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A non-perturbative real-space renormalization group scheme

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Abstract. Based on the original idea of the density matrix renormalization group (DMRG), i.e. to include the missing boundary conditions between adjacent blocks of the blocked quantum system, we present a rigorous and non-perturbative mathematical formulation for the real-space renormalization group idea conceived by Kadanoff and further developed by Wilson. This is achieved by using additional Hilbert spaces called auxiliary spaces in the construction of each single isolated block, which is then termed a superblock, in accordance with the original nomenclature. On this superblock we define two maps, called embedding and truncation, for successively integrating out the small-scale structure. Our method overcomes the known difficulties of the numerical DMRG, i.e. the limitation to zero temperature and one space dimension.

1. Introduction

Soon after Wilson's dramatic success in applying a momentum space formulation of the renormalization group (RG) method [1] to the theory of critical phenomena and the Kondo problem [2] there was a considerable amount of effort made to apply the same type of approach as the real-space formulation to a variety of quantum physical problems. Since the momentum space formulation, with a few exceptions [2, 3], in most cases relies on a perturbative expansion, real-space methods offer non-perturbative approaches and are therefore extremely important in applying RG ideas to complex and strongly correlated systems. It then transpired that for a variety of such physical models the real-space RG techniques give significantly poor results, the reason for which remained unknown for nearly 15 years. During this time some new real-space RG methods were discovered, some of which worked very well, while others failed without providing any insight into their failure. We refer the interested reader to the book by Burkhardt and van Leeuwen [4] for a summary of work on this topic.

Apart from these developments White and Noack published a series of papers containing a new idea for improving real-space RG techniques [5, 6]. Based on the understanding of the importance of boundary conditions for isolated blocks in real-space RG methods for quantum physical systems, a numerical approach was developed to take a sufficient number of boundary conditions into account during the RG procedure. Apart from the impressive accuracy of the numerical results this new approach also displays the characteristic universal character of an RG formulation, in that it is applicable, with some particular changes, to a variety of problems and was termed the density matrix RG (DMRG) [5, 6].

The dramatic success of the DMRG method has changed completely the picture of real-space RG techniques and, until now, has been applied in very different fields of scientific

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research [7–9]. The method itself is a rather complicated algorithm and a detailed description together with some examples is given by White [5].

In spite of the great excitement surrounding DMRG, the method has some important limitations which are given by the method itself and therefore cannot be removed by applying simple changes to the DMRG algorithm. Here we describe briefly the three main limitations

(a) The chief limitation of DMRG is dimensionality. Although higher-dimensional variations are not forbidden, in general, it becomes a complicated task. Recent applications of DMRG to finite-width strips in two dimensions show a declining accuracy with the width. Therefore, a successful approach for two dimensions, in general, or for even higher dimensions has not yet been worked out.
(b) DMRG is by definition an algorithm and therefore it is a purely numerical RG approach. Although this need not be a disadvantage we would like to have an analytical formulation of the DMRG method. In such a reformulation the numerical DMRG scheme will occur as one possible realization of a more general description. We would therefore expect to have a deeper insight into successful working RG approaches.
(c) DMRG is restricted to zero temperature and is usually applied for calculating ground state properties such as the ground-state magnetization or even the ground state itself. Finite-temperature results were obtained only in the low-lying spectrum but with very limited accuracy. In comparison with other real-space RG methods DMRG is different because it is designed to calculate ground-state quantities. Recently, based on the work of Wang and Xiang [10], a thermodynamic method was applied successfully, which combines White's DMRG idea [5] with the *transfer-matrix* technique [11], now referred to as TMRG. Although TMRG is also purely numerical, since it shares the basic idea of DMRG, it is an even more complicated algorithm [11]. Due to its close relationship with DMRG, the aim of TMRG is to give numerically accurate results for physical quantities and it does not predict RG flow behaviour. In contrast, our method is suitable for calculating the flow behaviour of the system, even analytically, although the main advantage of our RG scheme when compared with TMRG lies in its simple structure. This makes it easy to apply to a great variety of physical models.

This paper is organized as follows. In the next section we briefly review the key idea of DMRG. We begin by introducing the standard concepts of the real-space RG method in the language of spin chains in the way they were originally proposed. In section 3 we present a rigorous formulation of a real-space RG transformation. Each single block within the blocked chain is enlarged by an additional space, the auxiliary space. A single block together with its auxiliary space is called a superblock, for which a real-space RG transformation is defined by integrating out the small spatial structure. Constructing a global RG transformation for the complete quantum system from the concatenation of the local superblock RG transformations leads to the definition of exact and perfect RG transformations. In section 7 we make some final remarks on this work. Applications in terms of this new formulation are left entirely for a subsequent paper.

2. The idea of DMRG

The very standard real-space RG approach is best explained for a spin Hamiltonian H on a one-dimensional lattice, as shown in figure 1. The dots represent the individual spins which are grouped together by breaking up the chain into blocks, as shown in figure 2 for a particular

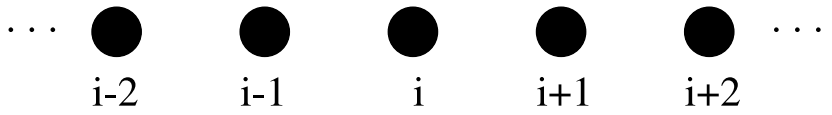


Figure 1. A one-dimensional spin chain.

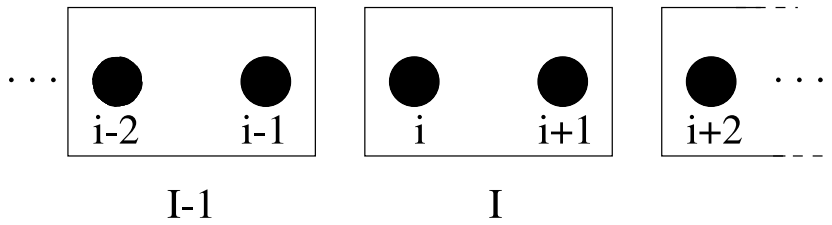


Figure 2. A one-dimensional chain divided into blocks where each block is composed of two single sites.

block composition of two sites. We will establish a notation in which small letters refer to the single-site spins and capital letters denote the blocks. The block Hamiltonian for the block with the index I is thus denoted as H_I. The idea of a real-space RG is then to replace each block of the single spins by one effective *block spin*, which leads to a renormalized block-spin Hamiltonian $H_{I'}$. The calculation of the block spins from the blocks composed of single-site spins is carried out by an *RG transformation* R, which can be defined in various ways [4]; for example, by projecting the block onto the low-lying spectrum [5]. In summary, an RG approach is designed to split the whole system into subsystems, called blocks, for which it is possible to reduce the degrees of freedom. Iterating this procedure leads to an *RG flow* in the parameter space of the model and the aim is to find a fixed point of this flow behaviour. Such a fixed-point Hamiltonian is helpful in determining the universal behaviour of the physical model.

As explained in the introduction, the boundary conditions of a block within the quantum system are essential for the calculation of an *RG step*, which is defined as one application of the renormalization group transformation (RGT). In fact, the different boundary conditions represent the correlations in the quantum chain between adjacent blocks which we refer to in the following as *system blocks*. To provide the opportunity to choose those boundary conditions that result in the most accurate representation of an isolated block, the fundamental idea of DMRG is to embed the system block into a 'bigger' block, termed a *superblock*. This nomenclature, as well as the term 'system block' derives from the original work of White [5]. In some sense this simulates the environment represented by the surrounding spin sites and effectively smooths out the sharp effects of the boundary conditions, as depicted in figure 3.

To construct a working approach from this overall picture we are immediately faced with two basic problems. How can we describe the embedding of the system block within the superblock and how can one include the boundary conditions during an RG step? Within the framework of DMRG these problems are overcome by focusing on one particular state, the *target state* $|\psi\rangle$, which is the ground state of the superblock Hamiltonian obtained by diagonalization. By using a complete set of eigenstates of the system block $\left\{|\psi_m^{\text{system}}\rangle,\ m = 1, \ldots, l_{\text{system}}\right\}$ and a complete set of eigenstates for the environment represented by the

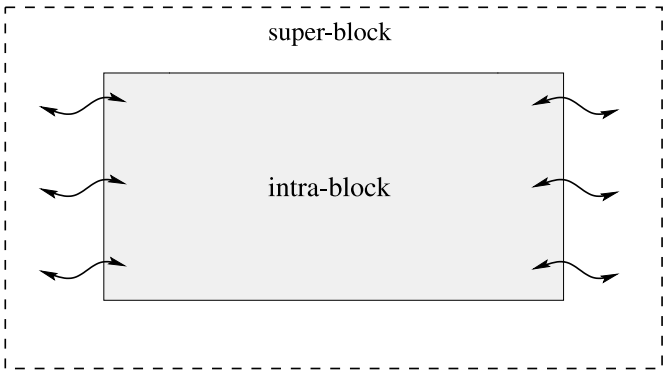


Figure 3. An isolated system block embedded into a superblock shown by broken lines.

superblock $\left\{|\psi_n^{\text{environment}}\rangle,\ n = 1, \ldots, l_{\text{environment}}\right\}$ we decompose the target state $|\psi\rangle$ according to

$$|\psi\rangle = \sum_{m}^{l_{\text{system}}} \sum_{n}^{l_{\text{environment}}} c_{m,n} |\psi_m^{\text{system}}\rangle \otimes |\psi_n^{\text{environment}}\rangle. \tag{1}$$

We are interested in those states that lead to an optimal representation of the target state $|\psi\rangle$ in a 'truncated' basis. Of course, in this way we lose the exactness of relation (1) and we therefore denote the new result as an *optimal approximation* expressed as

$$|\psi\rangle \approx |\psi^{\text{opt}}\rangle = \sum_{p}^{l_{\text{opt}}} \sum_{n}^{l_{\text{environment}}} \gamma_{p,n} |\psi_p^{\text{opt}}\rangle \otimes |\psi_n^{\text{environment}}\rangle \tag{2}$$

where the *optimal states* $\left\{|\psi_p^{\text{opt}}\rangle,\ p = 1, \ldots, l_{\text{opt}} < l_{\text{system}}\right\}$ are defined in terms of the original system block states by

$$|\psi_p^{\text{opt}}\rangle = \sum_{m}^{l_{\text{system}}} \alpha_{m,p}^{\text{opt}} |\psi_m^{\text{system}}\rangle \tag{3}$$

with some coefficients $\alpha_{m,p}^{\text{opt}}$. The coefficients $\gamma_{p,n}$ in (2) can be determined by examining the *reduced density matrix* of the system block within the superblock [5].

The two problems described above are therefore solved as follows. First, the embedding of the system block within the superblock is achieved by reconstructing the target state of the superblock in a basis, in which the basis vectors are given as a tensor product composition of states of the system block and the chosen environment. In this way the system block is described within the bigger superblock. Since we have not truncated the set of states which belong to the environment, the RG step for the system block is performed by taking into account all possible boundary conditions within the selected environment.

From the previous discussion it becomes clear that the coefficients $\gamma_{p,n}$ can only be determined numerically within real applications of this technique. To develop a complete analytic approach, a method for using a target state will be impractical and we can only use the overall picture represented in figure 3.

3. A rigorous real-space RG transformation

We start this section by giving a very general but well known definition of an RG transformation. An RGT R is a map defined on a set of physical variables $\{\sigma_l\}$ and a further set of parameters $\boldsymbol{K} = (K_1, K_2, \ldots)$

$$R\colon\ (\{\sigma_l\}, \boldsymbol{K}) \longrightarrow \left(\{\mu_m\}, \boldsymbol{K}'\right) \tag{4}$$

where $\{l\}$ and $\{m\}$ are not necessarily equal indexing sets and $\{\mu_m\}$ denotes the new set of blocked variables belonging to the larger scale. The quantitative prescription for the map (4) is then given in physical terms by including physical constraints such as, for example, the conservation of symmetries, the maintenance of the structure of the Lagrangian or the Hamiltonian or the preservation of physical quantities, such as, for example, the free energy of the system. Since in most cases it is a difficult task to define a transformation which combines all the necessary constraints, this has led to an enormous variety of approximate RG transformations developed over the last few decades [4].

The most common realization of the quantitative prescription is to apply the RG transformation R to the Lagrangian or the Hamiltonian as a functional, which then acts on the variables and parameters given in (4). In the special example of a one-dimensional quantum spin chain the new variables are the block spins and the new coupling constant belongs to the *renormalized* set of parameters $\boldsymbol{K}'$. For our case, we generalize this RGT to an arbitrary suitable functional dependence $\mathcal{O}$

$$R\,[\mathcal{O}(\{\sigma_l\}, \boldsymbol{K})] = \mathcal{O}(\{\mu_m\}, \boldsymbol{K}'). \tag{5}$$

By further mathematical analysis of a particular RGT R defined by (5) this hopefully yields to a dependence of the *renormalized* parameters $\boldsymbol{K}'$ on the old parameters $\boldsymbol{K}$, which is called the *flow behaviour* of the RGT. We emphasize that once the functional dependence $\mathcal{O}(\{\sigma_l\}, \boldsymbol{K})$ is known, we immediately know the functional dependence $\mathcal{O}(\{\mu_m\}, \boldsymbol{K}')$, which plays an important role in our construction.

We now make the ansatz that, in principle, each RGT R can be written as a composition of two maps, called *embedding* and *truncation* [12]. This terminology originates from a RG technique for Hamiltonian systems [13], which was then further developed and used for calculations of the flow behaviour [12]. Rephrasing equation (5) and focusing only on the renormalization of the set of parameters for determining the flow behaviour, we obtain

$$G^{+} \circ \mathcal{O}(\boldsymbol{K}) \circ G = \mathcal{O}(\boldsymbol{K}') \tag{6}$$

where we denote G^{+} as the *truncation map* and G as the *embedding map*.

As a quite intuitive example for the abstract definition of the operators G^{+} and G, in the special case of a functional dependence given by the Hamiltonian, we can construct G^{+} as a projection map from the space of all eigenvectors of the Hamiltonian to a space containing a reduced number of eigenvectors. A projection map from this truncated space back to the space containing all eigenvectors is a natural way of defining G. Although such an example illustrates a possible application of the abstract formulation given by (6), it raises the question of which eigenstates are necessary to keep for constructing the truncated space. In the case of zero temperature we can argue that the only eigenvectors that should be kept are those which correspond to the low-energy eigenvalues [4]. As pointed out previously, the aim of this paper should be to devise a real-space RG formulation which overcomes these limitations with a more abstract formulation.

Let us now assume that the functional dependence $\mathcal{O}$ is given by some operator, not necessarily the Hamiltonian, on the original Hilbert space $\mathcal{H}$ so that equation (6) can be written as the commuting diagram

$$\begin{array}{ccc} \mathcal{H}' & \xrightarrow{G} & \mathcal{H} \\ {\scriptstyle \mathcal{O}(\boldsymbol{K}')}\downarrow & & \downarrow{\scriptstyle \mathcal{O}(\boldsymbol{K})} \\ \mathcal{H}' & \xleftarrow[G^+]{} & \mathcal{H} \end{array} \tag{7}$$

where $\mathcal{H}'$ refers to the effective Hilbert space for the functional dependence of the truncated set of parameters.

We introduce the blocking concept discussed in the previous section as a tensor product decomposition of the Hilbert space

$$\mathcal{H} = \bigotimes_{I\in\mathfrak{I}} \mathcal{H}_I \tag{8}$$

where $\mathfrak{I}$ denotes some indexing set for the blocks. We are looking for an embedding and truncation map which respects the block decomposition by factorization

$$G_{\mathcal{H}'} = \bigotimes_{I\in\mathfrak{I}} G_{\mathcal{H}'_I} \qquad \text{and} \qquad {G^+}_{\mathcal{H}} = \bigotimes_{I\in\mathfrak{I}} {G^+}_{\mathcal{H}_I}. \tag{9}$$

Using this mathematical formulation of the blocking scheme we write the RG transformation for a block in an analogous way

$$\mathcal{O}_{\mathcal{H}'_I}(\boldsymbol{K}') = {G^+}_{\mathcal{H}_I} \circ \mathcal{O}_{\mathcal{H}_I}(\boldsymbol{K}) \circ G_{\mathcal{H}'_I} \tag{10}$$

due to (9). However, equation (10) is not an independent relation since we have to relate it to the *global* relation (6). To decompose (6) into the blocked pieces (10) we have to assume that the operator $\mathcal{O}_{\mathcal{H}}$ can be decomposed into commuting block operators $\mathcal{O}_{\mathcal{H}_I}$ which, in general, is not the case in quantum physics. Therefore, the problem at this stage is to find suitable functions $\mathcal{O}_{\mathcal{H}}(\boldsymbol{K})$ which respect the block decomposition of the Hilbert space within the RGT.

To find a solution for this problem our ansatz is to enlarge the Hilbert space $\mathcal{H}$ by an additional (auxiliary) Hilbert space $\mathcal{H}_{\text{aux}}$, due to the composition rule

$$\mathcal{H}_{\text{total}} = \mathcal{H} \otimes \mathcal{H}_{\text{aux}}. \tag{11}$$

We think of the space $\mathcal{H}_{\text{total}}$ as some kind of 'superspace' and the global operator $\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})$ is then embedded into the total space $\mathcal{H}_{\text{total}}$. The key idea is to recover a block decomposition for $\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})$ into blocked pieces of the form $\mathcal{O}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K})$ which we identify as superblocks, as described in section 2. The next step in our approach, following the basic principles of DMRG, is to outline a general construction for $\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})$ with a commuting block decomposition. This can be performed explicitly by starting with standard real-space RG concepts.

In the formulation of a *standard* block RG we consider a decomposition of $\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})$ into disconnected block functions given by

$$\mathcal{O}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) = \mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \qquad \text{with} \quad I \in \mathfrak{I}. \tag{12}$$

where we have neglected completely the non-commutativity or *correlations* between the blocks. A straightforward way to improve the standard RG method is to somehow include the correlations between adjacent system blocks. As shown in figure 4, we can refer to these

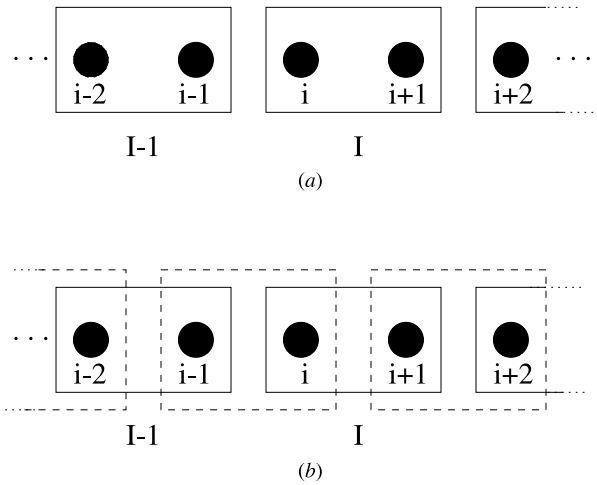


Figure 4. Successive blocks in a one-dimensional chain in (*a*) the commuting case and (*b*) the non-commuting case. In the non-commuting case the system blocks are connected by *correlation blocks* shown by a broken line.

correlations as blocks, which we denote therefore as *correlation blocks*. Using these correlation blocks enables us to represent the non-commutativities between the system blocks in a compact way and we denote these correlation blocks, using the overall notation given in the appendix, as

$$\mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}}(\boldsymbol{K}) \tag{13}$$

with

$$\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}\subset\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I\otimes\mathcal{H}_{I-1}\otimes(\mathcal{H}_{\text{aux}})_{I-1}\otimes\cdots.$$

The subspace

$$\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}=\mathcal{H}_i\otimes(\mathcal{H}_{\text{aux}})_i\otimes\mathcal{H}_{i-1}\otimes(\mathcal{H}_{\text{aux}})_{i-1}\otimes\cdots \tag{14}$$

denotes the tensor product composition of all the block Hilbert spaces used for the construction of the correlation block.

4. Decomposition rules

We are address the problem of how to include these correlation blocks into the RG transformation. One can find previous approaches where this is performed perturbatively [12] and would therefore be unsuitable in our case. To gain some insight into this problem let us start with the composition

$$\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})=\sum_{I\in\mathfrak{I}}\mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K})+\sum_{\substack{\{i,i-1,\ldots\}\\ \subset\{I,I-1,\ldots\}}}\mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}}(\boldsymbol{K}) \tag{15}$$

which is exact and, as always, $\{i, i-1, \ldots\}$ denotes the subset of all the product subspaces needed for constructing the correlation blocks. We stress that the decomposition (15) in sums of system blocks and correlation blocks is not unique. Later we examine another decomposition which, in contrast we will refer to as the product decomposition.

Let us apply the RG transformation (6) on the sum decomposition (15)

$$\mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}(\boldsymbol{K}') = G^{+}{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}} \circ \left[\sum_{I\in\mathfrak{I}} \mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K})\right] \circ G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}$$

$$+G^{+}{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}} \circ \left[\sum_{\substack{\{i,i-1,\ldots\}\\ \subset\{I,I-1,\ldots\}}} \mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}}(\boldsymbol{K})\right] \circ G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}} \tag{16}$$

and all quantities are used in the context of additional auxiliary spaces. Let us first consider the system block summand in (16), which can be rewritten as

$$\sum_{I\in\mathfrak{I}}\left[G^{+}{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}} \circ \mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \circ G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}\right]$$

$$= \sum_{I\in\mathfrak{I}}\left[G^{+}{}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I} \circ \mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \circ G_{\mathcal{H}'_I\otimes(\mathcal{H}'_{\text{aux}})_I}\right]$$

$$\times \prod_{\substack{J\in\mathfrak{I}\\ J\neq I}} G^{+}{}_{\mathcal{H}_J\otimes(\mathcal{H}_{\text{aux}})_J} \circ G_{\mathcal{H}'_J\otimes(\mathcal{H}'_{\text{aux}})_J}. \tag{17}$$

This is precisely the local RGT for the system blocks (10) if we neglect the last product term on the right-hand side of (17). We will refer to this factor as a correction term, which vanishes if we demand

$$G^{+}{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}} \circ G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}} = \mathbb{1}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}. \tag{18}$$

Inserting this constraint into (17), carrying out the same calculation for the correlation blocks and finally using relation (10) we obtain the renormalized version of equation (15) given by

$$\mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}(\boldsymbol{K}') = \sum_{I\in\mathfrak{I}} \mathcal{O}^{\text{system}}_{\mathcal{H}'_I\otimes(\mathcal{H}'_{\text{aux}})_I}(\boldsymbol{K}') + \sum_{\substack{\{i,i-1,\ldots\}\\ \subset\{I,I-1,\ldots\}}} \mathcal{O}^{\text{correlation}}_{\mathcal{H}'_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}'_{\text{aux}})_{\{i,i-1,\ldots\}}}(\boldsymbol{K}') \tag{19}$$

which leads to the renormalized set of parameters $\boldsymbol{K}'$. In (19) we used the reasonable definition

$$\mathcal{O}^{\text{correlation}}_{\mathcal{H}'_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}'_{\text{aux}})_{\{i,i-1,\ldots\}}}(\boldsymbol{K}') := \left[G^{+}{}_{\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}}\right]$$

$$\circ \mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,i-1,\ldots\}}}(\boldsymbol{K}) \circ \left[G_{\mathcal{H}'_{\{i,i-1,\ldots\}}\otimes(\mathcal{H}'_{\text{aux}})_{\{i,i-1,\ldots\}}}\right]. \tag{20}$$

Relation (18) introduces an additional constraint for the RGT and therefore restricts the variety of possible transformations.

In the case of a product decomposition of the operator $\mathcal{O}(\boldsymbol{K})$ we can write

$$\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K}) = \prod_{i\in I} \mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \cdot \prod_{\substack{\{i,i-1,\ldots\}\\ \subset\{I,I-1,\ldots\}}} \mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,j,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,j,\ldots\}}}(\boldsymbol{K}). \tag{21}$$

In analogy to the case of the sum decomposition (15), we can apply the RG transformation (6) to (21) which leads to the expression

$$\mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}(\boldsymbol{K}') = G^{+}{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}} \circ \left[\prod_{i\in I} \mathcal{O}^{\text{system}}_{\mathcal{H}_I\otimes(\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \cdot \prod_{\substack{\{i,i-1,\ldots\}\\ \subset\{I,I-1,\ldots\}}} \mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,j,\ldots\}}\otimes(\mathcal{H}_{\text{aux}})_{\{i,j,\ldots\}}}(\boldsymbol{K})\right]$$

$$\circ G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}. \tag{22}$$

Since this is already the final step in the calculation for this special case of a decomposition we are not able to write the result as a composition of the renormalized system block part and correlation block part as we did in (19) for the sum decomposition. By the considerations outlined so far the product decomposition, therefore, does not seem to be as useful as the sum decomposition for later applications. This is not the case as we will show in the following.

For the auxiliary space we distinguish between two different cases, an *active* role and a *passive* role. Here, active means that the auxiliary space is directly involved in the RGT, i.e. G and G^+ act non-trivially on this additional space. The commutative diagram describing the general active situation is given in (23):

$$\begin{array}{ccc} \mathcal{H}' \otimes \mathcal{H}'_{\text{aux}} & \xrightarrow{G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}} & \mathcal{H} \otimes \mathcal{H}_{\text{aux}} \\ {\scriptstyle \mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}(\boldsymbol{K}')}\downarrow & & \downarrow{\scriptstyle \mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})} \\ \mathcal{H}' \otimes \mathcal{H}'_{\text{aux}} & \xleftarrow[G^+_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}]{} & \mathcal{H} \otimes \mathcal{H}_{\text{aux}} \end{array}. \tag{23}$$

Relation (23) reduces to a rewriting of (7), if the transformation maps G and G^+ each operate as the identity on the auxiliary space and the functional dependence $\mathcal{O}(\boldsymbol{K})$ acts non-trivially only on $\mathcal{H}$. This gives us an example of the particular case of a passive role of the auxiliary space as depicted in (24).

$$\begin{array}{ccc} \mathcal{H}' \otimes \mathcal{H}'_{\text{aux}} & \xrightarrow{G_{\mathcal{H}'}\otimes \mathbb{1}_{\mathcal{H}'_{\text{aux}}}} & \mathcal{H} \otimes \mathcal{H}_{\text{aux}} \\ {\scriptstyle \mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}(\boldsymbol{K}')}\downarrow & & \downarrow{\scriptstyle \mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K}).} \\ \mathcal{H}' \otimes \mathcal{H}_{\text{aux}} & \xleftarrow[G^+_{\mathcal{H}}\otimes \mathbb{1}_{\mathcal{H}_{\text{aux}}}]{} & \mathcal{H} \otimes \mathcal{H}_{\text{aux}} \end{array} \tag{24}$$

In the case of (23) we can think of the auxiliary space as some kind of medium not changed during an RG step. The active and passive choice of the auxiliary space yield two different realizations of our RG, the 'general (real-space) RG' (GRG) and the corresponding RG transformation (GRGT).

5. The construction of the local GRG transformation

So far we have discussed different types of quantum decompositions and types of auxiliary spaces. We now turn to the question of how to construct the embedding map $G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}$ and the truncation map $G^+{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}$. In (5) we used the functional dependence $\mathcal{O}$ to introduce physical constraints within the RG transformation. To determine $G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}$ and $G^+{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}$ we introduce another constraint. In addition to keeping the structure of the operator $\mathcal{O}$ we relate $\mathcal{O}$ to a physical quantity $\mathcal{Z}(\mathcal{O})$ which acts as a physical invariant†. Equating the original physical quantity $\mathcal{Z}(\mathcal{O})$ calculated from the original quantum lattice and the effective physical quantity $\mathcal{Z}(\mathcal{O}')$ for the reduced lattice we obtain $G^+{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}$ and $G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}$ from

$$\mathcal{Z}\left[\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K})\right] = \mathcal{Z}\left[G^+{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}} \circ \mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}(\boldsymbol{K}) \circ G_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}\right] = \mathcal{Z}\left[\mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}(\boldsymbol{K}')\right]. \tag{25}$$

We refer to equation (25) as the *invariance relation* for the RGT. Finally, we have to decompose $G^+{}_{\mathcal{H}\otimes\mathcal{H}_{\text{aux}}}$ and $G_{\mathcal{H}'\otimes\mathcal{H}'_{\text{aux}}}$ according to (9).

† A possible example for such a quantity could be the partition function or the free energy of the physical system.

We are now able to give the precise definition of the local RGT in the form

$$\begin{array}{ccc} \mathcal{H}'_I \otimes \left(\mathcal{H}'_{\text{aux}}\right)_I & \xrightarrow{G_{\mathcal{H}'_I \otimes (\mathcal{H}'_{\text{aux}})_I}} & \mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I \\ \Big\downarrow {\scriptstyle \mathcal{O}_{\mathcal{H}'_I \otimes (\mathcal{H}'_{\text{aux}})_I}(\boldsymbol{K}')} & & \Big\downarrow {\scriptstyle \mathcal{O}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K})} \\ \mathcal{H}'_I \otimes \left(\mathcal{H}'_{\text{aux}}\right)_I & \xleftarrow[G^+{}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}]{} & \mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I \end{array} \tag{26}$$

where we refer to $G^+{}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}$ and $G_{\mathcal{H}'_I \otimes \left(\mathcal{H}'_{\text{aux}}\right)_I}$ as the generators of the transformation. By the explanations of section 4

$$\mathcal{O}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) = \mathcal{O}^{\text{system}}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \cdot \prod_{\substack{\{i,i-1,\ldots\} \\ \subset I}} \mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,j,\ldots\}} \otimes (\mathcal{H}_{\text{aux}})_{\{i,j,\ldots\}}}(\boldsymbol{K}) \tag{27}$$

or

$$\mathcal{O}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) = \mathcal{O}^{\text{system}}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) + \sum_{\substack{\{i,i-1,\ldots\} \\ \subset I}} \mathcal{O}^{\text{correlation}}_{\mathcal{H}_{\{i,j,\ldots\}} \otimes (\mathcal{H}_{\text{aux}})_{\{i,j,\ldots\}}}(\boldsymbol{K}) \tag{28}$$

and analogously for $\mathcal{O}_{\mathcal{H}'_I \otimes \left(\mathcal{H}'_{\text{aux}}\right)_I}(\boldsymbol{K}')$.

6. Perfect and exact local RG transformations

In this section we study the relationship between (26) and the global RGT

$$\begin{array}{ccc} \mathcal{H}' \otimes \mathcal{H}'_{\text{aux}} & \xrightarrow{G_{\mathcal{H}' \otimes \mathcal{H}'_{\text{aux}}}} & \mathcal{H} \otimes \mathcal{H}_{\text{aux}} \\ \Big\downarrow {\scriptstyle \mathcal{O}_{\mathcal{H}' \otimes \mathcal{H}'_{\text{aux}}}(\boldsymbol{K}')} & & \Big\downarrow {\scriptstyle \mathcal{O}_{\mathcal{H} \otimes (\mathcal{H}_{\text{aux}})}(\boldsymbol{K})} . \\ \mathcal{H}' \otimes \mathcal{H}'_{\text{aux}} & \xleftarrow[G^+{}_{\mathcal{H} \otimes \mathcal{H}_{\text{aux}}}]{} & \mathcal{H} \otimes \mathcal{H}_{\text{aux}} \end{array} \tag{29}$$

Diagram (29) represents an exact relation which implies all the necessary constraints for the RG procedure that can be verified from equation (25). We therefore choose relation (29) as the basic relation in defining local RGTs.

Decomposing the global RGT (29) into local RGTs given by (26) demands the decomposition of $\mathcal{O}$ into commuting blocks. From previous considerations we conclude that this is impossible for quantum chains due to the correlation blocks occurring in a decomposition of a quantum physical system. Therefore, the idea is to use the auxiliary space to decompose the chain into commuting blocks by storing the information about the correlations of adjacent system blocks within the auxiliary space. By the decompositions discussed so far we then decompose a chain into system blocks and try to find an auxiliary space $(\mathcal{H}_{\text{aux}})_I$ for each system block which takes over the role of the correlation blocks within the RGT, as shown in figure 5. This statement can be expressed more precisely.

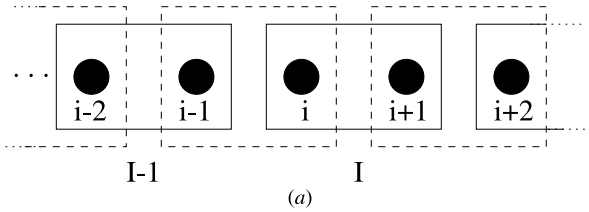
Definition 6.1. *A local RGT is said to be* perfect *if there exists a local operator*

$$\mathcal{O}_{\mathcal{H}'_I \otimes (\mathcal{H}'_{\text{aux}})_I}(\boldsymbol{K}') = \left[G^+{}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}\right] \circ \mathcal{O}^{\text{system}}_{\mathcal{H}_I \otimes (\mathcal{H}_{\text{aux}})_I}(\boldsymbol{K}) \circ \left[G_{\mathcal{H}'_I \otimes (\mathcal{H}'_{\text{aux}})_I}\right]$$

together with a global functional dependence $\tilde{\mathcal{O}}_{\mathcal{H}' \otimes \mathcal{H}'_{\text{aux}}}(\boldsymbol{K}')$ *defined by the decomposition*

$$\tilde{\mathcal{O}}_{\mathcal{H}' \otimes \mathcal{H}'_{\text{aux}}}(\boldsymbol{K}') := \sum_{I \in \mathfrak{I}} \mathcal{O}_{\mathcal{H}'_I \otimes (\mathcal{H}'_{\text{aux}})_I}(\boldsymbol{K}') \quad \textit{or} \quad \tilde{\mathcal{O}}_{\mathcal{H}' \otimes \mathcal{H}'_{\text{aux}}}(\boldsymbol{K}') := \prod_{I \in \mathfrak{I}} \mathcal{O}_{\mathcal{H}'_I \otimes (\mathcal{H}'_{\text{aux}})_I}(\boldsymbol{K}')$$

and there occurs no further local relation governing the renormalization of the correlation block part.



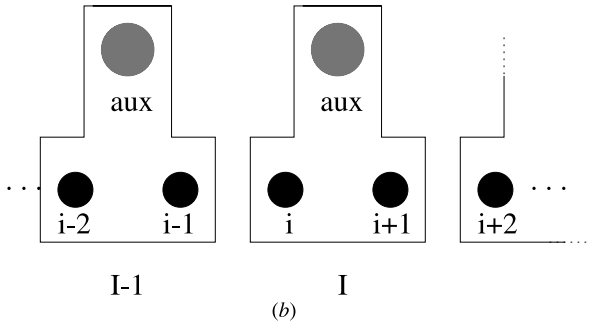


Figure 5. A rigorous blocked chain in the non-commuting case with (*a*) decomposition into system and correlation blocks, the latter shown by broken boxes and (*b*) decomposition into system blocks, each equipped with an auxiliary space suitable to take over the role of the correlation blocks during the RGT.

The main advantage of a perfect RGT is a rigorous mathematical description for a local RGT. Although the structure of the local operator $\mathcal{O}_{\mathcal{H}_I \otimes (\mathcal{H}_{\rm aux})_I}$ is conserved, a perfect RGT does not make use of the invariance relation (25).

Definition 6.2. *A local RGT is said to be* exact *if it is perfect and*

$$\mathcal{Z}\left[\mathcal{O}_{\mathcal{H}\otimes\mathcal{H}_{\rm aux}}(\boldsymbol{K})\right] = \mathcal{Z}\left[\mathcal{O}_{\mathcal{H}'\otimes\mathcal{H}'_{\rm aux}}(\boldsymbol{K}')\right] = \mathcal{Z}\left[\tilde{\mathcal{O}}_{\mathcal{H}'\otimes\mathcal{H}'_{\rm aux}}(\boldsymbol{K}')\right].$$

If an RGT is exact it includes all necessary constraints and therefore we can compare the RGT to the classical situation where non-commutativity effects are absent.

At this point we present some important remarks on perfect and exact RGTs. Although in both cases a rigorous mathematical formalism is used, a physical approximation usually enters the problem through the choice of an appropriate auxiliary space. Only for a certain class of models will we be able to find auxiliary spaces with a structure that allows for describing the non-commutativity effects without any approximation.

We stress again that in the exact as well as in the perfect RGT, $\mathcal{O}_{\mathcal{H}}$ and $\mathcal{O}_{\mathcal{H}'}$ are known so that we can determine G and G^+ in both cases according to the explanations in section 5.

If the auxiliary space is active it may happen that it vanishes by truncation during the RG procedure. In such a case no auxiliary space is available after the local transformation has been worked out and the previously provided information concerning the correlations between adjacent system blocks is lost. Therefore, the RGT is at its most perfect.

In the case of an auxiliary space which (only) allows for an approximate description of the correlations between adjacent system blocks we need insight into the accuracy of the approximation. Here we remember the numerical DMRG procedure in which convergence of

numerical values of ground state quantities by enlarging the superblock is used as an estimate for the accuracy of the method.

It is apparent that only in the case of an exact RGT are we able to calculate global quantities such as the total ground state energy shift. Since we are interested mainly in an overall effective coupling determining the RG flow we are looking for exact RGTs.

7. Conclusions

We have invented a non-perturbative quantum RG method based on the idea of an additional auxiliary space. The work was motivated by the success of the DMRG concerning numerical results and the open question of an underlying general mathematical framework.

The main ideas introduced in this paper concern the auxiliary space $\mathcal{H}_{\mathrm{aux}}$ and the two maps $G^{+}{}_{\mathcal{H}_I\otimes(\mathcal{H}_{\mathrm{aux}})_I}$ and $G_{\mathcal{H}'_I\otimes\left(\mathcal{H}'_{\mathrm{aux}}\right)_I}$ which generate the RGT. By using these quantities we have been able to give the definition of an exact local RGT which is the end result of this work. An exact local RGT involves all the information provided by the physical system.

In future work we will proceed by applying the abstract formalism presented here to quantum spin chains such as the Heisenberg models and compare our results with related work on these models [14]. This will lead to concrete and different examples of possible auxiliary spaces. As expected, the correct choice of the auxiliary space will be the main factor in the construction of the RGT, whereas the definition of the maps $G^{+}{}_{\mathcal{H}_I\otimes(\mathcal{H}_{\mathrm{aux}})_I}$ and $G_{\mathcal{H}'_I\otimes\left(\mathcal{H}'_{\mathrm{aux}}\right)_I}$ turns out to be rather straightforward. We also hope there will be further applications of the method introduced here.

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Appendix

Throughout this work blocks are denoted by capital indexing letters, corresponding to the block sites. The indexing set for the blocks is denoted by $\mathfrak{I}$. Neighbouring blocks are denoted by a sequence $I, I-1, I-2, \ldots \in \mathfrak{I}$, whereas arbitrary blocks are indexed by different letters $I, J, \ldots \in \mathfrak{I}$.

A block Hilbert space $\mathcal{H}_I$ contains a minimum of two single-site Hilbert spaces $\mathcal{H}_i$ and $\mathcal{H}_{i-1}$. Single site Hilbert spaces are denoted by the letters $i, j, k, \ldots$. To indicate that a single-site space $\mathcal{H}_i$ is contained in a block space $\mathcal{H}_I$ we write $\mathcal{H}_i \subset \mathcal{H}_I$ or, even more simply, $i \in I$ if it is clear that I refers to the block Hilbert space. We also use the abbreviation $\{i, i-1, \ldots\} \subset \{I, I-1, \ldots\}$ instead of $\mathcal{H}_{\{i,i-1,\ldots\}} \subset \mathcal{H}_{\{I\}} \otimes \mathcal{H}_{\{I-1\}}, \ldots$. Using this notation it is not clear which single-site space is contained in a certain block Hilbert space. If this is important it must be pointed out explicitly.

Expressions which are written in italics are either defined and used in this work or have a special physical meaning.

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