Frustrated spin -1/2 two-leg and three-leg antiferromagnetic Heisenberg ladders

Ningsheng Zhu
University of Nevada, Las Vegas

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FRUSTRATED SPIN-1/2 TWO-LEG AND THREE-LEG
ANTIFERROMAGNETIC HEISENBERG LADDERS

by

Ningsheng Zhu

Bachelor of Science
University of Science and Technology of China
1982

A dissertation submitted in partial fulfillment
of the requirements for

Doctor of Philosophy Degree
Department of Physics
College of Science

Graduate College
University of Nevada, Las Vegas
August 2000

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Frustrated Spin-1/2 Two-leg and Three-leg Antiferromagnetic Heisenberg Ladders

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Doctor of Philosophy

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ABSTRACT

Frustrated Spin-1/2 Two-Leg and Three-Leg Antiferromagnetic Heisenberg Ladders

by

Ningsheng Zhu

Dr. Changfeng Chen, Examination Committee Chair
Professor of Physics
University of Nevada, Las Vegas

The goal of this project is to study the ground-state properties of frustrated spin-1/2 two- and three-leg Heisenberg ladders, and to investigate possible effects of diagonal couplings on spin gaps. The ground-state and the first-excited-state energies of these two systems are calculated systematically by using the density matrix renormalization group method. The ground state phase diagrams for these two systems are obtained. For the frustrated two-leg ladder, we found that the spin gap is insensitive to the change of the FM diagonal coupling constant. This is in agreement with experimental suggestions. For the frustrated three-leg ladder, we conclusively proved that introducing AF diagonal couplings can not change the gapless property of the ground state.
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CHAPTER 1

INTRODUCTION

The study of ladder systems started in late 80's and early 90's. It has now developed into a well-established area of research within the context of strongly correlated electrons and condensed matter physics (Dagotto and Rice 1996, Rice 1997, Dagotto 1999). An \( n \)-leg ladder is defined as \( n \) parallel chains of ions, with bonds among them such that the interchain couplings are comparable in strength to the intrachain couplings. The particular case of \( n=2 \) and the interchain couplings are only through "rungs" motivates the use of the name "ladder" for this geometry.

A vast literature on this area has already accumulated and the investigations

---

Fig. 1 Schematic representation of the two-leg ladder compound \( \text{SrCu}_2\text{O}_3 \) and the three-leg ladder compound \( \text{Sr}_2\text{Cu}_3\text{O}_5 \). The black dots are Cu atoms, and the intersections of the solid lines are O locations.
continue at a rapid pace.

The main reason for this sudden interest in ladder systems is that ladders provide a “playground” for studies of high critical-temperature ($T_c$) cuprate superconductors (Bednorz and Müller 1986), which contain Cu$^{2+}$ spin-1/2 antiferromagnetic square lattice layers. Early theoretical studies of ladder models (Dagotto, Riera, and Scalapino 1992; Sigrist, Rice, and Zhang 1994) predicted that (i) in the absence of hole carriers even-leg ladders have a spin gap in their spin excitation spectrum, namely it costs a finite amount of energy to create spin excitations above the ground state; (ii) upon doping of holes the ground state of the even-leg ladders, in which two holes sharing a common rung forms a hole pair, becomes dominated by superconducting correlations, and this superconductivity for ladders should be in the d-wave channel, which is currently most accepted channel for superconductivity in the high-$T_c$ cuprates. This spin-gap property resembles the “pseudogap” feature that has been observed in the high-$T_c$ cuprates, particularly in the underdoped regime of low hole-density, while the d-wave channel superconductivity adds further evidence for strong similarities between doped-ladders and doped-plan. Besides, ladder systems are considerably easier to study theoretically than two-dimensional models because they are basically quasi-one-dimensional. A plethora of powerful many-body techniques, notably those involving computational methods, work well in one-dimension but lose their accuracy in two-dimensions (Dagotto 1994). By studying how physical properties of ladder systems evolve with increasing number of legs and/or couplings, we can obtain insights on the high-$T_c$ cuprate superconductors.

Another reason for this sudden interest in ladder systems is related with the explicit syntheses of ladder compounds. After an enormous experimental effort, several ladder materials have become available, such as the Cu-oxide ladder com-
pound SrCu$_2$O$_3$ (Azuma et al. 1994), the metallic ladder compound La$_{1-x}$Sr$_x$CuO$_{2.5}$ (Hiroi and Takano 1995), the superconducting ladder compound Sr$_{11-x}$Ca$_x$Cu$_{24}$O$_{41}$ (Uehara et al. 1996), the strong-coupling ladder compound Cu$_2$(C$_5$H$_{12}$N$_2$)$_2$Cl$_4$ (Chaboussant et al. 1997a, 1997b), vanadium-based ladder compound CaV$_2$O$_5$ (Iwase et al. 1996), and the ladder compound KCuCl$_3$ (Tanaka et al. 1996). A variety of exciting experiments have already been carried out on these materials (Dagotto 1999) and clear evidence has already accumulated that real ladder materials with an even (odd) number of legs, two (three) in particular, have a finite (have no) spin gap in their spectrum of spin excitations, in agreement with early theoretical predictions. In addition, superconductivity in one of the ladder compounds has been detected upon the introduction of hole carriers and using high pressure (Uehara et al. 1996). Furthermore, several recent experiments (Nagata et al. 1998) have shown that there are regions of parameter space where the resistivity of ladders is linear with temperature, a hallmark of the exotic normal state found in the two-dimensional cuprates, revealing additional close analogies between superconducting ladder compounds and high-T$_c$ superconductors.

The study of ladder systems is also interesting in its own right. Odd-leg ladders with AF couplings along legs ($J$) and rungs ($J'$) were predicted to have no spin gap; whereas, surprisingly, even-leg ladders were predicted to have a spin gap for any finite AF rung coupling $J'$ (Dagotto, Riera and Scalapino 1992, White, Noack and Scalapino 1994). A close relationship of these generic spin gap behaviors of spin-1/2 even- and odd-leg AF Heisenberg ladders was established with AF integer- and half-integer-spin Heisenberg chains, which are gapful and gapless, respectively (Sierra 1996). For even-leg ladders in which $J'/J \leq 1$, the spin gap decreases exponentially with increasing number of legs (Poilblanc, Tsunetsugu and Rice 1994). A spin gap also occurs for AF leg coupling if $J'$ is any finite ferromagnetic (FM) value, although
the dependence of the gap on the magnitude of $J'$ is different from the dependence of when $J'$ is AF: a second-order transition between the two spin-gapped ground state occurs when the spin gap is zero as the rung coupling passes from AF values through zero to FM values (Wang 1999).

<table>
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<th>Correlations</th>
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<td>gapped</td>
<td>exponential decay</td>
</tr>
<tr>
<td>odd</td>
<td>gapless</td>
<td>algebraic decay</td>
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Table 2 Behaviour of spin-1/2 $n$-leg ladders

<table>
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<td>odd</td>
<td>gapless</td>
<td>algebraic decay</td>
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It is now believed that the physics of isolated (i.e. without interladder coupling) regular (i.e. without intraladder frustrations) ladders are under reasonable theoretical control, and there is little controversy on their main properties: but it is also fair to say that the effects of interladder couplings and intraladder frustrations are still not very clear. To provide a basis for further understanding of the properties of ladder systems, it is important to study the effects of these intraladder and/or interladder interactions. The investigations of interladder couplings in two particular systems, the trellis layer compounds SrCu$_2$O$_3$ and CaV$_2$O$_5$, was reported by Normand, Penc, Albrecht and Mila (1997) and by Johnston’s group (2000). There were also some calculations including intraladder frustrations coursed by diagonal couplings, such as Xian’s composite operator method (1995); Zheng, Kotov, and Oitma’s series expansions (1997); and Wang’s DMRG calculation (1998). All these
works concentrate on two-leg ladders and assume a antiferromagnetic diagonal coupling. The purpose of this research is to study the effects of intraladder frustrations on spin-1/2 two-leg ladders with ferromagnetic diagonal couplings and three-leg ladders with antiferromagnetic diagonal couplings.

Since there is no general analytical method to solve the many-body problem of a strongly interacting lattice system, we have to resort to numerical methods. Three best known numerical methods for studying quantum lattice models are the exact diagonalization method (Dagotto 1994), the quantum Monte Carlo (QMC) method (von der Linden 1992), and the density matrix renormalization group (DMRG) method (White 1992 & 1993). I will use the DMRG method in this research because the exact diagonalization method can treat only very short ladders while the QMC method suffers from the sign problem in dealing with frustration couplings.

The organization of the dissertation is as follows. In chapter 2 the model Hamiltonians, the physical picture, and some related terminologies of spin-1/2 frustrated two- and three-leg Heisenberg ladders are introduced. Chapter 3 gives a detail description of the DMRG method. In chapter 4 the effect of the ferromagnetic diagonal coupling on the spin gap of a two-leg spin ladder is discussed based on extensive DMRG calculations. In chapter 5 the ground state phase diagram of a spin-1/2 frustrated three-leg Heisenberg ladder is provided. Chapter 6 contains a brief summary of the conclusions. The appendix A collects the numerical solution of the ground state energy (per rung) for the frustrated three-leg spin ladder.
CHAPTER 2

HEISENBERG LADDERS

The study of low-dimensional quantum magnetism has experienced a resurgence in the last decade with the synthesis of whole new families of organic and inorganic compounds containing spin-1/2 and spin-1 degrees of freedom, especially oxide compounds having spins arranged in two-dimensional planes, one-dimensional chains, quasi-one-dimensional ladders with both even and odd numbers of legs, and even two-dimensional arrays of intersecting one-dimensional chains. These new systems have fascinating properties and provide an excellent testing ground for theories of strongly correlated electronic systems. In this project, we will study two examples of these systems, i.e. frustrated spin-1/2 two- and three-leg Heisenberg ladders, and will concentrate on one interesting aspect of the problem – the effects of frustration on the low energy properties of these two systems.

In Section 2.1 we introduce the Heisenberg model and discuss the physical picture of ferromagnetic and antiferromagnetic couplings. In Section 2.2 we collect major results known for the “regular” Heisenberg ladders. In section 2.3, we write down our model Hamiltonians and give a brief summary of literatures on “frustrated” Heisenberg ladders.

2.1 The Heisenberg Hamiltonian

The Heisenberg Hamiltonian is a fundamental model for quantum magnetism, as well as other phenomena that can be effectively described by quantum spin op-
The Hamiltonian which describes the nearest-neighbor interactions of localized quantum spins is given by

\[ H = J \sum_{\langle ij \rangle} S_i \cdot S_j, \]  

where \( S_i \) is the spin operator at lattice site \( i \), \( \langle ij \rangle \) denotes the nearest-neighbor sites, and \( J \) is the exchange coupling constant that provides the energy scale in the problem. This scale is material dependent and ranges from a few millielectron volts to about 0.1 eV.

Generally speaking, if the valence electrons occupy nondegenerate s-orbitals, the ground state and the elementary excited states of the system are well described by an effective "Heisenberg Hamiltonian" which couples nearest-neighbor spins antiferromagnetically and neglects all the electronic degrees of freedom. If, on the other hand, two or more valence states are accessible to the conduction electrons on each atom, we might expect that an effective "Heisenberg Hamiltonian" with ferromagnetic coupling among nearest-neighbor spins will satisfactorily describe the magnetic degrees of freedom for the system, although not the electronic one of course.

Paradoxically, magnetism arises from electrostatic not magnetic forces. Magnetic dipolar interaction between the electron moments (which is of order \( 10^{-5} \) eV) is far too weak to explain the observed magnetic transition temperatures (which are of order \( 10^2 - 10^3 \) °K in transition metal and rare earth compounds). It was therefore realized in the early days of quantum mechanics that the coupling mechanism that gives rise to magnetism derives from the following fundamental properties of electrons:

- The electron's spin.
- The electron's kinetic (delocalization) energy.
- Pauli exclusion principle (Fermi statistics).
• Coulomb interactions between electrons and between electron and ionic core.

Imagine that the electrons being reasonably localized to their corresponding atoms, with these atoms carrying a net magnetic moment due to its having a net electronic spin. The electron in each atom which carries the net spin interacts with its counterparts on neighbouring atoms, resulting in an effective spin-spin interaction between these atoms. This spin-spin interaction can come about due to the exchange part of the Coulomb interaction, which arises due to the antisymmetrization of the wave function which is required because of the Fermi statistics of the electrons. The overall antisymmetry of the wave function for a pair of electrons requires that the spatial wave function be symmetric for spin singlet and antisymmetric for the spin triplet. If the spatial wave function is antisymmetric, it vanishes when two electrons are at the same location; thus the probability of close approach is reduced. This in turn reduces the mean Coulomb repulsion. However, this reduction in the potential energy comes at the expense of increased kinetic energy associated with the extra nodes in the spatial wave function.

Ferromagnetic (FM) ($J < 0$) coupling arises from the Coulomb repulsion of a pair of outer shell electrons on neighboring atoms. The electrons stay further apart in the parallel spin state, due to Fermi statistics. Antiferromagnetic (AF) ($J > 0$) coupling arises from the Coulomb attraction of neighboring electron to each other's ionic core. This attraction makes the electrons want to be closer to each other, which they achieve in the anti-parallel spin state.

If the $S_i$ were classical spins, i.e. fixed length classical vectors, the ground state of $H$ would be trivially parallel array of vectors for the $J < 0$ case and antiparallel array of vectors for the $J > 0$ case as shown in Figure 2. The classical antiferromagnetic ground state is known as the Néel state. It exists for any bipartite lattice; i.e. one with two sub-lattices such that the nearest neighbors of any point in one
sub-lattice are all in the other.

the classical ferromagnetic ground state

the classical antiferromagnetic ground state
(the Neel state)

Fig. 2 Classical ferromagnetic and antiferromagnetic ground states. The circles
represent atoms and the arrows stand for localized spins. In the Neel state, the
bipartite lattice is shown by circles with two different line styles.

In quantum mechanics S is an operator whose components obey the following
commutation relation

\[ [S^a, S^b] = i \epsilon^{abc} S^c, \quad S^2 = s(s + 1) \]  \hspace{1cm} (2)

where \( \epsilon^{abc} \), (a,b,c = x,y,z), is the Levi-Civita tensor; \( \hbar \) is chosen to be 1, and repeated
indices denote summation. It is easy to see that the ferromagnetic state is indeed
the quantum ground state, but the Neel state is not an eigenstate of the antiferro-
magnetic Heisenberg Hamiltonian. In fact, using raising and lowering operators

\[ S^\pm = S^x \pm i S^y, \] \hspace{1cm} (3)
we can rewrite the Heisenberg Hamiltonian (1) as follows

$$H = J \sum_{(i,j)} [S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)].$$

(4)

Since for the ferromagnetic ground state

$$S_i^+ S_j^- | \uparrow \uparrow \cdots \uparrow \rangle = 0.$$  
$$S_i^- S_j^+ | \uparrow \uparrow \cdots \uparrow \rangle = 0.$$

we have

$$H | \uparrow \uparrow \cdots \uparrow \rangle = N s^2 | \uparrow \uparrow \cdots \uparrow \rangle$$

where $N$ is the number of nearest-neighbor pairs in the system. This means that it is the ground state of $H$. For the Néel state, since

$$S_i^+ S_j^- | \uparrow \downarrow \cdots \uparrow \cdots \downarrow \cdots \uparrow \rangle \sim | \uparrow \downarrow \cdots \downarrow \cdots \uparrow \cdots \rangle.$$  
$$S_i^- S_j^+ | \uparrow \downarrow \cdots \uparrow \cdots \downarrow \cdots \uparrow \rangle \sim | \uparrow \downarrow \cdots \downarrow \cdots \uparrow \cdots \rangle.$$  

it is not an eigenstate of $H$.

2.2 Regular Heisenberg Ladders

By “regular” Heisenberg ladders we mean the coupled Heisenberg spin chains with interchain couplings only through the rungs. After many years theoretical as well as experimental investigations, the following consensuses are well established for the regular Heisenberg ladders: A ladder made from an even number of legs has

- a spin-liquid ground state, i.e. $S=0$ and no long range spin correlations,

- a finite spin gap in its excitation spectrum,

- an exponential decay of the spin-spin correlation function;

while a ladder made from an odd number of legs has
- a gapless spin excitation spectrum,
- a power-law decay of the spin-spin correlation function.

Two most-cited real-world examples of the 2-leg and the 3-leg regular spin ladders are SrCu₂O₃ and Sr₂Cu₃O₅ compounds, respectively. They are the first two members of the family Srₙ₋₁Cuₙ₊₁O₂ₙ (n = 3, 5, 7, 9, ...), a physical realizations of m-leg spin ladders with m = (n + 1)/2.

Since the basic method to synthesize Cu-oxide ladder compounds, for example the Srₙ₋₁Cuₙ₊₁O₂ₙ family, is to introduce arrays of parallel line defects into the CuO₂ planes of the corresponding cuprate, only when the interladder couplings across the defects and the distortions produced to the CuO₄ squares are negligible can we have a real regular Heisenberg ladder.

2.3 Frustrated Heisenberg Ladders

By frustration we mean that there are conflicts among various interaction terms in the Hamiltonian of a system. Most physical systems in condensed matter physics are "frustrated" in the sense that there usually exists several competing interactions, each favoring a different type of ordered state. Such competition can often be revealed by changing a parameter of the system (such as temperature, pressure, magnetic field, etc.), which serves to enhance the effect of a particular interaction and drive the system into a different ordered state (Diep 1994). In a frustrated system, local minimization of the energy is not compatible with the global energy minimum (or minima). A system is highly frustrated when the conflict interactions are of similar magnitude, which will result in a larger degeneracy of its ground states.

The triangular lattice with antiferromagnetic nearest-neighbor interactions appears to be the simplest example of lattice-geometry frustration. It is not possible
for all three spins at the corners of a triangle to satisfy the optimum antiparallel configuration which would minimize the energy of individual pair interactions.

![Diagram of a triangular lattice with spins](a) and the resulting 120° spin structure (b).

The principal effect of this frustration is that it gives rise to a noncollinear magnetic order, i.e. the 120° spin structure.

For low-dimensional quantum magnetism, the simplest example of frustration is the so-called $J_1 - J_2$ model given by the following Hamiltonian which describes the competition of nearest-neighbor ($nn$) and next-nearest-neighbor ($nnn$) interactions of localized spins.

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle ij' \rangle} \mathbf{S}_i \cdot \mathbf{S}_j'$$

Here $\langle ij \rangle$ and $\langle ij' \rangle$ represents summation over $nn$ and $nnn$ pairs on a one- or two-dimensional lattice. It is easy to see, as shown in Figure 4, that $J_1$ and $J_2$ cannot be both antiferromagnetic, so the spins are frustrated.

Since the properties of regular Heisenberg ladders are relatively clear, we will concentrate on frustrated Heisenberg ladders in this project. By frustrated Heisenberg ladders we mean those Heisenberg ladders which include diagonal couplings. We will concentrate on the following two systems, i.e. frustrated spin-1/2 two- and
three-leg AF Heisenberg ladders, respectively. They are the simplest but most important systems of frustrated Heisenberg ladders. Their Hamiltonians are as follows.

\[
H = \sum_i [J_{||}(S_{1,i} \cdot S_{1,i+1} + S_{2,i} \cdot S_{2,i+1}) + J_{\perp} S_{1,i} \cdot S_{2,i} \\
+ J_x (S_{1,i} \cdot S_{2,i+1} + S_{1,i+1} \cdot S_{2,i})]
\]

Fig. 5 Schematic structure of a frustrated two-leg ladder.

\[
H = \sum_i \{J_{||}(S_{0,i} \cdot S_{0,i+1} + S_{1,i} \cdot S_{1,i+1} + S_{2,i} \cdot S_{2,i+1}) + J_{\perp} S_{0,i} \cdot (S_{1,i} + S_{2,i}) \\
+ J_x [(S_{1,i} + S_{2,i}) \cdot S_{0,i+1} + S_{0,i} \cdot (S_{1,i+1} + S_{2,i+1})]\}
\]
Fig. 6 Schematic structure of a frustrated three-leg ladder.

where $S_{n,i}$ denotes a spin-1/2 operator at site $i$ of the $n$th chain. $J_{\parallel}$ is an intrachain coupling between two neighboring spins in each chain. $J_\perp$ an interchain coupling between two spins on each rung and $J_x$ an interchain coupling between two spins of neighboring rungs.

The diagonal coupling $J_x$ in the above Hamiltonians may introduce frustrations to the systems. Taking the two-leg ladder as an example, we have four possibilities ($J_{\parallel} = 1$) as shown in Figure 7.

The purpose of this project is to investigate the effect of frustrations caused by the diagonal coupling $J_x$.

There are several published papers dealing with frustrated spin ladders. Xian (1995) found some rigorous expressions and a partial phase diagram for Hamiltonian (7) using the so-called composite operators. Zheng, Kotov, and Oitmaa (1998) studied Hamiltonian (7) by using series expansions about two particular limit cases, the Ising and dimer limits. Lin and Shen (1998) found two exact solutions of Hamiltonian (7) in some particular parameter regions. Azaria, Lecheminant, and Nersesstan (1998) discussed the chiral universality class in a frustrated three-leg spin ladder described by Hamiltonian (8). Using the DMRG method, Wang (1998) obtained an
Fig. 7 Various frustrated and unfrustrated competitions caused by diagonal couplings.

unbiased numerical solution for Hamiltonian (7) with $J_x \geq 0$.

In this project, we will study the ground state properties for both Hamiltonian (7) and (8) with $J_x < 0$ for the former and $J_x > 0$ for the later. We make no simplification assumptions to our solutions. Our focus will be on the effect of frustration to the ground state properties of these systems.
CHAPTER 3

DENSITY MATRIX RENORMALIZATION GROUP

The Density Matrix Renormalization Group (DMRG) method (White 1992 & 1993) is a numerical technique for finding accurate approximations to the ground state and the low-lying excited states of strongly interacting quantum lattice systems such as the Heisenberg, $t - J$, and Hubbard models. DMRG traces its roots to Wilson's renormalization group (RG) treatment of Kondo problem (Wilson 1975) and is related to the block approach of real space renormalization group (Burkhardt and van Leeuwen 1982). It applies to almost any one-dimensional (1D) quantum lattice systems with local interactions and can provide a wide variety of static properties. (Peschel, Wang, Kaulke, and Hallberg 1999)

The reason for choosing the DMRG method is two fold. First, the other two best known numerical methods for strongly interacting systems are not suitable for studying frustrated ladder systems. The exact diagonalization method can handle only very short ladder length, while the QMC method suffers from the sign problem when dealing with frustrated system. Second, the DMRG method is the state-of-the-art numerical method to solve any 1D or quasi-1D strongly interacting lattice problems. It is remarkable in the accuracy that can be achieved for 1D systems.

In Section 3.1 we briefly describe the standard numerical RG procedure for 1D lattice systems. In Section 3.2 we introduce the superblock scheme and the density matrix projection approach. Then, in Section 3.3, we discuss DMRG algorithms for infinite system and finite system, respectively.
3.1 Standard Real-Space RG Procedure

In this section, we describe the standard numerical RG procedure in the simplest possible context, a real-space blocking approach for 1D lattice system. The aim of this section is to introduce some concepts as well as some notations which will be useful latter for our discussions of the DMRG.

The basic idea of any numerical RG procedure is to truncate away unimportant degrees of freedom iteratively using a succession of RG transformations. A typical iteration starts with a numerical representation of the Hamiltonian in a particular basis, then adds degrees of freedom by increasing the size of the system, and finally carries out a numerical RG transformation to truncate away unimportant degrees of freedom, i.e. transforms the representation of the Hamiltonian to a reduced basis.

In the 1D real-space blocking approach, one begins by breaking the 1D chain into finite identical blocks and proceeds by building larger blocks out of the smaller ones until the whole chain becomes one large block. We label the blocks $B$ and the block Hamiltonian $H_B$. $H_B$ contains all terms of $H$ involving only sites contained in $B$. In the first iteration, block $B$ should be chosen to be small enough so that $H_B$ can be diagonalized exactly. It is usually convenient to start at the first iteration with blocks consisting of just one site. A block is described by a list of $m$ many-body states on the block and by matrix elements between these states. This set of $m$ states forms the basis of matrix representations. We store the number $m$ and all quantum numbers used to describe a single many-body state. Under this basis $H_B$ is represented as an $m \times m$ matrix. Besides the $H_B$ matrix, other matrices which describe the interactions between two blocks also need to be stored.

Take the spin-1/2 Heisenberg chain as an example. If in the first iteration each block consists of just one site, then we can choose the two eigenstates of $S_z$, i.e. $|\uparrow\rangle$ and $|\downarrow\rangle$, to describe an initial one-site block. We store $m=2$ as the number of basis
states and use quantum numbers $S_z = \pm 1/2$ to label these two states. Under this basis, the block Hamiltonian and the end operators have the following matrix representations:

$$H_B = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \quad S_i^z = S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad S_i^+ = S_i^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Here $H_B$ is a zero matrix because the Heisenberg interaction (with $J = 1$)

$$S_i \cdot S_{i+1} = S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+), \quad (1)$$

involves two neighboring sites and our initial block contains only one site. $S_i^z, S_i^z$ are $S^z$ matrices at the right end of the left block, and at the left end of the right block, respectively. (Note, in the one site case, they are the same.) Note also that we do not store $S_i^-$ and $S_i^-$ matrices because they can be obtained by taking the Hermitian conjugate of $S_i^+$ and $S_i^+$, respectively.

The standard real-space RG procedure is summarized in Table 3. At the beginning of an iteration one forms the Hamiltonian matrix $H_{BB}$ for two blocks joined together. The joined block $BB$ has $m^2$ states labeled by two indices, $i_1 i_2$. The $m^2 \times m^2$ matrix $H_{BB}$ is given by

$$[H_{BB}]_{i_1,i_2,i_1',i_2'} = [H_B]_{i_1,i_1'} \delta_{i_2,i_2'} + \delta_{i_1,i_1'} [H_B]_{i_2,i_2'} + [H_{BB}^m]_{i_1,i_2,i_1',i_2'}. \quad (2)$$
For the Heisenberg interaction (1) the above $m^2 \times m^2$ interaction matrix $H_{BB}^{\text{int}}$ can be written as

$$[H_{BB}^{\text{int}}]_{i_1,i_2,i_1',i_2'} = [S^z_{i_1,i_1'}][S^z_{i_2,i_2'}] + \frac{1}{2}[S^+_r][S^-_r][S^z_{i_1,i_1'}][S^z_{i_2,i_2'}] + \frac{1}{2}[S^-_r][S^+_r][S^z_{i_1,i_1'}][S^z_{i_2,i_2'}],$$

(3)

where $r$ represents the right-most site of the left block, and $l$ the left-most site of the right block.

In diagonalizing $H_{BB}$ it is useful to separate the basis states by quantum numbers, since $H_{BB}$ is block diagonal. It is very simple to use $S_z$ in this way. Utilizing the total spin $S$ is more tedious. The value of $S$ for a state can easily be inferred by degeneracies for different values of $S_z$.

The lowest-lying eigenstates $u^\alpha_{i_1,i_2}, \alpha = 1, \ldots, m$, of $H_{BB}$ are the states used to describe $B'(BB \rightarrow B')$. The new block Hamiltonian matrix $H_{B'}$ is diagonal under this basis. However, in the more general case where the states kept, the $u^\alpha$, are not eigenstates of $H_{BB}$, we can write

$$H_{B'} = O H_{BB} O^\dagger,$$

(4)

where the $m \times m^2$ matrix $O$, the truncation matrix, is formed from the eigenstates $u^\alpha$:

$$[O]_{i_1,i_2} = u^i_{i_1,i_2},$$

(5)

i.e. the rows of $O$ are the states kept. If $O$ were square, this would be a unitary transformation. Since $O$ is not square, the transformation truncates away, or equivalently integrates out, the high-energy states.

In order to obtain end operators $S^z_i, S^\pm_r$, etc. for the new block $B'$, one must first construct the operators for the joined block $BB$, which we denote by $\tilde{S}^z_i, \tilde{S}^\pm_r$, etc. for example

$$[	ilde{S}^z_i]_{i_1,i_2,i_1',i_2'} = [S^z_i][S^z_{i_1,i_1'}][S^z_{i_2,i_2'}],$$

(6)

$$[	ilde{S}^\pm_i]_{i_1,i_2,i_1',i_2'} = \delta_{i_1,i_1'}[S^\pm_i][S^z_{i_2,i_2'}],$$

(7)

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and then use the truncating matrix $O$ again,

$$A = O\tilde{A}O^t.$$ \hspace{1cm} (8)

where $A$ stands for $S_x^2, S_y^2$, or $S_z^2$, etc.

**First Iteration**

Break the L-site chain into identical blocks $B_1$ and exactly diagonalize $B_1$.

$$B_1$$

**The $l$th Iteration ($l > 1$)**

- **Step 1.** Join two identical blocks.
  - \[ B_{l-1} \quad B_{l-1} \]
  - $B'_l$

- **Step 2.** Diagonalize $H_{B_{l-1} B_{l-1}}$ and use its $m$ lowest eigenvectors $u^\alpha$ to form the truncation matrix:
  - $O(\alpha; i_1, i_2) = u^\alpha (i_1, i_2)$

- **Step 3.** Truncate away unimportant degrees of freedom.
  - $B'_l = O B'_l O^+$

- **Step 4.** Goto Step 1. until L is large enough.

Fig. 8 A pictorial depiction of the standard real-space RG procedure.

After these new operator matrices are formed, we can replace $B$ by $B'$ and start the next iteration. The iteration is continued until the system is large enough to
represent the infinite system.

3.2 Superblock Approach and Density Matrix Projection

Although Wilson's momentum-space RG procedure achieved great success, its counterpart in real-space, the standard real-space RG procedure described above, turned out to be very unreliable. Except a few cases, it generally performs poorly. The two reasons for the failure of the standard real-space RG procedure are, as pointed out by White and Noack (1992), using isolated blocks $BB$ and choosing the eigenstates of $H_{BB}$ as the states kept. Since $H_{BB}$ contains no connections to the rest of the lattice, its eigenstates have inappropriate features at the block ends. Figure 9 illustrates the inconsistency in the groundstate wavefunction of two joined identical $B$ blocks, i.e. $\Psi_B \otimes \Psi_B$, and that of their fusion block $B' = BB$, i.e. $\Psi_{B'}$, for the particle-in-a-box problem. It can be seen that the groundstates of two identical $B$ blocks are a bad choice to describe the groundstate of the fusion block $B'$, since the latter is maximal at the node of the former.

Fig. 9 Illustration of the inconsistency in the groundstate wavefunctions of two isolated $B$ blocks and their fusion block $B' = BB$, i.e. $\Psi_B \otimes \Psi_B \neq \Psi_{B'}$.

To solve these two problems, White introduced the superblock approach and density matrix projection method (White 1992& 1993). In the superblock approach,
one diagonalizes a larger system called the *superblock* which includes the *system* we are interested in. The rest of the superblock is called the *environment*. The wavefunctions of the superblock are then projected onto the system block, and these projected states are the states kept for the system block. For a single-particle wavefunction, this projection is single-valued and trivial. However, for a many-particle wavefunction, the “projection” of a wavefunction onto the system block is many-valued, and in fact, a single many-particle state of the superblock generally “projects” onto a complete set of the system block states. However, some of these states are more important than others in investigating low-energy properties of the system: the density matrix tells us which states are the most important.

Here is a simple explanation. Let $|i\rangle$ be a complete set of many-body states of the system block, and $|j\rangle$ be that of the environment block. If $|\psi\rangle$ is a particular state of the superblock, probably the ground state, then

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle. \tag{9}$$

The reduced density matrix for the system block is then defined as

$$\rho_{\psi} = \sum_j \psi_{ij}^* \psi_{ij}. \tag{10}$$

If an operator $A$ acts only on the system block, its expectation value on the state $|\psi\rangle$ is given by

$$\langle A \rangle = \sum_{\alpha} w_{\alpha} \langle v_{\alpha}|A|v_{\alpha}\rangle. \tag{11}$$

where $w_{\alpha}$ are the eigenvalues of the reduced density matrix $\rho$ and $|v_{\alpha}\rangle$ are the corresponding eigenstates. Since $w_{\alpha} \geq 0$ and $\sum_{\alpha} w_{\alpha} = 1$, the $w_{\alpha}$ represents the probabilities of the states $|v_{\alpha}\rangle$ in the state $|\psi\rangle$ (Feynman 1972). This relation tells us that if for a particular $\alpha$, $w_{\alpha} \approx 0$, we make no error in $\langle A \rangle$ if we discard the state $|v_{\alpha}\rangle$, for any $A$; and we make no error in our ability to represent $|\psi\rangle$. Thus, the density matrix naturally gives a way to throw out states with minimal errors: throw
out the eigenstates of the density matrix with minimal eigenvalues; or equivalently, it tells us which states should be chosen as the states kept: choose the most probable eigenstates of the density matrix as the states kept to describe the system block. A more rigorous proof can be found in White's paper (1993).

3.3 DMRG Algorithms

In this section, we describe how to combine the superblock approach with the density matrix projection method in order to define efficient DMRG algorithms. There are three main ingredients needed to form a DMRG algorithm: first, we have to decide how to add degrees of freedom to the system, i.e. how to enlarge the system block; second, we have to determine the superblock configuration; or equivalently, we have to specify the form of the environment block; and finally, we must decide which superblock eigenstate or eigenstates to use to construct the density matrix.

Figure 10 shows the superblock configuration used in DMRG calculations. We adopt the notation $B_l \bullet B_R^R$ for this configuration, where $B_l$ represents a block composed of $l$ sites, $B_R$ is the reflected block of $B_l$, i.e. right interchanged with...
left, a solid circle • represents a single site, and the total length of the superblock is \( L = l + l' + 2 \).

For interacting systems, it is clear that one wants to add the minimum number of degrees of freedom to the system block at each step in order to keep as large a fraction of the system block states as possible, and to keep the size of the Hilbert space of the superblock as small as possible. Therefore, one usually build up the system block by adding a single site at a time, i.e. \( B_{t+1} = B_t \bullet \), instead of joining two identical blocks at each step as was used in the standard real-space RG procedure.

The algorithms then fall into two classes, depending on how the environment block is chosen to form the superblock: the infinite system algorithm where \( B_t^R \) is the reflection of \( B_t \), i.e. \( l' = l \); and the finite system algorithm where \( B_t^R \) is the reflection of some prestored \( B_t \) with \( l + l' + 2 = L \) (a fixed number). We will discuss these algorithms in detail in the following two subsections.

We will call the superblock state or states, used to form the reduced density matrix of the system block, the target state(s). If only ground state properties are desired, it is most accurate to target just the ground state of the superblock. (The superblock Hamiltonian matrix is usually block diagonal in particular quantum numbers, such as \( S_z \), the \( z \) component of the total spin; by ground state we will mean ground state for a particular quantum number.) If excited states or matrix elements between different states are required, more than one target can be used. However, for fixed number of states kept \( m \), the accuracy with which the properties of each individual state can be determined goes down as more states are targeted. For simplicity, we will assume that only the ground state is targeted in the following.
3.3.1 Infinite System DMRG Algorithm

In the infinite system algorithm, the environment block is formed by reflecting the system block, i.e. by relabeling the sites in the system block so that they are reflected onto the right part of the lattice as shown in Figure II.

Fig. II The superblock configuration for the infinite system DMRG algorithm in which block 4 is the mirror reflection of current block 1.

In the first iteration of the infinite system DMRG method, we start with a four site chain and diagonalize the Hamiltonian of the superblock configuration $B_1 \bullet B_1^R$, where $B_1$ and $B_1^R$ both represent a single site. Using the target state calculated with this configuration, we calculate a density matrix and form an effective Hamiltonian for $B_2 = B_1 \bullet$. In the second iteration we diagonalize $B_2 \bullet B_2^R$, where we have formed $B_2^R$ by reflecting $B_2$. We continue in this manner, diagonalizing the configuration $B_t \bullet B_t^R$, and setting $B_{t+1} = B_t \bullet$, and using $B_{t+1}$ and its reflection in the next iteration. At each iteration, we add one site to the system block and one site to the environment block; thus, the total length of the chain increases by two sites at each iteration. The infinite system DMRG algorithm is summarized in Table 4 and Figure 12.
The infinite-system DMRG algorithm is usually used when one is interested in ground state properties of the infinite chain. It converges in two senses simultaneously: in the length of $B_i$ going to infinity and in the sense that $B_i$ is adapted to respond to an infinite chain connected to it on the right.

Table 4 Infinite-system DMRG algorithm for a 1D lattice system

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1)</td>
<td>Set up matrices representing the block Hamiltonian and end operators for each of the initial four single-site blocks.</td>
</tr>
<tr>
<td>2)</td>
<td>Diagonalize the superblock Hamiltonian numerically using the Davidson or Lanczos method, obtaining only the ground state eigenvalue and eigenvector $\psi(i_1, i_2, i_3, i_4)$.</td>
</tr>
<tr>
<td>3)</td>
<td>Form the reduced density matrix $\rho$ for the system (block 1 + block 2) using formula (10).</td>
</tr>
<tr>
<td>4)</td>
<td>Diagonalize $\rho$ with a dense matrix diagonalization routine to find its $m$ largest eigenvalues $\omega_\alpha$ and eigenvectors $u_{i_1, i_2}^\alpha$.</td>
</tr>
<tr>
<td>5)</td>
<td>Form matrices representing the block Hamiltonian and end operators for the system from the block Hamiltonian and end operators of block 1 and block 2, using formula (2) and formulas similar to (6) and (7).</td>
</tr>
<tr>
<td>6)</td>
<td>Form a new block 1 by changing basis to the $u^\alpha$ using (4) and (8).</td>
</tr>
<tr>
<td>7)</td>
<td>Replace old block 4 with the reflection of new block 1.</td>
</tr>
<tr>
<td>8)</td>
<td>Go to step 2.</td>
</tr>
</tbody>
</table>
Initialization

Set up matrix representations for the initial four single-site block.

\[ B_1 \bullet \bullet \bullet B_1 \]

The \( i^{th} \) Iteration

Step 1. Diagonalize the superblock Hamiltonian,

\[ \begin{array}{c|c|c}
B_l & \bullet & B_l^R \\
\end{array} \]

obtaining only the ground state eigenvalue and eigenvector \( \psi(i_1,i_2,i_3,i_4) \).

Step 2. Form the reduced density matrix for the system block.

\[ \rho(i_1,i_2 ; i_1',i_2') = \sum_{i_3,i_4} \psi(i_1,i_2,i_3,i_4) \psi(i_1',i_2',i_3,i_4) \]

Step 3. Diagonalize \( \rho \) and keep its \( m \) largest eigenvalues \( \omega^\alpha \) & associated eigenvectors \( u^\alpha(i_1,i_2) \). Form the truncation matrix

\[ O(\alpha; i_1,i_2) = u^\alpha(i_1,i_2) \]

Step 4. Add a single site to block 1.

\[ \begin{array}{c|c|c}
B_l & \bullet \\
\end{array} \]

Step 5. Truncate away unimportant degrees of freedom.

\[ B_{l+1} = O B_{l+1}^R O^+ \]

Step 6. Reflect \( B_{l+1} \) to form a new block 4.

Step 7. Goto Step 1. until the size of the system is large enough.

Fig. 12 The DMRG infinite system interactions.
3.3.2 Finite System DMRG Algorithm

In the finite system algorithm, the environment block is chosen to be the reflection of some prestored block so that the size of the superblock is kept fixed at each iteration as shown in Figure 13.

![Diagram of superblock configuration for the finite system DMRG algorithm.]

Fig. 13 The superblock configuration for the finite system DMRG algorithm in which block 4 is the mirror reflection of some prestored block 1.

The finite system DMRG algorithm begins with the use of the infinite system algorithm for \( L/2 - 1 \) steps, so that the final superblock used is of size \( L \). In original infinite system algorithm, there is no need to store \( B_i \) once we have \( B_{i+1} \); we need to store only the latest block. In the finite system algorithm, however, we need to store \( L-3 \) blocks from \( B_1 \) to \( B_{L-3} \), and the infinite system method is used to get initial approximate versions of \( B_1 \) to \( B_{L/2} \). After the system \( B_{L/2-1} \bullet B_{L/2-1}^{R} \) is used to form \( B_{L/2} \), the next step is to use the configuration \( B_{L/2} \bullet B_{L/2-2}^{R} \) to form \( B_{L/2+1} \). This configuration, and all the other superblock configuration to follow, contains \( L \) sites. We continue to form the other blocks up to size \( L-3 \), using the the superblock \( B_i \bullet B_{L-1-2}^{R} \) to form \( B_{i+1} \). This sequence of steps is the first iteration of the finite system algorithm.
The second and subsequent iterations use the blocks obtained from the previous iteration as the right-hand reflected in each superblock. The first step starts by diagonalizing the superblock $B_1 \bullet B_{L-3}^R$, where $B_1$ is a single site and is always know exactly, and $B_{L-3}^R$ is obtained form the last step of the previous iteration. Once a new $B_1$ is formed, it replace the old $B_1$, so that only one set of blocks need be stored. Consequently, for the second-half of the iteration, starting with the superblock $B_{L/2-1} \bullet B_{L/2-1}^R$, we use a block formed in the current iteration, rather than the last iteration, as the right-hand block. On the very last iteration, we usually stop after the diagonalization of $B_{L/2-1} \bullet B_{L/2-1}^R$, and then use this wave function of the $L$-site system to measure various properties, such as the local magnetization or correlation functions. After a few iterations each $B_1$ accurately represents an $l$-site block which is the left-hand $l$ sites of an $L$-site chain.

The finite system DMRG algorithm is summarized in Table 5 and Figure 14. The superblock contains $L$ sites. The calculation consists of several iterations, indexed by $I$, with each iteration consisting of $L-3$ steps, indexed by $l$, where $l$ is the size of the first block.

A useful analogy is to think of this procedure as being like running a zipper repeatedly from left to right and then right to left through a superblock that is always the same size. Each time the zipper changes direction, a new set of stored blocks is used as the environment block. In this way, the representations of the stored blocks are iteratively improved and the zipping can be repeated until convergence is reached.

For a given system size $L$, the finite system algorithm almost always gives substantially more accurate results than the infinite system algorithm, and is therefore usually preferred unless there is a specific reason to go to the thermodynamic limit.
Table 5 Finite system DMRG algorithm for a 1D lattice system.

1) (First-half of I=1.) Use the infinite system algorithm for \( L/2 - 1 \) steps to build up the lattice of \( L \) sites. At each iteration store the block Hamiltonian and end operator matrices for block 1. Label the blocks by their size, \( B_l, l = 1, \ldots, L/2 \).

2) (Start of second-half of I=1) Set \( l = L/2 \). Use \( B_l \) as block 1, and the reflection of \( B_{L-l-2} \) as block 4.

3) Steps 2)-6) of the infinite system DMRG algorithm.

4) Store the new block 1 as \( B_{l+1} \), replacing the old \( B_{l+1} \).

5) Replace block 4 with the reflection of \( B_{L-l-2} \), obtained from the first half of this iteration.

6) If \( l < L - 3 \), set \( l = l + 1 \) and go to step 3).

7) (Start of iteration \( l, l \geq 2 \)) Make four initial blocks. the first three consisting of a single site, and the fourth consisting of the reflection of \( B_{l-3} \) from the previous iteration. Set \( l = 1 \).

8) Steps 2)-6) of the infinite system DMRG algorithm.

9) Store the new block 1 as \( B_{l+1} \), replacing the old \( B_{l+1} \).

10) Replace block 4 with the reflection of \( B_{L-l-2} \), obtained from the previous iteration (if \( l \leq L/2 - 1 \)) or the first half of current iteration (if \( l > L/2 - 1 \)).

11) If \( l < L - 3 \), set \( l = l + 1 \) and go to step 8). If \( l = L - 3 \), start a new iteration by going to step 7). (Stop after 2 or 3 iterations)
Fig. 14 The superblock configuration of the DMRG finite system algorithm in which block 4 is the mirror reflection of some prestored block 1 such that the superblock has a fixed length $L$. 

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Spin-1/2 AF Heisenberg ladders have been the subject of intense theoretical and experimental research in recent years. It is by now well established that the energy spectrum of an even-leg spin ladder has a finite gap, while that of an odd-leg spin ladder is gapless (White 1994, and Greven et al. 1996). This even-odd scenario sounds similar to the integer and half integer scenario of AF Heisenberg chains (Haldane 1983), but what is the difference between a spin ladder and a related spin chain, say a two-leg spin ladder and a spin-1 chain? After introducing a AF diagonal coupling $J_x$, Wang (1998) obtained a phase diagram characterized by two fixed points: (i) the “Haldane phase”, so named as it contains the limiting case $J_x = 1$ and $J_\perp = 0$, whose low-energy spectrum is identical to that of a spin-1 chain: (ii) the “singlet phase”, as it contains the case $J_\perp \gg 1$, in which the ground state consists a singlet on each rung and low-lying excitations is generated by creating triplets on rungs. In both cases, the system is gapped. However, a phase transition occurs in the parameter space as we cross from (i) to (ii). This distinguishes the two-leg ladder from the spin-1 chain whose low-energy spectra is sensitive to boundary conditions or impurity as can be observed by experiments (DiTusa 1994).

The above mentioned even-odd scenario is basically for isolated regular ladders. Whether a regular ladder is sufficient for the description of real world ladder materials, or equivalently, whether we need to include other coupling terms, is a problem
still under investigation. The problem has been readdressed by recent experimental
(Imai et al. 1999) and theoretical (Neaf and Wang 2000) NMR data, because the
NMR rate at finite temperature shows its sensitivity to local properties of materials.
On contrary, the low-temperature behavior of the spin susceptibility depends on the
value of the gap. In this regard, one may expect that the diagonal interaction $J_x$
induces non-negligible effects for the NMR rate rather than for the spin susceptibil­
ity up to intermediate temperature. According to Johnston et al. (Johnston 2000),
one should have $J_x < 0$, i.e. FM coupling, to describe materials SrCu$_2$O$_3$ and
La$_6$Ca$_8$Cu$_{24}$O$_{41}$. Up to date, the AF case $J_x > 0$ has been studied in great detail
2000). One of interesting results indicates that the spin gap might be insensitive
to some positive values of $J_x$ when $J_\perp = 1$. (Wang 1998). Concerning the ladder
materials interested in experiments, we needs to know whether and how the spin
gap depends on a FM diagonal interaction $J_x$ for $J_\perp = 0.5$.

In this chapter, we study a spin-1/2 two-leg AF Heisenberg ladder with FM diag­
onal couplings. By calculating spin gaps with respect to various coupling constants
for the system, we try to find out how the spin gap of an isolated two-leg AF Heisen­
berg ladder is affected by FM diagonal couplings. One motivation for studying such
a system comes from theoretical needs, such as fitting quantum Monte Carlo (QMC)
simulation data of magnetic susceptibilities $\chi(T)$ (Johnston 2000) or answering the
problem whether frustration can lead to some behavior not encountered by the above
“even-odd” scenarios. Another motivation comes from experimental hope that FM
diagonal interactions may exist in real two-leg ladder materials.
4.1 Model and Method

The spin-1/2 two-leg AF Heisenberg ladder with FM diagonal couplings is described by the Hamiltonian

\[ H = \sum_i [J_{||}(S_{1,i} \cdot S_{1,i+1} + S_{2,i} \cdot S_{2,i+1}) + J_\perp S_{1,i} \cdot S_{2,i} 
+ J_x (S_{1,i} \cdot S_{2,i+1} + S_{2,i} \cdot S_{1,i-1})] \tag{1} \]

where \( S_{n,i} \) denotes the spin-1/2 operator at site \( i \) of leg \( n \) (\( n=1,2 \)). \( J_{||} \) is the intrachain coupling between two neighboring spins in each chain, \( J_\perp \) the interchain coupling between two spins on each rung, and \( J_x \) the interchain coupling between two spins on the diagonal of a plaquette.

In the following discussion, we set \( J_{||} = 1, \ J_x < 0 \) and \( J_\perp > 0 \) or \( < 0 \). The system becomes frustrated only when \( J_\perp < 0 \) as shown in Section 2.3. We also note that the Hamiltonian is unchanged by exchanging \( J_x \) and \( -J_{||} \) and thus we only consider the case of \(-1 \leq J_x \leq 0\).

Numerical calculations in this paper were carried out using density matrix renormalization group (DMRG) method (White 1992 & 1993) which is very powerful and efficient for a systematic study of low-lying energy properties of low-dimensional lattice models. In our calculations, we typically keep 300 states and truncation error is about of the order of \( 10^{-8} \). Lengths up to 300 rungs are considered for open boundary conditions and finite size scaling is used to determine those quantities for the thermodynamic limit. For convenience, the number of rungs \( N \) is chosen to be even. The relative errors on physical quantities are estimated to be less than one percent in most cases.
4.2 Ground State Phase Diagram for FM Diagonal Couplings

To find the ground state phase diagram, we calculated the ground state energy per rung (GSEPR) for various combinations of the coupling constants $J_x$ and $J_\perp$. As shown in Figure 15, each GSEPR curve has a maximum.

Fig. 15 The ground state energy per rung for frustrated spin-1/2 two-leg Heisenberg ladders.

Plotting the $(J_x, J_\perp)$ pairs of these maximums in the $J_x$-$J_\perp$ plane, we obtained the ground state phase diagram for the FM diagonal interaction $J_x$. From the phase diagram, we found (1) When $J_\perp > 0$, i.e. the rung coupling is AF, there exists only one phase, the singlet phase, for all $J_x$ values between -1.0 and 0.0. When the rung coupling becomes FM, i.e. $J_\perp < 0$, frustration appears; if $|J_\perp|$ is large enough, the
system may get into the Haldane phase, in which the ground state is degenerated with the total spin $S^z = 0, 1$ for open boundary condition or is the singlet state for the periodic boundary.

Fig. 16 Ground state phase diagram for a two-leg Heisenberg ladder with FM diagonal couplings. The solid line indicates the phase boundary.

condition. (2) It is interesting to note that the phase boundary is a straight line $J_\perp = 2J_x$. Furthermore, this line is actually the extension of Wang's non-gaped line for $0 < J_x \leq 0.287$ and $J_\perp > 0$ (Wang 1998). (3) As it is illustrated for the ground state energy below, the quantum phase transition between these two phases is of second order. (4) We also notice that there is no regions in the parameter space where the midgap states occur in the Haldane phase or the first excitation state has $S^z = 0$ in the singlet phase. This is a difference for low-energy properties between
FM and AF diagonal interactions.

Apart from the sensitivity to the boundary conditions and impurity effects, the singlet phase and the Haldane phase can be further characterized by the singlet density for each rung. Under a given state $|\Psi\rangle$, one has the singlet density

$$\rho_s = \frac{1}{N} \sum_i \langle \Psi | S_i S_i^\dagger | \Psi \rangle.$$  \hspace{1cm} (2)

where

$$S_i = \frac{1}{\sqrt{2}} (|\alpha_1 \beta_2\rangle_i - |\beta_1 \alpha_2\rangle_i)$$ \hspace{1cm} (3)

is the singlet state formed by two spins on the $i$th rung. When $J_\perp = J_\parallel = 0$, one has $\rho_s = \frac{1}{4}$, while $\rho_s < \frac{1}{4}$ in the Haldane phase, and $\rho_s > \frac{1}{4}$ in the singlet phase. The results for the singlet density at $J_\parallel = -0.2$ and $-0.8$ are explicitly shown in Figures 17 and 18, together with corresponding GSEPR, denoted as $e_0$. One can see that $\rho_s$ changes continuously with respect to $J_\parallel$. On contrary, it changes abruptly for $J_\parallel > 0.287$ and $J_\perp > 0$ case (Wang 1998), indicating the first order transition there.
Fig. 17 The ground state energy (per rung) and the singlet density vs the rung coupling constant for the case of $J_x=-0.2$.

Fig. 18 The ground state energy (per rung) and the singlet density vs the rung coupling constant for the case of $J_x=-0.8$. 

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4.3 Effect of Diagonal Coupling on the Spin Gap

In this section we study the effect of the diagonal interaction on the spin gap. As relevant to real world materials Sr$_2$Cu$_3$O$_4$ and La$_6$Ca$_8$Cu$_{24}$O$_{41}$, we focus on the case of $J_\perp = 0.5$ and 1, respectively. Our DMRG results are shown in Figure 19.

The spin gap $\Delta$ for the singlet phase is given by $\Delta = E(S_z^s = 1) - E(S_z^s = 0)$, while for the Haldane phase it is defined as $\Delta = E(S_z^s = 2) - E(S_z^s = 1)$. As seen in Figure 19, for the case of $J_\perp = 0.5$, when $J_x \leq 0.28 \pm 0.01$, we has the singlet phase; otherwise, we has the Haldane phase. For the case of $J_\perp = 1$, the singlet phase appears when $J_x \leq 0.595 \pm 0.005$: otherwise the Haldane phase appears. Remarkably, the spin gap has maximum at $J_x \approx 0.25$ and -0.25 for $J_\perp = 1$ and 0.5, respectively, in the singlet phase; while it is a monotonical function of $J_x$ in the

Fig. 19 Spin gap $\Delta$ vs diagonal coupling constant $J_x$ for the case of $J_\perp = 0.5$ and $J_\perp = 1$, respectively. For each case, the left part corresponds to the singlet phase and the right to the Haldane phase.
Haldane phase. Moreover, we can see that the changes in the spin gap is very small within the range $0 \leq J_x \leq 0.4$ for $J_\perp = 1$ and $-1 \leq J_x \leq 0.0$ for $J_\perp = 0.5$. The latter case is particularly interesting for materials Sr$_1$Cu$_3$O$_4$ and La$_6$Ca$_4$Cu$_{24}$O$_{41}$.

Recently, Johnston's group has systematically investigated the fitting of their spin susceptibility calculations with the experimental data (Johnston 2000). They found that best fitting corresponds to $J_\perp \approx 0.5$ and the fitting is insensitive to the diagonal interaction $J_x$. In fact, for Sr$_1$Cu$_3$O$_4$ and La$_6$Ca$_4$Cu$_{24}$O$_{41}$, $J|| \approx 1900 K$, so the experimental data displays only low energy behavior of the spin susceptibility, which relies crucially on the value of the spin gap. Our results for the spin gap at $J_\perp = 0.5$ support this insensitivity to a FM $J_x$. On the other hand, the appearance of $J_x$ can more substantially change behaviors of other quantities such as NMR rate. Therefore, as Johnston et al. pointed out, much work remain to be done to establish a spin Hamiltonian for a self-consistent description of the spin susceptibility. NMR, and other experimental measurements probing the magnetism of the cuprate spin ladder materials.

4.4 Summary

To conclude, we have studied the low-energy properties of a two-leg AF Heisenberg ladder with FM diagonal couplings. Combining with Wang's results (Wang 1998), we found that the Haldane phase can be induced by sufficient strong diagonal interactions and the spin gap in the singlet phase is insensitive to the changes of FM diagonal coupling strength at least for the rung coupling strength related to cuprate ladder materials, i.e. $J_\perp = 0.5$
CHAPTER 5

GROUND STATE PHASE DIAGRAM OF A FRUSTRATED
SPIN-1/2 THREE-LEG HEISENBERG LADDER

The spin-1/2 three-leg AF Heisenberg ladder is the simplest odd-leg ladder system. A typical experimental realization is the strontium cuprate ladder compound Sr$_2$Cu$_3$O$_5$ (Takano et al. 1992). For “regular” spin-1/2 odd-leg AF Heisenberg ladders, extensive theoretical and experimental investigations give us a picture similar to that of half-integer Heisenberg chains, namely gapless spin excitations and a power-law falloff of the spin-spin correlation functions; but for their “frustrated” counterparts, no such consensus is established yet. In the 1D $J_1 - J_2$ model, the frustration caused by the nn coupling $J_1$ and the nnn coupling $J_2$ can lead to a dimerized ground state, as exemplified by the exactly soluble 1D Majumdar-Ghosh model (Majumdar and Ghosh 1969). In the 2D $J_1 - J_2$ model, the frustration caused by the competition of $J_1$ and $J_2$ may lead to the disappearance of the Néel’s order (Chandra and Doucôt 1988). Thus, a natural question is that what will be the effects of frustrations on spin ladders, the crossover systems between 1D and 2D.

The goal of this chapter is to study the ground-state properties of a spin-1/2 three-leg AF Heisenberg ladder with diagonal couplings. In Section 5.1 we introduce the Hamiltonian of the system and briefly describe the numerical method used in this chapter. Section 5.2 collects our DMRG results of the ground state energies (per rung) for various combinations of the coupling constants. Section 5.3 describes the two ground states found through numerical calculations, and gives the ground
state phase diagram of the system. Section 5.4 discusses the effects of frustration on the three-leg system. Finally, Section 5.5 provides a brief summary of our results.

5.1 Model and Method

The frustrated spin-1/2 three-leg AF Heisenberg ladder is described by the following Hamiltonian

\[
H = \sum_{i} \left\{ J_{||}(S_{1,i} \cdot S_{1,i+1} + S_{2,i} \cdot S_{2,i+1} + S_{3,i} \cdot S_{3,i+1}) + J_{\perp}(S_{1,i} + S_{3,i}) \cdot S_{2,i} + J_{x}(S_{1,i} + S_{3,i}) \cdot S_{2,i+1} + S_{2,i} \cdot (S_{1,i+1} + S_{3,i+1}) \right\},
\]

where \( S_{n,i} \) is the spin-1/2 operator on the \( n \)th leg and at the \( i \)th rung (\( n=1,2,3 \) and \( i=1,2,3,\ldots \)). \( J_{||} \) and \( J_{\perp} \) are the usual "leg" and "rung" coupling constants, respectively; \( J_{x} \) is the diagonal coupling constant responsible for the frustration. The labeling conventions of legs, rungs, and sites used in this chapter are shown in Figure 20.

Fig. 20 Labeling conventions for legs, rungs, and sites used in this chapter. Solid lines represent intrachain couplings between two \( n \) spins in each chain, long-dashed lines stand for interchain couplings between two spins on the same rung, and dotted lines describe interchain couplings between two \( nnn \) spins on the diagonal of a plaquette.

Since there is no general analytical method to solve many-body problems of a
strongly interacting lattice system, we have to resort to numerical methods. Three best known numerical methods for studying quantum lattice models are the exact diagonalization method (Dagotto 1994), the quantum Monte Carlo (QMC) method (von der Linden 1992), and the density matrix renormalization group (DMRG) method (White 1992 & 1993). We will use the DMRG method in this project because the exact diagonalization method can treat only very short ladders, while the QMC method suffers from the sign problem in dealing with frustration couplings.

The DMRG method is a real-space renormalization procedure where a quasi-1D lattice system is built up gradually to the desired length \( L \) and in the meantime by keeping only \( m \) most probable states of a reduced density matrix the truncated Hilbert space of the system is kept treatable numerically. In all the calculations of this chapter, we choose \( m=250 \) and \( L=200 \). The ground-state and the first-excited-state energies, as well as expectation values of some projectors, are first calculated to a finite ladder length \( L \) by the DMRG finite system algorithm and then extrapolated to their thermodynamic limits by the following formula

\[
Q(L) = Q(\infty) + a_1 L^{-1} + a_2 L^{-2} + \ldots.
\]  

Here \( Q \) can be the ground-state energy per rung (GSEPR), the spin gap \( \Delta \), or the density of state \( \langle P \rangle \) of some projector \( P \).

### 5.2 Ground State Energy Per Rung

Again, to find the ground state phase diagram, we calculated the ground state energies for various combinations of \( J_x \) and \( J_\perp \). Figure 21 summarizes our DMRG results for the ground state energy per rung (GSEPR). For each GSEPR curve where \( J_x > 0 \), there is a maximum point at which the derivative of GSEPR with respect to the rung coupling constant \( J_\perp \) equals zero. These points are the transition points
of quantum phase transitions at the corresponding diagonal coupling strengths as discussed in the next section. Table 6 lists the transition points corresponding to $J_x = 0.2, 0.4, 0.6, 0.8,$ and $1.0,$ respectively.

Fig. 21 The ground state energy per rung (GSEPR) vs the rung coupling constant $J_\perp$ at various diagonal coupling strengths for the frustrated spin-1/2 three-leg AF Heisenberg ladders.

The details of the extrapolated GSEPR and corresponding extrapolation coefficients are given in Appendix A for possible need of references. Using formula (2), we can reproduce the ground state energy for a frustrate spin-1/2 AF Heisenberg ladder of any finite length $L$. 

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Table 6 Transition points

<table>
<thead>
<tr>
<th>$J_x$</th>
<th>$J_\perp$</th>
<th>GSEPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.375</td>
<td>-1.333475526359312</td>
</tr>
<tr>
<td>0.4</td>
<td>0.715</td>
<td>-1.351166290104413</td>
</tr>
<tr>
<td>0.6</td>
<td>1.000</td>
<td>-1.391655207596632</td>
</tr>
<tr>
<td>0.8</td>
<td>1.220</td>
<td>-1.471094477409377</td>
</tr>
<tr>
<td>1.0</td>
<td>1.430</td>
<td>-1.647577768017481</td>
</tr>
</tbody>
</table>

5.3 Ground State Phase Diagram

Plotting the $J_x - J_\perp$ data pairs in Table 6, we obtained the following ground state phase diagram for the frustrated spin-1/2 three-leg AF Heisenberg ladders. Since both phase A and phase B are the ground states of the system, the phase transition between phase A and phase B should be a quantum phase transition.

![Phase Diagram](image)

Fig. 22 Ground state phase diagram of the frustrated spin-1/2 three-leg AF Heisenberg ladder.

In order to find out the difference of the two phases, we define the following six "probe" projectors:
(1) Rung quartet projector

\[ P_1 = |S_{123} = 3/2, S_{13} = 1 \rangle \langle S_{123} = 3/2, S_{13} = 1 | \]

where

\[ |S_{123} = 3/2, S_{13} = 1 \rangle = \left\{ \begin{array}{l}
\frac{1}{\sqrt{3}}(\alpha_1 \alpha_2 \alpha_3 + \beta_1 \alpha_2 \alpha_3 + \alpha_1 \beta_2 \alpha_3) \\
\frac{1}{\sqrt{3}}(\alpha_1 \beta_2 \beta_3 + \beta_1 \beta_2 \alpha_3 + \beta_1 \alpha_2 \beta_3) \\
\beta_1 \beta_2 \beta_3
\end{array} \right. \]

(2) Rung symmetric doublet projector

\[ H_2 = |S_{123} = 1/2, S_{13} = 1 \rangle \langle S_{123} = 1/2, S_{13} = 1 | \]

where

\[ |S_{123} = 1/2, S_{13} = 1 \rangle = \left\{ \begin{array}{l}
\frac{1}{\sqrt{3}}(2\alpha_1 \beta_2 \alpha_3 - \alpha_1 \alpha_2 \beta_3 - \beta_1 \alpha_2 \alpha_3) \\
\frac{1}{\sqrt{3}}(\alpha_1 \beta_2 \beta_3 + \beta_1 \beta_2 \alpha_3 - 2\beta_1 \alpha_2 \beta_3)
\end{array} \right. \]

(3) Rung antisymmetric doublet projector

\[ H_3 = |S_{123} = 1/2, S_{13} = 0 \rangle \langle S_{123} = 1/2, S_{13} = 0 | \]

where

\[ |S_{123} = 1/2, S_{13} = 0 \rangle = \left\{ \begin{array}{l}
\frac{1}{\sqrt{3}}(\alpha_1 \alpha_2 \beta_3 - \beta_1 \alpha_2 \alpha_3) \\
\frac{1}{\sqrt{2}}(\alpha_1 \beta_2 \beta_3 - \beta_1 \beta_2 \alpha_3)
\end{array} \right. \]

(4) Edge dimer projector

\[ H_4 = |S_{14} = 0 \rangle \langle S_{14} = 0 | \]

where

\[ |S_{14} = 0 \rangle = \frac{1}{\sqrt{2}}(\alpha_1 \beta_4 - \beta_1 \alpha_4) \]

(5) Centre dimer projector

\[ H_5 = |S_{25} = 0 \rangle \langle S_{25} = 0 | \]

where

\[ |S_{25} = 0 \rangle = \frac{1}{\sqrt{2}}(\alpha_2 \beta_5 - \beta_2 \alpha_3) \]

(6) Diagonal dimer projector

\[ H_6 = |S_{15} = 0, S_{24} = 0 \rangle \langle S_{15} = 0, S_{24} = 0 | \]

where

\[ |S_{15} = 0, S_{24} = 0 \rangle = \frac{1}{\sqrt{2}}(\alpha_1 \beta_5 - \beta_1 \alpha_5) \frac{1}{\sqrt{2}}(\alpha_2 \beta_4 - \beta_2 \alpha_4) \]
Note that, in the above expressions, \( S_{ij} = S_i + S_j \), \( S_{ij}^2 = S_{ij}(S_{ij} + 1)\hbar^2 \), \( S_{ijk} = S_i + S_j + S_k \), and \( S_{ijk}^2 = S_{ijk}(S_{ijk} + 1)\hbar^2 \); and the "symmetric" and "antisymmetric" are referred to the exchange of spins at site 1 and 3.

In order to find out the statistical weight for a particular spin state defined above, we can calculate its spin-state density defined below

\[
\langle P_i \rangle = \frac{1}{N} \sum_j \langle 0 | P_i(j) | 0 \rangle, \quad i = 1, 2, \ldots, 6
\]

where \( |0\rangle \) is the ground state of the system, \( P_i \) is one of the six projectors, and \( j \) runs over all rungs in the system.

Figure 23 plots the six spin-state densities versus the rung coupling constant \( J_\perp \) for \( J_x = 1.0 \) case. All six graphs show discontinuities at \( J_\perp = 1.43 \), the position at which the corresponding GSEPR reaches its maximum. For all other \( J_x > 0 \) cases, i.e., Figures 24 ~ 27, we have similar plots; but for \( J_x = 0 \) case, the Figure 28, no discontinuity appears in any one of the six plots.

On the left side of a transition point, the system is in the A phase: after crossing the transition point, the system becomes in the B phase. From the plots for \( \langle P_1 \rangle \) and \( \langle P_2 \rangle \), we see that phase A is predominantly in the rung quartet state \( |S_{123} = 3/2, S_{13} = 1\rangle \), while phase B is basically in the symmetric rung doublet state \( |S_{123} = 1/2, S_{13} = 1\rangle \). The other four expectation values are very small compared with \( \langle P_1 \rangle \) or \( \langle P_2 \rangle \). That means the statistical weights for the corresponding rung spin states to appear are very low. The difference between phase A and phase B is mainly the relative statistical weight of the rung quartet state and the rung symmetric doublet state. What have been changed in the phase transition is this relative statistical weight and the reason for the this change is the frustration caused by diagonal interactions.

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Fig. 23 Plots of the six spin-state densities versus the rung coupling constant $J_\perp$ for the $J_x=1.0$ case.
Fig. 24 Plots of the six spin-state densities versus the rung coupling constant $J_\perp$ for the $J_x=0.8$ case.
Fig. 25 Plots of the six spin-state densities versus the rung coupling constant $J_\perp$ for the $J_x=0.6$ case.
Fig. 26 Plots of the six spin-state densities versus the rung coupling constant $J_\perp$ for the $J_x=0.4$ case.
Fig. 27 Plots of the six spin-state densities versus the rung coupling constant $J_\perp$ for the $J_x=0.2$ case.
Fig. 28 Plots of the six spin-state densities versus the rung coupling constant $J_\perp$ for the $J_\parallel=0.0$ case.
5.4 Effect of the Diagonal Interaction

By plotting the same spin-state density for different diagonal coupling strengths, we can clearly see the effect of the diagonal interactions. Figures 29 is an example in the case of the rung quartet density. As we can see from Figures 29 that all

![Diagonal Interaction Diagrams](image)

Fig. 29 A comparison of the quartet densities \( P_1 \) for six different diagonal coupling strength 1.0, 0.8, 0.6, 0.4, 0.2 and 0.0.

five quartet densities for which \( J_x > 0 \) have discontinuities at their corresponding quantum phase transition points, while the quartet density for which \( J_x = 0 \) is continuous. At one side of the transition point we have a particular statistical weight for a rung spin state, at the other side the statistical weight has a drastic different value if \( J_x \) is large enough. Therefore it is the diagonal interaction \( J_x \).
which causes these changes in the internal spin symmetries and degeneracies.

The regular three-leg AF Heisenberg ladder does not have a spin gap in its excitation spectrum. To see whether frustration can introduce a spin gap, we calculated the spin gap $\Delta(L)$ for various coupling constant combinations and plot them versus the reciprocal of the ladder length $L$. The definition of the spin gap $\Delta(L)$ is

$$\Delta(L) = E_0(L,1) - E_0(L,0).$$

Here $E_0(L,S_z)$ is the ground state energy of the system containing $L$ rungs under open boundary condition and $z$ component of total spin $S_z$. A typical plot where $J_1=2.0$ and $J_x=0.0, 0.2, 0.4, 0.6, 0.8$ and $1.0$ is shown below.

As we can see that there is no spin gap opened for any strength of diagonal couplings considered in our calculations. The fitting of our DMRG data by the formula (2) gives $\Delta=0.0$ for all the coupling constant combinations. Our results confirms the results of exact diagonalization on much smaller ladder length.

5.5 Summary

From our systematic DMRG calculations for the ground-state and the first-excited-state energies of the frustrated spin-1/2 three-leg antiferromagnetic Heisenberg ladders, we found that the frustration caused by the diagonal interactions can create new ground-state, the rung quartet state, for the system and changing the diagonal coupling strength will lead to a quantum phase transition between these two ground states. Nevertheless, changing the diagonal coupling strength will not change the gapless structure of the excitation spectrum of the system in the thermodynamic limit.
Fig. 30 Spin gap $\Delta(L)$ vs the reciprocal of the ladder length $1/L$ for the case of $J_\perp=2.0$ and $J_x=0.0, 0.2, 0.4, 0.6, 0.8$ and 1.0.
CHAPTER 6
CONCLUSIONS

In this project, we have studied the ground state properties of frustrated spin-1/2 two-leg and three-leg antiferromagnetic Heisenberg ladders. The aim of this project is to investigate the effects of diagonal interactions on the ground state phase diagrams and on the spin gap structures of the systems. In the two-leg case, we assume a ferromagnetic diagonal coupling, while in the three-leg case an antiferromagnetic diagonal coupling. Through extensive DMRG calculations, we found the ground state and the first excited state energies for these two systems. Using these numerical solutions, we obtained the ground state phase diagrams for these systems, and found some relations among the spin gap and the diagonal coupling constants. We found

(1) Frustrations caused by the diagonal interaction can introduce new phase to the ground state. In the two-leg case, ferromagnetic diagonal coupling produces a Haldane phase and a singlet phase as antiferromagnetic diagonal coupling can do, but the phase diagrams are different. In the three-leg case, the diagonal coupling produces a quartet ground state and a symmetric doublet state. Here the effect of frustration is to change the internal symmetry of the system and to cause quantum phase transitions between different ground states.

(2) The spin gap of the two-leg ladder do vary with the diagonal coupling strength, but for ferromagnetic couplings the changes in spin gap is very small compared with that of antiferromagnetic couplings. For the three-leg ladder, no spin
gap was opened for the whole range of the diagonal coupling strength considered.

Our numerical calculations can not answer why ferromagnetic diagonal couplings can lead to different results compared with antiferromagnetic diagonal couplings. As an unbiased numerical experiment, our results can contribute to the understanding of the effect of frustration on spin ladder systems.
APPENDIX A

GSEPR FOR SPIN-1/2 THREE-LEG AF HEISENBERG LADDERS

This appendix collects the extrapolated GSEPRs (Ground-State Energy Per Rung) of our DMRG calculations for spin-1/2 three-leg AF Heisenberg ladders, together with their corresponding extrapolating coefficients $a_1, a_2, \ldots, a_6$. Using these data and the following finite size scaling formula

$$GSEPR(L) = GSEPR(\infty) + \frac{a_1}{L^1} + \frac{a_2}{L^2} + \frac{a_3}{L^3} + \cdots + \frac{a_6}{L^6},$$

we can reproduce the ground-state energy (per rung) for the system of any finite length $L$. 

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Table 7 GSEPR(∞) and corresponding extrapolating coefficients for $J_\perp=0.0$ case

<table>
<thead>
<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
<td>$a_6$</td>
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Table 8 GSEPR(∞) and corresponding extrapolating coefficients for Jx=0.2 case

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<tr>
<td>a1</td>
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<td>0.562436492253709</td>
</tr>
<tr>
<td>a2</td>
<td>0.274804321816191</td>
<td>0.094244203821290</td>
<td>1.005036987655330</td>
</tr>
<tr>
<td>a3</td>
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<td>-87.25785870477557</td>
</tr>
<tr>
<td>a4</td>
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<td>-323.8362910151482</td>
<td>1799.730207967818</td>
</tr>
<tr>
<td>a5</td>
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<td>3685.625245571136</td>
<td>-14507.25154256821</td>
</tr>
<tr>
<td>a6</td>
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<td>-9583.482393668591</td>
<td>34452.23122882843</td>
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</tr>
<tr>
<td>a1</td>
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<tr>
<td>a2</td>
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</tr>
<tr>
<td>a3</td>
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<td>-3.253614455461502</td>
<td>-2.355269614607096</td>
</tr>
<tr>
<td>a4</td>
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<td>-3.748877525329500</td>
<td>47.45707714557648</td>
</tr>
<tr>
<td>a5</td>
<td>2427.106978893280</td>
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</tr>
<tr>
<td>a6</td>
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</tr>
<tr>
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<tr>
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<tr>
<td>a1</td>
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<td>-0.205358654260635</td>
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<td>a3</td>
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<td>201.7505912780762</td>
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Table 9 GSEPR(∞) and corresponding extrapolating coefficients for $J_x = 0.4$ case

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<th>$J_\perp = 0.7$</th>
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<td>GSEPR(∞)</td>
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<td>$a_1$</td>
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<td>0.996671995206693</td>
<td>0.564133221234897</td>
</tr>
<tr>
<td>$a_2$</td>
<td>0.315258801216259</td>
<td>0.260905999399256</td>
<td>-0.58366925838012</td>
</tr>
<tr>
<td>$a_3$</td>
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</tr>
<tr>
<td>$a_4$</td>
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<td>80.22155201435089</td>
<td>-4896.171247839928</td>
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<tr>
<td>$a_5$</td>
<td>-2314.795143127441</td>
<td>-294.4819736480713</td>
<td>-14363.09709692001</td>
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<tr>
<td>$a_6$</td>
<td>5130.936068534851</td>
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<table>
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<th>$J_\perp = 1.2$</th>
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<td>-1.651601225695295</td>
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<tr>
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<tr>
<td>$a_2$</td>
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<td>0.112451550434343</td>
<td>-0.50764258950948</td>
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<tr>
<td>$a_3$</td>
<td>1.211192928254604</td>
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<td>-2.951289907097816</td>
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<td>104.4814241528511</td>
<td>57.61979347467422</td>
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<td>-450.0765562057495</td>
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<tr>
<td>$a_6$</td>
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<td>1549.665646553040</td>
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Table 10 GSEPR(∞) and corresponding extrapolating coefficients for $J_x$=0.6 case

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<tr>
<td>$a_1$</td>
<td>1.404161704221599</td>
<td>1.358488435614163</td>
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<tr>
<td>$a_2$</td>
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<td>0.261746920994482</td>
</tr>
<tr>
<td>$a_3$</td>
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<td>-18.09756449237466</td>
</tr>
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<td>356.8551985025406</td>
<td>169.8781157732010</td>
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<tr>
<td>$a_5$</td>
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<tr>
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<td>$a_1$</td>
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<tr>
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<td>-0.017442711163312</td>
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<tr>
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Table 11 GSEPR(\(\infty\)) and corresponing extrapolating coefficients for \(J_x=0.8\) case

<table>
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<th>(J_x=0.8)</th>
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<th>(J_\perp = 1.0)</th>
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<td>GSEPR((\infty))</td>
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<tr>
<td>(a_1)</td>
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<tr>
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<td>0.192717722384259</td>
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<td>-0.032695283531211</td>
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<td>-5.002000663429499</td>
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<td>(a_3)</td>
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<th>(J_\perp = 2.0)</th>
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<tbody>
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<td>(a_3)</td>
<td>-2.236139774322510</td>
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<td>(a_4)</td>
<td>42.74022996425629</td>
<td>10.54169809818268</td>
</tr>
<tr>
<td>(a_5)</td>
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</tr>
<tr>
<td>(a_6)</td>
<td>769.6185369415777</td>
<td>200.8307914733887</td>
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</table>
Table 12 GSEPR(∞) and corresponding extrapolating coefficients for \( J_x = 1.0 \)

<table>
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<th>( J_x =1.0 )</th>
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<th>( J_\perp =1.0 )</th>
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<td>( J_\perp =1.4 )</td>
<td>( J_\perp =1.6 )</td>
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</tr>
<tr>
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</tr>
<tr>
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<tr>
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<td>0.193430059822276</td>
</tr>
<tr>
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<td>-18.64130239188671</td>
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\( J_\perp =2.0 \)

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BIBLIOGRAPHY


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