A DMRG STUDY OF QUANTUM SPIN MODELS WITH RING EXCHANGE

A DENSITY-MATRIX RENORMALIZATION GROUP STUDY OF QUANTUM SPIN MODELS WITH RING EXCHANGE

By

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A Thesis Submitted to the School of Graduate Studies in Partial Fulfillment of the Requirements for the Degree Master of Science

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Abstract

In this thesis we discuss in detail the density-matrix renormalization group (DMRG) for simulating lowenergy properties of quantum spin models. We implement an original DMRG routine on the S = 1/2antiferromagnetic Heisenberg chain and benchmark its efficiency against exact results (energies, correlation functions, etc.) as well as conformal field-theoretical calculations due to finite-size scaling (ground-state energy and spin gap logarithmic corrections). Moreover, we apply the DMRG to a two-leg square ladder system, where in addition to bilinear exchange terms, we also consider an additional cyclic four-spin ringexchange. The transposition of four spins gives rise to biquadratic exchange terms which are non-trivial to implement in the DMRG. Intermediate results of the ring-exchange are presented along with the difficulties presently encountered.

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CHAPTER 1

INTRODUCTION

In condensed matter physics a theoretical investigation of magnetic behaviour often begins with writing down a sensible Hamiltonian. Within a solid, however, the types of atomic interactions which give rise to magnetism are generally complicated and difficult to model. Rather than obtain an exact Hamiltonian, which can be hard to do, we often resort to simplified effective descriptions of the interactions. In many cases the effective interactions within magnetic materials can often be described in terms of low-dimensional quantum spin models. Not only can these models provide insight into the microscopic physics, a large number of them in recent years have also been experimentally realized.

The simplest and perhaps most dominant interaction is a nearest-neighbour exchange of quantum spins. By quantum spins we mean the effective description used to model the magnetic moments of an atom. This formalism of quantum spin interaction was derived simultaneously by Heisenberg and Dirac in 1926. One of the most widely used and successful Hamiltonians describing a set of interacting quantum spins with nearest-neighbour exchange is the Heisenberg model [1]

$$H_{\text{Heis}} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \qquad (1.1)$$

where J denotes the strength of the interaction, and the quantum mechanical operators $\mathbf{S}_i = (\hbar/2)\boldsymbol{\sigma}_i$ are the Pauli matrices¹ for spins of magnitude $|\mathbf{S}| = 1/2, 1, 3/2, \ldots$ etc. We note that (1.1) is indeed one of the more "simpler" Hamiltonians one can use to describe magnetic phenomena.² Two immediate intuitive states we can think of are the ferromagnetic phase (J < 0) and the antiferromagnetic phase (J > 0), depicted in Figures 1.1a and 1.1b, respectively. But what of other phases? How well-suited is this model at describing experimental data? Should we consider other interactions terms, and if so, what can we expect to find?

¹See Eq. (A.1) in Appendix A for more details.

²It can be derived from the more general Hubbard model (see Appendix B).



Figure 1.1: (a) Ferromagnetic phase: all spins are aligned in parallel. (b) Antiferromagnetic phase: neighbouring spins are aligned in opposing orientations.

1.1 Modelling Magnetism in ³He

One of the earliest attempts at understanding the magnetic behaviour of solid ³He was through the Heisenberg model [2]. Helium atoms are practically impenetrable hard spheres with a weak attractive interaction potential. With high enough pressure solid ³He can be formed by decreasing the available space for each atom. As a solid, due to the small mass of helium, the mean-square displacement of the atoms is large compared to ordinary solids, thus making atom-atom exchange processes significant. Made of two protons and one neutron, solid ³He has an overall spin of S = 1/2 where, through atom-atom exchange, an effective interaction between nuclear spins is induced. From these exchange interactions it was observed that the nuclear spins ordered at ~1mK (see Figure 2 in Section II of reference [2]). At the time, the hope was to use the Heisenberg model to explain this behaviour and possibly more.

Among the first predictions were the magnetic exchange coefficients of solid ³He through high-temperature series expansions [2]. These coefficients were shown to agree reasonably well when compared with a number of experiments which included nuclear magnetic resonance (NMR) techniques [3, 4], pressure measurements in zero field [5] and specific-heat measurements [6]. Having thought to be well-understood as a Heisenberg antiferromagnetic [7], the model became inadequate when studied at low temperatures since several predictions were qualitatively wrong including the nature of the phase transition at ~1mK and the behaviour of the Curie-Weiss law [8, 9, 10]. This seemed to suggest that bilinear exchange, as in (1.1), was not sufficient to capture the magnetic behaviour of solid ³He.

The mechanism behind low-temperature magnetic phenomena turned out to be from higher-order exchange processes involving three- or four-atom permutations; not only do the electrons exchange places but whole atoms corresponding to real permutations of hard spheres. The actual exchange of atoms is about three orders of magnitude greater than magnetic dipole interactions [2]. The most general effective exchange Hamiltonian can be written as [11, 12]

$$H_{\rm ex} = -\sum_{P} (-1)^{\rm sgn(P)} J_P P,$$
(1.2)

where P is any permutation operator of the spins on the lattice, and J_P equals one-half of the positive tunnelling frequency associated with the permutation. An important consequence was that odd permutations, such as cyclic three-particle exchange, generally lead to ferromagnetism, while even permutations such as two and four, favour antiferromagnetism [12]. Subsequently, three- and four-spin exchange terms were shown to be at least the same order of magnitude as two-particle exchanges [13]. Moreover, the first-order phase transition could be accounted for at ~1mK, giving a qualitative description of the phase diagram [14] and explain the correct Curie-Weiss behaviour [15]. Eventually, it was deemed that an antiferromagnetic nearest-neighbour-only description was inadequate [16].

1.2 The Multiple-Spin Exchange in Two-Leg Ladders

Having established that biquadratic exchanges were essential to describing the magnetic behaviour of solid ³He [2], the concept of multiple-spin exchange (MSE) in the form of (1.2) can also be extended to other areas. For instance, the three-particle ferromagnetic exchange in two-dimensional high-density solid ³He films adsorbed on graphite [17] as well as in low-density calculations in the Wigner crystal of electrons [18]. As recent as the early 1990s it was suggested that strongly correlated systems involving cuprates [19, 20] and two-leg spin ladders [21] exhibit biquadratic exchange. In particular, a number of experiments on S = 1/2 two-leg spin ladder "telephone number compounds" $A_{14}Cu_{24}O_{41}$, have been realized to have non-negligible fourspin cyclic ring-exchange interactions. These works include measurements using inelastic neutron scattering $(A = Sr_{14})$ [22], NMR ($A = La_8Ca_6$, Sr_{14} , $Sr_{11}Ca_3$) [23] and optical conductivity ($A = Ca_{14}$, La_{14}) [24]. In addition, attempts to fit experimental data without MSE resulted in an unnaturally large ratio of Heisenberg couplings [23] which did not agree with electronic structure calculations nor the geometrical structure of the ladder [25], furthering the evidence of a ring-exchange contribution.

With experiments setting the pace, theory has spawned a number of studies on two-leg square ladders and triangular strips with four-spin ring-exchanges. These quantum spin systems, with additional frustration, should lead to new and exotic phases. The common form of the two-leg square ladder Hamiltonian is given by the following SU(2) invariant $S = 1/2 \mod^{13}$:

$$H_{\rm SL} = J_{\perp} \sum_{i} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} + J_{||} \sum_{i} \sum_{\alpha=1,2} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{i+1,\alpha} + K \sum_{\langle ijkl \rangle} \left(P_{ijkl}^{\circlearrowright} + P_{ijkl}^{\circlearrowright} \right), \tag{1.3}$$

where J_{\perp} and $J_{||}$ are the bilinear exchange couplings on the rungs and along the legs of the ladder, respectively, and K is the coupling of the cyclic four-spin permutation operator per plaquette (see Figure 1.2).

³The two-leg triangular strip can be defined analogously.

Roman subscripts denote the lattice positions while Greek subscripts number the two legs. Note that a bilinear cross-plaquette term can also be added to this Hamiltonian.



Figure 1.2: A schematic of a two-leg square ladder with Heisenberg interactions along the rungs and legs as well as an additional cyclic four-spin ring-exchange per plaquette.

The action of the P operator is a cyclic permutation of four spins, i.e.

$$P_{ijkl}^{\circlearrowright} \begin{vmatrix} i & j \\ l & k \end{pmatrix} = \begin{vmatrix} j & k \\ i & l \end{pmatrix} \quad \text{and} \quad P_{ijkl}^{\circlearrowright} \begin{vmatrix} i & j \\ l & k \end{pmatrix} = \begin{vmatrix} l & i \\ k & j \end{pmatrix}.$$
(1.4)

Through a bit of algebra (see Appendix A) it can be shown that P decomposes into spin operators involving bilinear and biquadratic terms:

$$P_{ijkl}^{\circlearrowright} + P_{ijkl}^{\circlearrowright} = \sum_{\mu < \nu} \mathbf{S}_{\mu} \cdot \mathbf{S}_{\nu} + 4\mathcal{G}_{ijkl} + \frac{1}{4},$$
(1.5)

where the sum $\sum_{\mu < \nu}$ is performed over all distinct pairs in a plaquette of four-spins and

$$\mathcal{G}_{ijkl} = (\mathbf{S}_i \cdot \mathbf{S}_j) \left(\mathbf{S}_k \cdot \mathbf{S}_l \right) + \left(\mathbf{S}_j \cdot \mathbf{S}_k \right) \left(\mathbf{S}_l \cdot \mathbf{S}_i \right) - \left(\mathbf{S}_i \cdot \mathbf{S}_k \right) \left(\mathbf{S}_j \cdot \mathbf{S}_l \right),$$
(1.6)

which carries the biquadratic terms.

In recent years an assortment of methods were used to explore the phase diagram and behaviour of (1.3). In both the strong and weak ring-exchange coupling regimes investigations have used a variety of perturbative expansions [21, 26], spin-wave analysis [27, 28], numerical exact diagonalization (ED) in conjunction with conformal field theory (CFT) [29], renormalization group (RG) analysis around different CFT solutions [30], the density-matrix renormalization group (DMRG) [31, 32, 33] and large scale exact diagonalizations supplemented with trial wavefunction variational Monte Carlo (VMC) [34]. Both analytical and numerical approaches have observed a variety of phases. The phase diagrams are quite exotic in that these phases are both unexpected and unconventional. The following two sections provides an overview of the phase diagrams for different ladder geometries.

1.2.1 Square Ladder

Starting with the two-leg square ladder, as in Figure 1.2, we show a schematic of the phase diagram in Figure 1.3 obtained from reference [33]. The phases captured within this study agree with most of the studies presented above. We briefly describe these phases and their properties.



Figure 1.3: A schematic of the phase diagram from reference [33] of the two-leg square ladder obtained from exact diagonalization and DMRG calculations. The couplings are set as $J_{\perp} = J_{||} = J = \cos(\theta)$ and $K = \sin(\theta)$ so that the energy scale $\sqrt{J^2 + K^2}$ is set to one. First- and second-order phase transitions are denote by squares and circles, respectively. The empty circle marks a phase transition of unknown nature while the dashed line indicates a crossover between two regions without a phase transition.

Valence-bond crystals. Around $\theta = 0$ (J = 1, K = 0), there is a phase in which the ground-state is well-approximated by the product of local rung singlets and all excitations are gapped. In this region, spin-spin correlations dominate and decay exponentially with distance. Since $K \approx 0$, this behaviour is perhaps expected. As θ becomes non-zero, there is a second-order phase transition to a staggered dimer phase where a finite gap to triplet excitations exists. The ground-state is two-fold degenerate and breaks translational symmetry. Furthermore, the system exhibits valence-bond long-range order (LRO), with the order parameter given by

$$\langle \mathbf{S}_{i-1,\alpha} \cdot \mathbf{S}_{i,\alpha} - \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{i+1,\alpha} \rangle.$$
 (1.7)

Phases with chirality. There are two phases characterized by the chirality in the order parameter. As

 θ becomes larger the dimerization vanishes and there is a phase transition (of unknown type) to a staggered scalar chirality phase with LRO. The symmetry breaking two-fold degenerate ground-state is described by the order parameter

$$\left\langle \mathbf{S}_{i,1} \cdot \left[\mathbf{S}_{i,2} \times \mathbf{S}_{i+1,1} \right] \right\rangle,$$
(1.8)

which breaks both spatial and time reversal symmetries but not SU(2). This discrete symmetry breaking is suggestive of a small finite gap to triplet excitations. The other phase, as θ continues to increase, is observed to have short-range order (SRO) and is characterized by vector chirality. Its order parameters are given by

$$\langle \mathbf{S}_{i,\alpha} \times \mathbf{S}_{i+1,\alpha} \rangle$$
 and $\langle \mathbf{S}_{i,\alpha} \times \mathbf{S}_{i,\alpha+1} \rangle$, (1.9)

which break translational symmetry. These can be visualized in a staggered circular arrangement along each plaquette and can be regarded as local spin current operators. Thus correlations between diagonal sites are weaker than the bonds on rungs or legs. It should be noted that these vector chirality correlations are seen to decay much slower than spin-spin correlations. Lastly, the system has a unique ground-state and a fully gapped excitation spectrum.

Polarization of spins. As we continue around in θ , we cross over into a region characterized by collinear spin-spin correlations on individual legs. That is, spins on the same (different) leg exhibit ferromagnetic (antiferromagnetic) correlations and have SRO. Similar to the vector chirality phase, the system has a unique ground-state with a fully gapped excitation spectrum. Finally, bound between two first-order phase transitions is a ferromagnetic phase where the energy for each plaquette is minimized separately.

1.2.2 Triangular Strip

Another ladder geometry with a cyclic four-spin ring-exchange that also has a rich phase diagram is the two-leg triangular strip. With this geometry, the Hamiltonian (1.3) can be written as a 1D $J_1 - J_2$ chain with an additional four-spin interaction. This system was studied [34] using a wide variety of numerical techniques including ED, DMRG, and VMC. Using the DMRG, four distinct phases were observed in the $J_2/J_1 - K/J_1$ plane (see Figure 2 on page 2 of [34]). For K = 0 the system is a conventional Bethe chain when $J_2 \leq 0.241167J_1$ and a period 2 valence bond solid (VBS-2) for larger J_2 . In a fairly wide region with $K > 0.2J_1$, $J_2 \neq 0$, a new phase exhibiting spin liquid behaviour is seen. This phase, called a spin Bose metal (SBM), is suggested to be a gapless spin liquid possessing spin correlations which are singular along surfaces in momentum space, i.e. "Bose surfaces". Signatures of this state are expected to manifest in quasi-one-dimensional (quasi-1D) ladder systems as in (1.3). This proposed SBM is believed to be a quasi-1D descendant state of the two-dimensional "boson-ring" model describing itinerant hard-core bosons hopping on a square lattice with a four-spin exchange term. Its ground-state is believed to be a gapless spin liquid, called a *d*-wave Bose liquid, where in momentum space the Bose surface is singular. It has been suggested that SBMs could be accessed by systemically approaching two dimensions through a sequence of quasi-1D

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ladder models [34, 35]. Surely enough, signatures of the SBM phase are observed via the DMRG and can be seen to dominate the intermediate $J_2/J_1 - K/J_1$ parameter space. We also note that in this study the DMRG found a VBS-3 as well as a partially ferromagnetic phase flanked between SBMs. These two phases result from instabilities of the SBM at special commensuration⁴. SBM has also been observed in four-leg triangular ladders [35].

Having access to an assortment of phases, an interesting property one can measure is the entanglement and how it differs between phases. For example, the entanglement entropy (EE) of a state, first introduced in the context of quantum information theory [36], has gained popularity within the field of strongly correlated systems. For a many-body quantum system the EE is defined as the von Neumann entropy (see Section 3.6.1). It is an easily attainable quantity using the DMRG and is one kind of entanglment we wish to study in detail.

We have organized this thesis into two main parts: Chapter 2 discusses in fair detail iterative numerical techniques for investigating 1D strongly correlated systems as well as briefly outlining Wilson's numerical renormalization group [37]. Chapter 3 focuses on the intricate details of the DMRG [38, 39]. We benchmark the efficiency of an original DMRG implementation on the S = 1/2 antiferromagnetic Heisenberg chain (1.1) by comparing with known theoretical results. This includes ground-state properties and CFT logarithmic corrections. Finally, in Chapter 4 we describe the technical issues associated with the DMRG when considering a ring-exchange Hamiltonian (1.3) on a two-leg square ladder.

⁴The system has developed order compatible with the lattice.

CHAPTER 2_{-}

NUMERICAL TECHNIQUES

In this chapter we discuss the Lanczos method [40], an iterative exact diagonalization technique used to treat quantum spin models such as the Heisenberg Hamiltonian (1.1), as well as provide a brief overview of Wilson's numerical renormalization group (NRG) [37].

A full investigation of a quantum many-body system requires a complete diagonalization of the matrix representation of the system's Hamiltonian. However, for strongly interacting quantum spin systems the Hilbert space grows exponentially with the system size. It is therefore not practical in terms of time consumption and memory storage to perform a complete diagonalization. Moreover, the simplest effective models which involve only nearest-neighbour interactions generate sparse¹ Hamiltonians presenting difficulties for standard algorithms. Be that as it may, the investigation of condensed matter systems is almost always targeted towards the low-energy properties, usually the ground-state and a few low-lying excited states. By projecting out those states which contribute to the low-energy spectrum we can restrict our analysis to what is known as a Krylov subspace [41] and reach larger system sizes.

2.1 Krylov Space

In general, the many-body matrix representation of a Hamiltonian is large and in particular sparse. For numerical routines which require the full Hamiltonian to solve the eigenvalue problem, such as Jacobi's rotation method [42], the large number of matrix-matrix operations puts limitations on practical computational efficiency and the system size. However, if the focus is to probe the low-energy physics of a strongly interacting system, in particular the ground-state, one can use iterative diagonalization techniques. The basic idea behind iterative diagonalization is to use successive matrix-vector operations (instead of matrix-matrix operations) to construct a linear subspace in such a way that the ground-state is well-approximated. It is

 $^{^{1}\}mathrm{A}$ matrix is said to be sparse if it is populated primarily with zeros.

an approximation due to the repeated application of the Hamiltonian through matrix-vector products, but it is numerically exact.

Consider an N-dimensional Hilbert space with Hamiltonian H and eigenbasis satisfying $H|n\rangle = E_n|n\rangle$. Let $|v\rangle$ be an initial state with random entries. Expanding $|v\rangle$ in terms of the eigenbasis and applying H with power M gives

$$H^{M}|v\rangle = H^{M}\sum_{n=1}^{N}c_{n}|n\rangle = \sum_{n=1}^{N}c_{n}E_{n}^{M}|n\rangle = c_{\max}E_{\max}^{M}\left[|n_{\max}\rangle + \sum_{n\neq\max}\frac{c_{n}}{c_{\max}}\left(\frac{E_{n}}{E_{\max}}\right)^{M}|n\rangle\right],$$
 (2.1)

where the constructed Krylov subspace is defined by

$$\mathcal{K} = \operatorname{span} \Big\{ |v\rangle, \ H|v\rangle, \ H^2|v\rangle, \ \dots, \ H^M|v\rangle \Big\}.$$
(2.2)

It is clear that if M is large enough and $c_{\max} \neq 0$, the eigenpair $(|E_{\max}|, |n_{\max}\rangle)$ will dominate the sum in Eq. (2.1) guaranteeing a ground-state². However, even if M is large, convergence to the ground-state may not occur; the difference between the ground-state and the first-excited state eigenvalues must be sufficiently large. It is otherwise unclear as to whether we have found the true ground-state. Although useful, this power method is limited to finding only one eigenvalue (the one with the greatest absolute value) and the speed at which it converges also varies. In the proceeding section we discuss the Lanczos method which not only optimizes this power method but is also capable of targeting excited states. For a more detailed discussion see Cullum and Willoughby [43].

2.2 Lanczos Method

The Lanczos method is an iterative numerical technique where a special orthonormal basis is constructed via a Krylov subspace $\{|v_0\rangle, |v_1\rangle, \dots, |v_{M-1}\rangle\}$. Using this basis, an $N \times N$ -dimensional Hermitian Hamiltonian (likely sparse) is transformed into a simple tridiagonal matrix where its matrix elements are generated through an iterative procedure. In this form, it can be diagonalized by dense matrix algorithms.

Similar to the power method, we start with a normalized initial state $|v_0\rangle$ of dimension N with random entries. In general, no a priori information about the ground-state is known and thus random entries are used to ensure a finite overlap between the initial state and the actual ground-state, i.e. $\langle v_0 | \Psi_0 \rangle \neq 0$. On the other hand, if information about the ground-state is known, e.g. the total spin number, total spin in the z-direction, total charge, etc., the initial state can be chosen (also with random entries) to lie in a reduced subspace belonging to that conserved quantity. It is therefore advantageous to know a priori some information about the ground-state as both the speed of convergence and precision can be increased. Note that this initial state can also be chosen to target excited states. Having chosen $|v_0\rangle$ we

²The ground-state can be ensured by using $(H-c)^{M}$ instead of H^{M} , for c > 0 and large enough, so that $|E_{0}-c| > |E_{M-1}-c|$.

perform M iterations of the recursion relation

$$\beta_{i} = \langle v_{i-1} | H | v_{i} \rangle$$

$$\alpha_{i} = \langle v_{i} | H | v_{i} \rangle$$

$$|v_{i+1} \rangle = H | v_{i} \rangle - \alpha_{i} | v_{i} \rangle - \beta_{i} | v_{i-1} \rangle$$

$$|v_{i-1} \rangle = |v_{i} \rangle$$

$$|v_{i} \rangle = \frac{|v_{i+1} \rangle}{\sqrt{\langle v_{i+1} | v_{i+1} \rangle}}, \quad \text{for} \quad i = 0, 1, \dots, M-1$$

$$(2.3)$$

with $|v_{-1}\rangle \equiv 0$. Note that the vectors $|v_i\rangle$ are normalized in this formulation. By construction, the Gram-Schmidt process guarantees the orthogonality condition $\langle v_i | v_j \rangle = \delta_{ij}$. The resulting tridiagonal matrix can be read off as

$$T = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & & \\ & \beta_2 & \alpha_2 & \ddots & & \\ & & \ddots & \ddots & & \beta_{M-1} \\ & & & & & \beta_{M-1} & \alpha_{M-1} \end{pmatrix}.$$
 (2.4)

The main advantage the Lanczos method has over dense matrix algorithms is not due to the tridiagonal form of H but rather that only three vectors $|v_{i-1}\rangle, |v_i\rangle$, and $|v_{i+1}\rangle$ of size N need to be stored in memory, making this method very efficient. Typically, for quantum spin systems, $M \sim \mathcal{O}(10) - \mathcal{O}(100)$ for convergence. The most time-consuming step is the implementation of the matrix-vector product $H|v_i\rangle$, which should be written as efficiently as possible. Equation (2.4) can be diagonalized (via standard linear algebra subroutine libraries) to yield approximate eigenvalues $(\lambda_0, \lambda_1, \ldots, \lambda_{M-1})$ of H, and eigenvectors $(|\phi_0\rangle, |\phi_1\rangle, \ldots, |\phi_{M-1}\rangle)$, represented the Lanczos basis.

In order to calculate quantities such as quantum mechanical observables the eigenvectors need to be in the original basis $|n\rangle$. There are two ways to perform a change of basis. The first approach is to store the basis vectors $|v_i\rangle$ generated at each iteration creating a transformation matrix

$$V = \begin{pmatrix} \langle 0 | v_0 \rangle & \langle 0 | v_1 \rangle & \dots & \langle 0 | v_{M-1} \rangle \\ \langle 1 | v_0 \rangle & \langle 1 | v_1 \rangle & \dots & \langle 1 | v_{M-1} \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N - 1 | v_0 \rangle & \langle N - 1 | v_1 \rangle & \dots & \langle N - 1 | v_{M-1} \rangle \end{pmatrix}.$$
(2.5)

The ground-state in the original basis can then be obtained by carrying out the change of basis

$$\left|\phi_{0}\right\rangle = \sum_{i=0}^{M-1} \left|v_{i}\right\rangle \left\langle v_{i}\left|\phi_{0}\right\rangle\right. = \sum_{n=0}^{N-1} \sum_{i=0}^{M-1} \left|n\right\rangle \left\langle n\left|v_{i}\right\rangle \left\langle v_{i}\left|\phi_{0}\right\rangle\right.$$
(2.6)

which is equivalent to performing the matrix-vector multiplication $V|\phi_0\rangle$. In practice, and in particular for larger system sizes, the transformation matrix (2.5) would require storing a matrix of size $N \times M$ and is therefore not usually implemented. The second and more memory efficient approach is to run the Lanczos subroutine twice; the first iteration as described above, while during the second iteration the basis vectors $|v_i\rangle$ would be systematically reconstructed to give the coefficients $\langle n | v_i \rangle$ to form the ground-state in the original basis $|n\rangle$.

As we have seen, the Lanczos method approximates the extremal eigenvalue and eigenvector by systematically improving upon a variational state that is used to represent the ground-state. For most systems convergence to the ground-state is reached roughly on the order of 10-100 iterations. If excited states are required then additional iterations are needed to ensure their convergence. In exact arithmetic, the set of basis vectors $\{|v_0\rangle, |v_1\rangle, \ldots, |v_{M-1}\rangle\}$ are mutually orthogonal and at most only M-1 iterations are needed; the eigenvalues and eigenvectors of Eq. (2.4) are then exact. However, as the number of iterations grows, the Lanczos method suffers from finite machine precision leading to a loss of mutual orthogonality among the basis vectors. This loss of orthogonality can lead to the appearance of spurious eigenvalues which are not part of the original eigenvalue spectrum. Figure 2.1 shows an example of this behaviour. This loss in orthogonality is intrinsic to the algorithm. There are, however, ways to restore lost orthogonality by modifying the original Lanczos method (see [44] and references therein).

The basic Lanczos method is one of many iterative diagonalization procedures. Each method shares a common idea: project the Hamiltonian onto a subspace smaller than the original Hilbert space and generate a set of orthonormal bases spanning a Krylov subspace. In doing so the original matrix is transformed into a convenient representation and dense matrix algorithms can be used for diagonalization. The resulting extremal eigenpairs are known as Ritz eigenvalues and Ritz eigenvectors. In quantum mechanics, given a trial wavefunction $|\phi\rangle$, the Ritz variational principle asserts that

$$E_0 \le \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}.$$
(2.7)

That is, the true ground-state energy E_0 is always bounded from above by λ_0 . Nevertheless, the efficiency and convergence rate of the Lanczos method makes it a common tool in studying quantum spin systems.

Finally, a number of software packages are available such as the ALPS project [45] and ARPACK [46, 47] which have optimized implementations of various iterative diagonalization routines. A matrix-vector product routine $H|v\rangle$ must be provided by the user and should be implemented efficiently for best results.



Figure 2.1: Convergence of the ten lowest-lying energies as a function of the number of iterations M for a 10-site isotropic S = 1/2 antiferromagnetic Heisenberg chain. The ground-state converges in less than 10 iterations while excited states require more. In this example, additional iterations cause the appearance of spurious eigenvalues which skews the multiplicity of certain states.

2.3 Numerical Renormalization Group

The major problem when treating a many-body quantum system is the exponential growth of the Hilbert space with the system size. While iterative methods are capable of handling surprisingly large matrices they are ultimately limited by maximum system sizes³. Moreover, numerical instabilities cause the structure of the energy spectrum to be determined incorrectly. Nevertheless, in a strongly-interacting system, there will be large parts of the Hilbert space which are irrelevant if focus is solely on the low-energy spectrum. By throwing away states which do not contribute an effective Hamiltonian can be formed to capture the essential low-energy physics. The question is how do we decide which states to keep? In this chapter we give a brief discussion of the NRG approach developed by Wilson to solve the Kondo impurity problem [37].

From statistical physics, the scaling hypothesis states that the singular behaviour of physical quantities at the critical point is controlled by the competition between long-range correlations and fluctuation of the order parameters at all length scales up to the correlation length. Given that these fluctuations exist at every energy scale, an RG scheme can be developed to find the underlying hierarchical structure from which the RG flow can be studied. The basic idea behind lattice RG techniques is to increase the system size iteratively

 $^{{}^{3}}L \sim 40$ sites for the S = 1/2 Heisenberg chain.

while keeping the number of basis states constant. The computational approach is analogous to Kadanoff's block-spin RG [48] where the lattice Hamiltonian can be split into "blocks". Rather than discussing the details of the Kondo problem Wilson's NRG will be presented in the context of 1D real-space blocking.

Starting with a chain small enough to be treated exactly we isolate two identical blocks AA as in Figure 2.2. We then diagonalize the Hamiltonian matrix H_{AA} , corresponding to two blocks joined together, and retain m of its lowest-lying eigenstates. These eigenstates are used to transform H_{AA} into a new Hamiltonian $H_{A'}$ representing a block A' which is now twice as large. With the new block and new effective Hamiltonian $H_{A'}$ we continue this procedure iteratively until a desired length is reached. The NRG algorithm is summarized in Table 2.1.



Figure 2.2: Blocking scheme for real-space numerical renormalization group.

Table 2.1: Numerical renormalization group in real-space.

0. Construct the full Hamiltonian H_{AA} from two identical isolated blocks AA .
1. Diagonalize H_{AA} and obtain the <i>m</i> lowest eigenstates.
2. Form matrix representations of all relevant operators H_{AA} , Q_{AA} , etc., for AA from the corresponding matrices for A.
3. Perform a change of basis via $H_{A'} = O^{\dagger} H_{AA}O$, etc., where O is an $N \times m$ matrix and N is the dimension of H_{AA} . The columns of O are the m lowest eigenstates of H_{AA} .
4. Replace A with A' .
5. Go to step 0 .

It is clear that for the system to remain treatable the Hilbert space at each iteration must be decreased. This reduction is the RG step and is done by projecting the Hamiltonian H_{AA} onto the basis spanned by the m < N lowest-lying eigenstates of H_{AA} . Thus, the idea is to enlarge the system iteratively by doubling its size at each iteration without having to increase the Hilbert space. While the NRG method succeeds in capturing the physics of the Kondo problem it fails when applied to 1D quantum lattice models. To illustrate this we consider the elementary problem of a single particle confined to a box (block) of length L. The Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = E\psi(x),\tag{2.8}$$

where from the boundary conditions, the states of this Hamiltonian are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \quad n = 1, 2, \dots$$
(2.9)

Depicted in Figure 2.3 (as points) are the ground-state and first-excited state wavefunctions for an isolated block A of a given length L. When two identical isolated blocks are joined together to form a block AAtwice as large, the ground-state results in a node at the centre. However, we know that for a box of length 2L the ground-state wavefunction is at a maximum when x = L (Figure 2.3 solid line). Hence, from this example we see that it is incorrect to assume that only those states which are energetically the lowest-lying contribute to the ground-state of the final (infinite) system. In other words, the eigenstates which are kept to form the new basis are likely to have inappropriate features at the boundaries for building up the blocks. The effect of the boundary conditions on real-space RG methods was eventually understood by White and



Figure 2.3: Two isolated blocks A are connected to form a block twice as large AA. The lowest-lying eigenstates of A do not approximate well the eigenstate of the larger block AA.

Noack [49]. Several solutions were proposed, each with a different treatment of the boundary conditions. It was shown that errors could be eliminated, at least for single particle problems.

In summary, we have seen that the standard RG approach is not particularly effective when applied to

strongly correlated systems. It works remarkably well for the Kondo problem because the couplings between adjacent layers (sites) decreases exponentially, whereas in 1D systems the couplings remain constant. We have also demonstrated that the two key aspects in the renormalization procedure need refining: enlargement of the block and the criterion in how we choose which states to keep.

CHAPTER 3

DENSITY-MATRIX RENORMALIZATION GROUP

As the main focus of this thesis, this chapter aims to provide both a theoretical and computational understanding of the DMRG approach developed by White [38, 39]. In the concluding remarks of Chapter 2 we stated that the two most important aspects of numerical renormalization group techniques are the way in which we enlarge the system (connecting blocks together) and how we decide which states to keep (decreasing the dimension of the Hilbert space as the system grows). In this chapter we will see that both aspects are one in the same when viewed from the perspective of the DMRG. In the standard NRG approach, we chose the *m* lowest-lying eigenstates of H_{AA} as the new basis for the next iteration. However, these eigenstates contain no information about the rest of the system (the new block it connects to) and is therefore the principal issue. The superblock method (analogous to "supercell" as used in electronic structure calculations) suggested by White and Noack, where the system is embedded in an environment, is the basis for the density matrix approach. The idea is to optimize the basis which describes the system allowing for a "smoother" connection to a new block.

In a standard DMRG calculation, the focus is a single target state of the superblock Hamiltonian, usually the ground-state (although it is possible to target multiple states simultaneously). The density matrix is constructed from the target state where from its properties an optimal basis can be found. We begin the DMRG discussion by reviewing density matrices. For a more complete analysis see Feynman's introduction to density matrices [50].

3.1 The Reduced Density Matrix

To motivate the use of density matrices, let us consider a statistical mechanical problem where the universe is divided into two parts: system and environment. From this perspective we can think of the environment as a large heat bath in contact with a system. Using the notation in Figure 3.1, let $|i\rangle$ and $|j\rangle$ be a complete set of states describing the system and environment, respectively.



Figure 3.1: A typical superblock configuration divided into system and environment blocks with basis $|i\rangle$ and $|j\rangle$, respectively.

A general wavefunction of the universe can be written in a direct product basis as

$$|\psi\rangle = \sum_{i} \sum_{j} \psi_{ij} |i\rangle \otimes |j\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle, \qquad (3.1)$$

where we have dropped the \otimes notation which is henceforth implied. Let A be an operator which acts only on the system, i.e.

$$A = \sum_{ii'} \sum_{j} A_{ii'} |i\rangle |j\rangle \langle j|\langle i'|.$$
(3.2)

Taking the expectation value of A, we have

$$\begin{split} \langle A \rangle &= \langle \psi | A | \psi \rangle = \sum_{ij} \sum_{i'j'} \psi_{ij} \psi_{i'j'}^{\dagger} \langle j | \langle i | A | i' \rangle | j' \rangle \\ &= \sum_{ij} \sum_{i'j'} \psi_{ij} \psi_{i'j'}^{\dagger} \langle i | A | i' \rangle \langle j | j' \rangle \\ &= \sum_{ii'} \sum_{j} \psi_{ij} \psi_{i'j}^{\dagger} \langle i | A | i' \rangle \\ &= \sum_{ii'} \rho_{ii'} \langle i | A | i' \rangle \\ &= \operatorname{tr} (\rho A), \end{split}$$
(3.3)

where we have defined the reduced density matrix

$$\rho_{ii'} = \sum_{j} \psi_{ij} \psi^{\dagger}_{i'j} . \qquad (3.4)$$

Let us define an operator ρ such that $\rho_{ii'} = \langle i | \rho | i' \rangle$. Using the hermiticity of $\rho_{ii'}$ and the completeness relation $\sum |i\rangle\langle i| = 1$, ρ can be diagonalized as

$$\rho = \sum_{\alpha} w_{\alpha} |u^{\alpha}\rangle \langle u^{\alpha}|, \qquad (3.5)$$

where $|u^{\alpha}\rangle$ is a complete orthonormal basis with corresponding eigenvalues w_{α} . If we let the operator A = 1and use Eqs. (3.3) and (3.5) we see that

$$\sum_{\alpha} w_{\alpha} = \operatorname{tr} \rho = \langle A \rangle = \langle \psi | \psi \rangle = 1.$$
(3.6)

On the other hand, since the trace is representation-independent, we can let $A = |u^{\alpha}\rangle\langle u^{\alpha}|$ and conclude that

$$w_{\alpha} = \operatorname{tr} (\rho A) = \langle A \rangle = \langle \psi | A | \psi \rangle$$

$$= \langle \psi | u^{\alpha} \rangle \langle u^{\alpha} | \psi \rangle$$

$$= \sum_{j} \langle \psi | u^{\alpha} \rangle | j \rangle \langle j | \langle u^{\alpha} | \psi \rangle$$

$$= \sum_{j} \left| (\langle j | \langle u^{\alpha} |) | \psi \rangle \right|^{2}$$

$$\geq 0.$$
(3.7)

In summary, any universe composed of a system and environment can be described by a density matrix ρ in the form of Eq. (3.5) with the following properties:

- 0. Hermitian, $\rho^{\dagger} = \rho$.
- 1. $|u^{\alpha}\rangle$ is a complete orthonormal basis.
- 2. Eigenvalues are non-negative $w_{\alpha} \ge 0$ with $\sum_{\alpha} w_{\alpha} = 1$.
- 3. Probability interpretation: Recall that

$$\langle A \rangle = \operatorname{tr} (\rho A)$$

$$= \sum_{\alpha} \langle u^{\alpha} | \rho A | u^{\alpha} \rangle$$

$$= \sum_{\alpha\beta} \langle u^{\alpha} | \rho | u^{\beta} \rangle \langle u^{\beta} | A | u^{\alpha} \rangle$$

$$= \sum_{\alpha\beta} w_{\alpha} \langle u^{\alpha} | u^{\beta} \rangle \langle u^{\beta} | A | u^{\alpha} \rangle$$

$$= \sum_{\alpha} w_{\alpha} \langle u^{\alpha} | A | u^{\alpha} \rangle.$$

$$(3.8)$$

Hence w_{α} can be interpreted as the probability that the system is in state $|u^{\alpha}\rangle$.

The above density operator formalism describes qualitatively the physical state of an ensemble. By this we mean an ensemble which is either pure or mixed. A pure ensemble is a state in which the collection of all interacting parts can be described by the same basis, i.e. all but one of the w_{α} are zero. In contrast, in a mixed ensemble, for example, the system would be described by one set of bases while the environment in

another. In other words, a mixed ensemble is a collection of pure ensembles. Using this prescription we can view quantum mechanics in a different light. Rather than describe a quantum mechanical system in terms of the wavefunction, we can instead use the density matrix. This turns out to be very convenient because for a general state $|\psi\rangle$, the eigenvalues w_{α} of the reduced density matrix carry important information about the entanglement of the system with the environment. That is, given that the universe is in a state $|\psi\rangle$, w_{α} is the probability that the system is in state $|u^{\alpha}\rangle$. This is precisely the criterion we need for deciding which states to keep. In the context of the DMRG, by projecting the Hamiltonian onto those states which carry the most weight in describing the target state, the blocks are better suited to be connected to new blocks at the next iteration. It is therefore very natural to use the density matrix.

To compare this with the standard RG approach, consider an isolated block with Hamiltonian H at finite temperature T. Assume that we know all the states $|n\rangle$ to $H|n\rangle = E_n|n\rangle$. The probability that the block is in an eigenstate $|n\rangle$ is given by the Boltzmann weight

$$p_n = \frac{1}{Z} \exp(-\beta E_n), \tag{3.9}$$

where Z is the partition function and $\beta = (k_B T)^{-1}$ is the thermodynamic beta. For an isolated block, its density matrix is not Eq. (3.4) but rather given by the expression

$$\rho_{\rm iso} = \sum_{n} p_n |n\rangle \langle n| = \frac{1}{Z} \sum_{n} \exp(-\beta E_n) |n\rangle \langle n|.$$
(3.10)

The Boltzmann weight is clearly an eigenvalue of the density matrix since

$$\rho_{\rm iso}|n\rangle = \frac{1}{Z} \sum_{n'} \exp(-\beta E_{n'})|n'\rangle \langle n'|n\rangle = \frac{1}{Z} \exp(-\beta E_n)|n\rangle.$$
(3.11)

Thus an eigenstate of the Hamiltonian is also an eigenstate of the density matrix. Therefore, under the assumption that the block is isolated, choosing the m lowest-lying eigenstates to represent the block is equivalent to viewing the new block connections as a heat bath at an effective inverse temperature β , to which the system is very weakly coupled. However, since the system is in fact not isolated and strongly-interacting with its environment, the more appropriate choice is to use the density matrix Eq. (3.4) and its eigenstates to describe the system.

3.2 The Optimal States

We now show that a target state of the universe, which we assume for the moment to be pure, can be accurately represented by keeping the m lowest-lying eigenstates of both the system and environment density matrices. Mathematically, we wish to minimize the error

$$S = \left| \left| \psi \right\rangle - \left| \psi' \right\rangle \right|^2,\tag{3.12}$$

where $|\psi\rangle$ is the target state in the original basis, Eq. (3.1), and $|\psi'\rangle$ is the target state in the density matrix basis, Eq. (3.5). Let $|i\rangle$, i = 1, 2, ..., I and $|j\rangle$, j = 1, 2, ..., J be complete sets of states for the system and environment, respectively. From Eq. (3.5) the following eigenstate expansions

$$|u^{\alpha}\rangle = \sum_{i} u_{i}^{\alpha}|i\rangle \quad \text{and} \quad |v^{\alpha}\rangle = \sum_{j} v_{j}^{\alpha}|j\rangle,$$
(3.13)

are where we choose the m < I, J states to keep. Thus, the approximation for $|\psi\rangle$ is

$$|\psi\rangle \approx |\psi'\rangle = \sum_{\alpha=1}^{m} u_i^{\alpha} v_j^{\alpha} |u^{\alpha}\rangle |v^{\alpha}\rangle = \sum_{\alpha=1}^{m} a_{\alpha} |u^{\alpha}\rangle |v^{\alpha}\rangle.$$
(3.14)

Switching to matrix notation, the error is

$$S = \sum_{ij} \left(\psi_{ij} - \sum_{\alpha=1}^{m} a_{\alpha} u_i^{\alpha} v_j^{\alpha} \right)^2, \qquad (3.15)$$

where minimization is over all $|u^{\alpha}\rangle$, $|v^{\alpha}\rangle$ and a_{α} . In this form we can invoke a theoretical result from linear algebra to obtain the desired solution. The superblock state vector $|\psi\rangle$, with possibly complex coefficients, may be thought of as a rectangular matrix ψ_{ij} . We may write it as a singular value decomposition

$$\psi = UDV^{\dagger}, \tag{3.16}$$

where U and D are $I \times I$ matrices, and V^{\dagger} is $I \times J$. Specifically, U and V are unitary and D is a diagonal matrix containing the singular values of ψ^1 . This is made clear by noticing that

$$\psi\psi^{\dagger} = UDV^{\dagger}VDU^{\dagger} = UD^{2}U^{\dagger} \implies D^{2} = U^{\dagger}\psi\psi^{\dagger}U$$
(3.17a)

$$\psi^{\dagger}\psi = VDU^{\dagger}UDV^{\dagger} = VD^{2}V^{\dagger} \implies D^{2} = V^{\dagger}\psi^{\dagger}\psi V$$
(3.17b)

and thus the elements of D are the square roots of the eigenvalues of $\psi\psi^{\dagger}$ or $\psi^{\dagger}\psi$, the reduced density matrices of the system or environment. Moreover, the matrices U and V are column orthogonal eigenvectors corresponding to $\psi\psi^{\dagger}$ and $\psi^{\dagger}\psi$, respectively. It is now clear how we minimize S: the m largest-magnitude diagonal elements of D are the a_{α} and the corresponding columns of U and V are the u_i^{α} and v_j^{α} . Therefore, an optimal basis is found for a given m < I, J.

Comparing Eqs. (3.4) and (3.17a) we see that the reduced density matrix for the system is (the environment is analogous)

$$\rho_{ii'} = \sum_{j} \psi_{ij} \psi^{\dagger}_{i'j} = U D^2 U^{\dagger}, \qquad (3.18)$$

¹Singular values are defined as the square roots of the eigenvalues of $\psi\psi^{\dagger}$ or $\psi^{\dagger}\psi$ and are non-negative real numbers.

where U diagonalizes $\rho_{ii'}$. The eigenvalues $w_{\alpha} = a_{\alpha}^2$ represent the probability of the system being in state $|u^{\alpha}\rangle$, and hence the optimal states u_i^{α} to keep are the eigenvectors with the largest eigenvalues. We note the deviation from unity

$$\varepsilon = 1 - \sum_{\alpha=1}^{m} w_{\alpha} , \qquad (3.19)$$

measures the error in the truncation to m states.

The generalization can be made to a universe in a mixed state, in other words, an ensemble at finite temperature. As defined earlier, a mixed state is a collection of pure states, thus we write the mixed state wavefunction as an expansion of pure state wavefunctions Eq. (3.1)

$$|\psi\rangle = \frac{1}{Z} \sum_{k} \exp(-\beta E_k) |\psi^k\rangle = \sum_{k} W_k |\psi^k\rangle, \qquad (3.20)$$

where the W_k are normalized Boltzmann weights. The appropriate definition of the error is now

$$S_k = \sum_k W_k \sum_{ij} \left(\psi_{ij}^k - \sum_{\alpha=1}^m a_\alpha^k u_i^\alpha v_j^{k,\alpha} \right)^2, \qquad (3.21)$$

where the interest is in obtaining a single set of system optimal states u_i^{α} while allowing the environment to vary over k. The reduced density matrix is simply

$$\rho_{ii'} = \sum_{k} W_k \sum_{j} \psi_{ij} \psi^{\dagger}_{i'j}, \qquad (3.22)$$

where the eigenvalues are analogously

$$w_{\alpha} = \sum_{k} W_k \left(a_{\alpha}^k \right)^2. \tag{3.23}$$

Thus the conclusion we draw is identical to that of the pure state: for a universe in a mixed state the optimal states to keep are the eigenvectors of the reduced density matrix with the largest eigenvalues.

3.3 DMRG Algorithms

Having demonstrated the advantage in using density matrices, we now formulate DMRG algorithms for investigating one-dimensional lattice models. The general idea is to follow the standard NRG approach whereby an iterative diagonalization technique is applied to the superblock and a target state is obtained. To represent the target state appropriately at the next iteration, we form a new truncated basis by choosing the m lowest-lying eigenstates of the reduced density matrices. However, in order to construct a sensible algorithm we must address the details of how the superblock is constructed and how new degrees of freedom
are added. The former element deals with how we build the superblock from the system and environment blocks whereas the latter is concerned with how the blocks are enlarged.

At this point, how we build up the superblock seems rather arbitrary. One approach is to follow the NRG and double the system size at each iteration. However, for an efficient DMRG algorithm employing an iterative diagonalization technique, the number of degrees of freedom should be minimized. For that reason it is not computationally efficient to double the size but instead to grow the superblock by adding only a single site to the system and environment blocks at each iteration. This freedom in how we construct the superblock leads to two classes of algorithms which depend on how we evolve the superblock at each iteration: the infinite and finite system procedures. The two proceeding sections outline the details and uses of each method in a pedagogical fashion.

It will be useful to introduce some terminology to avoid any confusion that may arise. The infinite and finite "system" algorithms refer to the superblock as a whole (the system block plus the environment block), hence the system and environment blocks will always be referred to explicitly. When discussing the algorithms, in particular the finite system, the left and right blocks (made clear in Figure 3.2) will refer to all operators associated with that block defined as matrix representations in the current basis that is relevant. We will adopt the following matrix notation

$$\left[M_i\right]_{a;a'}^b,\tag{3.24}$$

where M is the operator, i a specific site location, b the block the operator belongs to, and a is the basis. As previously mentioned, it is possible to target multiple states simultaneously, however, for simplicity we shall target only the ground-state. Finally, forthcoming figures will depict the DMRG applied to block schematics corresponding to one-dimensional lattice models, and even though originally developed for one dimension the technique is not strictly limited by the dimensionality.

3.3.1 Infinite System Build

The following refers to Figure 3.2. We start with a chain of L sites as depicted in Figure 3.2a, small enough to be treated exactly from which the superblock Hamiltonian \mathcal{H} is formed². It is convenient to separate the superblock into four smaller blocks as in Figure 3.2b: a left block, two central blocks which are typically single sites, and a right block³. We label the states of the elementary unit site, denoted by a solid circle \bullet , by $|s_d\rangle$ $(d = 1, \ldots, D)$, where D is the number of accessible configurations⁴. The blocks $\mathcal{B}_{l,m}$ and $\mathcal{B}'_{l',m'}$ contain l and l' sites such that L = l + l' + 2. In addition the blocks are labeled by a m-dimensional⁵ basis, $|a_l\rangle$, $a_l = 1, \ldots, (s_d)^l$ and $|b_{l'}\rangle$, $b_{l'} = 1, \ldots, (s_d)^{l'}$, i.e. $m = (s_d)^l$ and $m' = (s_d)^{l'}$, to reflect the number of sites contained. Finally, Figure 3.2c shows one particular choice in distinguishing the system from the

² "Forming the superblock" is to be interpreted as constructing the Hamiltonian \mathcal{H} in sparse form via iterative diagonalization. ³This configuration is for open boundary conditions. See Section 3.3.3 for periodic boundary conditions.

⁴For example, in the Heisenberg model D = 2: $|s_1\rangle = |\uparrow\rangle$, $|s_2\rangle = |\downarrow\rangle$ in the S^z basis.

⁵In general, m is chosen so that the Hilbert space does not grow with the system size but at this stage it is exact.

environment. It is usually the case that for the infinite system algorithm the environment block is chosen to be a reflection of the system block which includes a single site. With (l', m') = (l, m) the superblock grows by two sites per iteration until a desired "infinite" length is reached. For the proceeding discussion (l', m')are not necessarily equal to (l, m).



Figure 3.2: (a) One-dimensional chain of L sites with open ends. (b) A typical superblock configuration broken into four separate blocks. Rectangles represent blocks containing l and l' sites, while solid circles • represent single sites. (c) One choice in isolating the system from the environment.

Having defined an appropriate basis, the first step in the infinite system algorithm is to construct the Hamiltonian \mathcal{H} for the superblock configuration $\mathcal{B}_{l,m} \bullet \bullet' \mathcal{B}'_{l',m'}$. To illustrate how we construct \mathcal{H} , let us assume for simplicity that the chain interacts through a nearest-neighbour exchange J and is subjected to an on-site field term h. The superblock Hamiltonian can then be written as

$$\mathcal{H} = H^{B} \otimes \mathbb{1}^{\bullet \bullet' B'} + \mathbb{1}^{B \bullet \bullet'} \otimes H^{B'} + J \left(H^{B \bullet} \otimes \mathbb{1}^{\bullet' B'} + \mathbb{1}^{B} \otimes H^{\bullet \bullet'} \otimes \mathbb{1}^{B'} + \mathbb{1}^{B \bullet} \otimes H^{\bullet' B'} \right) + h \left(\mathbb{1}^{B} \otimes H^{\bullet} \otimes \mathbb{1}^{\bullet' B'} + \mathbb{1}^{B \bullet} \otimes H^{\bullet'} \otimes \mathbb{1}^{B'} \right).$$
(3.25)

Using the Lanczos method, or any other sparse matrix diagonalization routine, we calculate the ground-state wavefunction in the superblock basis

$$|\psi\rangle = \sum_{a_l, s_d, s_{d'}, b_{l'}} \psi_{a_l s_d s_{d'} b_{l'}} |a_l s_d s_{d'} b_{l'}\rangle.$$
(3.26)

To extend the length of the superblock to L+2 and simultaneously suppress the growth of the Hilbert space, we form an effective Hamiltonian $\widetilde{\mathcal{H}}$ for the superblock configuration $\mathcal{B}_{l+1,m} \bullet \bullet' \mathcal{B}_{l'+1,m'}$ from an optimal basis obtained through diagonalizing the system and environment reduced density matrices

$$\left[\rho\right]_{a_{l}s_{d};a_{l}'s_{d}'}^{\rm sys} = \sum_{s_{d'},b_{l'}} \psi_{a_{l}s_{d}s_{d'}b_{l'}} \psi_{a_{l}'s_{d}'s_{d'}b_{l'}}^{\dagger}, \tag{3.27a}$$

$$\left[\rho\right]_{s_{d'}b_{l'};s_{d'}'b_{l'}'}^{\text{env}} = \sum_{a_{l},s_{d}} \psi_{a_{l}s_{d}s_{d'}b_{l'}} \psi_{a_{l}s_{d}s_{d'}'b_{l'}'}^{\dagger}.$$
(3.27b)

From Eqs. (3.27a)-(3.27b) the optimal bases $u^{\alpha}_{a_ls_d}$ and $v^{\beta}_{s_{d'}b_{l'}}$ satisfy

$$\sum_{a_{l}',s_{d}'} \left[\rho\right]_{a_{l}s_{d};a_{l}'s_{d}'}^{\text{sys}} u_{a_{l}s_{d}}^{\alpha} = w_{\alpha}u_{a_{l}s_{d}}^{\alpha} , \qquad (3.28a)$$

$$\sum_{s'_{d'},b'_{l'}} \left[\rho\right]_{s_{d'}b_{l'};s'_{d'}b'_{l'}}^{\text{env}} v^{\beta}_{s_{d'}b_{l'}} = w_{\beta}v^{\beta}_{s_{d'}b_{l'}}, \qquad (3.28b)$$

where the set of eigenvectors u^{α} and v^{β} are expanded in terms of the superblock basis. Retaining the m(m') largest-magnitude eigenvalues⁶ and associated eigenvectors of the system (environment) density matrix, we construct the following truncation matrices

$$[O]_{a_l s_d; \alpha}^{\text{sys}} = u_{a_l s_d}^{\alpha}, \quad \alpha = 1, 2, \dots, m , \qquad (3.29a)$$

$$[O]_{s_{d'}b_{l'};\beta}^{\text{env}} = v_{s_{d'}b_{l'}}^{\beta}, \quad \beta = 1, 2, \dots, m'.$$
(3.29b)

Note that if all the states are retained then $O^{\dagger}O = 1$. These will be used to "renormalize", or rather, transform the blocks $\mathcal{B} \bullet$ and $\bullet'\mathcal{B}'$ to an appropriate basis to represent the ground-state at the next iteration. To apply the transformation we form matrix representations of the system (left+central) and environment (central+right) block Hamiltonians

$$\left[\widetilde{H}\right]_{\alpha;\alpha'}^{\mathcal{B}} = O^{\mathrm{sys},\dagger} H^{\mathcal{B}\bullet} O^{\mathrm{sys}} = \sum_{a_l,s_d,a_l',s_d'} O_{\alpha;a_l s_d} H_{a_l s_d;a_l' s_d'} O_{a_l' s_d';\alpha'} , \qquad (3.30a)$$

$$\left[\widetilde{H}\right]_{\beta;\beta'}^{\mathcal{B}'} = O^{\mathrm{env},\dagger} H^{\bullet'\mathcal{B}'} O^{\mathrm{env}} = \sum_{s_{d'},b_{l'},s_{d'}',b_{l'}'} O_{\beta;s_{d'}b_{l'}} H_{s_{d'},b_{l'};s_{d'}',b_{l'}'} O_{s_{d'}'b_{l'}';\beta'} , \qquad (3.30b)$$

as well as any other relevant operators such as a spin component⁷

$$\left[\tilde{S}^{\sigma}_{\bullet}\right]_{\alpha;\alpha'} = O^{\mathrm{sys},\dagger} \left(\mathbb{1}^{\mathcal{B}} \otimes S^{\sigma}_{\bullet}\right) O^{\mathrm{sys}} = \sum_{\sigma,a_l,s_d,a_l',s_d'} O_{\alpha;a_ls_d} \left[\hat{S}^{\sigma}_{\bullet}\right]_{a_ls_d;a_l's_d'} O_{a_l's_d';\alpha'} , \qquad (3.31a)$$

$$\left[\tilde{S}_{\bullet'}^{\sigma}\right]_{\beta;\beta'} = O^{\mathrm{env},\dagger}\left(S_{\bullet'}^{\sigma}\otimes\mathbb{1}^{\mathcal{B}'}\right)O^{\mathrm{env}} = \sum_{\sigma,s_{d'},b_{l'},s_{d'}',b_{l'}'}O_{\beta;s_{d'}b_{l'}}\left[\hat{S}_{\bullet'}^{\sigma}\right]_{s_{d'}b_{l'};s_{d'}'b_{l'}'}O_{s_{d'}'b_{l'}';\beta'} . \tag{3.31b}$$

⁶The values of m and m' should be chosen sufficiently large to accurately represent the ground-state at the next iteration but also sufficiently small to maximize efficiency.

⁷Eqs. (3.31a)-(3.31b) show that for a chain with nearest-neighbour interactions, it is necessary to reconstruct the appropriate "link" needed between the rightmost (leftmost) site of the system (environment) block and a free site.

The superblock Hamiltonian $\widetilde{\mathcal{H}}$ of size L + 2 is formed using $\widetilde{H}^{\mathcal{B}}$, two single sites and $\widetilde{H}^{\mathcal{B}'}$, plus any other local operators needed to connect the blocks. For example, if the Hamiltonian is of the form

$$\mathcal{H} = J \sum_{i=1}^{L-1} \mathbf{S}_i \cdot \mathbf{T}_{i+1} + h \sum_{i=1}^{L} \mathbf{V}_i , \qquad (3.32)$$

where \mathbf{S}_i , \mathbf{T}_i and \mathbf{V}_i are operators acting on the *i*th site, then the effective superblock Hamiltonian is

$$\begin{aligned} \widetilde{\mathcal{H}} &= \left[\widetilde{H}\right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbf{1}_{s_{d}s_{d'}\beta;s_{d'}s_{d'}\beta'}^{\bullet\bullet'\mathcal{B}'} + \mathbf{1}_{\alpha s_{d}s_{d'};\alpha's_{d}'s_{d'}'}^{\mathsf{B}\bullet\bullet'} \otimes \left[\widetilde{H}\right]_{\beta;\beta'}^{\mathcal{B}'} \\ &+ J\left(\left[\widetilde{\mathbf{S}}_{l+1}\right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbf{T}_{s_{d};s_{d}'}^{\bullet} \otimes \mathbf{1}_{s_{d'}\beta;s_{d'}'\beta'}^{\bullet'} \\ &+ \mathbf{1}_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbf{S}_{s_{d};s_{d}'}^{\bullet} \otimes \mathbf{T}_{s_{d'};s_{d'}'}^{\bullet'} \otimes \mathbf{1}_{\beta;\beta'}^{\mathcal{B}'} \\ &+ \mathbf{1}_{\alpha s_{d};\alpha's_{d}'}^{\mathfrak{B}\bullet} \otimes \mathbf{S}_{s_{d'};s_{d'}'}^{\bullet'} \otimes \left[\widetilde{\mathbf{T}}_{l}\right]_{\beta;\beta'}^{\mathcal{B}} \\ &+ h\left(\mathbf{1}_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbf{V}_{s_{d};s_{d}'}^{\bullet} \otimes \mathbf{1}_{s_{d'}\beta;s_{d'}'\beta'}^{\bullet'\mathcal{B}'} + \mathbf{1}_{\alpha s_{d};\alpha's_{d}'}^{\mathcal{B}\bullet} \otimes \mathbf{V}_{s_{d'};s_{d'}'}^{\bullet'} \otimes \mathbf{1}_{\beta;\beta'}^{\mathcal{B}'} \right), \end{aligned}$$

$$(3.33)$$

and has a reduced Hilbert space of size D^2mm' . Note the similarity in form between Eqs. (3.25) and (3.33). The calculation is then repeated substituting $\tilde{\mathcal{H}}$ for \mathcal{H} , until a desired length is reached. We summarize the infinite system algorithm in Table 3.1.

Table 3.1: Infinite system density-matrix algorithm.

0.	Form the superblock Hamiltonian \mathcal{H} (in sparse form) from four initial blocks: a left block, two central blocks and a right block.
1.	Using a sparse matrix diagonalization routine, diagonalize \mathcal{H} and obtain the target state (usually the ground-state) in the superblock basis $\psi(a_l, s_d, s_{d'}, b_{l'})$.
2.	Form the reduced density matrices ρ^{\flat} and diagonalize to obtain the m^{\flat} largest-magnitude eigenvalues and corresponding eigenvectors u_{\flat}^{α} .
3.	Construct the appropriate truncation matrices $O_{b;\alpha}^{\flat} = u_b^{\alpha}$, $\alpha = 1, 2, \ldots, m^{\flat}$, such that the columns are the m^{\flat} retained eigenvectors of ρ^{\flat} .
4.	Form matrix representations of all relevant operators H^{\flat} , $S^{\sigma,p}$, etc., and truncate to the new basis of m^{\flat} states via $\tilde{H}^{\flat} = O^{\flat,\dagger} H^{\flat} O^{\flat}$, etc.
5.	Form the next iteration superblock Hamiltonian $\widetilde{\mathcal{H}}$ of length $L + 2$ (in sparse form) using $\widetilde{\mathcal{H}}^{\mathcal{B}}$, two single sites and $\widetilde{\mathcal{H}}^{\mathcal{B}'}$, plus any other local operators.
6.	Is the desired length L_{\max} ? If not, go to step 0 . substituting $\widetilde{\mathcal{H}}$ for \mathcal{H} .

As illustrated by Eq. (3.33) and Figure 3.3 the new sites replace the old central ones, effectively pushing the ends of the chain apart. It is important to note that these new sites are in the original superblock



Figure 3.3: Three infinite system DMRG steps. Central sites are absorbed (red and blue dashed boxes) with each successive iteration, pushing them outward towards the ends of the chain.

basis as they have had no previous connection to the system. When a desired length L_{max} is reached, each block approximately represents one-half of an infinite chain but both are neither completely isolated in the standard NRG sense; the effective Hamiltonian formed contains a system block which depends strongly on the environment block.

We emphasize that the infinite system algorithm can increase the total number of sites by two at each iteration without increasing the Hilbert space. For a strongly-interacting system of L sites each with D degrees of freedom, the Hilbert space is reduced to D^2mm' at each iteration provided m and m' are chosen appropriately. Clearly, the more states kept the better the representation. However, the precision of the end result is, in some sense, predetermined since each block is always described by m states regardless of the number of sites it contains. Hence, for a reliable DMRG calculation m should be chosen by inspecting the truncation error Eq. (3.19) at each iteration and ensuring that ε remains sufficiently small $\sim 10^{-5} - 10^{-8}$. In particular, for critical one-dimensional systems where the correlation length $\xi = \infty$, ε decays algebraically in m whereas for non-critical $\xi < \infty$, ε decays exponentially. This decay behaviour characterizes how entangled the system is: a critical system is more entangled and requires more states to be kept.

3.3.2 Finite System Sweep

The infinite system algorithm is used to build up the size of the superblock to a "thermodynamic limit" by systematically introducing new sites between the system and environment blocks. There is, however, a slight setback due to the nature of the algorithm; at each step as we truncate all operators to an *m*-dimensional basis superficial errors are introduced in the description of the wavefunction for the next iteration. As the algorithm iterates, these errors are compounded leading to poor convergence⁸ of the wavefunction. The result is an unsatisfactory wavefunction for a superblock of length L_{max} . The underlying physical reason is because the wavefunction of the final lattice size is completely different from the initial size.

 $^{^8\}mathrm{Not}$ in the sense of converging to the wrong state.

In this section we describe how to overcome the issue of different lattice sizes by using a finite system sweep procedure on a superblock of length L_{max} . This procedure optimizes, to a degree, the bases in both blocks by varying the size of the environment block while keeping the superblock length fixed. By optimizing the bases most of the compounded superficial errors can be eliminated as well as reducing some of the truncation error. As a direct consequence, measurements of observables can be adjusted to be more accurate and in some cases change the overall qualitative behaviour.

The finite system algorithm is summarized in Table 3.2 and a schematic is presented in Figure 3.4. We start with a slightly modified infinite system DMRG for a chain of L sites, where for simplicity we assume the environment block has been chosen to be a reflection of the system block $\mathcal{B}_{l,m} \bullet \bullet \mathcal{B}'_{l,m}$. Ordinarily, $\mathcal{B}_{l+1,m}$ would replace $\mathcal{B}_{l,m}$ at each step; instead we store in memory the block Hamiltonian and any other relevant operators of $\mathcal{B}_{l,m}$ so that we may recall them later. Aside from this addition, we carry out the infinite system DMRG as normal until the superblock becomes $\mathcal{B}_{L_{\max}/2-1,m} \bullet \bullet \mathcal{B}'_{L_{\max}/2-1,m}$, the starting point of the finite system DMRG.

 Table 3.2: Finite system density-matrix algorithm.

- 0. Use the infinite system algorithm on a chain of L sites to build up a superblock of length L_{max} , storing at each iteration the block Hamiltonian and any relevant operators for the left and right blocks. Here, $l = l' = L_{\text{max}}/2 1$.
- 1. Left-to-right. Carry out steps 2. 4. of Table 3.1 enlarging only the left block to $\mathcal{B}_{l+1,m}$. Store the block. Now l = l+1 and l' = l'-1.
- 2. Form the superblock $\mathcal{B}_{l,m} \bullet \bullet \mathcal{B}'_{l',m}$ of length L_{\max} , where the right block is obtained from step [0,].
- 3. Repeat steps 1. 2. until $l = L_{\text{max}} L/2 1$ and l' = L/2 1.
- 4. Right-to-left. Carry out steps 2. 4. of Table 3.1 reversing the roles of the left and right blocks, that is, enlarge only the right block to $\mathcal{B}_{l'+1,m}^{'}$ using the stored $\mathcal{B}_{l,m}$ as the environment. Store $\mathcal{B}_{l'+1,m}^{'}$. Now l = l 1 and l' = l' + 1.
- 5. Form the superblock $\mathcal{B}_{l,m} \bullet \bullet \mathcal{B}'_{l',m}$ of length L_{\max} , where the left block is obtained from the previous sweep.
- 6. Repeat steps 3. 4. until l = L/2 1 and $l' = L_{\text{max}} L/2 1$.
- 7. Go to step 1. until convergence has been obtained, in which case terminate with a symmetric superblock configuration $\mathcal{B}_{L_{\max}/2-1,m} \bullet \bullet \mathcal{B}'_{L_{\max}/2-1,m}$.

The finite system algorithm improves the convergence of the wavefunction by carrying out a "sweep" procedure. The idea is to systematically grow the left block by one site while reducing the right block correspondingly. In the first step we diagonalize the superblock configuration $\mathcal{B}_{L_{\max}/2-1,m} \bullet \bullet \mathcal{B}'_{L_{\max}/2-1,m}$ but enlarge only the left block to $\mathcal{B}_{L_{\max}/2,m}$ in the usual way. Like before we store this block in memory. In



Figure 3.4: A schematic of the finite system algorithm completing a full system sweep. Dashed boxes (red) denote the direction of the sweep.

the next step, we take the right block from memory and form the configuration $\mathcal{B}_{L_{\max}/2,m} \bullet \mathcal{B}'_{L_{\max}/2-2,m}$, where again we enlarge only the left block to $\mathcal{B}_{L_{\max}/2+1,m}$ and store it to memory. We continue this until the number of sites in the right block reaches the minimum size of L/2 - 1, comprising one finite system sweep.

We now reverse the roles of the blocks and sweep in the opposite direction. Note that subsequent iterations will use blocks which have been obtained from the previous sweep. The second sweep starts by diagonalizing the configuration $\mathcal{B}_{L_{\max}-L/2-1,m} \bullet \bullet \mathcal{B}'_{L/2-1,m}$ to obtain an enlarged right block $\mathcal{B}'_{L/2,m}$. Here, $\mathcal{B}'_{L/2-1,m}$ is always known exactly and $\mathcal{B}_{L_{\max}-L/2-1,m}$ is taken from memory. From this point the remainder of the second sweep is equivalent to the first sweep in that we iterate until the superblock configuration is $\mathcal{B}_{L/2-1,m} \bullet \bullet \mathcal{B}'_{L_{\max}-L/2-1,m}$. We continue sweeping back and forth in this manner, improving the ground-state with each sweep, until the ground-state energy converges. Although in some cases the energy will not show any sign of improvement until after a few sweeps. For one-dimensional systems a typical number of sweeps is of $\mathcal{O}(1)$. The last sweep should end in the symmetric configuration $\mathcal{B}_{L_{\max}/2-1,m} \bullet \bullet \mathcal{B}'_{L_{\max}/2-1,m}$.

where the wavefunction can then be used to calculate observables.

By keeping the superblock length fixed, each finite system sweep improves the overall accuracy of the block matrix representations, leading to a more desirable description of the ground-state. However, because of the truncation to m basis states, the reduced Hilbert space of the Hamiltonian will always yield a ground-state energy higher than the exact value. By sweeping back and forth, the finite system DMRG is equivalent to a variational method whereby the trial wavefunction at each step is automatically constructed under the restriction of the m basis states.

Throughout the discussion of the two algorithms we focused our attention on the ground-state of the Hamiltonian. However, because we employ a sparse matrix diagonalization routine, it is possible to target more than one state using both DMRG algorithms. After each diagonalization step, reduced density matrices for each extracted target state must be calculated leading to separate truncation matrices. Thus, for every target state acquired each operator must be kept and updated accordingly during the entirety of the calculation. In this way, the DMRG is capable of representing the Hilbert spaces around each target state very efficiently.

3.3.3 Periodic Boundary Conditions

The DMRG algorithms described in the two previous sections were in terms of open boundary conditions (OBC). To use DMRG with periodic boundary conditions (PBC), the correct superblock configuration is $\mathcal{B}_{l,m} \bullet \mathcal{B}'_{l',m'} \bullet'$, which helps to reduce the sparseness of the superblock Hamiltonian. This is useful since most one-dimensional strongly correlated systems are studied using PBC. For smaller system sizes PBC are mainly preferred to OBC since finite-size effects can be kept to a minimum. Be that as it may, even with this configuration the periodic case yields less accurate results [51]. Thus, OBC are mainly used since better results are obtained for a given computational effort, i.e. if a certain accuracy is obtained by keeping m states for OBC, then m^2 states need to be kept to achieve the same accuracy for PBC.

3.4 Measurements

Once the superblock of L_{max} sites has been swept through, the improved wavefunction(s) can be used to calculate expectation values of quantum observables. In addition to the energy, the DMRG is capable of evaluating expectation values of the form

$$\langle A \rangle = \langle \psi | A | \psi \rangle, \tag{3.34}$$

using the ground-state (or an excited-state) wavefunction $|\psi\rangle$ from the diagonalization of the L_{max} – site superblock. Note that the most accurate results will come from diagonalizing the symmetric configuration $l = l' = L_{\text{max}}/2 - 1$, where both left and right blocks have an equal number of sites.

Although seemingly a straightforward task, one cannot just simply carry out Eq. (3.34). The problem

lies in the basis of the obtained wavefunction $|\psi\rangle$. The states which describe the left and right blocks have been transformed many times over, evolving in such a way that cannot be easily deciphered. That is to say, any quantum observable we wish to measure must also evolve in exactly the same manner as the blocks. For example, to measure the expectation value of the on-site spin density S_i^z for a site *i* in the left block, the matrix representation $[\tilde{S}_i^z]_{\alpha;\alpha'}^{\mathcal{B}}$ must be tracked throughout the entire calculation and updated at each subsequent DMRG step. Suppose we have added the site *i* to the left block as in Eq. (3.31a). When a new site is added at the next iteration the matrix representation must be adjusted properly according to

$$\left[\widetilde{S}_{i}^{z}\right]_{\alpha;\alpha'}^{\mathcal{B}} \longleftarrow \sum_{a_{l},s_{d},a_{l}',s_{d}'} O_{\alpha;a_{l}s_{d}} \left(\left[\widetilde{S}_{i}^{z}\right]_{a_{l};a_{l}'}^{\mathcal{B}} \otimes \mathbb{1}_{s_{d};s_{d}'}^{\bullet}\right) O_{a_{l}'s_{d}';\alpha'} .$$

$$(3.35)$$

where the measurement can then be carried out as

$$\langle \psi | S_i^z | \psi \rangle = \sum_{a_l, a_l'}^m \sum_{s_d, s_{d'}, b_l} \psi_{a_l s_d s_{d'} b_l}^{\dagger} \left[\widetilde{S}_i^z \right]_{a_l; a_l'}^{\mathcal{B}} \psi_{a_l' s_d s_{d'} b_l}^{\mathcal{B}} , \qquad (3.36)$$

giving an exact evaluation of $\langle \psi | S_i^z | \psi \rangle$ for an approximate eigenstate $| \psi \rangle$.

For a non-local measurement such as the two-point correlation function $C_{ij} = \langle \psi | S_i^z S_j^z | \psi \rangle$ extra care must be taken. If the sites *i* and *j* are located on different blocks, say the left block and the right block respectively, the expectation value is a direct application of Eq. (3.36) with an intermediate step:

$$\left\langle \psi | S_i^z S_j^z | \psi \right\rangle = \sum_{a_l, b_l, a_l', b_l'}^m \sum_{s_d, s_{d'}} \psi_{a_l s_d s_{d'} b_l}^{\dagger} \left[\widetilde{S}_i^z \right]_{a_l; a_l'}^{\mathcal{B}} \left[\widetilde{S}_j^z \right]_{b_l; b_l'}^{\mathcal{B}'} \psi_{a_l' s_d s_{d'} b_l'}^{\mathcal{B}'} \left. \right.$$
(3.37)

However, if i and j are located on the same block, say the left block, the expression is not

$$\left\langle \psi | S_i^z S_j^z | \psi \right\rangle \neq \sum_{a_l, a_l', a_l''}^m \sum_{s_d, s_{d'}, b_l} \psi_{a_l s_d s_{d'} b_l}^{\dagger} \left[\widetilde{S}_i^z \right]_{a_l; a_l'}^{\mathcal{B}} \left[\widetilde{S}_j^z \right]_{a_l'; a_l''}^{\mathcal{B}} \psi_{a_l' s_d s_{d'} b_l}^{\mathcal{B}} , \qquad (3.38)$$

but is rather given by the compound object

$$\left\langle \psi | S_i^z S_j^z | \psi \right\rangle = \sum_{a_l, a_l'}^m \sum_{s_d, s_{d'}, b_l} \psi_{a_l s_d s_{d'} b_l}^{\dagger} \left[\widetilde{S_i^z S_j^z} \right]_{a_l; a_l'}^{\mathcal{B}} \psi_{a_l' s_d s_{d'} b_l} , \qquad (3.39)$$

which must also be updated analogous to Eq. (3.35). To see why this is the case, consider a symmetric configuration where l' = l = L/2, and i = l + 1 and j = l + 2 belonging to the system block with a basis

indexed by $a_l = 1, \ldots, m$. The on-site spin density matrix representations are then

$$\left[\widetilde{S}_{i}^{z}\right]_{\alpha;\alpha'}^{\mathcal{B}} = O^{\mathrm{sys},\dagger}\left(\mathbb{1}^{\mathcal{B}_{i}} \otimes \mathbb{1}_{2;2}^{j} \otimes S_{i}^{z}\right)O^{\mathrm{sys}} = \sum_{a_{l},s_{d},a_{l}',s_{d}'} O_{\alpha;a_{l}s_{d}}\left[\widehat{S}_{i}^{z}\right]_{a_{l}s_{d};a_{l}'s_{d}'}O_{a_{l}'s_{d}';\alpha'}, \quad (3.40a)$$

$$\left[\tilde{S}_{j}^{z}\right]_{\alpha;\alpha'}^{\mathcal{B}} = O^{\mathrm{sys},\dagger}\left(\mathbb{1}^{\mathcal{B}_{j}} \otimes S_{j}^{z} \otimes \mathbb{1}_{2;2}^{i}\right)O^{\mathrm{sys}} = \sum_{a_{l},s_{d},a_{l}',s_{d}'} O_{\alpha;a_{l}s_{d}}\left[\hat{S}_{j}^{z}\right]_{a_{l}s_{d};a_{l}'s_{d}'}O_{a_{l}'s_{d}';\alpha'}, \quad (3.40b)$$

$$\left[\widetilde{S_i^z S_j^z}\right]_{\alpha;\alpha'}^{\mathcal{B}} = O^{\text{sys},\dagger} \left(\mathbbm{1}^{\mathcal{B}_{ij}} \otimes S_i^z \otimes S_j^z\right) O^{\text{sys}} = \sum_{a_l,s_d,a_l',s_d'} O_{\alpha;a_l s_d} \left[\widehat{S_i^z S_j^z}\right]_{a_l s_d;a_l' s_d'} O_{a_l' s_d';\alpha'} , \quad (3.40c)$$

where \mathcal{B}_i , \mathcal{B}_j and \mathcal{B}_{ij} label the appropriate dimensions for the respective identity matrices. Applying Eqs. (3.38)-(3.39) we have

$$\begin{split} \left\langle \tilde{S}_{i}^{z} \tilde{S}_{j}^{z} \right\rangle &= \left\langle \sum_{a_{l},a_{l}',a_{l}''}^{m} \left[\tilde{S}_{i}^{z} \right]_{a_{l};a_{l}'}^{\mathcal{B}} \left[\tilde{S}_{j}^{z} \right]_{a_{l}';a_{l}''}^{\mathcal{B}} \right\rangle \\ &= \left\langle \sum_{a_{l},a_{l}',a_{l}''}^{m} \sum_{s_{d},s_{d}',s_{d}''} \left(O_{a_{l};a_{l}s_{d}} \left[\hat{S}_{i}^{z} \right]_{a_{l}s_{d};a_{l}'s_{d}'} O_{a_{l}'s_{d}';a_{l}'} \right) \left(O_{a_{l}';a_{l}'s_{d}'} \left[\hat{S}_{j}^{z} \right]_{a_{l}'s_{d}';a_{l}''} O_{a_{l}''s_{d}''} \right) \right\rangle \\ &= \left\langle \sum_{a_{l},a_{l}',a_{l}''}^{m} \sum_{s_{d},s_{d}',s_{d}''}^{\mathcal{D}} O_{a_{l};a_{l}s_{d}} \left[\hat{S}_{i}^{z} \right]_{a_{l}s_{d};a_{l}'s_{d}'} O_{a_{l}'s_{d}';a_{l}'} O_{a_{l}';a_{l}'s_{d}'} \left[\hat{S}_{j}^{z} \right]_{a_{l}'s_{d}';a_{l}''s_{d}''} O_{a_{l}''s_{d}''} \right) \right\rangle \\ &\neq \left\langle \sum_{a_{l},a_{l}'}^{m} \left[\widetilde{S}_{i}^{\widetilde{z}} S_{j}^{z} \right]_{a_{l}'a_{l}'}^{\mathcal{B}} \right\rangle. \end{split}$$

$$(3.41)$$

We see that the product of two truncated operators results in a non-unitary inner multiplication of $O^{\dagger}O$. We stress that this kind of multiplication leads to incorrect measurements. The solution is to multiply the two operators as soon as possible guaranteeing the sum to run over a complete set of states, i.e. $O^{\dagger}O = 1$. Generally speaking, one should choose points *i* and *j* located on different blocks, preferably a block and a free site. If possible, avoid choosing *i* and *j* such that they are separated across the centre as this generally leads to a larger error (since both the left and right blocks have been truncated). In Chapter 4 we will see that multiplications occurring on the same block as well as different blocks are unavoidable when applying the DMRG to Hamiltonians with higher-order interactions.

3.5 Improving Efficiency

The most time-consuming part of any DMRG calculation is the multiplication of the Hamiltonian with an arbitrary vector $\mathcal{H}|v\rangle$ during the iterative diagonalization step. The Lanczos method, discussed in Section 2.2, converges to a target state typically on the order of $\mathcal{O}(10) - \mathcal{O}(100)$ iterations. Of course, if a sufficiently large basis is generated, then we are guaranteed a numerically exact result. However, in a typical DMRG calculation where the number of matrix-vector multiplications could be several hundred, reducing the number of steps to reach convergence would lead to a proportional speedup of the diagonalization. Moreover, depending on the complexity of the interactions in the system several of these bonds may need to be reconstructed to form the superblock Hamiltonian. In such an instance, because each operator is $m \times m$ in size, the number of operations scales linearly with the overall time $\mathcal{O}(Nm^2)$ needed to perform one matrix-vector multiplication. In this section we discuss the properties of both the Hamiltonian and the finite system algorithm which can be exploited in order to construct an efficient implementation.

3.5.1 Exploiting Symmetries

For an overall increase in speed and precision it is essential to exploit a system's symmetries. By truncating to m basis states we have thrown away bits and pieces of the description of the target state which seemingly, according to the density matrices, are not all that important. However, to ensure that we are as precise as possible it is necessary that we minimize the degrees of freedom which do not contribute. In condensed matter we often use models which exhibit Abelian symmetries, i.e. conserved quantities. These could be a rotational symmetry, parity inversion, square of the total spin, total spin in the z direction, total particle number, etc. For example, if a Hamiltonian H preserves symmetry A, i.e.

$$\left[H,A\right] = 0,\tag{3.42}$$

then the eigenvalues of H and A are simultaneous good quantum numbers. Once good quantum numbers are identified we can choose to work in a representation where the symmetry operators are always diagonal, i.e. working in a basis which simultaneously diagonalizes H and A. In one-dimensional systems where shortranged interactions are the norm, the matrix representations of operators are populated mostly by zeros. Depending on the target state, most of these zeros will not contribute and thus should be ignored from the entire calculation. By choosing an appropriate symmetry sector for the target state, i.e. keeping only relevant states, we can do away with large sparse matrices and instead work with smaller dense matrices. The target state is then always computed within a set of good quantum numbers and not in the superblock Hilbert space, thus leading to a significant reduction in the computational effort. The payoff is a faster and more precise DMRG implementation.

3.5.2 Preconditioning: Transforming the Wavefunction

We emphasize that the following procedure improves only the speed at which the target state is computed while the precision remains unchanged. To reduce the time needed to perform the matrix-vector multiplications and to ensure convergence to the actual target state, we make use of the fact that the starting vector can be preconditioned. Typically, the operation $\mathcal{H}|v\rangle$ requires ~ $\mathcal{O}(40) - \mathcal{O}(100)$ iterations to converge to the target state with sufficient accuracy. In the Lanczos method where the starting vector is random, a large number of iterations are needed to ensure convergence to the target state. The solution to ensuring that the DMRG always remains stable and accurate is to modify the starting vector. The basic principle behind preconditioning is to provide the Lanczos method with an initial starting wavefunction that is a good approximation to the desired target state. Not only will this will ensure convergence to the correct target state, but more importantly it will reduce the overall computational time. Since the lattice size remains fixed during the finite system DMRG, an ideal starting wavefunction would be the state $|\psi\rangle$ obtained from the previous step. However, this wavefunction is in a different basis corresponding to a different superblock. To transform the wavefunction into an appropriate basis to describe the superblock at the next finite system step, we make use of the truncation matrices Eqs. (3.29a)-(3.29b) obtained after step $\overline{3}$ of Table 3.1.

Following [52] we present the wavefunction transformation using the four-block superblock description of fixed size L. We begin with the left-to-right finite system sweep. At step l of the sweep the wavefunction in the superblock basis is given by

$$|\psi\rangle = \sum_{\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}} \psi_{\alpha_l s_{l+1} s_{l+2} \beta_{l+3}} |\alpha_l\rangle \otimes |s_{l+1}\rangle \otimes |s_{l+2}\rangle \otimes |\beta_{l+3}\rangle, \tag{3.43}$$

where $|\alpha_l\rangle$ is the basis of the left block containing l sites, $|s_{l+1}\rangle$ and $|s_{l+2}\rangle$ are the bases of the two single sites l+1 and l+2, and $|\beta_{l+3}\rangle$ is the basis of the right block containing L-l-2 sites. The transformation of the wavefunction into the new superblock basis for step l+1 is carried out in two steps: absorb a site into the left block and "spit out" a site from the right block. After enlarging the left block in the usual manner, we use the constructed truncation matrix $[O]_{\alpha_l s_{l+1};\alpha_{l+1}}^{sys}$ to form the new left block basis

$$|\alpha_{l+1}\rangle = \sum_{\alpha_l, s_{l+1}} \left[O\right]_{\alpha_l s_{l+1}; \alpha_{l+1}}^{\text{sys}} |\alpha_l\rangle \otimes |s_{l+1}\rangle.$$
(3.44)

The right block basis $|\beta_{l+3}\rangle$ was formed with the truncation matrix $[O]_{s_{l+3}\beta_{l+4};\beta_{l+4}}^{\text{env}}$ at an earlier DMRG step⁹ and is similarly written as

$$|\beta_{l+3}\rangle = \sum_{s_{l+3},\beta_{l+4}} \left[O\right]_{s_{l+3}\beta_{l+4};\beta_{l+4}}^{\text{env}} |s_{l+3}\rangle \otimes |\beta_{l+4}\rangle.$$
(3.45)

To transform the wavefunction into the appropriate basis for the next step, $|\alpha_{l+1}s_{l+2}s_{l+3}\beta_{l+4}\rangle$, we make use of the approximations¹⁰

$$\sum_{\alpha_{l+1}} |\alpha_{l+1}\rangle \langle \alpha_{l+1}| \approx 1 \quad \text{and} \quad \sum_{\beta_{l+3}} |\beta_{l+3}\rangle \langle \beta_{l+3}| \approx 1.$$
(3.46)

With these the coefficients of the wavefunction in the new basis are obtained through two steps:

⁹Either from the infinite system DMRG or a previous finite system sweep.

 $^{^{10}\}mathrm{They}$ are approximate simply because we have truncated to m states.

3.6. BENCHMARKING AND ANALYSIS

0. Form the intermediate result

$$\left\langle \alpha_{l+1} s_{l+2} \beta_{l+3} \middle| \psi \right\rangle \approx \sum_{\alpha'_{l+1}} \left\langle \alpha_{l+1} \middle| \alpha'_{l+1} \right\rangle \left\langle \alpha'_{l+1} s_{l+2} \beta_{l+3} \middle| \psi \right\rangle$$

$$= \sum_{\alpha_{l}, s_{l+1}} \left[O \right]_{\alpha_{l} s_{l+1}; \alpha_{l+1}}^{\text{sys}, \dagger} \left\langle \alpha_{l} s_{l+1} s_{l+2} \beta_{l+3} \middle| \psi \right\rangle.$$

$$(3.47)$$

1. Followed by the final result

$$\left\langle \alpha_{l+1}s_{l+2}s_{l+3}\beta_{l+4} \middle| \psi \right\rangle \approx \sum_{\beta_{l+3}} \left\langle \alpha_{l+1}s_{l+2}s_{l+3}\beta_{l+4} \middle| \beta_{l+3} \right\rangle \left\langle \beta_{l+3} \middle| \psi \right\rangle$$
$$= \sum_{\beta_{l+3}} \sum_{s'_{l+3},\beta'_{l+4}} \left\langle \alpha_{l+1}s_{l+2}s_{l+3}\beta_{l+4} \middle| [O]_{s'_{l+3}\beta'_{l+4}}^{\mathrm{env}} \middle| s'_{l+3}\beta'_{l+3} \right\rangle \left\langle \beta_{l+3} \middle| \psi \right\rangle$$
$$= \sum_{\beta_{l+3}} \left\langle \alpha_{l+1}s_{l+2}\beta_{l+3} \middle| \psi \right\rangle [O]_{s_{l+3}\beta_{l+4};\beta_{l+4}}^{\mathrm{env}} . \tag{3.48}$$

Therefore, the complete transformation sweeping left-to-right is

$$\left\langle \alpha_{l+1}s_{l+2}s_{l+3}\beta_{l+4} \middle| \psi \right\rangle \approx \sum_{\alpha_l s_{l+1}\beta_{l+3}} \left[O \right]_{\alpha_l s_{l+1};\alpha_{l+1}}^{\mathrm{sys},\dagger} \left\langle \alpha_l s_{l+1}s_{l+2}\beta_{l+3} \middle| \psi \right\rangle \left[O \right]_{s_{l+3}\beta_{l+4};\beta_{l+4}}^{\mathrm{env}}, \tag{3.49}$$

and analogously for the right-to-left sweep

$$\left\langle \alpha_{l-1} s_l s_{l+1} \beta_{l+2} \middle| \psi \right\rangle \approx \sum_{\alpha_l s_{l+2} \beta_{l+3}} \left[O \right]_{s_{l+2} \beta_{l+3}; \beta_{l+3}}^{\text{env},\dagger} \left\langle \alpha_l s_{l+1} s_{l+2} \beta_{l+3} \middle| \psi \right\rangle \left[O \right]_{\alpha_{l-1} s_l; \alpha_l}^{\text{sys}} . \tag{3.50}$$

Indeed, preconditioning requires storing all truncation matrices to memory but is comparatively less than the blocks themselves. The overall gain in speed during the diagonalization procedure more than accounts for the time spent transforming the wavefunction, which is considerably small when compared to say, diagonalizing a reduced density matrix. Preconditioning is thus an essential part in any efficient implementation of the DMRG.

3.6 Benchmarking and Analysis

In this section we benchmark the efficiency of an original DMRG implementation through a variety of calculations. We use a symmetric configuration (l', m') = (l, m) for the infinite system DMRG with open boundary conditions (OBC) and benchmark with the S = 1/2 antiferromagnetic Heisenberg chain. In some cases we add a next-nearest-neighbour coupling J_2 . In addition to using ARPACK for the iterative diagonalization, we also exploit the SU(2) spin-rotation invariance of the Heisenberg model by restricting our calculations to $\sum_i S_i^z = \text{const}$ subspaces. Properties of the low-lying excitations are compared with well-established theoretical results, where in particular we focus on logarithmic corrections (due to finite-size

effects) which are obtained from conformal field-theoretical approaches. Note that all calculations use a nearest-neighbour coupling strength of $J_1 = 1$.

3.6.1 Observables

Accuracy and precision. $J_2 = 0$; Shown in Figure 3.5 are the reduced density matrix eigenvalues w_{α} of the system block for the ground-state and first-excited state of a 32-site chain. Comparing with the Bethe ansatz results [53], the relative error (inset) in the ground-state energy $|\Delta E/E| = |1 - E_0^{\text{DMRG}}/E_0^{\text{BA}}|$ is seen to falloff slower than the density matrix eigenvalues, reflecting that higher precision is attained when more states are kept. One way to ensure a desired accuracy of the target state is to check that the truncation error $\varepsilon(m) = 1 - \sum_{\alpha=1}^{m} w_{\alpha}$ at each step meets a specific cutoff.



Figure 3.5: Reduced density matrix eigenvalues w_{α} for the ground-state and first-excited state plotted against the index number α for a 32-site isotropic Heisenberg chain. These eigenvalues were obtained from a 14-site superblock keeping m = 64 states at each iteration. The step-like structure is the result of spin degeneracies. Inset shows the relative error in the ground-state energy $|\Delta E/E|$ as a function of the states kept m, and is seen to falloff slower than the w_{α} .

Target-state energy. $J_2 = 0$; We compare the ground-state energy of a 100-site chain with the Bethe ansatz result as a function of the finite system sweep position. In Figure 3.6a, one sees the energy improve with sweeping. In this example with m = 128, the precision of the ground-state energy is improved roughly by one order of magnitude after 3 sweeps while no significant improvement was observed with additional sweeps. Figure 3.6b is a similar result but as a function of the sweep iteration. When m is too small no amount of sweeping will improve the description of the wavefunction, whereas for large enough m, there is a clear emphasis on the improvement of the wavefunction per iteration.



Figure 3.6: (a) The ground-state energy E_0^{DMRG} output from a 3-sweep finite system DMRG procedure compared with the Bethe ansatz result E_0^{BA} for a 100-site isotropic Heisenberg chain. Position refers to the location of the finite system sweep. (b) Same as (a) but as a function of the sweep iteration for different values of m. Only every third point is plotted.

Entanglement Entropy. With access to the density matrix weights, one can measure how entangled the system is with its environment. First introduced in the context of quantum information [36], the entanglement entropy (EE) of a subsystem embedded in a larger system is defined as the von Neumann entropy [54] of the reduced density matrix:

$$S_{\rm vN}(\rho) = -{\rm tr}(\rho \,\ln\rho) = -\sum_{\alpha} w_{\alpha} \,\ln w_{\alpha}. \tag{3.51}$$

For a one-dimensional isotropic Heisenberg chain, the EE of a semi-infinite subsystem of size x including the open end has been shown to follow the universal form [55, 56]

$$S(x,L) = \frac{c}{6}\ln x + k,$$
 (3.52)

where c is the central charge of the associated CFT [57, 58] and k is a non-universal constant. For critical systems such as the Heisenberg chain where the correlation length is infinite, we should expect the ground-state entanglement to extend to all length scales. We can see this reflected in Figure 3.7 where the EE diverges logarithmically with L. We also notice that the EE of the 100-site system block disagrees with the CFT fit (red line) (3.52); it does not account for the alternating behaviour. The use of OBC breaks translational symmetry which causes an additional slowly decaying alternating term or dimerization to the



Figure 3.7: The von Neumann entropy of the system block (environment block is the same) of a 200-site chain obtained from reduced density matrices of the ground-state. The alternating behaviour is due to open boundary conditions and therefore does not obey the CFT prediction (red line).

entropy [59]. This alternating behaviour can be understood in terms of a resonating valence bond picture. An example of a valence bond state is

$$|\Phi\rangle = \frac{1}{2^{L/2}} \otimes_{x=1}^{L/2} \left[|\uparrow_{2x-1}\downarrow_{2x}\rangle - |\downarrow_{2x-1}\uparrow_{2x}\rangle \right], \tag{3.53}$$

where the valence bonds are nearest-neighbours. Since any singlet state can be written as a linear combination of all valence bond states (with no bonds crossing each other), there is naturally a higher EE associated with paired spins than with unpaired. We therefore end up with a staggering structure for the EE where every odd (even) bond has an enhanced (reduced) entropy.

Spin-spin correlations. One of the defining characteristics of any quantum spin system is the two-point spin-spin correlation function, a measure of the similarity of the states of spins separated by a distance r. For the spin-isotropic Heisenberg chain the correlation function can be written as

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle = 3 \langle S_i^z S_{i+r}^z \rangle, \qquad (3.54)$$

where r is the distance from a reference site i. For the ground-state of the isotropic Heisenberg chain, Figure 3.8 shows the corresponding correlation function for one-half of the superblock where the left free site is taken as the reference and the measurement is out towards the end of the system block. For large r, the correlation function decays to zero with the distance algebraically $C(r) \sim (-1)^r/r$, up to a multiplicative logarithmic correction $(\ln r)^{1/2}$ [60, 61]. This power law behaviour is indicative of a critical ground-state which does not order magnetically (is spin-disordered and has quasi-long-ranged order), in agreement with the Mermin-Wagner-Hohenberg theorem [62, 63], i.e. the global SU(2) spin-rotation symmetry under short-ranged interactions is not spontaneously broken at zero temperature. From the staggering structure we can conclude that the ground-state of the isotropic Heisenberg chain is of antiferromagnetic nature.



Figure 3.8: The ground-state spin-spin correlation function of the isotropic Heisenberg chain. The staggering behaviour confirms that the ground-state is antiferromagnetically ordered. For large r, the multiplicative logarithmic correction $(\ln r)^{1/2}$ is small and not shown.

3.6.2 Logarithmic Corrections

While it is remarkable that Bethe ansatz [64] solves the S = 1/2 antiferromagnetic Heisenberg chain exactly, there is no implied understanding of how finite-size corrections come about. Through an appropriate twodimensional CFT the use of marginally irrelevant operators has shown that there are logarithmic corrections to finite-size calculations where the associated coupling constant scales as $g(L) \sim 1/\ln L$, and L is the characteristic length or energy scale [65]. Due to this slowly vanishing g(L) logarithmic corrections are expected to appear in virtually all measurable quantities. In this section we show that there are indeed logarithmic corrections, particularly to the ground-state energy and spin gap of the Heisenberg chain [60, 61]. In addition we also show that these corrections can vanish when we consider the $J_1 - J_2$ Hamiltonian

$$\mathcal{H} = J_1 \sum_{i=1}^{L-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_{i=1}^{L-2} \mathbf{S}_i \cdot \mathbf{S}_{i+2} , \qquad (3.55)$$

at a critical next-nearest-neighbour coupling of J_2^{crit} .

3.6.2.1 Ground-State Energy

For any one-dimensional Hamiltonian which renormalizes to a CFT, i.e. at some energy scale the Hamiltonian becomes conformally invariant, the ground-state energy of a finite chain of length L with open ends can be written as the general expression

$$E_0(L) = e_0 L + e_1 - \frac{\pi v}{24L}c, \qquad (3.56)$$

where e_0 is the ground-state energy per spin in the limit $L \to \infty$, e_1 is some non-universal surface energy arising from OBC, v is the spin-wave velocity, and c is the central charge. The expression with logarithmic corrections, obtained through a perturbative expansion in powers of the marginally irrelevant coupling constant g(L), is given by

$$E_0(L) \approx e_0 L + e_1 - \frac{\pi v}{24L} \Big[1 - 24\pi^2 g(L)^2 \Big].$$
 (3.57)

For the S = 1/2 antiferromagnetic Heisenberg chain, we have from the Bethe ansatz $e_0 = 1/4 - \ln 2$, and $e_1 = (\pi - 1 - 2 \ln 2)/4$ which can be exactly calculated for the two open ends of the chain [61]. To capture the logarithmic scaling we rearrange Eq. (3.57) and fit against the function f(L, v, a):

$$E_0(L) - \left(\frac{1}{4} - \ln 2\right)L - \frac{1}{4}\left(\pi - 1 - 2\ln 2\right) \approx -\frac{\pi v}{24L} + \frac{\pi^3 v}{L} \left(\frac{a}{\ln L}\right)^2 = f(L, v, a).$$
(3.58)

In Figure 3.9 we see that there is indeed a universal O(1/L) and additive $O(1/\ln L)$ logarithmic dependence. In particular the DMRG calculation shows excellent agreement with the prediction. We have also extracted a central charge $c \approx 1$ and spin-wave velocity $v \approx \pi/2$, which also agrees with the Weiss-Zumino-Witten non-linear σ model (c = 1) [66] and Bethe ansatz solution ($v = \pi/2$). We note that a better fit (red line) is made if v is treated as a variable and we find that it varies smoothly to $\pi/2$ with increasing length.

3.6.2.2 Spin Gaps

Finite-size logarithmic corrections can also be observed with excited states. The spin gap Δ of an antiferromagnet is a characteristic of the spin excitation spectrum where its magnitude is the difference between the energies of the ground-state, usually expected to be of spin S = 0, and an excited state of spin S. To emphasize the finite-size scaling of the gap we consider three cases: $J_2 = 0$, 0.241167, and 0.4. The point



Figure 3.9: The modified ground-state energy expression $E_0^{\text{DMRG}} - e_0 L - e_1$ versus the system length L. The number of states kept is m = 128. A logarithmic correction to the energy is clearly visible from the fit f(L, v, a) (red line), with $v = 1.44592 \approx \pi/2$, and a = 0.06398.

 $J_2^{\text{crit}} = 0.241167$ is known as the dimerization transition point which distinguishes two phases:

$$\begin{split} J_2 < J_2^{\rm crit} : \text{unique } |\psi_0\rangle & J_2 > J_2^{\rm crit} : \text{doubly degenerate } |\psi_0\rangle \\ & \text{antiferromagnetic quasi order} & \text{valence bond order} \\ & \text{power law } C(r) \sim (-1)^r/r & \text{exponential } C(r) \sim (-1)^r \exp(-r/\xi)/r \\ & \text{gapless } \Delta = 0 & \text{gapped } \Delta \neq 0 \end{split}$$

where ξ is the correlation length, a measure of the distance over which fluctuations in one region influence another region, i.e. how correlated two regions/points are. Hence, two points which are separated by a distance larger than ξ will be relatively uncorrelated. The transition across J_2^{crit} is analogous to the Kosterlitz-Thouless transition for the classical two-dimensional XY model and is of infinite order [67].

Using the DMRG we plot in Figure 3.10 the spin gap of the Heisenberg chain between the ground-state, which has $\sum_i S_i^z = 0$, and the first-excited state, which has $\sum_i S_i^z = 1$, as a function of the inverse lattice size for different values of J_2 . When $J_2 = 0 < J_2^{\text{crit}}$ the gap scales to zero as 1/L, agreeing with Haldane's conjecture that Heisenberg chains with half-integral spin are gapless $\Delta = 0$ in the thermodynamic limit $L \to \infty$ [68, 69]. On the other hand by introducing frustration, the gap opens up when $J_2 > J_2^{\text{crit}}$ leading to



Figure 3.10: Spin gaps of the Heisenberg and $J_1 - J_2$ chains as functions of the inverse lattice size. For $J_2 < J_2^{\text{crit}}$ the gap converges to zero as 1/L in the limit $L \to \infty$, and non-zero for $J_2 > J_2^{\text{crit}}$. Inset shows the gap multiplied by the length. If $J_2 \neq J_2^{\text{crit}}$ long-distance spin-spin correlations remain enhanced.

valence bond ordering.

The gap behaviour has also been predicted to scale with an additive $1/\ln L$ correction term which is made clear when multiplied by the lattice length L (inset of Figure 3.10). For $J_2 \neq J_2^{\text{crit}}$ this effect is clearly visible while not as distinct when $J_2^{\text{crit}} = 0.241167$. At the critical value the leading order logarithmic correction vanishes, as can be seen by the (almost) 1/L behaviour; a pure 1/L dependence can only be expected in the limit $L \to \infty$. Analytically, with an additive logarithmic correction, the spin gap expression between states of spin S = 0 and S = 1, is given by [61]

$$\Delta = E_1(L) - E_0(L) \approx \frac{\pi v}{L} \left[1 - \frac{4\pi}{\sqrt{3}} g(L) \right],$$
(3.59)

where again we expect that $g(L) \sim 1/\ln L$. As with the ground-state energy of the Heisenberg chain, we find that the spin gap matches the predicted behaviour of Eq. (3.59). This agreement can be seen in Figure 3.11. Again, the spin-wave velocity is $v \approx \pi/2$, however, the prefactor of $4\pi^2 v/\sqrt{3}$ for g(L) is significantly off. For this we adopt the reasoning in reference [61]: there are various corrections at higher orders in the coupling constant for different energy levels. This varying behaviour is plotted in Figure 3.12 where we have calculated g(L) from Eqs. (3.57) and (3.59). When L is small (not of exponential length) the estimates of g(L) clearly



Figure 3.11: DMRG calculation of the isotropic Heisenberg chain spin gap. The gap is between the groundstate and first-excited state. From the fit (red line) it is clear the DMRG verifies very accurately the CFT finite-size scaling prediction of the gap.

do not agree but are seen to approach zero as $L \to \infty$. Since CFT predicts $g(L) \to 0$ in the large L limit, both estimates indeed coalesce into one value which approaches zero. To show this is the case, we compare the one-loop renormalization group CFT prediction of the coupling constant [60]

$$g(L) = \frac{g_0(l_0)}{1 + (4\pi/\sqrt{3})g_0(l_0)\ln\left(L/l_0\right)},$$
(3.60)

where $g_0(l_0)$ is an average dependent on the chain length l_0 , to the DMRG extrapolation of g(L). The full line is the CFT prediction Eq. (3.60) with $g_0(l_0)$ determined by averaging the DMRG calculation of the ground-state's g(L) at a chain length of $l_0 = 200$. We see that the two logarithmic corrections of the Heisenberg chain both merge with the CFT g(L) at large L. We have thus confirmed the logarithmic corrections predicted by CFT through an efficient implementation of the DMRG.



Figure 3.12: The marginally irrelevant coupling constant g(L) calculated from the expressions for the ground-state energy and the spin gap of the isotropic Heisenberg chain as predicted by CFT. The full line is the one-loop renormalization group prediction $g(L) = g_0(l_0)/[1 + \pi b g_0(l_0) \ln(L/l_0)]$ with $b = 4/\sqrt{3}$. We have determined $g_0(l_0)$ by averaging the ground-state's g(L) at a chain length of $l_0 = 200$.

CHAPTER 4 ______CYCLIC FOUR-SPIN RING-EXCHANGE

The simplest geometry to study a cyclic four-spin ring-exchange model is on a two-leg square ladder. Coupling two chains together, the seemingly two-dimensional structure is effectively a one-dimensional chain with extended interactions. In this thesis we apply the DMRG to such a spin ladder as described by Hamiltonian (1.3). We discuss the difficulties encountered in applying the DMRG, where in particular the effective Hamiltonian at each step is highly non-trivial. In regards to this, only preliminary results are presented.

For the following analysis we take the couplings to be $J_{\perp} = J_{||} = 0$ and K = 1. The Hamiltonian is then given by

$$H_{\text{Ring}} = \sum_{\langle ijkl \rangle} \left(P_{ijkl}^{\circlearrowright} + P_{ijkl}^{\circlearrowright} \right)$$

$$= \sum_{\langle ijkl \rangle} \left(\sum_{\mu < \nu} \mathbf{S}_{\mu} \cdot \mathbf{S}_{\nu} + 4\mathcal{G}_{ijkl} + \frac{1}{4} \right)$$

$$= \sum_{\langle ijkl \rangle} \left[\sum_{\mu < \nu} \mathbf{S}_{\mu} \cdot \mathbf{S}_{\nu} + 4 \left(\left(\mathbf{S}_{i} \cdot \mathbf{S}_{j} \right) \left(\mathbf{S}_{k} \cdot \mathbf{S}_{l} \right) + \left(\mathbf{S}_{j} \cdot \mathbf{S}_{k} \right) \left(\mathbf{S}_{l} \cdot \mathbf{S}_{i} \right) - \left(\mathbf{S}_{i} \cdot \mathbf{S}_{k} \right) \left(\mathbf{S}_{j} \cdot \mathbf{S}_{l} \right) \right) + \frac{1}{4} \right], \quad (4.1)$$

and is illustrated in Figure 4.1.



Figure 4.1: A schematic of a two-leg square ladder with a cyclic four-spin ring-exchange per plaquette.

At the end of Section 3.4 we noted that multiplications occurring on the same block require more care. With the introduction of biquadratic terms, same block multiplications are unavoidable and one must carry a set of compound operators, updating them accordingly at each DMRG step, similar to the correlation function. This will be made clear below.

In a standard DMRG calculation, two new sites are added and the Hamiltonian governs which bonds need to be formed. For a Hamiltonian with only bilinear interactions, the implementation is straightforward. It is not the case when biquadratic terms are present. To understand where the difficulty lies, we consider a symmetric configuration in which the environment is a reflection of the system. If L (taken to be even) is the total number of sites then depending on the parity of L/2 (odd or even) we have the following scenarios as depicted in Figure 4.2. As we can see, the way \mathcal{G}_{ijkl} is formed for a given parity is affected by the lattice



Figure 4.2: Even (a) and odd (b) DMRG schematics for the two-leg ladder when two sites are added for the first time. Solid (open) circles denote original (new) sites and solid lines denote exact local Hamiltonians. The labelling scheme of the sites indicates the environment is a reflection of the system. The three dashed, dashed-dotted, and dotted line pairs denote the dimer-dimer bonds that are needed to form \mathcal{G}_{iikl} .

geometry at each DMRG step. In the even case there are two sites, S_1 and S_2 , which are on the same block whereas in the odd case there are three as well as a cross-block multiplication between S_1 and $S_{1'}$. We have emphasized before (see Eq. (3.41)) that by multiplying truncated operators residing on the same block the result is non-unitary. This is precisely the issue at hand for the Hamiltonian (4.1). The solution, to state again, is to multiply them before hand to guarantee a summation over a complete set of states, i.e. $O^{\dagger}O = 1$. What this means is a decomposition into spin components.

Following the labelling scheme in Figure 4.2 we give an alternate formulation of the biquadratic terms in \mathcal{G}_{ijkl} for a given DMRG step. Each of the three terms in \mathcal{G}_{ijkl} (for either system or environment) can be written as 0. Even

$$(\mathbf{S}_1 \cdot \mathbf{S}_2)(\mathbf{S}_i \cdot \mathbf{S}_j) \longrightarrow (O^{\dagger} \mathbf{S}_1 \cdot \mathbf{S}_2 O)(\mathbf{S}_i \cdot \mathbf{S}_j), \tag{4.2a}$$

$$(\mathbf{S}_1 \cdot \mathbf{S}_i)(\mathbf{S}_2 \cdot \mathbf{S}_j) = (S_1^a S_i^a)(S_2^b S_j^b) = S_1^a S_2^b S_i^a S_j^b \longrightarrow (O^{\dagger} S_1^a S_2^b O) S_i^a S_j^b,$$
(4.2b)

,

-

$$(\mathbf{S}_1 \cdot \mathbf{S}_j)(\mathbf{S}_2 \cdot \mathbf{S}_i) = (S_1^a S_j^a)(S_2^b S_i^b) = S_1^a S_2^b S_j^a S_i^b \longrightarrow (O^{\dagger} S_1^a S_2^b O) S_j^a S_i^b,$$
(4.2c)

1 1.

where

$$S_{k}^{a}S_{l}^{b}S_{i}^{a}S_{j}^{b} = S_{k}^{z}S_{l}^{z}S_{i}^{z}S_{j}^{z} + \frac{1}{2}\left(S_{k}^{z}S_{l}^{+}S_{i}^{z}S_{j}^{-} + S_{k}^{z}S_{l}^{-}S_{i}^{z}S_{j}^{+}\right) + \frac{1}{2}\left(S_{k}^{+}S_{l}^{z}S_{i}^{-}S_{j}^{z} + S_{k}^{-}S_{l}^{z}S_{i}^{+}S_{j}^{z}\right) + \frac{1}{4}\left(S_{k}^{+}S_{l}^{+}S_{i}^{-}S_{j}^{-} + S_{k}^{-}S_{l}^{-}S_{i}^{+}S_{j}^{+}\right) + \frac{1}{4}\left(S_{k}^{+}S_{l}^{-}S_{i}^{-}S_{j}^{+} + S_{k}^{-}S_{l}^{+}S_{i}^{+}S_{j}^{-}\right).$$
(4.3)

1. Odd

$$(\mathbf{S}_2 \cdot \mathbf{S}_3)(\mathbf{S}_1 \cdot \mathbf{S}_j) = (\mathbf{S}_2 \cdot \mathbf{S}_3)(S_1^a S_j^a) \longrightarrow (O^{\dagger} \mathbf{S}_2 \cdot \mathbf{S}_3 S_1^a O) S_j^a,$$
(4.4a)

$$(\mathbf{S}_3 \cdot \mathbf{S}_1)(\mathbf{S}_2 \cdot \mathbf{S}_j) = (\mathbf{S}_3 \cdot \mathbf{S}_1)(S_2^a S_j^a) \longrightarrow (O^{\dagger} \mathbf{S}_3 \cdot \mathbf{S}_1 S_2^a O) S_j^a,$$
(4.4b)

$$(\mathbf{S}_1 \cdot \mathbf{S}_2)(\mathbf{S}_3 \cdot \mathbf{S}_j) = (\mathbf{S}_1 \cdot \mathbf{S}_2)(S_3^a S_j^a) \longrightarrow (O^{\dagger} \mathbf{S}_1 \cdot \mathbf{S}_2 S_3^a O) S_j^a,$$
(4.4c)

where

$$\mathbf{S}_{k} \cdot \mathbf{S}_{l} S_{i}^{a} S_{j}^{a} = \mathbf{S}_{k} \cdot \mathbf{S}_{l} \bigg[S_{i}^{z} S_{j}^{z} + \frac{1}{2} (S_{i}^{+} S_{j}^{-} + S_{i}^{-} S_{j}^{+}) \bigg].$$
(4.5)

Note that the cross-block multiplications of \mathcal{G}_{ijkl} occurring in the centre plaquette with sites \mathbf{S}_1 and $\mathbf{S}_{1'}$ is straightforward and does not require a rewrite of matrices.

In Table 4.1 we give the ground-state energies for one iteration of the infinite system DMRG. Indeed by decomposing the interactions into spin components we were able to obtain results which are in good agreement with exact diagonalization.

Table 4.1: Ground-state energy from one DMRG iteration of the ring-exchange Hamiltonian.

$L \rightarrow L+2$	Parity	m	$E_0^{\rm ED}(L+2)$	$E_0^{\rm DMRG}(L+2)$
$14 \rightarrow 16$	odd	64	-12.04957305280811	$\underline{-12.0495}2454957575$
$16 \rightarrow 18$	even	128	-13.73377982355355	$\underline{-13.73377}127051409$

We now discuss the main problem we have encountered during the implementation of the DMRG. In the next and subsequent iterations the new sites must be absorbed into the system and environment blocks. It is in this step where the formation of the effective local Hamiltonians for each block presents some confusion.

It is unclear for the even case as to how one should absorb spin \mathbf{S}_j since there is no four-spin plaquette to reconstruct the ring-exchange. We will, however, attempt to understand this process for the odd case. Following the notation used in Section 3.3.1, the system (and similarly the environment) Hamiltonian will be comprised of the previous local Hamiltonian, six bilinear Heisenberg terms and three biquadratic terms:

$$\begin{split} \left[\widetilde{H}\right]_{2\alpha;2\alpha'}^{\mathcal{B}\bullet_{j}} &\longleftarrow \left[\widetilde{H}\right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbb{1}_{2;2}^{\bullet_{j}} + \frac{1}{4} \quad (\text{previous Hamiltonian} \ + \ \text{constant}) \\ &+ \sum_{n=1}^{3} \left[\widetilde{\mathbf{S}}_{n}\right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbf{S}_{2;2}^{\bullet_{j}} + \sum_{\substack{\mu,\nu=1\\\mu<\nu}}^{3} \left[\widetilde{\mathbf{S}}_{\mu} \cdot \mathbf{S}_{\nu}\right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbb{1}_{2;2}^{\bullet_{j}} \quad (\text{bilinear terms}) \\ &+ 4 \left(\left[\widetilde{\mathbf{S}_{2} \cdot \mathbf{S}_{3}} S_{1}^{a}\right]_{\alpha;\alpha'}^{\mathcal{B}} + \left[\widetilde{\mathbf{S}_{3} \cdot \mathbf{S}_{1}} S_{2}^{a}\right]_{\alpha;\alpha'}^{\mathcal{B}} - \left[\widetilde{\mathbf{S}_{1} \cdot \mathbf{S}_{2}} S_{3}^{a}\right]_{\alpha;\alpha'}^{\mathcal{B}} \right) \otimes S_{2;2}^{a,\bullet_{j}}. \quad (\text{biquadratic terms}) \quad (4.6) \end{split}$$

Notice that in the second summation of the bilinear terms we are required to have three Heisenberg terms previously calculated. Moreover, by absorbing a new spin \mathbf{S}_j we need to update the individual spins \mathbf{S}_1 , \mathbf{S}_2 , etc. for the next iteration. This is accomplished by pushing them inward $\mathbf{S}_1 \leftarrow \mathbf{S}_j$, $\mathbf{S}_2 \leftarrow \mathbf{S}_1$, etc. analogous to Eq. (3.35). We now transform (4.6) according to (3.30a) (updating individual spins as well) and repeat. However, now that L/2 is even, one needs to compute the appropriate set of biquadratic terms similar to those of Eqs. (4.2a)-(4.2c) for the next diagonalization step:

Eq. (4.2a)
$$\longrightarrow O_{\mathrm{II}}^{\dagger} \left(\left[\widetilde{\mathbf{S}}_{1} \right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes \mathbf{S}_{2;2}^{\bullet_{j}} \right) O_{\mathrm{II}},$$
 (4.7a)

Eqs. (4.2b)
$$- (4.2c) \longrightarrow O_{\mathrm{II}}^{\dagger} \left(\left[\widetilde{S}_{1}^{a} \right]_{\alpha;\alpha'}^{\mathcal{B}} \otimes S_{2;2}^{b,\bullet,\flat} \right) O_{\mathrm{II}},$$
 (4.7b)

where the subscript II on the truncation matrices indicates the DMRG iteration. We have done this and the results are shown in Table 4.2 for two iterations of the DMRG starting with the odd case L = 14. We see

Iteration	L	$E_0^{ m ED}(L)$	$E_0^{\mathrm{DMRG}}(L)$
0	14	-10.45040854700329	exact
1	16	-12.04957305280811	$\underline{-12.0495}2454957575$
2	18	-13.73377982355355	$\underline{-13.733}52838489993$

Table 4.2: Two DMRG iterations of the ring-exchange starting with odd parity.

that the ground-state energy for L = 18 is in good agreement with exact calculations. We note that at the time, complications arose when updating these biquadratic terms (at least for the case presented) in which resulting matrices were not strictly Hermitian. This issue has since been resolved.

With these preliminary ground-state energies we have confirmed that decomposing the spins of the biquadratic terms serves to give the correct result. Currently we are moving forward with the rest of the implementation. Once a working DMRG routine is in place we hope to confirm the phase diagrams of previous studies (see Sections 1.2.1 and 1.2.2), where in particular we would like to understand the entanglement properties of the various phases.

chapter 5

CONCLUSION AND FUTURE WORK

In this thesis we have shown that the DMRG captures very accurately the low-energy physics of strongly correlated one-dimensional systems. We accomplished this by using the infinite system algorithm on the S = 1/2 Heisenberg model to iteratively build up a lattice of sites to a desired chain length. A finite system sweep was then used to optimize the blocks so that accurate measurements of observables could be made. These measurements (see Section 3.6) are supported by well-known theoretical results such as the Bethe ansatz, Haldane's spin gap conjecture and conformal field-theoretical calculations.

With an understanding of the DMRG, we applied the algorithm to a S = 1/2 two-leg square ladder with an additional cyclic four-spin ring-exchange. However, due to the non-trivial biquadratic terms in the ring-exchange, a number of difficulties were encountered leading to preliminary results in the ground-state energy. We are currently in the stages of completing a full implementation. The goal is to study the phase diagrams of previous works where the primary focus will be on the entanglement properties of the different phases.

5.1 Extending to Higher Dimensions

Although the DMRG is tailored for one-dimensional systems an extension to two dimensions is possible. At the cost of long-range interactions two-dimensional systems can be investigated through an appropriate choice in path, as seen in Figure 5.1. To minimize the number of long-range interactions one should choose a path such that the width of the system is traversed before the length. Of course, depending on the lattice one path may be more optimal over another. As with the one-dimensional case, two sites are added at each DMRG step. It is, however, not a straightforward extension of the infinite system DMRG mentioned above; there no longer exists any reflection symmetry between the system and environment blocks. The implication is that both the system and environment blocks must be built separately requiring additional storage.



Figure 5.1: A superblock schematic of a two-dimensional system with a one-dimensional path traced out. Such a mapping introduces long-range interactions.

Another factor one must consider is the boundary between the two blocks. Whatever the schematic one chooses to employ there is a fundamental limitation the DMRG suffers from. The number of interactions along the boundary (scaling with the width of the lattice) leads to large entanglement between the system and the environment. A direct consequence is a slower fall-off of the density-matrix weights, requiring more states to be kept in order to attain a given accuracy. In practice, an upper bound is established on the system sizes one can simulate. Nevertheless, through a variety of techniques, issues concerning ground-state convergence, finite-size limitations and excited states have been addressed [70], resulting in a successful extension into two dimensions.

5.2 Real-Time Dynamics

One can take the approach a step further by studying the real-time dynamics of one- or two-dimensional systems using the DMRG. In practice, such as in the lab via inelastic neutron scattering, it is important to understand how a material scatters incident radiation. For example, the dynamical structure factor (a frequency-dependent quantity) contains information on the evolution of inter-particle correlations. Such quantities have applications in material science and engineering.

Time evolution in DMRG can be accomplished by realizing that as a wavefunction evolves through time its density matrix samples a region of a continuously changing Hilbert space. The idea is to evolve the wavefunction through a series of time steps to generate an accurate basis at a later desired time. To this end, the evolution is carried out through a modified finite system sweep procedure which makes use of the classical fourth-order Runge-Kutta (RK) method [71]. During each step in a half sweep¹, one calculates the set of four RK vectors,

$$|k_{1}\rangle = \tau \tilde{H}(t)|\psi(t)\rangle,$$

$$|k_{2}\rangle = \tau \tilde{H}(t+\tau/2)[|\psi(t)\rangle + |k_{1}\rangle/2],$$

$$|k_{3}\rangle = \tau \tilde{H}(t+\tau/2)[|\psi(t)\rangle + |k_{2}\rangle/2],$$

$$|k_{4}\rangle = \tau \tilde{H}(t+\tau)[|\psi(t)\rangle + |k_{3}\rangle],$$

(5.1)

for the time-dependent Hamiltonian $\tilde{H}(t) = H(t) - E_0$. Using the density matrix four states are targeted, $|\psi(t)\rangle$, $|\psi(t + \tau/3)\rangle$, $|\psi(t + 2\tau/3)\rangle$, and $|\psi(t + \tau)\rangle$, which can be approximated by the RK vectors as

$$\begin{split} \psi(t+\tau/3) &\approx |\psi(t)\rangle + \frac{1}{162} \big[31|k_1\rangle + 14|k_3\rangle + 14|k_3\rangle - 5|k_4\rangle \big], \\ \psi(t+2\tau/3) &\approx |\psi(t)\rangle + \frac{1}{81} \big[16|k_1\rangle + 20|k_3\rangle + 20|k_3\rangle - 2|k_4\rangle \big], \\ \psi(t+\tau) &\approx \frac{1}{6} \big[|k_1\rangle + 2|k_3\rangle + 2|k_3\rangle + |k_4\rangle \big], \end{split}$$
(5.2)

giving an overall error $\mathcal{O}(\tau^4)$. The advancement in time is then done on the last step of a half sweep. We conclude by noting that this is just one approach to time-dependent DMRG.

 $^{^{1}}A$ half sweep is defined as a finite system sweep over the left or right block, as opposed to over the entire superblock.

Appendix A

TWO-, THREE-, AND FOUR-SPIN CYCLIC PERMUTATIONS

In this appendix we provide a short summary of the Pauli matrices and their relation to transposition of quantum spins. Defined under the permutation operator between two spins, we derive expressions for threeand four-spin cyclic exchanges.

A.1 Pauli Matrices

The Pauli matrices σ are a set of three 2 × 2 complex, Hermitian and unitary matrices given by

$$\sigma^{x} = \sigma^{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^{y} = \sigma^{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^{z} = \sigma^{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
 (A.1)

These matrices have the following properties:

0. Commutation and anticommutation identities:

$$\left[\sigma^{a},\sigma^{b}\right] = 2i\epsilon^{abc}\sigma^{c} \quad \text{and} \quad \left\{\sigma^{a},\sigma^{b}\right\} = 2\delta^{ab} , \qquad (A.2)$$

where ϵ^{abc} is the Levi-Civita symbol and δ^{ab} is the Kronecker delta. Moreover, (A.2) is equivalent to

$$\sigma^a \sigma^b = \delta^{ab} + i \epsilon^{abc} \sigma^c. \tag{A.3}$$

1. Completeness relation:

$$\boldsymbol{\sigma} \cdot \boldsymbol{\sigma} = \sum_{i=1}^{3} \sigma^{i}_{\alpha\beta} \sigma^{i}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}. \tag{A.4}$$

The permutation (transposition) operator $P_{ij}^{\circlearrowright}$ between two spins σ_i and σ_j can be written as

$$P_{ij}^{\circlearrowright} = \frac{1}{2} \left(1 + \boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}} \right).$$
(A.5)

One can then check that the action of (A.5) satisfies $P_{ij}^{\bigcirc} |\sigma_i \sigma_j\rangle = |\sigma_j \sigma_i\rangle$. Note that (A.5) also satisfies

$$\left(P_{ij}^{\circlearrowright}\right)^2 = 1 \quad \text{and} \quad \left(P_{ij}^{\circlearrowright}\right)^{-1} = P_{ij}^{\circlearrowright}.$$
 (A.6)

A.2 Three- and Four-Spin Cyclic Permutations

For a three-spin cyclic exchange the permutation operator can be written as the product of two transposition operators

$$P_{ijk}^{\circlearrowright} = P_{ij}^{\circlearrowright} P_{ik}^{\circlearrowright} = \frac{1}{4} \left(1 + \boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}} \right) \left(1 + \boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}} \right) = \frac{1}{4} \left[1 + \boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}} + \boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}} + \left(\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}} \right) \left(\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}} \right) \right], \quad (A.7)$$

where

$$(\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}}) (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}}) = \sigma_{i}^{a} \sigma_{j}^{a} \sigma_{i}^{b} \sigma_{k}^{b} = \sigma_{j}^{a} \sigma_{k}^{b} \left(\delta^{ab} + i \epsilon^{abc} \sigma_{i}^{c} \right) = \boldsymbol{\sigma}_{\mathbf{j}} \cdot \boldsymbol{\sigma}_{\mathbf{k}} + i \epsilon^{abc} \sigma_{j}^{a} \sigma_{k}^{b} \sigma_{i}^{c} .$$
(A.8)

The imaginary terms end up cancelling when we perform the summation:

$$P_{ijk}^{\circlearrowright} + P_{ijk}^{\circlearrowright} = \frac{1}{2} \left(1 + \boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}} + \boldsymbol{\sigma}_{\mathbf{j}} \cdot \boldsymbol{\sigma}_{\mathbf{k}} + \boldsymbol{\sigma}_{\mathbf{k}} \cdot \boldsymbol{\sigma}_{\mathbf{i}} \right).$$
(A.9)

The four-spin cyclic exchange can be written as the product of three transposition operators

$$P_{ijkl}^{\circlearrowright} = P_{ij}^{\circlearrowright} P_{ik}^{\circlearrowright} P_{il}^{\circlearrowright}$$

$$= \frac{1}{8} \bigg[1 + \boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{j} + \boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{k} + \boldsymbol{\sigma}_{l} \cdot \boldsymbol{\sigma}_{i} + (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{j}) (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{k})$$

$$+ (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{j}) (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{l}) + (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{k}) (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{l}) + (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{j}) (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{k}) (\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{l}) \bigg].$$
(A.10)

The triple product can be simplified as follows:

$$(\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}}) (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}}) (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{l}}) = \sigma_{i}^{a} \sigma_{j}^{a} \sigma_{k}^{b} \sigma_{i}^{c} \sigma_{i}^{c}$$

$$= \sigma_{i}^{a} \sigma_{j}^{a} \sigma_{k}^{b} \sigma_{i}^{c} \left(\delta^{bc} + i\epsilon^{bcd} \sigma_{i}^{d}\right)$$

$$= (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}}) (\boldsymbol{\sigma}_{\mathbf{k}} \cdot \boldsymbol{\sigma}_{\mathbf{l}}) + i\epsilon^{bcd} \sigma_{j}^{a} \sigma_{k}^{b} \sigma_{i}^{c} \left(\delta^{ad} + i\epsilon^{ade} \sigma_{i}^{e}\right)$$

$$= (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}}) (\boldsymbol{\sigma}_{\mathbf{k}} \cdot \boldsymbol{\sigma}_{\mathbf{l}}) - \sigma_{j}^{a} \sigma_{k}^{b} \sigma_{i}^{c} \sigma_{i}^{e} \epsilon^{bcd} \epsilon^{ade} + i\epsilon^{bcd} \sigma_{j}^{a} \sigma_{k}^{b} \sigma_{i}^{c} , \qquad (A.11)$$

where upon using the relation

$$\epsilon^{ade}\epsilon^{bcd} = -\epsilon^{dae}\epsilon^{dbc} = -\left(\delta_{ab}\delta_{ec} - \delta_{ac}\delta_{eb}\right),\tag{A.12}$$

we obtain

$$(\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}}) (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}}) (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{l}}) = (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{j}}) (\boldsymbol{\sigma}_{\mathbf{k}} \cdot \boldsymbol{\sigma}_{\mathbf{l}}) + (\boldsymbol{\sigma}_{\mathbf{j}} \cdot \boldsymbol{\sigma}_{\mathbf{k}}) (\boldsymbol{\sigma}_{\mathbf{l}} \cdot \boldsymbol{\sigma}_{\mathbf{i}}) - (\boldsymbol{\sigma}_{\mathbf{i}} \cdot \boldsymbol{\sigma}_{\mathbf{k}}) (\boldsymbol{\sigma}_{\mathbf{j}} \cdot \boldsymbol{\sigma}_{\mathbf{l}}) + i\epsilon^{bcd}\sigma_{j}^{a}\sigma_{k}^{b}\sigma_{l}^{c}.$$

$$(A.13)$$

Combining relations (A.8) and (A.13) we have

$$P_{ijkl}^{\circlearrowright} + P_{ijkl}^{\circlearrowright} = \frac{1}{4} \left(\sum_{\mu < \nu} \boldsymbol{\sigma}_{\mu} \cdot \boldsymbol{\sigma}_{\nu} + \mathcal{G}_{ijkl} + 1 \right), \tag{A.14}$$

where the sum $\sum_{\mu < \nu}$ is performed over all distinct pairs in $\{i,j,k,l\}$ and

$$\mathcal{G}_{ijkl} = (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \left(\boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \right) + \left(\boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_k \right) \left(\boldsymbol{\sigma}_l \cdot \boldsymbol{\sigma}_i \right) - \left(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k \right) \left(\boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_l \right).$$
(A.15)

Finally, in terms of quantum spin operators we let $\boldsymbol{\sigma}=2\mathbf{S}~(\hbar=1)$ giving

$$P_{ij} \to \frac{1}{2} \left(1 + 4\mathbf{S}_i \cdot \mathbf{S}_j \right), \tag{A.16}$$

where (A.3) becomes

$$S^{a}S^{b} = \frac{1}{4} \left(\delta^{ab} + 2i\epsilon^{abc}S^{c} \right). \tag{A.17}$$

It is then straightforward to show that

$$P_{ijk}^{\circlearrowright} + P_{ijk}^{\circlearrowright} = 2\sum_{\mu < \nu} \mathbf{S}_{\mu} \cdot \mathbf{S}_{\nu} + \frac{1}{2} , \qquad (A.18)$$

and

$$P_{ijkl}^{\circlearrowright} + P_{ijkl}^{\circlearrowright} = \sum_{\mu < \nu} \mathbf{S}_{\mu} \cdot \mathbf{S}_{\nu} + 4\mathcal{G}_{ijkl} + \frac{1}{4} .$$
(A.19)

APPENDIX B_{-}

FROM HUBBARD TO HEISENBERG

We often study the microscopic details of solids by confining electrons to lattice models, for example, the Heisenberg model (1.1). These are often great approximations to physical systems since the atomic structure determines the possible locations of where electrons are allowed to be. Sharing of electrons is possible if two neighbouring atoms at roughly equal energies have overlapping electronic orbitals. On the other hand the strong repulsion between electrons gives rise to an on-site Coulomb potential. The Hubbard model consists of these two competing interactions and is the simplest model of interacting particles in a lattice. In this appendix, starting from the one-band Hubbard model, we apply second order Brillouin-Wigner perturbation theory in the atomic limit to obtain the low-energy effective Heisenberg Hamiltonian.

B.1 The Hubbard Model

Let t_{jk} be the matrix element denoting the tunnelling amplitude from lattice site j to k and U the strength of the on-site repulsive potential, the generalized Hubbard model can be written as

$$H_{\text{Hubb}} = \sum_{j,k=1}^{L} \sum_{\alpha=\uparrow,\downarrow} t_{jk} \left(c_{j\alpha}^{\dagger} c_{k\alpha} + c_{k\alpha}^{\dagger} c_{j\alpha} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow} , \qquad (B.1)$$

where $c_{j\alpha}^{\dagger}(c_{j\alpha})$ is the creation (annihilation) fermionic operator of an electron with spin $\alpha = \uparrow, \downarrow$ in a Wannier orbital at lattice site j. If the local particle number operator $n_{j\alpha} = c_{j\alpha}^{\dagger}c_{j\alpha}$ counts the number of electrons of spin α at site j then the total particle number can be written as

$$\hat{N} = \sum_{j=1}^{L} \left(n_{j\uparrow} + n_{j\downarrow} \right).$$
(B.2)

The fermionic operators obey the anticommutation relations

$$\{c_{j\alpha}, c_{k\beta}\} = \{c_{j\alpha}^{\dagger}, c_{k\beta}^{\dagger}\} = 0, \tag{B.3}$$

$$\{c_{j\alpha}, c_{k\beta}^{\dagger}\} = \delta_{jk}\delta_{\alpha\beta}.\tag{B.4}$$

The creation operators $c_{j\alpha}^{\dagger}$ generate the Hilbert space \mathcal{H} of the Hubbard model by acting on the vacuum state $|0\rangle$ defined by the condition

$$c_{j\alpha}^{\dagger}|0\rangle = 0, \quad j = 1, 2, \dots, L, \quad \alpha = \uparrow, \downarrow.$$
 (B.5)

The number of linearly independent Wannier basis states for a fixed number of particles N is equal to $\binom{2L}{N}$ giving the dimension of the Hilbert space to be

$$\dim \mathcal{H} = \sum_{N=0}^{2L} \binom{2L}{N} = 4^L, \tag{B.6}$$

since the four states

$$|0\rangle, \quad c^{\dagger}_{j\uparrow}|0\rangle, \quad c^{\dagger}_{j\downarrow}|0\rangle, \quad c^{\dagger}_{j\uparrow}c^{\dagger}_{j\downarrow}|0\rangle, \tag{B.7}$$

are the associated states with every lattice site. That is, on a lattice of L sites each site has four possible configurations: empty, one electron with either of the two spin orientations, or two electrons with opposite signs. From the anticommutation relations (B.3)-(B.4) and (B.7), it follows that

$$\left[n_{j\alpha}, c_{k\beta}^{\flat}\right] = n_{j\alpha}c_{k\beta}^{\flat} - c_{k\beta}^{\flat}n_{j\alpha} = \delta_{jk}\delta_{\alpha\beta}c_{k\beta}^{\flat}, \tag{B.8}$$

for $\flat = \text{empty}, \dagger$.

In Appendix A we introduced the quantum spin operators as a set of three 2×2 complex, Hermitian and unitary matrices. Equivalently, using fermionic operators we define the site-specific total spin operator as

$$\mathbf{S}_{j} = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} c^{\dagger}_{j\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{j\beta}, \tag{B.9}$$

where the components satisfy the commutation relation

$$\left[S^a, S^b\right] = i\epsilon^{abc}S^c, \quad a, b, c = x, y, z.$$
(B.10)

Using the above definitions it can be shown that the Hubbard model conserves the total particle number and the z-component of the total spin, i.e. $[H_{\text{Hubb}}, \hat{N}] = [H_{\text{Hubb}}, S^z] = 0.$

Following [72] in our derivation of the Heisenberg model we define for convenience the 2×2 operator-
valued matrix

$$S_{jk} \equiv c_{j\alpha}^{\dagger} c_{k\beta} = \begin{bmatrix} c_{j\uparrow}^{\dagger} c_{k\uparrow} & c_{j\uparrow}^{\dagger} c_{k\downarrow} \\ c_{j\downarrow}^{\dagger} c_{k\uparrow} & c_{j\downarrow}^{\dagger} c_{k\downarrow} \end{bmatrix},$$
(B.11)

such that

$$S_{jk}^{a} = \operatorname{tr}\left(\sigma^{a}S_{jk}\right) \quad \text{and} \quad S_{jk}^{0} = \operatorname{tr}\left(S_{jk}\right).$$
 (B.12)

These definitions will come in handy later. With these the familiar local spin density and particle number operators are $S_j^a = \frac{1}{2}S_{jj}^a$ and $S_{jj}^0 = n_{j\uparrow} + n_{j\downarrow} = n_j$, respectively.

B.2 Brillouin-Wigner Perturbation Theory

The ground-state of the Hubbard model is highly degenerate making the familiar Rayleigh-Schrödinger perturbation theory unusable. Fortunately, with a weak perturbation, i.e. the hopping parameter, the ground-state energy splits into singly- and doubly-occupied states. Since the perturbation is assumed to be small, we can project out the doubly-occupied states and obtain a well-approximated effective Hamiltonian.

Consider any general Hamiltonian H acting on a Hilbert space \mathcal{H} . Let P be a projection on the subspace \mathcal{PH} of \mathcal{H} and $Q = \mathbb{1} - P$. Now $|\psi\rangle$ is a solution to the Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle,\tag{B.13}$$

if and only if

$$(PHP + PHQ)|\psi\rangle = EP|\psi\rangle,\tag{B.14}$$

$$(QHP + QHQ)|\psi\rangle = EQ|\psi\rangle. \tag{B.15}$$

We begin by solving for $Q|\psi\rangle$ from (B.15):

$$Q|\psi\rangle = (E - QH)^{-1} QHP|\psi\rangle, \tag{B.16}$$

which upon substitution into (B.14) gives

$$PHP|\psi\rangle + PH (E - QH)^{-1} QHP|\psi\rangle = EP|\psi\rangle,$$

$$PH \left[\mathbb{1} + (E - QH)^{-1} QH\right] P|\psi\rangle = EP|\psi\rangle,$$

$$PH \left[\mathbb{1} + (E - QH)^{-1} QH\right] |\phi\rangle = E|\phi\rangle, \quad (|\phi\rangle = P|\psi\rangle) \quad (B.17)$$

$$\hat{H}(E)|\phi\rangle = E|\phi\rangle. \quad (B.18)$$

Thus, $|\phi\rangle \in P\mathcal{H}$ is a solution to the spectral problem (B.18) with eigenvalue *E*. Moreover, if $|\phi\rangle \in P\mathcal{H}$ solves (B.18) then

$$|\psi\rangle = \left[\mathbb{1} + (E - QH)^{-1} QH\right] |\phi\rangle \tag{B.19}$$

is a solution to the full stationary Schrödinger equation (B.13) with eigenvalue also E.

We now consider now a bare hamilton with a weak perturbation of the form

$$H = H_0 + \lambda H_1, \tag{B.20}$$

where the spectral decomposition of $H_0 = \sum_n E_n P_n$ is known. We now let $P \to P_n$ so that the Hamiltonian

$$\hat{H}_n(E) = P_n H \left[\mathbb{1} + (E - Q_n H)^{-1} Q_n H \right] P_n,$$
(B.21)

in subspace $P\mathcal{H}$ acts non-trivially only on the degenerate subspace corresponding to the n^{th} energy level E_n of H_0 .

We first focus on simplifying the non-linear term in the energy. The ground-state of the Hubbard model is highly degenerate but the first-excited state in comparison is quite large. To extract an effective Hamiltonian which captures the low-lying excitations we make use of a little trick. Let us define the resolvent operators

$$G = (E - Q_n H)^{-1}$$
 and $G_0 = (E - Q_n H_0)^{-1}$. (B.22)

Using these definitions notice that

$$\mathcal{G}_0^{-1}\mathcal{G} = (E - Q_n H_0)\mathcal{G}$$

= $(E - Q_n H_0 - \lambda Q_n H_1 + \lambda Q_n H_1)\mathcal{G}$
= $(E - Q_n H_0 - \lambda Q_n H_1)\mathcal{G} + \lambda Q_n H_1\mathcal{G}$
= $1 + \lambda Q_n H_1\mathcal{G}.$ (B.23)

We therefore have a recursion relation for \mathcal{G} given by

$$\mathcal{G} = \mathcal{G}_0 + \lambda \mathcal{G}_0 Q_n H_1 \mathcal{G},\tag{B.24}$$

where upon iteration we obtain the series expansion

$$\mathcal{G} = \mathcal{G}_0 + \lambda \mathcal{G}_0 Q_n H_1 \mathcal{G}_0 + \lambda^2 \mathcal{G}_0 Q_n H_1 \mathcal{G}_0 Q_n H_1 \mathcal{G}_0 + \mathcal{O}\left(\lambda^3\right). \tag{B.25}$$

From the elementary relations

$$P_m P_n = \delta_{mn} P_n, \quad (\text{i.e. } P^2 = P) \tag{B.26}$$

$$P_n H_0 = H_0 P_n = E_n P_n \tag{B.27}$$

$$Q_n H_0 = H_0 Q_n = \sum_{m \neq n} E_m P_m \tag{B.28}$$

$$P_n H Q_n = \lambda P_n H_1 Q_n \tag{B.29}$$

$$Q_n H P_n = \lambda Q_n H_1 P_n \tag{B.30}$$

it can be shown easily that

$$(E - Q_n H_0)^{-1} = \left(E - \sum_{m \neq n} E_m P_m\right)^{-1} = \left(\begin{array}{cc}E - E_0 P_0 & & \\ & E - E_1 P_1 & \\ & & \ddots & \\ & & & E - E_L P_L\end{array}\right)^{-1}.$$
 (B.31)

Since the projectors $P_n^{-1}=P_n$ are invertible within their respective subspaces we may write

$$(E - Q_n H_0)^{-1} = \left(E - \sum_{m \neq n} E_m P_m\right)^{-1} = \sum_{m \neq n} \frac{P_m}{E - E_m},$$
(B.32)

where using (B.26) gives

$$(E - Q_n H)^{-1} = \sum_{m \neq n} \frac{P_m}{E - E_m} + \lambda \sum_{m \neq n} \frac{P_m}{E - E_m} H_1 \sum_{m \neq n} \frac{P_m}{E - E_m} + \lambda^2 \sum_{m \neq n} \frac{P_m}{E - E_m} H_1 \sum_{m \neq n} \frac{P_m}{E - E_m} H_1 \sum_{m \neq n} \frac{P_m}{E - E_m} + \mathcal{O}\left(\lambda^3\right).$$
(B.33)

Therefore, upon substitution and using (B.27)-(B.30) we obtain

$$\begin{aligned} \hat{H}_{n}(E) &= P_{n}HP_{n} + P_{n}H\left(E - Q_{n}H\right)^{-1}Q_{n}HP_{n} \\ &= P_{n}\left(H_{0} + \lambda H_{1}\right)P_{n} + P_{n}\left(H_{0} + \lambda H_{1}\right)\left(E - Q_{n}H\right)^{-1}\lambda Q_{n}H_{1}P_{n} \\ &= P_{n}H_{0}P_{n} + \lambda P_{n}H_{1}P_{n} + \lambda P_{n}H_{0}\left(E - Q_{n}H\right)^{-1}Q_{n}H_{1}P_{n} + \lambda^{2}P_{n}H_{1}\left(E - Q_{n}H\right)^{-1}Q_{n}H_{1}P_{n} \\ &= E_{n}P_{n} + \lambda P_{n}H_{1}P_{n} + \lambda P_{n}H_{0}\sum_{\substack{m\neq n}}\frac{P_{m}}{E - E_{m}}Q_{n}H_{1}P_{n} + \lambda^{2}P_{n}H_{1}\sum_{\substack{m\neq n}}\frac{P_{m}}{E - E_{m}}Q_{n}H_{1}P_{n} + \lambda^{2}P_{n}H_{1}\sum_{\substack{m\neq n}}\frac{P_{m}}{E - E_{m}}Q_{n}H_{1}P_{n} + \cdots \\ &= E_{n}P_{n} + \lambda P_{n}H_{1}P_{n} + \lambda^{2}P_{n}H_{1}\sum_{\substack{m\neq n}}\frac{P_{m}}{E - E_{m}}H_{1}P_{n} + \cdots \\ &= E_{n}P_{n} + P_{n}H_{1}\sum_{\substack{k=0}}^{\infty}\lambda^{k+1}\left(\sum_{\substack{m\neq n}}\frac{P_{m}H_{1}}{E - E_{m}}\right)^{k}P_{n} \\ &= \left[E_{n} + P_{n}H_{1}\sum_{\substack{k=0}}^{\infty}\lambda^{k+1}\left(\sum_{\substack{m\neq n}}\frac{P_{m}H_{1}}{E - E_{m}}\right)^{k}\right]P_{n}. \end{aligned}$$
(B.34)

And thus the spectral problem (B.18) about energy level E_n becomes

$$P_n H_1 \sum_{k=0}^{\infty} \lambda^{k+1} \left(\sum_{m \neq n} \frac{P_m H_1}{E - E_m} \right)^k |\phi\rangle = (E - E_n) |\phi\rangle, \tag{B.35}$$

for $|\phi\rangle \in P_n \mathcal{H}$. It is now clear that perturbation theory around an energy level E_n is an iterative solution. Clearly, when $\lambda = 0$, $E = E_n$. We expect that corrections to the energy will be of the form

$$E = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \mathcal{O}\left(\lambda^3\right),$$
(B.36)

thus the spectrum of (B.20), which evolves from the energy level E_n as λ is turned on, is given by

$$P_n H_1 \sum_{k=0}^{\infty} \lambda^{k+1} \left(\sum_{m \neq n} \frac{P_m H_1}{E_n - E_m} \right)^k P_n |\phi\rangle = \left(\lambda E_n^1 + \lambda^2 E_n^2 + \cdots \right) |\phi\rangle,$$

$$\left(\lambda P_n H_1 P_n + \lambda^2 P_n H_1 \sum_{m \neq n} \frac{P_m H_1}{E_n - E_m} P_n + \cdots \right) |\phi\rangle = \left(\lambda E_n^1 + \lambda^2 E_n^2 + \cdots \right) |\phi\rangle,$$

$$\left(P_n H_1 P_n + \lambda \sum_{m \neq n} \frac{P_n H_1 P_m H_1 P_n}{E_n - E_m} + \cdots \right) |\phi\rangle = \frac{E - E_n}{\lambda} |\phi\rangle,$$
(B.37)

where on the left hand side we have what is known as an effective Hamiltonian restricted to $P_n \mathcal{H}$.

B.3 Hubbard Model in the Large U Limit

The following calculation was done with reference [72] as a supplement. We now consider the Hubbard model with a large on-site Coulomb potential and the tunnelling strength to be a small perturbation. This corresponds to the atomic limit where the electrons are confined to their lattice positions. To apply the perturbative theory from the previous section we first rescale the Hubbard model as

$$H/U = D + T/U, \tag{B.38}$$

where

$$D = \sum_{j=1}^{L} n_{j\uparrow} n_{j\downarrow} \quad \text{and} \quad T = \sum_{j,k=1}^{L} t_{jk} c_{j\alpha}^{\dagger} c_{k\alpha}.$$
(B.39)

We assume that $t_{jj} = 0$, $t_{kj} = t_{jk}^*$, U > 0, and $|t_{jk}|^2 \ll U$ for j, k = 1, 2, ..., L. A sum over the spin index α is also assumed. We now use the fact that D is diagonal in the Wannier basis (it counts the number of doubly occupied sites) where its eigenvalues are simply n = 0, 1, ..., L. Denoting by P_n the projectors onto eigenspaces \mathcal{H}_n , we decompose the Hubbard Hilbert space into $\mathcal{H}^{(L)} = \mathcal{H}_0 \oplus \cdots \oplus \mathcal{H}_L$ allowing us to write D in the convenient form

$$D = \sum_{n=1}^{L} n P_n. \tag{B.40}$$

We restrict our analysis to the condition that $N \leq L$. The number of ground-states for a fixed number of electrons N is $2^N \binom{L}{N}$, yielding a Hilbert space with no doubly occupied sites a dimension of

$$\dim \mathcal{H}_0 = 3^L. \tag{B.41}$$

Under the small perturbation T this degeneracy is partially lifted, splitting the lowest energy level of D. However, as long as $|t_{jk}|^2 \ll U$ remains true, the first-excited state will be well-separated from the ground-state. This splitting of the ground-state via second-order Brillouin-Wigner perturbation theory is described by an effective Hamiltonian know as the t - J model, which we now derive.

Let $H_0 = D$, $H_1 = T$ and $\lambda = U^{-1}$. With only singly-occupied sites we set n = 0 and have to first-order

$$\left(P_0 T P_0 - \frac{1}{U} \sum_{m \neq n} \frac{P_0 T P_m T P_0}{m}\right) |\phi\rangle = E |\phi\rangle,\tag{B.42}$$

where the energy UE as also been rescaled to E. The operator on the left hand side is the t - J model. It describes the splitting of the ground-state energy $E_0 = 0$ of the Hubbard Hamiltonian in the atomic limit when hopping amplitudes are small. We now simplify the t - J model.

First, we need expressions for the projection operators P_n in a fermionic representation. They can be obtained through the generating function

$$G(\alpha) = \prod_{j=1}^{L} \left(1 - \alpha n_{j\uparrow} n_{j\downarrow} \right), \tag{B.43}$$

where

$$P_n = \frac{(-1)^n}{n!} \partial_\alpha^n G(\alpha) \Big|_{\alpha=1}, \quad n = 0, 1, \cdots, L.$$
(B.44)

In particular we are interested in the projection operator which projects onto the space with no doubly occupied sites

$$P_0 = \prod_{j=1}^{L} \left(1 - n_{j\uparrow} n_{j\downarrow} \right). \tag{B.45}$$

From this definition we can conclude the following: since $n_{j\uparrow}n_{j\downarrow} = 1$ if site j has a fermion and $(1-n_{j\uparrow}n_{j\downarrow}) = 0$ if not, then it must be true that

$$n_{j\uparrow}n_{j\downarrow}P_0 = P_0 n_{j\uparrow}n_{j\downarrow} = 0 \tag{B.46}$$

is always true, and vice versa. To simplify (B.42) we first compute the $P_m T P_0/m$ term. This can be done by direct application of (B.44):

$$\sum_{m=1}^{L} \frac{P_m T P_0}{m} = \left(P_1 + \frac{1}{2} P_2 + \dots + \frac{1}{L} P_L \right) T P_0$$
$$= \left[-\partial_\alpha G(\alpha) \Big|_{\alpha=1} + \frac{1}{2} \frac{1}{2!} \partial_\alpha^2 G(\alpha) \Big|_{\alpha=1} + \dots + \frac{1}{L} \frac{1}{L!} \partial_\alpha^L G(\alpha) \Big|_{\alpha=1} \right] T P_0.$$
(B.47)

The result of this expression turns out to be equivalent for all values of L. Below is a short calculation for L = 2.

$$\begin{split} \sum_{m=1}^{L=2} \frac{P_m T P_0}{m} &= \left(P_1 + \frac{1}{2} P_2 \right) T P_0 \\ &= \left[-\partial_\alpha \prod_{j=1}^{L=2} \left(1 - \alpha n_{j\uparrow} n_{j\downarrow} \right) \Big|_{\alpha=1} + \frac{1}{2} \frac{1}{2!} \partial_\alpha^2 \prod_{j=1}^{L=2} \left(1 - \alpha n_{j\uparrow} n_{j\downarrow} \right) \Big|_{\alpha=1} \right] T P_0 \\ &= \left[-\left(\left\{ \partial_\alpha \left(1 - \alpha n_{1\uparrow} n_{1\downarrow} \right) \right\} \left(1 - \alpha n_{2\uparrow} n_{2\downarrow} \right) \right. \right. \right. \\ &+ \left(1 - \alpha n_{1\uparrow} n_{1\downarrow} \right) \partial_\alpha \left\{ \left(1 - \alpha n_{2\uparrow} n_{2\downarrow} \right) \right\} \right) \Big|_{\alpha=1} \\ &+ \frac{1}{4} \partial_\alpha \left(\left\{ \partial_\alpha \left(1 - \alpha n_{1\uparrow} n_{1\downarrow} \right) \right\} \left(1 - \alpha n_{2\uparrow} n_{2\downarrow} \right) \right. \right. \\ &+ \left(1 - \alpha n_{1\uparrow} n_{1\downarrow} \right) \partial_\alpha \left\{ \left(1 - \alpha n_{2\uparrow} n_{2\downarrow} \right) \right\} \right) \Big|_{\alpha=1} \right] T P_0 \\ &= - \left[- n_{1\uparrow} n_{1\downarrow} (1 - n_{2\uparrow} n_{2\downarrow}) + (1 - \alpha n_{1\uparrow} n_{1\downarrow}) (-n_{2\uparrow} n_{2\downarrow}) \right] \\ &+ \frac{1}{4} \partial_\alpha \left[- n_{1\uparrow} n_{1\downarrow} (1 - \alpha n_{2\uparrow} n_{2\downarrow}) + (1 - \alpha n_{1\uparrow} n_{1\downarrow}) (-n_{2\uparrow} n_{2\downarrow}) \right] \Big|_{\alpha=1} T P_0 \\ &= \left(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow} - \frac{3}{2} n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow} \right) \left(t_{12} c_{1a}^{\dagger} c_{2a} + t_{21} c_{2a}^{\dagger} c_{1a} \right) P_0 \\ &= \sum_{j,k=1}^{L=2} t_{jk} n_{j\uparrow} n_{j\downarrow} c_{ja}^{\dagger} c_{ka} P_0 . \end{split}$$
(B.48)

The term with the factor of 3/2 is zero because we are projecting onto singly occupied sites. Moreover, the terms where the first index of t and the index of n do not match also result in zero due to (B.8) and (B.46). Therefore, the result for general L is

$$\sum_{m=1}^{L} \frac{P_m T P_0}{m} = \sum_{j,k=1}^{L} t_{jk} n_{j\uparrow} n_{j\downarrow} c_{ja}^{\dagger} c_{ka} P_0.$$
(B.49)

B.3.1 The t - J Model

With the result from the previous section we now have an explicit form for the t - J model:

$$H_{t-J} = P_0 \left(\sum_{j,k=1}^{L} t_{jk} c_{ja}^{\dagger} c_{ka} - \frac{1}{U} \sum_{j,k,k',l=1}^{L} t_{jk} t_{k'l} c_{ja}^{\dagger} c_{ka} n_{k'\uparrow} n_{k'\downarrow} c_{k'b}^{\dagger} c_{lb} \right) P_0,$$
(B.50)

as the effective Hamiltonian for the low-energy regime of the Hubbard model in the atomic limit. We may further simplify the second sum. Most calculations below use (B.8). Each simplification is given by

$$c_{ja}^{\dagger}c_{ka}n_{k'\uparrow}n_{k'\downarrow} = \begin{cases} c_{ja}^{\dagger} \left(n_{k'\uparrow}c_{ka} - \delta_{kk'}\delta_{\uparrow a}c_{ka} \right) n_{k'\downarrow}, \\ c_{ja}^{\dagger}c_{ka}n_{j\uparrow}n_{j\downarrow}, \\ c_{ja}^{\dagger}c_{ka}n_{j\uparrow}n_{j\downarrow}, \end{cases}$$
$$= \begin{cases} n_{k'\uparrow}n_{k'\downarrow}c_{ja}^{\dagger}c_{ka} = 0, \qquad k' \neq j, k, \\ c_{ja}^{\dagger}n_{j\uparrow}c_{ka}n_{j\downarrow} = c_{ja}^{\dagger}c_{ka}n_{j\uparrow}n_{j\downarrow} \text{ by (B.46)}, \qquad k' = j \neq k, \\ \left(n_{j\uparrow} + n_{j\downarrow} \right) n_{j\uparrow}n_{j\downarrow} = 2n_{j\uparrow}n_{j\downarrow} = 0 \text{ by (B.46)}, \qquad k' = j = k. \end{cases}$$
(B.51)

Only when k' = j = k is there a non-vanishing contribution in the sum:

$$H_{t-J} = P_0 \left(\sum_{j,k=1}^{L} t_{jk} c_{ja}^{\dagger} c_{ka} - \frac{1}{U} \sum_{j,k,l=1}^{L} t_{jk} t_{kl} c_{ja}^{\dagger} c_{ka} n_{k\uparrow} n_{k\downarrow} c_{kb}^{\dagger} c_{lb} \right) P_0.$$
(B.52)

We now consider the term

$$c_{ka}n_{k\uparrow}n_{k\downarrow}c_{kb}^{\dagger} = \begin{cases} c_{ka}c_{k\uparrow}^{\dagger}c_{k\uparrow}\left(1-c_{k\downarrow}c_{k\downarrow}^{\dagger}\right)c_{k\downarrow}^{\dagger} = c_{ka}c_{k\uparrow}^{\dagger}c_{k\uparrow}c_{k\downarrow}^{\dagger}, \quad b = \downarrow, \\ c_{ka}\left(1-c_{k\uparrow}c_{k\uparrow}^{\dagger}\right)c_{k\uparrow}^{\dagger}c_{k\downarrow}^{\dagger}c_{k\downarrow} = c_{ka}c_{k\downarrow}^{\dagger}c_{k\downarrow}c_{k\uparrow}^{\dagger}, \quad b = \uparrow, \\ = c_{ka}n_{kb'}c_{kb}^{\dagger}, \quad b' \neq b, \end{cases}$$
(B.53)

where by the same method,

$$c_{ka}n_{kb'}c_{kb}^{\dagger} = \begin{cases} c_{ka}\left(1 - c_{ka}c_{ka}^{\dagger}\right)c_{kb}^{\dagger} = c_{ka}c_{kb}^{\dagger}, & a = b' \neq b, \\ c_{kb}n_{kb'}c_{kb}^{\dagger} = c_{kb}c_{kb}^{\dagger}n_{kb'} = \left(1 - n_{kb}\right)n_{kb'}, & a = b \neq b'. \end{cases}$$
(B.54)

Then in general,

$$c_{ja}^{\dagger}c_{ka}n_{k\uparrow}n_{k\downarrow}c_{kb}^{\dagger}c_{lb} = c_{ja}^{\dagger} \left[c_{ka}c_{kb}^{\dagger} + (1 - n_{kb})n_{kb'} \right] c_{lb}$$
$$= c_{ja}^{\dagger}c_{ka}c_{kb}^{\dagger}c_{lb} + c_{jb}^{\dagger}n_{kb'}c_{lb} - c_{ja}^{\dagger}n_{kb}n_{kb'}c_{lb}.$$
(B.55)

For the last term, if $j \neq k$ then

$$c_{ja}^{\dagger} n_{kb} n_{kb'} c_{lb} = n_{kb} c_{ja}^{\dagger} n_{kb'} c_{lb} = n_{kb} n_{kb'} c_{ja}^{\dagger} c_{lb} = 0,$$
(B.56)

by (B.46). On the other hand, if j = k then

$$c_{ja}^{\dagger}n_{kb}n_{kb'}c_{lb} = c_{ja}^{\dagger}c_{jb}^{\dagger}c_{jb'}c_{jb'}c_{lb} = \begin{cases} n_{jb}c_{ja}^{\dagger}c_{jb'}^{\dagger}c_{jb'}c_{lb} = 0, & a = b' \neq b, \\ 0, & a = b \neq b'. \end{cases}$$
(B.57)

Putting it all together and using (B.8) on the second term of (B.55) we arrive at

$$H_{t-J} = P_0 \left[\sum_{j,k=1}^{L} t_{jk} c_{ja}^{\dagger} c_{ka} - \frac{1}{U} \sum_{j,k,l=1}^{L} t_{jk} t_{kl} \left(c_{ja}^{\dagger} c_{ka} c_{kb}^{\dagger} c_{lb} + c_{ja}^{\dagger} c_{la} c_{kb}^{\dagger} c_{kb} \right) \right] P_0,$$
(B.58)

where the former term in the second sum can be rewritten as

$$c_{ja}^{\dagger}c_{ka}c_{kb}^{\dagger}c_{lb} = -c_{ja}^{\dagger}c_{kb}^{\dagger}c_{ka}c_{lb} = c_{ja}^{\dagger}c_{kb}^{\dagger}c_{lb}c_{ka} = c_{ja}^{\dagger}\left(\delta_{kl} - c_{lb}c_{kb}^{\dagger}\right)c_{ka} = -c_{ja}^{\dagger}c_{lb}c_{kb}^{\dagger}c_{ka}, \tag{B.59}$$

since $a \neq b$ and $k \neq l$. The reason for this will be made clear in just a moment. From Eqs. (B.9) and (B.12) we have the following the products

$$S_{jk}^{a} \cdot S_{lm}^{a} = c_{j\alpha}^{\dagger} \sigma_{\alpha\beta}^{a} c_{k\beta} \cdot c_{l\gamma}^{\dagger} \sigma_{\gamma\delta}^{a} c_{m\delta} = \left(\sigma_{\alpha\beta}^{a} \cdot \sigma_{\gamma\delta}^{a}\right) c_{j\alpha}^{\dagger} c_{k\beta} c_{l\gamma}^{\dagger} c_{m\delta}, \tag{B.60}$$

$$S_{jk}^{0} \cdot S_{lm}^{0} = c_{j\alpha}^{\dagger} \sigma_{\alpha\beta}^{a} c_{k\beta} \cdot c_{l\gamma}^{\dagger} \sigma_{\gamma\delta}^{a} c_{m\delta} = \delta_{\alpha\beta} \delta_{\gamma\delta} \ c_{j\alpha}^{\dagger} c_{k\beta} c_{l\gamma}^{\dagger} c_{m\delta}. \tag{B.61}$$

For (B.60) we use the completeness relation (A.4) to consider the non-vanishing contributions given by

$$S^{a}_{jl} \cdot S^{a}_{kk} = \left(2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}\right)c^{\dagger}_{j\alpha}c_{l\beta}c^{\dagger}_{k\gamma}c_{k\delta} = 2c^{\dagger}_{j\alpha}c_{l\beta}c^{\dagger}_{k\beta}c_{k\alpha} - c^{\dagger}_{j\alpha}c_{l\alpha}c^{\dagger}_{k\gamma}c_{k\gamma}, \tag{B.62}$$

$$S_{jl}^0 \cdot S_{kk}^0 = c_{j\alpha}^\dagger c_{l\alpha} c_{k\gamma}^\dagger c_{k\gamma}. \tag{B.63}$$

Thus, with (B.59) the second sum in (B.58) becomes

$$c_{j\alpha}^{\dagger}c_{l\beta}c_{k\beta}^{\dagger}c_{k\alpha} - c_{j\alpha}^{\dagger}c_{l\alpha}c_{k\gamma}^{\dagger}c_{k\gamma} = \frac{1}{2}\left(S_{jl}^{a} \cdot S_{kk}^{a} - S_{jl}^{0} \cdot S_{kk}^{0}\right).$$
(B.64)

With this result we express the t - J model conveniently as

$$H_{t-J} = P_0 \left[\sum_{j,k=1}^{L} t_{jk} c_{ja}^{\dagger} c_{ka} + \frac{1}{U} \sum_{j,k,l=1}^{L} t_{jk} t_{kl} \left(c_{ja}^{\dagger} c_{lb} c_{kb}^{\dagger} c_{ka} - c_{ja}^{\dagger} c_{la} c_{kb}^{\dagger} c_{kb} \right) \right] P_0$$

$$= P_0 \left[\sum_{\substack{j,k=1\\j\neq k}}^{L} t_{jk} S_{jk}^{0} + \frac{1}{2U} \sum_{\substack{j,k,l=1\\j\neq k\neq l}}^{L} t_{jk} t_{kl} \left(S_{jl}^{a} \cdot S_{kk}^{a} - S_{jl}^{0} \cdot S_{kk}^{0} \right) \right] P_0$$

$$= P_0 \left[\sum_{\substack{j,k=1\\j\neq k}}^{L} t_{jk} S_{jk}^{0} + \frac{1}{2U} \sum_{\substack{j,k,l=1\\j\neq k\neq l=j}}^{L} |t_{jk}|^2 \left(S_{jj}^{a} \cdot S_{kk}^{a} - S_{jj}^{0} \cdot S_{kk}^{0} \right) \right] P_0, \quad (B.65)$$

where using the definitions of the total particle number (B.2) and total spin (B.9) the form becomes

$$H_{t-J} = P_0 \left[\sum_{\substack{j,k=1\\j\neq k}}^{L} t_{jk} S_{jk}^0 + \frac{1}{2U} \sum_{\substack{j,k,l=1\\j\neq k\neq l=j}}^{L} |t_{jk}|^2 \left(4\mathbf{S}_j \cdot \mathbf{S}_k - n_j n_k \right) + \frac{1}{U} \sum_{\substack{j,k,l=1\\j\neq k\neq l\neq j}}^{L} t_{jk} t_{kl} \left(c_{ja}^{\dagger} \sigma_{ab}^{\alpha} c_{lb} \cdot \mathbf{S}_k - \frac{1}{2} c_{ja}^{\dagger} c_{la} n_k \right) \right] P_0.$$
(B.66)

B.3.2 The Antiferromagnetic Heisenberg Model

Another useful representation of the t - J model is obtained when we move the left projector P_0 through the sums. In doing so the first sum in (B.66) becomes

$$P_0 c_{ja}^{\dagger} c_{ka} = \left(1 - n_{j\uparrow} n_{j\downarrow}\right) c_{ja}^{\dagger} c_{ka} = c_{ja}^{\dagger} c_{ka} - n_{j\uparrow} n_{j\downarrow} c_{ja}^{\dagger} c_{ka}, \tag{B.67}$$

where

$$n_{j\uparrow}n_{j\downarrow}c_{ja}^{\dagger}c_{ka} = \begin{cases} n_{j\uparrow}\left(c_{ja}^{\dagger} + c_{ja}^{\dagger}n_{j\downarrow}\right)c_{ka} = n_{j\uparrow}c_{ja}^{\dagger}c_{ka} = c_{ja}^{\dagger}c_{ka}n_{j\uparrow}, & a = \downarrow, \\ n_{j\uparrow}c_{ja}^{\dagger}n_{j\downarrow}c_{ka} = \left(c_{ja}^{\dagger} + c_{ja}^{\dagger}n_{j\uparrow}\right)n_{j\downarrow}c_{ka} = c_{ja}^{\dagger}c_{ka}n_{j\downarrow}, & a = \uparrow. \end{cases}$$
(B.68)

Hence

$$P_{0}c_{ja}^{\dagger}c_{ka} = c_{ja}^{\dagger}c_{ka} - c_{ja}^{\dagger}c_{ka}n_{j\uparrow} - c_{ja}^{\dagger}c_{ka}n_{j\downarrow} = c_{ja}^{\dagger}c_{ka}\left(1 - n_{j}\right).$$
(B.69)

The second sum is unaffected while the third becomes

$$P_{0}\left(c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k}-\frac{1}{2}c_{ja}^{\dagger}c_{la}n_{k}\right) = P_{0}c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k}-\frac{1}{2}P_{0}c_{ja}^{\dagger}c_{la}n_{k}$$
$$=\left(1-n_{j\uparrow}n_{j\downarrow}\right)c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k}-\frac{1}{2}\left(1-n_{j\uparrow}n_{j\downarrow}\right)c_{ja}^{\dagger}c_{la}n_{k}.$$
(B.70)

Simplifying the former term with $n_{j\uparrow}n_{j\downarrow}$ we obtain

$$\begin{split} n_{j\uparrow}n_{j\downarrow}c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k} &= n_{j\uparrow}\left(c_{ja}^{\dagger}+c_{ja}^{\dagger}n_{j\downarrow}\right)\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k} \\ &= n_{j\uparrow}c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k}, \ a = \downarrow, \\ &= c_{ja}^{\dagger}\sigma_{ab}^{\alpha}n_{j\uparrow}c_{lb}\cdot\mathbf{S}_{k} \\ &= c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}n_{j\uparrow}\cdot c_{kc}^{\dagger}\sigma_{cd}^{\alpha}c_{kd}, \ l \neq j, \\ &= c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k}n_{j\uparrow}, \ j \neq k. \end{split}$$
(B.71)

Similarly, if $a = \uparrow$ then

$$n_{j\uparrow}n_{j\downarrow}c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k} = c_{ja}^{\dagger}\sigma_{ab}^{\alpha}c_{lb}\cdot\mathbf{S}_{k}n_{j\downarrow}.$$
(B.72)

Therefore,

$$P_0 c_{ja}^{\dagger} \sigma_{ab}^{\alpha} c_{lb} \cdot \mathbf{S}_k = c_{ja}^{\dagger} \sigma_{ab}^{\alpha} c_{lb} \cdot \mathbf{S}_k \left(1 - n_j \right).$$
(B.73)

The other term with $n_{j\uparrow}n_{j\downarrow}$ is similar in calculation. We obtain

$$\begin{split} n_{j\uparrow}n_{j\downarrow}c_{ja}^{\dagger}c_{la}n_{k} &= n_{j\uparrow}\left(c_{ja}^{\dagger} + c_{ja}^{\dagger}n_{j\downarrow}\right)c_{la}n_{k} \\ &= n_{j\uparrow}c_{ja}^{\dagger}c_{la}n_{k}, \ a = \downarrow, \\ &= c_{ja}^{\dagger}c_{la}n_{j\uparrow}n_{k}, \ a = \downarrow, \ l \neq j, \\ &= c_{ja}^{\dagger}c_{la}n_{k}n_{j\uparrow}, \ k \neq j. \end{split}$$
(B.74)

Similarly, if $a=\uparrow$ then

$$n_{j\uparrow}n_{j\downarrow}c_{ja}^{\dagger}c_{la}n_{k} = c_{ja}^{\dagger}c_{la}n_{k}n_{j\downarrow}, \tag{B.75}$$

and thus

$$\frac{1}{2}P_0 c_{ja}^{\dagger} c_{la} n_k = \frac{1}{2}c_{ja}^{\dagger} c_{la} n_k \left(1 - n_j\right).$$
(B.76)

Under the application of P_0 the t - J model now takes on the form

$$H_{t-J} = \sum_{\substack{j,k=1\\j\neq k}}^{L} t_{jk} c_{ja}^{\dagger} c_{la} \left(1-n_{j}\right) + \frac{1}{2U} \sum_{\substack{j,k,l=1\\j\neq k\neq l=j}}^{L} |t_{jk}|^{2} \left(4\mathbf{S}_{j} \cdot \mathbf{S}_{k} - n_{j}n_{k}\right) + \frac{1}{U} \sum_{\substack{j,k,l=1\\j\neq k\neq l\neq j}}^{L} t_{jk} t_{kl} \left(c_{ja}^{\dagger} \sigma_{ab}^{\alpha} c_{lb} \cdot \mathbf{S}_{k} - \frac{1}{2} c_{ja}^{\dagger} c_{la}n_{k}\right) \left(1-n_{j}\right).$$
(B.77)

Note that since $H_{t-J} \in P_0 \mathcal{H}$ the right P_0 may be left out.

At half-filling, when the number of electrons equals the number of lattice sites L, all the eigenstates of H_{t-J} must be pure spin states. That is, every lattice site is occupied precisely by one electron $n_j = 1$. Therefore, the t - J model reduces down to the Heisenberg model

$$H_{\text{Heis}} = \sum_{\substack{j,k=1\\j\neq k}}^{L} \frac{2|t_{jk}|^2}{U} \left(\mathbf{S}_j \cdot \mathbf{S}_k - \frac{1}{4} \right).$$
(B.78)

If we consider only nearest-neighbour hopping then

$$t_{jk} = -t \left(\delta_{j,k-1} + \delta_{j,k+1} \right), \tag{B.79}$$

and we obtain the isotropic antiferromagnetic Heisenberg model

$$H_{\text{Heis}} = \frac{4t^2}{U} \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right). \tag{B.80}$$

Finally, we note that the cyclic four-spin ring-exchange term is obtained at the next non-vanishing order of Eq. (B.37) at half-filling. The result is an interaction exchange of $20t^4/U^3$.

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