Numerical Renormalization Group Methods

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Licenciate thesis

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Abstract

This thesis deals with the general properties of numerical Real-Space Renormalization Group methods (RSRG) and, in particular, the Density-Matrix Renormalization Group (DMRG). We provide an introduction to these methods and discuss the properties of the approximate states obtained from them. We only consider the so called infinite lattice algorithms.

In the paper we deal with the question of how the DMRG describes gapless systems, i.e. systems with quasi long-ranged correlations. To do this, we focus on a system consisting of free fermions on a lattice, with a staggered on-site potential. We study the convergence properties of the DMRG and find that the method converges to a fixed point, thus producing finitely correlated states. Furthermore, we investigate the DMRG correlation functions as the number of kept states, m, is changed. We find that the particle-hole correlation length scales as $\xi \propto m^{1.3}$. Moreover, we discuss how symmetries restrict the possibility of long range order in the system.

Key-words: Renormalization Groups, DMRG, Variational states.

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1 Introduction

When the first theories of condensed matter systems were put forward in the beginning of this century by Drude and Sommerfeld [1], the theories were mathematically tractable. The electrons were assumed to move independently of each other and the only effect of the ionic lattice was that sometimes electrons scattered against the fixed ions, this being the origin of the electrical resistivity. However, these simple models were not able to answer some of the fundamental questions one had about the solid state. For example, what distinguishes a metal from an insulator? This question could not be answered until Felix Bloch proved his theorem concerning electrons moving in a perfect periodic potential, due to the ionic lattice. Bloch's theory made it possible to understand most of the basic properties of solids, even though the electrons were still being regarded as independent. In the 50's, Landau [2] was able to give a phenomenological explanation of why the independent electron approximation works so well.

A rigorous treatment of electrons moving in a periodic potential, taking into account electron-electron interactions means solving a huge many-body problem, that is a non-linear partial differential equation with $6N$ variables, where N is the number of electrons in a system. One way to take the interactions into account is to start from non-interacting system and assume the interactions to weak, allowing for approximations of a pertubative nature. From the resulting equations, it is then possible to calculate corrections to the independent electron model. Using such a pertubative expansion one could (in principle) systematically compute corrections up to any order.

During the 50's, the main problem in the solid state community was to understand superconductivity. Many ingenious minds worked on this problem and one lesson that was learned on the path to the BCS-theory [3] was that the transition to a superconducting state could not be described within the usual pertubative approach starting from the free electron gas. The reason is that the superconducting state is so strongly correlated that a pertubative expansion is not valid, one can not obtain the superconducting ground state by changing the state continuously. Since then, a lot of work in condensed matter physics has been related to such strongly correlated systems and hence also methods that are of a non-pertubative nature. Numerical methods are often useful in these cases and the methods that this thesis is concerned with belong to the class of non-pertubative methods. The research on strongly correlated systems is perhaps more active today than ever and solid state theorists every day talks about Hubbard models, Heisenberg models, Kondo systems etc, all being examples of strongly correlated quantum systems. Other examples of strongly interacting electron systems are the fractional quantum Hall effect, the subject of this years Nobel prize, and also high-temperature superconductivity.

The problem with interacting quantum systems is that the complexity of such a system increases exponentially with the size of the system (or the number of particles). Since our ambition is to describe a real system, often consisting of a macroscopic number of particles, it is evident that the complexity is enormous. Even though there exist some analytical results for many systems, in general, analytical calculations often leave many questions open and one has to adopt

numerical methods to complement the analytical results. Furthermore, numerical calculations have been used to check predictions of analytical methods, like different field theories, one of the most famous examples being Haldanes conjecture of a the gap in the spin-1 antiferromagnetic Heisenberg model [4].

Numerical methods in condensed matter physics have become more and more important as both the complexity of the problems being studied and the computational power of the computers have increased rapidly. In this thesis we will focus on one particular type of numerical methods, the Real Space Renormalization Group methods (RSRG). These methods have their origin back in the 70's when Kenneth Wilson invented them to study the effects of electrons in a metal scattering against magnetic impurities, known as the Kondo problem [5]. Using RSRG, together with a large amount of tricks and genius, he was able to deduce unprecedented information about the behavior of this system. That some of these results could be exactly calculated a few years later does not diminish his accomplishment.

After Wilsons successful application of his numerical renormalization group scheme to the Kondo problem, a lot of attempts were made to apply his ideas to other systems as well [6]. However, the outcome was not as good as one could hope for, and it took another fifteen years before the reason for this was understood. In 1992, Steven White and Reinhardt Noack [7] investigated an RSRG approach to a simple system, consisting of a single massive particle moving freely in a lattice (a strategy proposed by Wilson). Using this simple model, they were able to figure out the problems with the RSRG and when this was done, they could also come up with more efficient algorithms. One of these algorithms lead White to the invention of the Density-Matrix Renormalization Group (DMRG) method later on in 1992 [8]. This method turned out to give astonishing results and in the years to follow people applied and extended the method to a wide range of problems. Originally, the method was designed to deal with one-dimensional quantum systems [9, 10], but today it is used to compute properties of two dimensional classical statistical mechanics systems [11], one dimensional quantum systems at finite temperature [12], finite two dimensional quantum systems [13] and the list can be made longer, with these being perhaps the most important areas of application so far.

The aim of this thesis is to introduce the RSRG and DMRG methods, describe their structures, similarities, and differences. Focusing on the theory underlying the methods, and not so much on how to make the algorithms computationally efficient exploiting different tricks, the hope is that the thesis will give an understanding of how the methods work and why they work as well as they do. The text will also serve as an introduction to the paper, which discusses the application of the DMRG to a gapless system. Since one of the ambitions has been to try to complement the existing texts on these topics, the discussion is quite detailed at some points, while at other points the discussion is more "handwaving" and we refer to the references for more complete treatments.

In Chapter 2, we introduce the ideas and basic concepts needed in a numerical RSRG method. We describe and discuss both the RSRG and DMRG algorithms. Furthermore we investigate the properties of the projection operator, the fundamental object in the numerical renormalization group methods. Next, in Chapter 3, we proceed with the discussions on the projection operator, now focusing on the convergence properties and the fixed point structure of the method in terms of so called matrix product states. The last chapter serves as an introduction to the paper. We describe the model we have used, how the matrix product formalism has been adapted to this problem, and finally there is a brief discussion of our results.

2 Numerical renormalization group methods

2.1 General ideas

The general idea behind renormalization group methods [6,7,14] is that in a large system, states that locally correspond to a high energies are not important in describing the low-energy physics of the system. This means that we can build a large system from smaller sub-systems where only the low-energy degrees of freedom are kept. An RSRG algorithm consists of two parts: a method to glue small systems together to form larger ones, and a method to throw away unimportant information from the description of the systems. Let us start with the second part.

Suppose that at some stage, say iteration n, in a renormalization group scheme, the system is described by the states $\{|i'\rangle\}_{i'=1}^{m'}$, spanning the Hilbert space $\mathcal{H}'_n$. Now we want to throw away states that we regard as, in some sense, "unimportant" in describing the low-energy physics of the system. Let us denote the effective Hilbert space, consisting of the m most important states in $\mathcal{H}'_n$, by $\mathcal{H}_n$. Let $A_n : \mathcal{H}'_n \longmapsto \mathcal{H}_n$ denote the operator that performs the truncation, the operator $A_n^\dagger : \mathcal{H}_n \longmapsto \mathcal{H}'_n$ can then be interpreted as an embedding operator of $\mathcal{H}_n$ into $\mathcal{H}'_n$. To simplify our notation, we will from now on drop the index n, refering to the number of iterations that have been performed. When needed, we will put this index back into the expressions. If we demand A to preserve orthonormal basis states we have the restriction, $AA^\dagger = \mathbb{1}_{\mathcal{H}}$. Of course, in general $A^\dagger A \neq \mathbb{1}_{\mathcal{H}'}$ since $\ker A \neq 0$.

Let us assume that the importance of a state $|i'\rangle$ can be measured by some operator ρ', and that the $|i'\rangle$'s are eigenstates of ρ'. A reasonable operator could be the Hamiltonian, and in that case we would keep the m energetically lowest states in $\mathcal{H}'$. In the renormalization group to be discussed later, the operator that will actually be used is a density operator, which explains the notation ρ'. At the moment it is however not important to understand what the operator ρ' really is, we simply assume that it is a good choice and that the importance of a state is larger the larger the corresponding ρ'-eigenvalue is. Our A matrix will be determined by the fact that $\mathcal{H}'$ and $\mathcal{H}$ should have the upper part of the spectrum of the corresponding operators ρ' and ρ in common, where ρ is the operator acting on $\mathcal{H}$. This fact is expressed by

$$\rho A = A\rho'. \tag{2.1}$$

To check this, assume $|i'\rangle \notin \ker A$. Then we have

$$\rho|i\rangle = \rho A|i'\rangle = A\rho'|i'\rangle = \rho'_i A|i'\rangle = \rho'_i|i\rangle.$$

The defining relation, Eq. (2.1), can also be expressed through the commutative diagram

$$\begin{array}{ccc} & \mathcal{H}' & \xrightarrow{A} & \mathcal{H} & \\ \rho' & \downarrow & & \downarrow & \rho \\ & \mathcal{H}' & \xrightarrow{A} & \mathcal{H} & \end{array} .$$

A solution to the equation for the projection operator, Eq. (2.1), together with the condition $AA^\dagger = \mathbb{1}_{\mathcal{H}}$ is provided by

$$A = \sum_{i=1}^{m} |i\rangle\langle i'|, \tag{2.2}$$

where we assumed that the states $|i\rangle$ ($|i'\rangle$) are enumerated in decreasing order of their ρ (ρ') eigenvalues.

The effective operator ρ can be obtained by operating with $A^\dagger$ from the right on Eq. (2.1) which results in

$$\rho = A\rho' A^\dagger. \tag{2.3}$$

Similarly, any operator $\mathcal{O}'$ acting on $\mathcal{H}'$ induces an effective operator $\mathcal{O}$ acting on $\mathcal{H}$ via

$$\mathcal{O} = A\mathcal{O}' A^\dagger. \tag{2.4}$$

Note that this does not imply that $\mathcal{O}A = A\mathcal{O}'$ and hence the spectrum of $\mathcal{O}$ is not identical to part of the spectrum of $\mathcal{O}'$.

2.2 Mathematics of the projection operator

If we did not know how to create the projection operator A using the operator ρ' which tells us which states we should keep, we could still implement a numerical renormalization group scheme. In principle the method works with any A that preservers orthonormal basis states and we could think of using some variational method where we find the "most suitable" matrix elements of A under the constraint $AA^\dagger = \mathbb{1}$. By "most suitable" we mean that an energy or some other quantity should be optimized. A reasonable question to ask is, how many free parameters are there in the projection operator A? Naively, this is the number of parameters needed to parametrise an arbitrary embedding of the set of m-dimensional planes in $\mathbb{R}^{m'}$, which is nothing but the Grassmannian manifold, $G_{m,m'}(\mathbb{R})$. Thus, the number of free parameters is $\dim G_{m,m'}(\mathbb{R}) = m(m'-m)$. In many cases it is possible to further reduce the number of degrees of freedom in the projection operator. This is when the Hamiltonian possesses some symmetries.

Suppose that the Hamiltonian is invariant under some group of transformations $\mathcal{G}$. For example $\mathcal{G}$ could be the $\mathsf{SU(2)}$ symmetry of an isotropic spin chain, or, as in the model we used in the paper, $\mathsf{U(1)}$ (particle number conservation) together with $\mathbb{Z}_2$ particle-hole symmetry. The Hilbert space $\mathcal{H}'$ is formed out of irreducible representations of the symmetry group $\mathcal{G}$. Normally, when working with renormalization group methods, one demands the transformation to preserve the symmetries of the system [15]. The reason for this is that which universality class a system belongs to depends on the symmetries of the system, which means that we must preserve the symmetries to make sure that the critical behavior of the system is not changed by the transformations [15]. Such a restriction will also be put on the projection operator of our RSRG method. This restriction implies that we must choose an operator ρ that is invariant under the same set of symmetry transformations as the Hamiltonian H, otherwise we cannot use good quantum numbers to label the states and it will be difficult to make sure that the symmetries of the system are preserved.

To state the above ideas more formally, decompose the Hilbert space $\mathcal{H}'$ into a direct sum of r' irreducible representations π'_i of $\mathcal{G}$, i.e. $\mathcal{H}' = \bigoplus_{i=1}^{r'} \pi'_i$. If we want our new effective Hilbert space to preserve the symmetries of the original one, we must make sure that we only project

out complete irreducible representations of $\mathcal{G}$. Thus, we may decompose $\mathcal{H}$ as $\mathcal{H} = \bigoplus_{i=1}^{r} \pi_i$, where $r \leq r'$ and $A : \pi_i' \longmapsto \pi_i$, the projection operator maps irreducible representations in $\mathcal{H}'$ to irreducible representations in $\mathcal{H}$.

2.3 Enlarging the lattice, different algorithms

As mentioned in the beginning of this chapter, an RSRG algorithm consists of two parts, the enlarging of the lattice and the truncation process. The previous sections have solely dealt with the second question and we will now turn our attention to the first one.

The renormalization group methods used in classical statistical mechanics [15,16] are mainly block-methods. In these methods a cluster of lattice sites containing a certain number of degrees of freedom is replaced by a new renormalized site carrying a few effective degrees of freedom, approximately describing the properties of the cluster. A couple of these renormalized clusters are then grouped together to form a new cluster which is renormalized and so on. In this way, the lattice is enlarged by grouping together small blocks are effective descriptions of larger blocks. Wilson used another method in his pioneering work on the Kondo problem [5], instead of joining clusters of sites he added a single site to a cluster, thus letting the lattice grow linearly (instead of exponentially) with the number of iterations. Many RSRG algorithms use Wilson's method to increase the lattice. Eq. (2.5) below illustrates how these RSRG algorithms are constructed,

$$\boxed{\mathcal{H}_{n-1}} \overset{add}{\longmapsto} \boxed{\mathcal{H}_{n-1}} \otimes \mathcal{H}_0 = \boxed{\mathcal{H}_n'} \overset{A}{\longmapsto} \boxed{\mathcal{H}_n}. \tag{2.5}$$

$\mathcal{H}_0$ denotes the Hilbert space of the single site being added to the lattice. Furthermore, we have used boxes to denote when Hilbert spaces describe clusters of sites. This can be compared to the block-methods, having the structure

$$\boxed{\mathcal{H}_n} \overset{add}{\longmapsto} \boxed{\mathcal{H}_n} \otimes \boxed{\mathcal{H}_n} = \boxed{\mathcal{H}_{2n}'} \overset{A}{\longmapsto} \boxed{\mathcal{H}_{2n}}. \tag{2.6}$$

In a practical calculation, the blocks are represented by the matrix elements of the relevant operators. Such operators are the Hamiltonian, and also operators that are needed in the increment of the lattice, that is operators in the block that are part of the interactions between the block and the piece of the system to be added. In a computer, the operators are represented as sparse matrices in a block-form, where good quantum numbers are used to label the different blocks. Enlarging the system then means constructing new operators describing the old block together with the new part of the system. This is done using tensor products. For example, the new Hamiltonian for an isotropic spin-s chain with nearest neighbor interactions is constructed as follows

$$H_{n+1}' = H_n \otimes \mathbb{1}_{s\times s} + \mathbf{S}_n^e \otimes \mathbf{S}, \tag{2.7}$$

where $\mathbf{S}_n^e$ represents the spin operators on the edge of the block, which hence must be part of the description of the block, and $\mathbf{S}$ is the spin-operator of the site being added to the block. The next step is to form the projection operator A_n using some prescription and then to form effective operators acting in the truncated Hilbert space through the construction given in Eq. (2.4). More details on the implementation of RSRG methods can be found in the excellent introductions by White [8,17] and we will not discuss the subject in more details.

Let us end this section with some comments on the relationship between the above described numerical renormalization and the "ordinary" renormalization used in the area of critical phenomena. The underlying ideas are similiar, we get rid of high-energy degrees of freedom since

we consider them to be unimportant for the description of low-energy physics. However, there is a main difference in the way we remove the high-energy states. In the ordinary renormalization group approach, the high-energy degrees of freedom are summed over in the partition function, leaving a smaller set of states coupled via renormalized interactions. The renormalization group transformation is defined in such a way that the partition function is invariant under the transformation. However, in our RSRG algorithms, we simply truncate the Hilbert space and hence the partition function is not invariant since

$$Z = \mathrm{tr} e^{-\beta H} \geq \mathrm{tr}[A e^{-\beta H} A^\dagger]. \tag{2.8}$$

To get the inequality we used that $e^{-\beta H}$ is a positive definite operator and hence its diagonal elements are always positive.

Thus there is an important difference between the RSRG algorithms and the ordinary renormalization group methods. A more appropriate name for the RSRG algorithms would perhaps be "iterative truncated basis algorithms".

2.4 The density-matrix renormalization group

In 1992 Steven White developed the density-matrix renormalization group (DMRG), which is basically an RSRG method, but with some very important differences. First of all, since the boundaries of the system are important [7], the method is constructed to deal with these in a simple but efficient way. The way DMRG does this, is by letting the system interact with an environment, which provides natural boundary conditions on the system and hence avoids the problem of having states in the system that are strongly depending on the boundary conditions and for this reason not appropriate for describing bulk properties of a large system. At each iteration the size of the system is increased by a single lattice site, meaning that the standard DMRG implementation is not a block-method. In the end of this section we mention another algorithm, the four-block method due to Bursill, which is a block-method. Figure 2.1 shows the DMRG block-configuration, the superblock. The upper part of the figure, consisting of an old system block, B, together with a single site • which are joined to form a new system block to the next iteration. The lower part of the figure is a copy of the upper part and it is the environment that provides the boundary conditions to the system block. As the figure shows, usually the system block and environment blocks are only connected in one end, and the combined system, the superblock, has open boundary conditions.

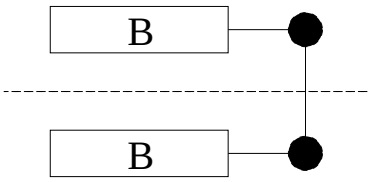

Figure 2.1: The superblock configuration used in the DMRG. The upper part corresponds to the system, while the lower part constitutes the environment. Note that the system- and environment-blocks are only connected in one end. Furthermore we note that the parity operator is simply a reflection through the line between the blocks, and hence parity is easy to use as a good quantum number in the calculations.

We have not yet said anything about how the optimal states of the new system block are chosen, i.e. how we perform the truncation of the Hilbert space. To begin with, we compute

the target state which, if we are interested in ground state properties, simply is the ground state of the superblock. We denote the target state by $|\Psi'\rangle$. This state can be decomposed as $|\Psi'\rangle = \sum_{i',j'} \psi'_{i',j'} |i'\rangle \otimes |j'\rangle$, where $\{|i'\rangle\}$ and $\{|j'\rangle\}$ form complete bases of the system and the environment respectively. A density operator ρ'_{tot} is formed by $\rho'_{tot} = |\Psi'\rangle\langle\Psi'|$. Taking a trace over the environment degrees of freedom of ρ'_{tot} we obtain a reduced density-matrix, $\rho' = \mathrm{tr}_{env}|\Psi'\rangle\langle\Psi'|$, or explicitly using the i'-j'-representation above, $\rho' = \psi'^{*}\psi'^{t}$. Feynman has written a nice introduction to density operators [18] and we refer to his book for the properties of these objects. The key point is that the eigenvalues of the reduced density-matrix for the system block are the probabilities of finding the system block in the corresponding eigenstates given that the superblock system is in the target state, $|\Psi'\rangle$. This means that the density operator provides us with a measure of the importance of the states in the system block and furthermore it has the same symmetries as the Hamiltonian. Note however that $[\rho', H'] \neq 0$, and hence the kept states will, in general, not be energy eigenstates. When we know which states to keep, we proceed as in the RSRG methods by constructing the projection operator A and truncating all the operators describing the system. In this way we achieve an iterative algorithm.

As argued by White [8], a simple error measure is the truncated weight of the density-matrix, $1 - \sum_{i=1}^{m} \rho'_i$ (we know $\mathrm{tr}\rho' = 1$), where ρ'_i is the i'th largest eigenvalue of ρ'. The DMRG is constructed to maximize the overlap between the exact target state $|\Psi'\rangle$ and the optimal description of the target state, using the truncated basis.

The procedure described above is called the infinite system method since the idea is to run the algorithm until the size of the system is so large that it effectively describes an infinite system, i.e. the thermodynamic limit. White also suggested another algorithm, the finite size method [8], which is constructed to give an optimal description of a system of a certain, finite, length. This method is more accurate than the infinite system method and it is often better to use the finite size method to compute, say the gap, for a certain number of fixed lengths of the system and then extrapolate the result to the thermodynamic limit, rather than using the infinite system method to compute the gap in the thermodynamic limit directly.

A drawback with this type of iterative enlarging of the lattice is that a possible translational invariance of the system cannot be used explicitly, i.e. we cannot use momentum as a good quantum number in our algorithms. Attempts have been made [19] to implement DMRG in momentum space contrary to real space, but these ideas have not received much attention. Parity, on the other hand, is easy to use as a good quantum number in the algorithms and can be used to reduce the needed computational effort.

Recently, Bursill [20] modified the prescription for enlarging the lattice, having a superblock containing four copies of the system block with periodic boundary conditions. A new system block is then formed by joining two system blocks, so this is really a block method because the size of the lattice increases exponentially. Using this blocking-procedure it is possible to partly preserve the translational invariance since it is now possible to target states with momentum $k = 2\pi/N$ directly, where N is the size of the superblock. Thus we see that as we iterate the procedure we can target excitations with small momentum, which often are the most interesting ones.

2.5 Why does the DMRG work so well?

After its appearance, the DMRG has produced a large amount of extremely accurate results [8,9]. Why is the DMRG so accurate? First of all, as White and Noack argued [7], the boundary conditions on the systems are crucial in the renormalization group methods, and the idea of a

superblock is a simple and effective way to take these into account. Moreover, White [8] proved that DMRG maximizes the overlap between the exact target state and the one obtained after truncation of the Hilbert space. Another approach is to consider DMRG as a variational method optimizing the ground state energy of the system [21]. Even though all of these arguments indicate that DMRG is a good way to implement a numerical renormalization group scheme, they do not answer the question of why the method is so accurate.

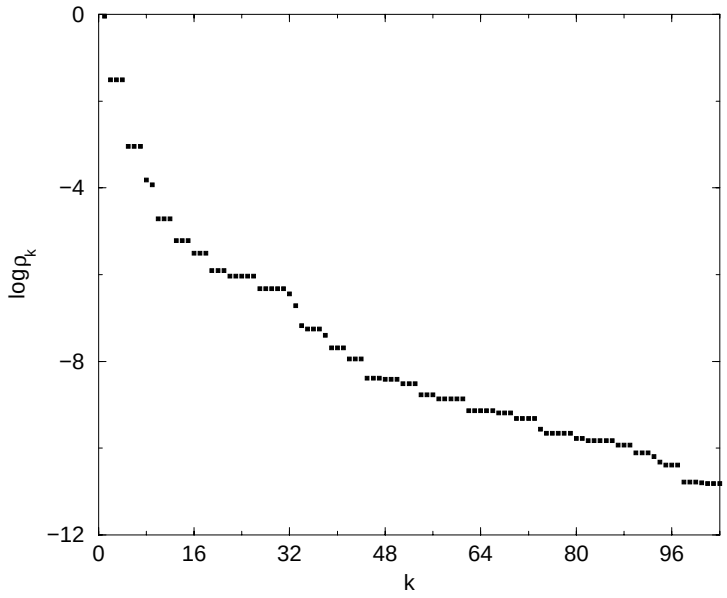

Figure 2.2: Upper part of the density-matrix spectrum of a spin-1/2 antiferromagnetic Heisenberg model with next nearest neighbor interaction $J_2 = 0.75$ ($J_1 = 1.0$) consisting of 64 sites. The figure shows how the spectrum is split up into multiplets corresponding to irreducible representations of the total spin. In the calculation we have kept 400 states in the basis.

The key to the success of DMRG, lies in the decay rate of the eigenvalues of the density-matrix. In Figure 2.2, part of the spectrum of the density-matrix for a gapped spin-1/2 antiferromagnetic Heisenberg model with next nearest neighbor interactions is shown. It is clear from the figure that the eigenvalues of the density-matrix decrease rather rapidly, showing that the truncation error decreases rapidly with the number of kept states. Recently Peschel *et. al.* [22] and Okunishi *et. al.* [23] studied the decay rate of the density-matrix using analytical methods. Their approach is based on the fact that a one-dimensional quantum system is related to a two-dimensional classical statistical mechanics system in such a way that the Hamiltonian of the quantum system can be related to the transfer matrix of the classical system and, furthermore, the ground state of the Hamiltonian is also the eigenvector corresponding to the maximum eigenvalue of the transfer matrix [24].

It can then be argued that the density-matrix is related to a so called corner transfer matrix, a construction due to Baxter, at least for non-critical systems where boundary effects can be neglected. For integrable systems the spectrum of the corner transfer matrix is known and hence also the spectrum of the corresponding density-matrix is known. Using this as a starting point, Okunishi *et. al.* [23] conjecture an asymptotic form of the density-matrix spectrum for a non-integrable system. The conjecture is that the k'th eigenvalue, ρ_k, of the density-matrix is

given by the universal form

$$\ln\left[k\left(\frac{\ln\rho_k}{\ln z}\right)^{1/4}\right] = B\sqrt{\frac{\ln\rho_k}{\ln z}}, \tag{2.9}$$

where z and B are two parameters that are known only for integrable models so they must be numerically determined for the non-integrable cases. The form Eq. (2.9) leads to the following asymptotic form of the spectrum

$$\rho_k \propto \exp[-A(\ln k)^2], \tag{2.10}$$

where the constant $A = |\ln z|/B^2$. In Figure 2.3 we have used the numerical data presented in Figure 2.2 and plotted $\ln[k|\ln\rho_k|^{1/4}]$ versus $|\ln\rho_k|^{1/2}$. As can be seen, the numerical spectrum fits the form given by Eq. (2.9) well, thus supporting the conjecture in this specific case. From the fitted line we can read off the model specific parameters $B \approx 0.0625$ and $z \approx 0.998$, which in turn implies that $A \approx 0.51$ for this model.

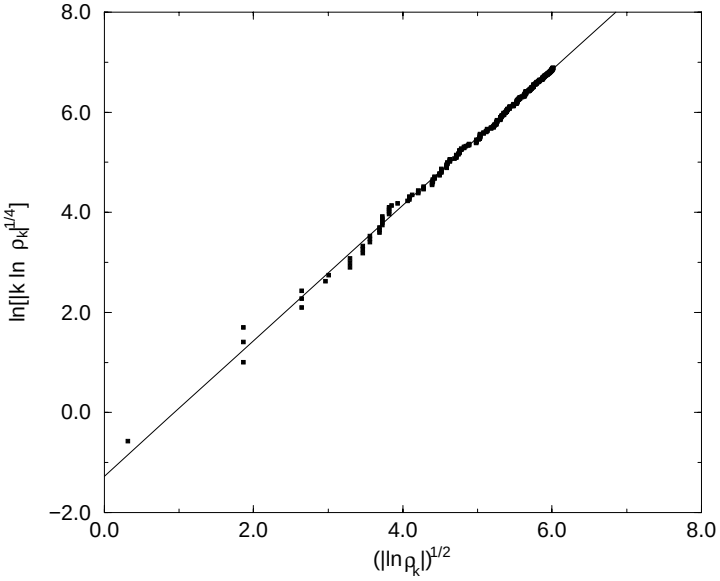

Figure 2.3: The spectrum of the density-matrix for the 64-site spin-1/2 Heisenberg model with next nearest neighbor interaction $J_2 = 0.75$ ($J_1 = 1.0$). The data are plotted in a form such that the asymptotic behavior of the spectrum is clear. In the calculation 400 states have been kept and the figure also contains 400 eigenvalues.

This work by Okunishi *et. al.* has useful consequences. If the asymptotic form, Eq. (2.10), is correct, we can use it to determine the truncation error of the density-matrix as a function of the number of kept states and the model specific parameters B and z. As mentioned above, these have to be determined from some DMRG calculation. The truncation error is then given by

$$\epsilon = \sum_{k=m+1}^{\infty} \rho_k \approx \frac{\int_m^\infty \exp[-A(\ln k)^2]dk}{\int_1^\infty \exp[-A(\ln k)^2]dk}$$

where we have replaced the sum by an integral and normalized the eigenvalues so that they sum up to 1. The integrals in the above equation may be evaluated in terms of the error-function

$\mathrm{erf}(x)$, which results in

$$\epsilon \approx \frac{1-\mathrm{erf}(\sqrt{A}\ln m - 1/2\sqrt{A})}{1+\mathrm{erf}(1/2\sqrt{A})}, \tag{2.11}$$

where we have assumed $\ln m \geq 1/2A$ which should be true if the system is not very close to a critical point (i.e. $z \approx 1$) in which case the conjecture Eq. (2.9) is not expected to hold anyway. Note that the inequality is satisfied when $m > 3$ in our numerical example.

We may also invert Eq. (2.11) to express the number of states we need to keep given a certain truncation error ϵ. The result is

$$\begin{aligned} m &\approx \exp[1/2A]\exp\Big[\mathrm{erf}^{-1}\Big(1-\epsilon(1+\mathrm{erf}(1/2\sqrt{A}))\Big)/\sqrt{A}\Big] \\ &\approx \exp[1/2A]\exp\Big[\sqrt{-A^{-1}\ln[\epsilon\sqrt{\pi}(1+\mathrm{erf}(1/2\sqrt{A}))]}\Big] \\ &\approx \exp\Big[\frac{1}{2A}+\sqrt{\frac{-\ln\epsilon}{A}}\Big] \end{aligned} \tag{2.12}$$

where we in the second line used the asymptotic form of the error-function [25]. In the last line have used that $\sqrt{\pi}(1+\mathrm{erf}(1/2\sqrt{A})) = O(1)$ which means that we may neglect this term compared to ϵ. Eq. (2.12) could be quite useful since it relates the accuracy of a calculation to the needed computational effort. Thus, if the conjecture is true, we have a nice picture of how DMRG performs for non-critical systems. How it behaves for critical systems is still not known. The intention with our paper was to improve the understanding of DMRG for gapless, critical systems.

3 More on numerical renormalization group methods

3.1 Reaching a fixed point

In the previous chapter, we have discussed RSRG algorithms and in particular the DMRG algorithm. An interesting question one can ask is what kind of approximate states do the methods produce, and what are the properties of these? The way to deal with these questions is to consider the structure of the states in the thermodynamic limit. This analysis was performed by Östlund and Rommer [21] and we will refer to the literature for a detailed discussion.

Suppose that at iteration n the projection operator is given by A_n, i.e. $A_n : \mathcal{H}_{n-1} \otimes \mathcal{H}_0 \longmapsto \mathcal{H}_n$. If the matrix A_n converges in the thermodynamic limit $n \to \infty$,

$$\lim_{n\to\infty} A_n = A, \tag{3.1}$$

important conclusions can be drawn. More generally, we can allow the projection operator to be cyclic, in the sense that we have a finite number, p, of projection operators repeating themselves with periodicity p. This is the case in for example a translationally invariant spin-1/2 system where the period is $p = 2$ (more details on this can be found in the paper). The following discussion assumes $p = 1$, but this is mainly a question of notation. Thus we have reduced all degrees of freedom of the approximate states to those of the projection operator. Since these, as was shown in the previous chapter, can be reduced further by exploiting the symmetries of the system, it is practically possible to treat the problem of finding A as a variational problem, at least for relatively small numbers of kept states.

As we discussed in the previous chapter, to make optimal use of the symmetries of the system we decompose the Hilbert space into a direct sum of irreducible representations of the symmetry group. If the Hilbert space $\mathcal{H}_{n-1}$ is decomposed as $\mathcal{H}_{n-1} = \bigoplus_{i=1}^{r} \mathbf{s}_i$, the domain of A_n is $\mathcal{H}_{n-1} \otimes \mathcal{H}_0 = \bigoplus_{i=1}^{r} \mathbf{s}_i \otimes \mathbf{s} = \bigoplus_{i=1}^{r'} \mathbf{s}'_i$. Thus the operator A_n must perform this tensor product decomposition and it must also select the appropriate subspace to keep as a description of the system.

3.2 Matrix product states

As was shown in reference [21], if the projection operator converges to a fixed point, the states generated by iterating the renormalization group procedure has the matrix product form

$$|\beta\rangle_n = \sum_{\{s_i\}} (A[s_1] \cdots A[s_n])^{\beta_n,\beta_0} |s_1 \cdots s_n\rangle \otimes |\beta_0\rangle. \tag{3.2}$$

A state in the bulk can be described as

$$|Q\rangle_n = \sum_{\{s_i\}} \mathrm{tr}[QA[s_1] \cdots A[s_n]]|s_1 \cdots s_n\rangle, \tag{3.3}$$

where Q is an $m \times m$ matrix specifying β_n and β_0 which can be viewed as boundary conditions on the system. If we want our state to have momentum k we must look for a matrix Q such that $QA[s] = e^{ik}A[s]Q$ for all s.

Defining the $\widehat{\ }$-mapping from a local $s \times s$ matrix M to an $m^2 \times m^2$ matrix $\widehat{M}$ via

$$\widehat{M} = \sum_{s,s'} M_{s,s'} A^*[s'] \otimes A[s], \tag{3.4}$$

it becomes a trivial task to compute expectation values in the Q-states. With $\widehat{Q} = Q^* \otimes Q$ we have

$$\langle Q|M^1_{i_1} \cdots M^k_{i_k}|Q\rangle = \frac{\mathrm{tr}[\widehat{Q}\widehat{1}^{i_1-1}\widehat{M^1}\widehat{1}^{i_2-i_1-1}\widehat{M^2}\cdots\widehat{M^k}\widehat{1}^{n-i_k}]}{\mathrm{tr}[\widehat{Q}\widehat{1}^n]}, \tag{3.5}$$

where $\widehat{1}$ is the $\widehat{\ }$-mapping of the identity matrix. Actually, the form of this expression depends on the statistics (commutation relations) of the operators in the expectation value. This topic is discussed in chapter 4 and as well as in the paper. We solve the problem by introducing the matrix $\widehat{F}$ which is the $\widehat{\ }$-mapping of the matrix $F = \mathrm{diag}(-1, 1)$ and which takes care of the fermionic operators in a system of spinless fermions. This operator has its origin in the string-operator of the Jordan-Wigner transformation.

In particular, Eq. (3.5) allows us to compute the energy of the Q-states. Making use of symmetries of the model to reduce the number of free parameters, we can use the above equation to perform a variational calculation to find the optimal (the one that minimizes the ground state energy) projection operator A. In Figure 3.1, we show the energy-landscape obtained for an isotropic spin-1 Heisenberg antiferromagnet keeping two total spin representations. The matrix Q is chosen as the $m \times m$ identity matrix in order to get a translationally invariant state (it trivially satisfies $QA[s] = A[s]Q$ for all s).

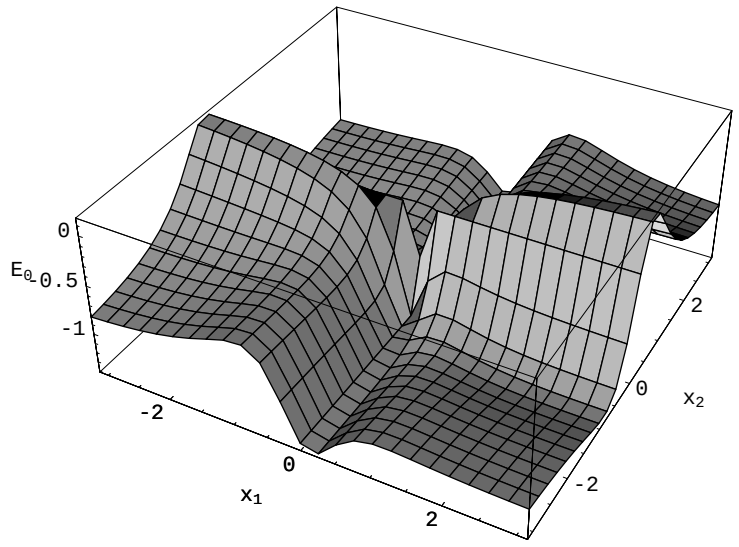

Figure 3.1: A typical energy landscape $E_0(\{x\})$ for the spin-1 antiferromagnetic Heisenberg model. This figure corresponds to a variational calculation using two free parameters corresponding to two total-spin representations, $(\frac{1}{2} \oplus \frac{3}{2})$.

Another method to obtain the A-matrices is of course to make a DMRG calculation where the iterations proceed until the projection operator has converged to some accuracy. Performing calculations within the matrix product basis is, in a sense, much more convenient than calculating expectation values within the DMRG method, since all the input we need is the projection operator and once we have found and stored it, we can always go back and compute additional quantities. If we computed the quantities within the DMRG we would have to restart the calculation and run through the whole procedure again, which takes a lot of time.

As it will turn out when we continue the investigation of the matrix product states, the properties of the matrix $\widehat{1}$ are very important. The spectrum of this matrix turns out to contain all possible correlation lengths in the system. Therefore, we will now discuss some important properties of this matrix.

First of all it is non-symmetric, which means that we must distinguish between left and right eigenvectors. When thinking about this matrix it is often useful to recall that the indices of A are states and hence also the indices of the $\widehat{\ }$-operators correspond to states (or rather pairs of states). This implies that we can think of the indices as carrying quantum numbers. In the paper we use symmetry arguments to make conclusions about the properties of the eigenstates of $\widehat{1}$. We also show that the matrix $\widehat{F}$ is closely related to $\widehat{1}$, actually they are equal up to a phase-factor and a unitary transformation.

We will now discuss some intrinsic properties of the spectrum of $\widehat{1}$. First of all, all eigenvalues λ of $\widehat{1}$ satisfy $|\lambda| \leq 1$. To show this we use the matrix norm $||\cdot||_2$ which has the property [26]

$$||M||_2 = \sigma_{max}(M) = \sqrt{\max \mathrm{eval}(M^t M)}, \tag{3.6}$$

where $\sigma_{max}(M)$ is the maximum singular value of M and $\mathrm{eval}(M)$ denotes eigenvalues of M. We may rewrite the equation $\widehat{1}v = \lambda v$ as

$$A(v \otimes \mathbb{1}_{s\times s})A^t = \lambda v \tag{3.7}$$

where we interpret v as an $m \times m$ matrix. Taking the norm of both sides we have

$$|\lambda|||v||_2 = ||A(v \otimes \mathbb{1}_{s\times s})A^t||_2 \leq ||A||_2||v \otimes \mathbb{1}_{s\times s}||_2||A^t||_2.$$

Recalling that $AA^t = \mathbb{1}$ has the maximum eigenvalue 1 (all the eigenvalues are 1) we have $||A^t||_2 = 1$. Thus we also have $\sigma_{max}(A^t) = 1$ which, since $\sigma_{max}(A) = \sigma_{max}(A^t)$, yields $||A||_2 = 1$. Finally, noting that $||v \otimes \mathbb{1}||_2 = ||v||_2$ we are left with the result $|\lambda| \leq 1$. Moreover, choosing $v = \mathbb{1}$ in Eq. (3.7) and making use of $AA^t = \mathbb{1}$, we find that $\widehat{1}$ always has an eigenvalue equal to 1.

The matrix product formalism allows us to draw qualitative conclusions concerning the properties of the states produced by the DMRG. If we, for example, consider the spin-spin correlation function in a spin-chain, it has the structure

$$\langle S_i^z S_{i+l}^z \rangle_Q \propto \mathrm{tr}[\widehat{Q}\widehat{1}^{i-1}\widehat{S^z}\widehat{1}^{l-1}\widehat{S^z}\widehat{1}^{n-i-l}] = \mathrm{tr}[\widehat{\mathcal{O}}\widehat{1}^{l-1}].$$

In the last step we introduced the shorthand notation $\widehat{\mathcal{O}} = \widehat{S^z}\widehat{1}^{n-i-l}\widehat{Q}\widehat{1}^{i-1}\widehat{S^z}$ which is valid under the assumption that $n \gg i + l$ so that we can replace $\widehat{1}^{n-i-l}$ by $\widehat{1}^{\infty}$, independent of l. If we now diagonalize the matrix $\widehat{1} = U\widehat{1}_D U^{-1}$ and introduce $\widehat{\mathcal{O}}_D = U^{-1}\widehat{\mathcal{O}}U$ we find

$$\langle S_i^z S_{i+l}^z \rangle_Q \propto \mathrm{tr}[\widehat{\mathcal{O}}_D \widehat{1}_D^{l-1}] = \sum_{i=1}^{m^2} (\widehat{\mathcal{O}}_D)_{i,i} \lambda_i^{l-1}. \tag{3.8}$$

From Eq. (3.8) it follows that the correlation functions obtained from the matrix product states are sums of exponentially decaying functions. The correlation length is given by the dominant eigenvalue λ of $\widehat{1}$ which corresponds to a non-zero amplitude $a_i = (\widehat{\mathcal{O}}_D)_{i,i}\lambda_i^{-1}$. Explicitly, we have $\xi = -1/\ln|\lambda|$, i.e. as long as $|\lambda| < 1$ the correlation length is finite and the correlation function decays exponentially. This means that the matrix product states cannot asymptotically describe quasi long range correlations correctly. Either the correlation functions decay exponentially $\lambda < 1$ or they show true long range order $\lambda = 1$. Algebraic correlations can only be obtained asymptotically as the number of kept states is increased to infinity.

Let us, for the sake of curiosity, think about what the spectrum of $\widehat{1}$ must look like in order to get correlation functions that decay algebraically. Suppose that the set of (real) eigenvalues of $\widehat{1}$ is $\{\lambda_i\}$, and that the amplitudes of the respective eigenvalues are a_i, i.e. we can write the correlation function as

$$C(l) = \sum_i a_i \lambda_i^l = \int_{-1}^{1} d\lambda \rho(\lambda) a(\lambda) \lambda^l, \tag{3.9}$$

where we have defined a "density of eigenvalues" $\rho(\lambda)$. Let us introduce the weight function $f(\lambda) = \rho(\lambda)a(\lambda)$. What functional form must the weight function $f(\lambda)$ take to create a correlation function that decays algebraically? Does such a form exist? Suppose we know that $C(l) = l^{-q}$ where q is some positive number. We will put an index q on the functions f in order to stress their dependence on q.

Taking a derivative of Eq. (3.9) with respect to l, one finds the recursion relation

$$f_{q+1}(\lambda) = -\frac{\ln|\lambda|}{q} f_q(\lambda),$$

which, together with the trivial solution $f_1(\lambda) = \lambda^{-1}$, provides us with the solution

$$f_{q+1}(\lambda) = \frac{(-1)^q}{q!} \frac{\ln^q|\lambda|}{\lambda}. \tag{3.10}$$

In this way we have obtained solutions for all positive integers q and this shows that the matrix product states consistently can describe algebraically decaying correlation functions in the limit where we keep an infinite number of states. The above solutions $f_q(\lambda)$ also give the correct asymptotic behavior for any real number $q > 0$. What really determines the asymptotic behavior of $C(l)$ as $l \to \infty$ is the analytic structure of the function $f(\lambda)$ in the limit $|\lambda| \to 1$. The interior of the disk $|\lambda| \leq 1$ only contributes to the behavior of short-range correlations. To be more precise; a sufficient condition on the function $f_q(\lambda)$ is that its asymptotic behavior as $|\lambda| \to 1^-$ is given by

$$f_q(\lambda) \propto (1 - |\lambda|)^{q-1}. \tag{3.11}$$

This statement is true even if the eigenvalues are not distributed along the real axis, they may be distributed along rays through the origin, giving rise to a periodicity in the phase of the correlation function.

Now, when the basic properties of the matrix product states are understood, it is possible to extend the formalism to generate excited states. Assuming periodic boundary conditions on the system we can form states with a definite momentum k by constructing a linear combination of Q-states. These Bloch-states have the form

$$|Q,k\rangle_n = \sum_{j=1}^{n} \sum_{\{s_i\}} e^{ijk} \mathrm{tr}[A[s_1]\cdots A[s_{j-1}]QA[s_j]\cdots A[s_n]]|s_1\cdots s_n\rangle. \tag{3.12}$$

The ansatz seems to describe excitations accurately and has the great advantage over the excitations found from DMRG that we can specify the momentum k. A drawback with this ansatz is that the calculations become very cumbersome as the number of kept states in A is increased. Furthermore it is difficult to know how accurate these excitations are, even though all cases we have studied has shown good agreement with the best available results. In the paper we use an ansatz of the above form to look at the excitation spectrum of a system of free fermions. We prove that the spectrum obtained this way has a certain symmetry that also exist in the exact solution, namely $E(k) = E(\pi - k)$. The crucial point for the existance of this symmetry is the spin of the model, (the free fermions are mapped onto spin-1/2 objects) and we believe this symmetry to be a rather general feature of half-integer spin systems.

4 DMRG for gapless systems

4.1 A model problem

With the aim of investigating the behavior of DMRG for a gapless system, we had to choose an appropriate model to work with. We wanted the model to be simple and exactly solvable and furthermore we wanted a simple parameter that we could use to tune the size of the gap.

The simplest gapless model one can think of is a model of free spinless fermions on a lattice. In this section we will assume that the lattice has periodic boundary conditions and lattice spacing $a = 1$. Note that the DMRG calculations discussed in the next chapter are performed assuming open boundary conditions, since open boundary conditions are more easy to treat numerically and the choice of boundary conditions is not crucial to the physics of the model. It is possible to introduce a gap in this model, without destroying the existence of an exact solution, by introducing a staggered on-site potential on the lattice. Let N be the size of the lattice, ϵ the strength of the on-site potential, and t the hopping amplitude. The Hamiltonian then takes the form

$$H = -\frac{t}{2}\sum_{j=1}^{N}[c_j^\dagger c_{j+1} + \text{h.c.}] + \epsilon\sum_{j=1}^{N}(-1)^j c_j^\dagger c_j, \tag{4.1}$$

with the c's being fermionic annihilation operators. Before we go on and diagonalize the Hamiltonian, let us take a more careful look at the model. If $\epsilon = 0$, we are simply left with a system of free fermions, having a finite size gap that scales as N^{-1}, leading to a gapless system in the thermodynamic limit. When the on-site interaction is strong, $|\epsilon/t| \gg 1$, the system will try to pile up electrons on odd or even sites, depending on the sign of ϵ, creating a charge density wave (CDW). This charge density wave will have gapfull excitations with a gap scaling linearly with $|\epsilon|$.

Other important properties are the symmetries of the model, as we have discussed in previous chapters, these can be exploited in the numerical renormalization group approach to reduce the amount of computational effort. The Hamiltonian, Eq. (4.1), has different symmetries depending on the parameters t and ϵ.

1. H is invariant under the global $\mathsf{U}(1)$ transformation $c_j \to e^{i\theta}c_j$. This simply means that the total number of particles in the system is conserved.

2. Translational symmetry. When $\epsilon = 0$, the system is invariant under any lattice translation, i.e. $[\mathcal{T}, H] = 0$, and hence the momentum is a good quantum number. When $\epsilon \neq 0$, the translational symmetry is reduced to $[\mathcal{T}^2, H] = 0$, the system is only invariant under a translation of an even number of lattice sites, hence the size of the first Brillouin zone is halfed, and we will have two energy bands, since there are two sites per primitive cell.

3. For any ϵ, the system is invariant under the "shifted" particle-hole transformation, $c_j \to (-1)^j c_{j+1}^\dagger$.

4. When $\epsilon = 0$ the system is invariant under the particle-hole transformation $c_j \to (-1)^j c_j^\dagger$.

In the paper we only exploit the symmetries 1 and 4.

Solving this model exactly is easy, but we will nevertheless sketch the solution. Since the Hamiltonian is invariant under translations by two lattice sites, we introduce the two-component vector $\Phi_j = (c_{2j-1}, c_{2j})$, with $j = 1, \ldots, N/2$. Next, we introduce collective coordinates

$$\Phi_j = \sqrt{\frac{2}{N}} \sum_k \Phi_k e^{2ijk},$$

with $k \in \{\frac{2\pi}{N} n\}_{n=0}^{\frac{N}{2}-1}$. Rewriting the Hamiltonian in terms of the Φ_k-operators we find

$$H = \sum_k \Phi_k^\dagger H(k) \Phi_k, \text{ where } H(k) = \begin{pmatrix} -\epsilon & -\frac{t}{2}[1 + e^{-2ik}] \\ -\frac{t}{2}[1 + e^{2ik}] & \epsilon \end{pmatrix}. \tag{4.2}$$

To compute the dispersion relation, all we have to do is to diagonalize the 2×2 matrix $H(k)$. We find

$$E^\pm(k) = \pm\sqrt{\epsilon^2 + t^2 \cos^2 k}. \tag{4.3}$$

The corresponding eigenstates are $f_k^{\pm\dagger}|0\rangle_k$, with $|0\rangle_k$ denoting the vacuum in the k-sector of the full Hilbert space, and

$$\begin{aligned} f_k^- &= a_k^- \phi_k^1 + b_k^- \phi_k^2 \\ f_k^+ &= a_k^+ \phi_k^1 + b_k^+ \phi_k^2, \end{aligned}$$

where $a_k^\pm$ and $b_k^\pm$ are coefficients depending on k, ϵ, and t.

We obtain the groundstate by filling up all negative energy states, i.e. all states in the $(-)$ band,

$$|\text{gnd}\rangle = \prod_k f_k^{-\dagger}|0\rangle. \tag{4.4}$$

Going to the thermodynamic limit, $N \to \infty$, the energy per site of the ground state is

$$\lim_{N\to\infty} \frac{E_0}{N} = \lim_{N\to\infty} \frac{1}{2\pi} \sum_k E^-(k)\Delta k = -\frac{1}{\pi} \int_0^{\frac{\pi}{2}} \sqrt{\epsilon^2 + t^2 \cos^2 k} dk = -\frac{\sqrt{\epsilon^2 + t^2}}{\pi} E\Big[\frac{t}{\sqrt{\epsilon^2 + t^2}}\Big], \tag{4.5}$$

where E is the complete elliptic integral of the second kind. From the dispersion relation, Eq. (4.3), we can read off the gap to the first excited state. This gap is simply the gap between the $(-)$ and the $(+)$ band at the Fermi-points $k_F = \pm\frac{\pi}{2}$, this is $\Delta = 2|\epsilon|$. The size of the gap is related to the range of the correlation functions, which is the next topic we will consider.

The structure of the correlation functions played an important role in the discussion in the preceding chapters and to really test our renormalization group methods it is important to check the structure of the numerical correlation functions versus exact results. We will mainly focus on the correlation length of the correlation functions. There are in principle two interesting correlation functions in our model system, the particle-hole and density-density correlation functions. These are defined via

$$\begin{aligned} C_{ph}(l) &= \langle c_j^\dagger c_{j+l} \rangle_0 \\ C_{dd}(l) &= \langle n_j n_{j+l} \rangle_0 - \langle n_j \rangle_0 \langle n_{j+l} \rangle_0, \end{aligned} \tag{4.6}$$

where $n_j = c_j^\dagger c_j$ is the particle-number operator and $\langle \cdot \rangle_0$ denotes ground state expectation value. To extract the correlation length we will take the asymptotic limit $l \to \infty$ and consider only the leading term in the expressions we obtain. Assuming l to be odd (the even l's give zero correlations) we find

$$C_{ph}(l) = -\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{dk}{\pi} e^{ikl} \frac{a_k^+ (b_k^+)^*}{|a_k^- b_k^+ - a_k^+ b_k^-|^2}.$$

Investigating the pole-structure of the denominator, one finds that it has poles at the points $k = \pm\frac{\pi}{2} + ik_0$, where $k_0 = \ln[\epsilon/t + \sqrt{1 + (\epsilon/t)^2}]$. The leading behavior is picked up at the poles and will therefore be governed by the exponential factor containing l with the k-value given by the poles. This implies that

$$C_{ph}(l) \propto e^{-k_0 l} = e^{-l/\xi_{ph}}$$

which allows us to read off $\xi_{ph} = k_0^{-1}$, or

$$\begin{aligned} \xi_{ph} &= \frac{1}{\ln\left[\epsilon/t + \sqrt{1 + (\epsilon/t)^2}\right]} \\ \xi_{dd} &= \xi_{ph}/2. \end{aligned} \tag{4.7}$$

where ξ_{dd} can be computed similarly.

From Eq. (4.7), it is clear that the correlation lengths are finite everywhere except at the point $\epsilon = 0$, where they diverge. This is perfectly consistent with the previously obtained result that the gap of the system goes to zero as $\epsilon \to 0$. At the point $\epsilon = 0$, the system will show algebraically decaying correlation functions and the exact form can be calculated to be

$$\begin{aligned} C_{ph}(l) &= \frac{1}{\pi l} \sin \pi l/2 \\ C_{dd}(l) &= -C_{ph}(l)^2. \end{aligned} \tag{4.8}$$

This will conclude our discussion of the exact properties of the model.

4.2 Adjusting the formalism

With the purpose of investigating the DMRG behavior for the model just described, using the matrix product formalism, the first thing that must be done is to verify that the projection operator reaches a fixed point in the thermodynamic limit. This turns out to be the case and the projection operator has periodicity $p = 2$ due to odd-even effects of the lattice size.

In the matrix product formalism we use the Jordan-Wigner transformation to write our fermionic operators as hard-core boson-operators connected to a string counting the number of particles left to the site. More explicitly the connection is

$$c_j = \exp\Big[i\pi \sum_{k=1}^{j-1} S_k^+ S_k^-\Big] S_j^- = \Big[\bigotimes_{k=1}^{j-1} F\Big] \otimes S_j^-, \tag{4.9}$$

where we have introduced the operator $F = -2S^z = \mathrm{diag}(-1, 1)$. Thus the local fermionic operators are represented as non-local bosonic operators. Working with these bosonic operators, a typical correlation function takes the form

$$C_{ph}(l) = \langle c_j^\dagger c_{j+l} \rangle_f = \langle S_j^+ F_{j+1} \cdots F_{j+l-1} S_{j+l}^- \rangle_b$$

with f and b denoting expectation values with respect to the fermionic- and bosonic ground states respectively. Using the matrix product formalism this expectation value is

$$C_{ph}(l) = \frac{\mathrm{tr}[\widehat{1}^{j-1}\widehat{S^+}\widehat{F}^{l-1}\widehat{S^-}\widehat{1}^{n-l-j}]}{\mathrm{tr}\widehat{1}^n}$$

where we have chosen the ground state $Q = \mathbb{1}$. This motivates the introduction of the operator $\widehat{F}$ which is used throughout the paper. It governs correlation functions between fermionic operators, just as $\widehat{1}$ governs the correlation functions between bosonic operators. In the paper we show that the spectrum of these two operators are equal up to a factor i, which means that they yield the same set of possible correlation lengths.

Working in spin-language, the 2-periodic projection operator has the block-structure

$$A[s] = \begin{pmatrix} 0 & A_{\mathtt{hi}\to\mathtt{i}}[s] \\ A_{\mathtt{i}\to\mathtt{hi}}[s] & 0 \end{pmatrix},$$

with `i` and `hi` denoting integer- and half-integer total S^z representations respectively. From the construction of the $\widehat{\ }$-mapping, it is clear that this block-structure gives rise to a block-structure in the $\widehat{\ }$-operators as well. In particular it implies that the eigenvalues of $\widehat{1}$ (and hence also $\widehat{F}$) appear in pairs $\pm\lambda$. The paper provides a proof of this result.

As was argued in Chapter 3, the existence of a fixed point of the DMRG projection operator implies that the states produced by DMRG will have exponentially decaying correlation functions, even though the system is at criticality. An interesting issue to study is therefore how the correlation length obtained from DMRG for the gapless system of free fermions, depends on the number of kept states in Hilbert space. One would expect that as the number of kept states is increased, the description of the ground state becomes better and better and hence the correlation length should increase. In the paper we justify this behavior and we also make a quantitative statement of how the correlation length depends on the number of kept states.

A nice way to compute the correlation length from a DMRG calculation is to use the matrix product formalism. Suppose we want to compute the particle-hole correlation length. The set of possible correlation lengths are then given by the spectrum of the matrix $\widehat{F}$, but we could equally well use $\widehat{1}$ since we know that the spectra of these matrices only differ by a factor i. The spectrum of $\widehat{1}$ is found by solving the eigenvalue problem $\widehat{1}v = \lambda v$ which can be recast into the form

$$\sum_s A[s]vA^t[s] = \lambda v,$$

with v interpreted as an $m \times m$ matrix instead of an m^2 vector. In this way we do not need to store the huge matrix $\widehat{1}$ but it is sufficient to store the much smaller matrices $A[s]$. To solve this generalized eigenvalue problem, we use an iterative method that can handle the non-symmetric property of $\widehat{1}$. Our choice of eigenvalue routine was the Arnoldi algorithm [27].

Normally, using only the DMRG, it is in principle impossible to compute the overlap between two states obtained from two different DMRG calculations. This is because the basis states are renormalized differently and to be able to compare them we need to keep track of all the renormalization group transformations that have been performed. However, using the matrix product method this becomes an almost trivial task. Suppose we have two states $|\mathbb{1}, m\rangle$ and $|\mathbb{1}, m'\rangle$ where we consider the translationally invariant states $Q = \mathbb{1}$ and where m and m' are the number of states that have been kept in the respective Hilbert spaces. We denote the corresponding projection operators by $A_m[s]$ and $A_{m'}[s]$. The overlap between these (unnormalized)

states is given by

$$\begin{aligned}\langle \mathbb{1}, m|\mathbb{1}, m'\rangle &= \sum_{\{s_i\},\{s_i'\}} \mathrm{tr}[A_m^*[s_1]\cdots A_m^*[s_n]]\mathrm{tr}[A_{m'}[s_1']\cdots A_{m'}[s_n']]\langle s_1\cdots s_n|s_1'\cdots s_n'\rangle \\ &= \sum_{\{s_i\}} \mathrm{tr}[(A_m^*[s_1]\otimes A_{m'}[s_1])\cdots(A_m^*[s_n]\otimes A_{m'}[s_n])] \\ &= \mathrm{tr}\widehat{1}_{m,m'}^n,\end{aligned}$$

where we have defined the generalized $\widehat{1}$-matrix $\widehat{1}_{m,m'}$ via

$$\widehat{1}_{m,m'} = \sum_s A_m^*[s]\otimes A_{m'}[s]. \tag{4.10}$$

Thus, the matrix product formalism provides a simple way to compute overlap between different DMRG states. In the paper we briefly discuss the possibility of using these overlaps as an error measure, to be compared with the usual measure, i.e. the truncation error of the density-matrix. Note that the method devised to compute the eigenvalues of the $\widehat{1}$ matrix can be used to compute the eigenvalues of the generalized matrix $\widehat{1}_{m,m'}$ as well. We note from Eq. (4.10) that the overlap decreases exponentially as $\langle \mathbb{1}, m|\mathbb{1}, m'\rangle \propto \lambda_{m,m'}^n$, with $\lambda_{m,m'}$ being the leading eigenvalue of $\widehat{1}_{m,m'}$.

The DMRG code we have used throughout the paper is mainly written in Mathematica, but to improve the performance, we have written a C-program that finds the target state of the superblock Hamiltonian, this being the computationally most demanding part of the algorithm. We have however not used parity as a good quantum number and neither have we used particle-number conservation to store the operators in a sparse form (as block-matrices labeled by the particle number). Using this very "primitive" code we have kept at most $m = 76$ states in the Hilbert space basis.

4.3 The results

As mentioned above, first of all we have checked that the DMRG projection operator converges to a fixed point, justifying the use of the matrix product formalism. The rate of convergence of the A-matrix depends strongly on the gap of the system, the larger the gap the faster the convergence. The ground state energy density of the system converges much faster than the projection operator so this is not a useful measure of whether the projection operator has converged or not. A more relevant measure is the spectrum of the density-matrix.

In order to find out how DMRG accounts for infinite correlation lengths we have computed the particle-hole correlation length using the matrix product formalism for different number of kept states. We find that as the number of kept states, m, increases, the correlation length also increases. More precisely, we find that the correlation length scales as

$$\xi_{ph} \propto m^{1.3}, \tag{4.11}$$

with a coefficient being $O(1)$. Thus, even though the DMRG manifestly produces a correlation function that is qualitatively wrong (exponential instead of algebraic decay), we can find out whether the system is critical or not by considering how the correlation length depends on the number of kept states. Furthermore, one finds that the DMRG correlation functions approximate the exact ones well for short distances and increasing the number of kept states make the

approximate correlation function look like a power-law for larger l, but in the end as $l \to \infty$ it will always decay exponentially no matter how large we make the number of kept states as long as it is finite.

Closely related to the correlation length is the gap of the system, and to investigate this we have used the Bloch-wave form Eq. (3.12) as an ansatz for the excitations. Using this ansatz, keeping only 8 states, we have computed the one-particle excitation spectrum. The reason that we only keep 8 states is that the calculations using the ansatz become very cumbersome as we increase the number of kept states. The size of the matrices involved is $m^2 \times m^2$. We find that the excitations close to the Fermi points have a negative energy, which signals that something is wrong with our ground state. The size of this negative energy gap seems to decrease as the number of kept states is increased, even though our data are not conclusive. We do not understand why these negative energy states occur, or in which way they are energetically more favorable than the ground state. Hopefully this will be understood some day, and probably one would gain important information about the DMRG ground states by solving this problem.

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