $|A\rangle$ will be in the even sector $\{|00\rangle, |11\rangle\}$, while the next to the largest one, say $|B\rangle$, will be in the odd sector $\{|01\rangle, |10\rangle\}$. According to this analysis, we may write those states as,

$$|A\rangle = x_{00}|00\rangle + x_{11}|11\rangle \quad (4.110)$$

$$|B\rangle = x_{01}|01\rangle + x_{10}|10\rangle \quad (4.111)$$

where $x_{00}, x_{11}, x_{01}, x_{10}$ are the components to be determined. Expressing the states $|00\rangle, |11\rangle \dots$ in the basis of $\{|+\rangle, |-\rangle\}$, the diagonalization of the density matrix (4.108) yields the following eigenvalues:

$$w_0 = \frac{1}{4(\cosh \alpha)^3} [\cosh \alpha (1 + \cosh^2 \alpha) + \sqrt{\cosh^2 \alpha (1 + \cosh^2 \alpha)^2 - \sinh^4 \alpha}] \quad (4.112)$$

$$w_1 = \frac{1}{4(\cosh \alpha)^3} [\cosh \alpha (1 + \cosh^2 \alpha) - \sqrt{\cosh^2 \alpha (1 + \cosh^2 \alpha)^2 - \sinh^4 \alpha}] \quad (4.113)$$

$$w_3 = \frac{1}{4(\cosh \alpha)^3} e^\alpha \sinh^2 \alpha \quad (4.114)$$

$$w_4 = \frac{1}{4(\cosh \alpha)^3} e^{-\alpha} \sinh^2 \alpha \quad (4.115)$$

For α small it is easy to see that the eigenvalues are sorted according to

$$w_0 > w_3 > w_1 > w_4 \quad (4.116)$$

For arbitrary values of α , which in turn amounts to arbitrary values of the coupling constant $g = J/2\Gamma$ due to the variational equations to be given bellow, we have plotted these 4 eigenvalues in Fig. 6 observing that there are not level crossings in the whole range of variation of α and that the sorting in Eq.(4.116) holds all over, not just for small α . It is very important for our DMRG(PV) method to work properly that this property holds up, for when we truncate to the eigenstates of the largest eigenvalues, w_0 and w_3 , the physics will not change qualitatively when varying the coupling constant g .

Moreover, it is also possible to show that the eigenvectors $|A\rangle$ (of w_1) and $|B\rangle$ (of w_3) are given by:

$$|A\rangle = \frac{|00\rangle + a^{PV}|11\rangle}{\sqrt{1 + (a^{PV})^2}} \quad (4.117)$$

$$|B\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}} \quad (4.118)$$

with the function a^{PV} now the following function of the parameter α (after some tedious algebra),

$$a^{PV} = \frac{\sqrt{\cosh^2 \alpha (1 + \cosh^2 \alpha)^2 - \sinh^4 \alpha - 2 \cosh \alpha}}{\sinh \alpha (1 + \cosh^2 \alpha)} \quad (4.119)$$

Notice that these states which now come from a DMRG(PV) analysis have the same form as the states $|G\rangle$, $|E\rangle$ of the block Hamiltonian H_B Eqs.(3.37)-(3.38), the difference being in the dependence of the function a upon the coupling constant. This means that we have again the same structure as in the BRG analysis where the intertwiner operator T_0 was fully determined, and consequently the whole RG procedure, by a single function $a = a(g)$ of the coupling constant. To obtain $a^{PV} = a^{PV}(g)$ we need the variational equation relating g with α . This can be found in [7] and is given by,

$$g = \frac{J}{2\Gamma} = \tanh \alpha \quad (4.120)$$

Observe that when $J/\Gamma \ll 1$ then $\alpha = J/2\Gamma$ and thus $a^{PV} \sim \alpha/2 = J/4\Gamma$. Now it is possible to eliminate the intermediate parameter α between Eqs. (4.119) and (4.120) yielding the desired formula,

$$a^{PV}(g) = \frac{\sqrt{1 - g^2 + \frac{g^6}{4}} - (1 - g^2)}{g(1 - \frac{g^2}{2})} \quad (4.121)$$

Therefore we may appreciate that this function shares the same qualitative properties as a_{BRG} (3.42) does, Eq.(3.56), namely it goes to zero linearly when $g \rightarrow 0$ and it is bounded below 1, i.e., $0 < a^{PV} < 1$ for $0 < g < 1$. In addition, it has a singularity at $g = \sqrt{2}$ which prevents the extension of this method beyond that singular point. The origin of this singularity is due to the variational nature of the method (see [7]). Nevertheless the critical region lies within the region of applicability of the PV method.

Furthermore, it is also possible to define a variational DMRG method valid for the whole range of variation of the coupling constant. To do this, we simply recall that for small α the coupling constant depends linearly on the variational parameter,

$$g \sim \alpha, \quad \text{for } \alpha \text{ small} \quad (4.122)$$

Thus, we may define another function say $a^{PV'}(g)$ by simply substituting α by g in $a(\alpha)$ (4.119),

$$a^{PV'} = \frac{\sqrt{\cosh^2 g (1 + \cosh^2 g)^2 - \sinh^4 g - 2 \cosh g}}{\sinh g (1 + \cosh^2 g)} \quad (4.123)$$

In this fashion, $a^{PV'}(g)$ shares the same properties with a_{BRG} , without any singularity in the range of g . In fact, $a^{PV'}(g)$ has a horizontal asymptote at 1 as a_{BRG} does (see Fig 7).

4.2 Fokker-Planck DMRG.

This is another approximated version for preparing the target state to be projected onto the block-system in order to construct another analytical DMRG method based upon a blocking procedure. The details of how the Fokker-Planck (FP) method is applied to construct an approximate version of the real ground state of the ITF model are given in the original paper [8]. Briefly stated, what the FP method does is to start with an exponential ansatz as in the variational method Eq. (4.94), but instead the parameter α is fixed by demanding that a certain Fokker-Planck Hamiltonian H^{FP} (to be determined

along the way) satisfies the eigenvalue equation to a certain order ν in the perturbative expansion of the parameter α , that is,

$$H^{FP}(\alpha)\Psi^{FP}(\alpha) = E^{FP}(\alpha)\Psi^{FP}(\alpha) \quad (4.124)$$

such that the exact ITF Hamiltonian H_{ITF} and its Fokker-Planck approximation version $H^{FP}(\alpha)$ differ in operators say V_I which involve interactions between lattice sites $\nu + 1$ distant apart or larger. Schematically,

$$H_{ITF} - H^{FP}(\alpha) = \sum_{I>\nu} C_I(\alpha)V_I \quad (4.125)$$

Correspondingly, the FP-energy $E^{FP}(\alpha)$, although incorporating non-perturbative effects, should agree with the exact ground state energy up to order $\nu + 1$ in α . In a sense, this gives the best “exact” approximation to the Hamiltonian H_{ITF} to order ν in perturbation theory [8].

It is possible to show that these conditions fix the relationship between α and g . To lowest order this is given by [8],

$$g = \frac{1}{2} \sinh(2\alpha) \quad (4.126)$$

Again we see that for small coupling constant α and g are equal as in the variational method.

In order to obtain the Fokker-Planck function, say $a^{FP}(g)$, we first notice that as in this FP method we start with the same exponential ansatz (4.94) as in the variational method, the same function $a(\alpha)$ in Eq. (4.119) is valid here. The new feature is that we have to use the relation (4.126) now to express the function $a^{FP}(g)$ in terms of the coupling constant. After some tedious algebra we arrive at the following expression:

$$a^{FP}(g) = \frac{\sqrt{(8 + 26g^2 + 4g^4) + (8 + 6g^2)\sqrt{1 + 4g^2}} - 2(1 + \sqrt{1 + 4g^2})}{g(3 + \sqrt{1 + 4g^2})} \quad (4.127)$$

This function contains all the information which upon inserted in the intertwiner operator T_0 gives rise to what we denote by a DMRG(FP) method. By looking at Fig.7 we notice again that $a^{FP}(g)$ has the same qualitative properties as a_{BRG} does.

In this section we have introduced 3 functions $a(g)$ namely, $a^{PV}(g)$, $a^{PV'}(g)$ and $a^{FP}(g)$, related to different analytical realizations of the density matrix RG ideas. It is our purpose now to check the goodness of those methods by comparing their predictions for the critical exponents with the exact values already found by the standard BRG method in Sect.3.

In Fig.7 we have plotted the 4 functions $a(g)$ along with the universal function $a(g_c)$ introduced in Eq. (3.58) whose cuts with the functions $a(g)$ gives the predictions on the location of the critical point g_c for each method. Recalling that the exact value is $g_c^{exact} = 1/2$, we see that the closest value to this one is produced by the Fokker-Planck version of the DMRG method, even better than the standard BRG. Nevertheless, we may appreciate from Fig.7 that the 4 methods lie rather close to one another within the critical region, the major differences being present off criticality when entering the strong coupling region. The particular values of g_c are gathered in Table 2.

Another interesting function to be plotted is the beta function $\beta(g)$ obtained for each method according to the analysis of Sect.3, Eq. (3.61). We show these results in Fig.8 where we observe that the 3 new beta functions introduced in this section by means of variational and Fokker-Planck DMRG methods have the same qualitative behaviour as the standard BRG beta function of Sec.3. We know that in particular this means that the unstable character of the fixed point g_c is preserved by these new methods. Moreover, we notice again that in the critical region the differences are small, namely, the

cut with the g -axis and the slope at the corresponding g_c . These two latter properties are related to critical exponents.

As far as the critical exponents is concerned, we have collected in Table 2 the exponents computed previously for the standard BRG method: correlation length exponent ν , dynamical exponent z , magnetic exponent β and the gap exponent s . Notice first that the 3 new DMRG methods also satisfy the scaling relation,

$$\beta = \frac{1}{2}z\nu$$

which we know does not hold for the exact solution of the ITF model.

From Table 2 we arrive at the following conclusions,

- The best correlation length exponent ν is provided by the DMRG Perturbative-Variational method.
- The best dynamical exponent z is provided by the DMRG Fokker-Planck method.
- The best magnetic exponent β is provided by the DMRG Perturbative-Variational method.
- The best gap exponent s is provided by the DMRG Fokker-Planck method.

From these results we may draw the conclusion that the RG methods based on block density matrix, either variational or Fokker-Planck, provide an improvement respect to the standard BRG methods, though it is not a major improvement. One of the reasons why this improvement is not as good as the numerical results obtained by White [1] relies on the fact that we have just kept 2 states in our analytical DMRG method while in the numerical treatment quite a lot states are kept.

5 Conclusions

We have presented in this paper an analytic formulation of the recently proposed Density Matrix RG method [1]. This method was originally developed in a numerical fashion mainly because it relies on the Wilsonian procedure of enlarging lattice sizes in the real-space RG. As this Density Matrix RG method has become a powerful tool to compute static and dynamic properties of quantum lattice systems at zero temperature, we find interesting to devise an analytic formulation of this method to be tested against the old procedures based upon the standard Block RG method introduced by Drell et al. [10] to study QCD.

The new feature of the DMRG method is its ability to take into account the unavoidable interaction between the block selected for truncating states and the rest of the lattice. This feature is the more relevant the more strongly correlated is the system under study, such as lattice QCD and strongly correlated electrons in High- T_c materials.

We have been able to devise an analytic formulation of the DMRG method by combining the idea of “interacting blocks” (that is, “non-isolated”) with two other approaches. One approach is the old idea of blocking “a la Kadanoff” instead of the Wilsonian procedure. To this end we have presented an unified formulation of the old BRG method (sect.3) in terms of what we call the intertwiner operator. This facilitates the task of bringing together the Kadanoff blocking with the DMRG. The second approach has been to devise an analytical method to produce “target states” which are the basic ingredients in the DMRG calculations. To this purpose we have used two recently proposed methods to deal with quantum lattice Hamiltonians: the Perturbative-Variational method [7] and the Fokker-Planck method [8]. We have coined the names DMRG(PV) and DMRG(FP), respectively, for the density matrix RG methods coming out of these two approaches ².

²After we finished this work we have been aware of references [17] where those authors also propose new extensions of the DMRG method.

In order to facilitate the task of testing these two new DMRG methods, we have chosen the simple ITF model where previous work with the BRG method is available. The results of computing several critical exponents are described in Sect.4 where we have seen that either of the new DMRG methods perform better than the old BRG, although the improvement we get is not as good as White's numerical DMRG for we keep a much lower number of states during the truncation among other reasons.

In addition, there is another line of work in order to improve our analytical DMRG methods. This is via the exact diagonalization of the block density matrix corresponding to 4 lattice sites (starting from the exact ground state for 4 lattice sites) and then to proceed in the usual fashion to construct the corresponding new $a(g)$ function which would allow us to carry the blocking method. We leave this possibility open for future work.

Another reason to seek analytical formulations of the DMRG method is the possibility of generalizing the current one-dimensional algorithms to higher dimensions. We consider our DMRG(PV) and DMRG(FP) methods as a first attempt at this goal. As a matter of fact, it is possible to use them to prepare 2-dimensional target states in the ITF model and to proceed with a DMRG analysis. Moreover, as far as fermion systems is concerned, it is also possible to apply the new density matrix methods using the perturbative-variational techniques described in [18].

Finally, the renormalization group method is one of the basic concepts in several branches of Physics and we believe that we are currently facing a reconsideration of the old renormalization group ideas which will certainly have implications in areas such as Field Theory, Statistical Mechanics and Condensed Matter.

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Table captions

Table 1 : Block Renormalization Group Method BRG1 (n_B, k').

Table 2 : Critical exponents for the ITF model according to different RG methods and exact solution.

Figure captions

Figure 1: Pictorial decomposition of the Hamiltonian H into single-site part H_S and two-nearest-neighbour-site part H_{SS} .

Figure 2 : Block decomposition of the open chain into blocks with $n_B = 3$ sites.

Figure 3 : Pictorial representation of the block Hamiltonian H_B and the interblock Hamiltonian H_{BB} for the ITF model.

Figure 4 : Pictorial representation of the truncation procedure for the block and interblock Hamiltonians in the ITF model.

Figure 5 : Lattice decomposition into “system”- and “universe”-parts.

Figure 6 : The 4 eigenvalues w_0, w_1, w_3 and w_4 of the block density matrix corresponding to the variational DMRG method.

Figure 7 : Plot of the functions $a(g)$ according to the methods: BRG (solid line), DMRG(PV) (grey line), DMRG(FP) (dashed line), DMRG(PV’).

Figure 8 : Plot of the beta functions $\beta(g)$ according to the methods: BRG (solid line), DMRG(PV) (grey line), DMRG(FP) (dashed line), DMRG(PV’).

Table 1: Block Renormalization Group Method BRG1 (n_B, k')

Steps of the BRG1 Method	
1) Blocking Transformation:	$H = H_B + H_{BB}$
2) Diagonalization of H_B	
3) Truncation within each block:	T_0
4) Renormalization of H_B and H_{BB}	
	$H'_{s'} = T_0^\dagger H_B T_0$
	$H'_{s's'} = T_0^\dagger H_{BB} T_0$
5) Iteration: Repeat 1) \rightarrow 4)	for $H' = H'_{s'} + H'_{s's'}$

Table 2: Critical exponents for the ITF model according to different RG methods and exact solution.

Method	g_c	ν	z	β	s
BRG	0.3916	1.4820	0.5515	0.4086	0.8173
DMRG(PV)	0.3790	1.4073	0.5353	0.3767	0.7534
DMRG(FP)	0.4011	1.5177	0.5647	0.4285	0.8570
DMRG(PV')	0.3874	1.4579	0.5459	0.3980	0.7958
Exact Solution	0.5	1	1	0.125	1