Studies on Frustrated Spin Models and Superconductivity in Strongly Correlated Electronic Systems

A Thesis Submitted for
the Degree of Doctor of Philosophy
in the Faculty of Science
by

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To

my respected teachers
I hereby declare that the work reported in this thesis is entirely original, and has been carried out by me independently in the Department of Physics, Indian Institute of Science, Bangalore, under the supervision of Professor B. Sriram Shastry. I further declare that this work has not formed the basis for the award of any degree, diploma, fellowship, associateship or similar title of any University or Institution.

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Acknowledgment

It is not so much of an acknowledgment. Rather, it is an expression of an experience. A confession of the fact that I owe a great deal to the place and the people who supported me, and cared for me for all these years that I have spent as a graduate student at the Indian Institute of Science; that the life here has been an enlightening experience; that this place means very special to me.

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Chapter 1

Introduction

The nature of the problems, whose studies constitute the present thesis, and their physical settings are briefly described. A summary of the main results is presented.

The physics of interacting many particle systems offers a wide range of challenging problems. The nature of a problem and its solution, in general, depends upon the nature of the constituent particles and interaction among them. In real life, every problem is a many body problem, be it within the domains of the natural sciences or otherwise. Our interest here is, of course, in the rich variety of interesting phenomena observed in the condensed matter laboratories, and in the questions raised thereby. The fact that each constituent strongly influences other constituents, and the number of constituents in a given system is infinitely large, gives rise to new states of matter which otherwise would not have existed. In short, ‘More is Different’ is the basic theme of the condensed matter physics which brings excitement in pursuing the many body problems, despite the fact that they are usually very difficult [1].

The strongly correlated electronic systems form an important area of the condensed matter research. The physical systems where electron-electron interaction is strong enough to bring about drastic changes in the electronic properties, in comparison to the Landau’s Fermi liquid description, come under this category. The most exciting example of this class of materials is the family of cuprate superconductors. These are more familiarly known as the high temperature superconductors because of the higher values of their superconducting transition temperatures. The questions related to the mechanism of superconductivity in cuprates and many unusual phenomena in their normal state, are still very puzzling [2]. The rare-earth manganese oxides and their divalent doped vari-
ants form another interesting class of materials with extremely rich phase diagram in the temperature-doping plane [3]. Among the large variety of materials which come under the heading of strongly correlated systems, a large portion consists of the transition metal oxides. The categorization, however, is purely phenomenological, as one can not \textit{a priori} be sure of whether a certain system is necessarily of this type or not.

An important aspect of the physics of real materials is the nature of their magnetic properties. The magnetism is an ancient subject which still continues to fascinate us. The frustrated quantum antiferromagnets form an exciting research area of current interest. On one hand, the advancements in material chemistry have made it possible to synthesize interesting new materials; on the other, theoretical studies of frustrated spin models provide better insight into the nature of complex quantum states of spin systems [4]. Ever since the discovery of the high-$T_C$ superconductivity in cuprates, the question of unconventional mechanism of superconductivity and the studies of spin-liquid quantum phases, have been treated with related interests. This makes the studies of frustrated spin systems, together with the search for new mechanisms of superconductivity, a topic of great current physical interest. The discoveries of new materials make these studies equally more desirable and exciting.

In the present thesis, we have worked on three distinct problems, which fall under two broad categories, viz. \textit{frustrated spin models} and \textit{superconductivity in strongly correlated electronic systems}. In one of these problems, we construct spin models of quantum antiferromagnets with frustrating exchange interactions [6]. They are so constructed that it becomes possible to find their ground states exactly. These quantum spin models have exact singlet dimer ground states. The other two problems are concerned with superconductivity in correlated electronic systems. In one of these, we do some useful calculations for materials of current interest, within the framework of the resonating valence bond (RVB) mean field theory [13, 14]. And the last problem deals with a formal question of superconductivity in the models of interacting electrons with pure repulsion. The central idea here is a mechanism called \textit{order by projection}. We do some calculations on simple models which show the phenomenon of order by projection explicitly [19]. Now, we briefly describe each of these problems.

\subsection*{1.1 Frustrated quantum antiferromagnets}

In a given material spin, charge and lattice degrees of freedom are all coupled together. But there are situations, for example in a magnetic insulator, where the gap for the charge excitations is sufficiently large so that the low energy physics is primarily governed by the excitations of magnetic nature. We may, then, safely investigate such systems with
1.1 Frustrated quantum antiferromagnets

an effective ‘spin-only’ description. The standard approach to this kind of studies is in terms of the Heisenberg spin-exchange model whose Hamiltonian can be written as:

\[ H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]  

(1.1)

where \( J_{ij} \) is the exchange interaction between spins at sites \( i \) and \( j \). Though we may ignore the dynamical effects of lattice (phonons) in many simple situations, the topology of the (infinitely rigid) lattice can still influence the physical state of the system, and we can have interesting effects arising purely due to the lattice geometry. For example, the lattice topology may give rise to what is called frustration. To illustrate this point, consider a standard example of three Ising spins, sitting at the corners of a triangle, and interacting pairwise via a uniform antiferromagnetic exchange. In order to achieve the lowest energy state, each pair of spins would like to attain the anti-parallel configuration. On a triangular plaquette, however, it is simply not possible to satisfy all three pairs of spins simultaneously. One of the pairs can never achieve the lowest energy state. And hence, the frustration. Here, we are interested in quantum spins, where frustration due to the lattice geometry or the competing exchange interactions may lead to interesting quantum phases.

It is often desirable and also challenging to be able to solve the Heisenberg Hamiltonian exactly for a certain choice of \( J_{ij} \). The exact solution, however, is not always guaranteed. And there are only handful of such models which are exactly solvable. The Majumdar-Ghosh (MG) model of spin-1/2 quantum antiferromagnetic chain is one of them, for which the ground state is known exactly [5]. Inspired by the ground state solution of the solvable MG model, we construct a new class of quantum spin models in one dimension (1D) whose ground states can be found exactly. The idea of construction is also applied to two (2D) and three (3D) dimensions. This forms the subject matter of Chapter 2, which is mainly based on Reference [6].

The exchange coupling of 1D family of models that we construct, varies linearly with separation between the coupled spins. Therefore, we call them the linear exchange spin models. The basic idea behind their construction is that of the completely and identically exchange-coupled spin blocks. We call them the fundamental spin blocks, and denote as \( \mathcal{B}_\mathcal{R} \), where \( \mathcal{R} \) is the number of spins in the block. This is motivated by the three-spin block structure of the solvable MG chain. All this will be discussed in great detail in Chapter 2. The Hamiltonian of a spin chain (with periodic boundary condition) made up of \( \mathcal{B}_\mathcal{R} \) blocks, can be written as:

\[ H_\mathcal{R} = J \sum_{i=1}^{L} \sum_{n=1}^{\mathcal{R}-1} (\mathcal{R} - n) \mathbf{S}_i \cdot \mathbf{S}_{i+n} \]  

(1.2)
where $L$ is the number of sites, and $J$ is positive. For $R = 3$, this is same as the MG model. We prove that for all odd integer values of $R$, the exact ground state of $H_R$ (for spin-$1/2$) consists of the two degenerate dimer configurations, one of which is given below. The other is related to this by a lattice translation.

$$|\psi_g\rangle = [1, 2] \otimes [3, 4] \otimes \cdots \otimes [L - 1, L]$$  \hspace{1cm} (1.3)$$

The notation $[i, j]$ denotes a singlet state of a pair of spins at sites $i$ and $j$. It is pointed out that these ground state dimer configurations have a property called superstability. The spin-spin correlation in the ground state is ultra-short ranged (only nearest neighbour). Thus we have a family of frustrated quantum spin models with exact spin-liquid ground state. The propagating domain wall (or kink) forms a good variational choice for an elementary excitation in these models. The excitation spectrum is shown to be gapped.

It is important to note, however, that the exact ground state solution is not possible for even integer values of $R$ (except for $R = 2$). Thus we have two sub-families within the family of linear exchange spin chains, the odd and the even. The Hamiltonian $H_2$ is the nearest neighbour Heisenberg antiferromagnet, which is a well-known integrable model with algebraically decaying spin-spin correlation. Though we do not know the exact nature of the ground state of higher members of the even sub-family, we have checked through the exact diagonalization of small chains that they have spin correlations similar to that of $H_2$, albeit with rapid decay for larger values of $R$. This presents a case of even-odd differences for finite $R$ in the linear exchange models. However, we are able to prove rigorously that in the limit when $R \sim O(L/2)$, and $L \to \infty$, the above mentioned singlet dimer configurations (Equation 1.3 and its lattice translated partner) also form the exact ground state of the even sub-family. Though it may sound inappropriate to distinguish between even and odd in this limit, the above result, however, is not necessarily obvious. We also point the similarity between the 1D Coulomb problem and our linear exchange models.

Using this block construction, we are also able to make models with finite entropy density in the ground state. This is contrary to the standard statement of the third law of the thermodynamics. In such models, the ground state consists of exponentially large number of dimer configurations (exponential in the number of lattice sites). We also apply this scheme for constructing models in 2D and 3D. A rather well know example, which fits well in our scheme, is the Shastry-Sutherland model [7], which is a 2D construction using generalized $B_3$ blocks. We construct more such models with exact dimer ground states, using bigger spins blocks. Here too, we have models with finite entropy density in their ground states. We find that in higher dimensions things do not differ so very significantly for models constructed using even or odd sized spin blocks. We make models using both
1.2 RVB superconductivity on frustrated lattices

The idea of RVB superconductivity was proposed soon after the discovery of high-$T_C$ superconductivity in cuprates [8, 9]. It is a new approach to superconductivity where super-exchange between electrons provides the mechanism for singlet pair formation. Its novelty lies in the fact that it is a purely electronic mechanism for superconductivity, unlike the BCS mechanism where electron-phonon interaction is essential. Though its applicability to high-$T_C$ cuprates may still be debatable, it nevertheless inspires the search for an RVB superconductor. The central theme of this approach is that it may be possible to derive a superconducting state by doping an RVB insulating state.

Originally, the notion of RVB was conceived by Linus Pauling. Later, it was proposed as a possible choice for the ground state of the Heisenberg antiferromagnet on triangular lattice [10]. This led to the useful notion of spin-liquid state, where there is no magnetic long ranged order in the ground state of an interacting spin system (similar to the usual liquid state of the interacting matter). The physical picture of an RVB spin liquid state is that of “freely” moving singlet pairs of electrons in real space. However, there are no (low-energy) charge fluctuations due to the Mott gap. The hope is that by doping such an insulating state, these real space singlet pairs may develop some phase coherence, and finally condense to form a superconductor.

In Chapter 3, we study two kinds of materials as the possible RVB superconductors. One of these is the doped variant of SrCu$_2$(BO$_3$)$_2$ (which is yet to be synthesized), and the other is a new low-$T_C$ cobaltate superconductor, Na$_x$CoO$_2$ · $y$H$_2$O ($x \sim 0.35$ and $y \sim 1.3$) with $T_C \sim 5K$ [12]. The orthoborate SrCu$_2$(BO$_3$)$_2$ is a quasi 2D spin-1/2 insulating material with layers of CuBO$_3$ separated by Sr$^{2+}$ ions. The copper lattice in these layers is topologically equivalent to the Shastry-Sutherland (SS) lattice (see Figures 3.1 and 3.2). The low temperature behaviour of SrCu$_2$(BO$_3$)$_2$ is very well explained by the dimer state (which is the exact ground state of the SS model) [11]. We believe that its doped variants (either with monovalent or trivalent dopant) may be good candidates for searching RVB superconductivity [13], and emphasize on the need for synthesizing these materials.

The cobaltate Na$_x$CoO$_2$ · $y$H$_2$O also has a highly anisotropic structure having layers of CoO$_2$ with cobalt ions forming a triangular lattice (see Figure 3.10). We interpret the superconductivity in the cobaltate as the RVB superconductivity, since there exists an antiferromagnetic exchange between electrons, and the triangular lattice is a frustrated lattice. Though at half filling, the three sublattice magnetically ordered state makes a better ground state, the RVB state may become stable for finite carrier concentration.
away from half filling. A CoO$_2$ layer acts as a half filled reference system, which is doped by the electrons from the sodium. Thus, we make a case for the cobaltate superconductor as an electron doped RVB superconductor [14].

We take the one band t-J model on the triangular and the SS lattice as the simple starting model for the respective materials. We perform simple RVB mean field calculations on the t-J models, and make some useful predictions. The RVB mean field theory on the SS lattice is exact at half filling since it gives the correct dimer state for the SS model. From the RVB calculations on the SS lattice, we make some predictions for the doped SrCu$_2$(BO$_3$)$_2$. Away from half filling, the RVB superconducting phase is appropriately interpreted. The symmetry of the order is d-wave like (between the dimer-forming bonds on the SS lattice). Very close to the half filling, the quasi-particle excitations are gapped (as it should be with the persistence of spin-gapped phase at very low doping). The energy gap, however, vanishes for sufficiently high doping. Therefore, the superconducting phase (if realized in doped SrCu$_2$(BO$_3$)$_2$) is predicted to be gap-less. The superconducting $T_C$ is found to be of the order of 10 K (which is reasonable since the super-exchange in SrCu$_2$(BO$_3$)$_2$ is almost one-tenth of that in high-$T_C$ cuprates). Since the SS lattice is frustrated, the different signs of the hopping parameters present different cases, which are carefully discussed.

From the triangular lattice RVB mean field calculations, we find that the symmetry of the superconducting order parameter is $d_1 + id_2$ type. The complex order parameter can be written as:

$$\Delta(k) = \Delta \left[ \cos(k_x) + e^{i\theta} \cos \left( \frac{k_x + \sqrt{3}k_y}{2} \right) + e^{i\phi} \cos \left( \frac{k_x - \sqrt{3}k_y}{2} \right) \right]$$

where $\theta$ and $\phi$ are the internal phases along two different directions. The mean field energy is found to be lowest (away from half filling) when $\theta = 2\pi/3$ and $\phi = 4\pi/3$ (and five more points reflecting the symmetry of the Brillouin zone). The quasi-particle spectrum is gapped. Since there is no particle-hole symmetry on the triangular lattice, the sign of the hopping ‘$t$’ becomes very important. We find that “$t < 0$ and hole doping” or equivalently “$t > 0$ and electron doping” is a robust case for the RVB superconductivity. The other case is weak. It is known from an earlier work that the same case ($t < 0$, hole doping) also presents robustness towards the ferromagnetic state (Nagaoka-Kanamori ferromagnetism) [15]. Putting all these facts together, we present a rough phase diagram in the temperature-doping plane, and predict the RVB superconductivity for moderate doping, which gives way to the ferromagnetic state at sufficiently high doping at low temperatures. It is also pointed that the high frequency Hall constant in the metallic phase of this system (sodium-cobaltate) is predicted to grow linearly with temperature for
temperatures much greater than $t$ [16]. Since the value of $t$ in these cobaltates is expected to be small, even the weak case ($t > 0$, hole doping) may support the RVB superconducting state. The Hall constant prediction will still go through, but the ferromagnetic state is no more stable.

1.3 Order by projection in repulsive lattice fermions

The question of superconductivity in a system of electrons with purely repulsive interaction has always been an interesting one. The Kohn-Luttinger result is probably the only compelling demonstration of superconductivity in a repulsive continuum electronic system [17]. There is a considerable renewed interest in models exhibiting superconductivity starting from pure repulsion, because superconductivity in cuprates appears in the close vicinity of the Mott insulating phase. The parent cuprates are Mott insulators with long ranged Néel order. Knowing the fact that strong local electron correlation is the dominant factor in Mott insulators, and these insulating parents become superconducting at small carrier concentrations, it is rather prudent to ask what effects strong local repulsion has on superconducting correlations. Why does the system pick up non-local pairing channels for Cooper pair formation? Also, the fermions on a lattice have an extra property of commensuration, which is very significant. It is therefore important to develop new non-perturbative methods to investigate rigorously the cooperative behaviour of lattice fermions. In this context, a general idea termed order by projection has been proposed recently [18].

The model introduced in this context contains pairing terms, as in the reduced BCS Hamiltonian, but with large and repulsive interaction. When transformed to the Wannier basis in real space, these pairing terms correspond to an infinite ranged hopping of local (s-wave) pairs of particles. The corresponding Hamiltonian is written as:

\[
H = \sum_{\langle i,j \rangle} \sum_{\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + U_s B^\dagger B \tag{1.4}
\]

The first two terms in the above Hamiltonian form the Hubbard model. It is a typical starting point for the physical systems with competing kinetic energy and the local electron correlation. The last term in Equation 1.4 is the infinite ranged pair hopping term. The operator $B$ is the local (s-wave) pairing operator which is defined as:

\[
B = \sum_i c_{i\downarrow} c_{i\uparrow} = \sum_k c_{-k\downarrow} c_{k\uparrow} \tag{1.5}
\]

Similarly, we can also define the extended s-wave and the d-wave pairing operators in the
following way.

\[ A = \sum_{i} \sum_{\delta} c_{i\downarrow} c_{i+\delta\uparrow} \]  \hspace{1cm} (1.6)

\[ = 2 \sum_{\mathbf{k}} (\cos(k_x) + \cos(k_y)) c_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \]

\[ D = \sum_{i} \sum_{\delta} e^{i\delta(0,\pi)} c_{i\downarrow} c_{i+\delta\uparrow} \]  \hspace{1cm} (1.7)

\[ = 2 \sum_{\mathbf{k}} (\cos(k_x) - \cos(k_y)) c_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \]

Here, \( n.n. \) stands for the nearest neighbour; \( A \) is the extended s-wave pairing operator, and \( D \) is the d-wave pairing operator.

The pair hopping term in Equation 1.4 is an important term, which for \( U_s < 0 \) and \( \sim \mathcal{O}(1/L) \) favours the s-wave (BCS) superconductivity. For \( U_s > 0 \) and \( \sim \mathcal{O}(1) \), however, if the ground state were to have local pairing, then \( \langle B \rangle \) is non-zero and \( \sim \mathcal{O}(L) \), which makes the contribution from the pairing term in the Hamiltonian positive super-extensive (\( \sim \mathcal{O}(L^2) \)). Thus, in this case, the new term suppresses the s-wave pairing or in other words it projects out the local pairing. This lattice fermion system, as shown in Reference [18], attains enhanced extended s-wave superconducting fluctuations close to half filling, which is briefly described below. The underlying principle behind this enhancement is the uncertainty principle, since the s-wave and the extended s-wave pairing operators are recognized to be conjugates.

For the nearest neighbour hopping operator \( T \), the extended s-wave pairing operator \( A = [T, B] \) (with an extra factor of \( 2t \) in comparison to the definition in Equation 1.6). It is in this sense (like \( p = [H, x] \)) we call \( A \) and \( B \) as the conjugate variables. With the suppression of s-wave pairing, two things happen in the thermodynamic limit. One, the ground state energy density remains unaffected by the presence of \( B^\dagger B \) term. That is, the ground state energy density with the repulsive pairing term and without this terms are the same. And the second thing that happens is the enhancement in \( \langle A^\dagger A \rangle \) in the close vicinity of the half filling. In the thermodynamic limit, \( \langle (B + B^\dagger)^2 \rangle / L = 1 - \rho \), where \( \rho \) is the lattice filling. Making use of the uncertainly principle and some other inequalities, one arrives at the following enhancement inequality for \( \langle A^\dagger A \rangle \) for \( \rho < 1 \).

\[ \langle A^\dagger A \rangle \geq \frac{2|\langle T \rangle|^2}{L(1-\rho)} - \frac{\langle \chi_A \rangle}{2} \]  \hspace{1cm} (1.8)

where \( |\langle T \rangle| \) and \( \langle \chi_A \rangle \) are some numbers of order \( L \). This inequality clearly shows an unbounded (from above) enhancement in the extended s-wave pairing correlation near half
1.2 Order by projection

filling. It is an interesting combined effect of the projection due to repulsion, uncertainty principle and the lattice commensuration.

At half filling, \( \rho = 1 \), the right hand side of Inequality 1.8 is divergent, and does not give us any guidance with reference to the question of how system behaves at half filling. Does it attain long ranged order (LRO) in the extended s-wave channel or what else happens? These are some of the questions that need to be answered explicitly. In Chapter 4, we do some calculations to clarify of these queries [19]. We introduce and solve simple spin models, derived from the original model (Equation 1.4) through pseudo-spin mapping and simplified dispersion relation. Through explicit calculation, we find that at half filling, system does not attain the true LRO in the extended s-wave channel. It rather acquires only a quasi LRO\(^1\), since \( \langle A^\dagger A \rangle \sim L^{3/2} \). It is not discouraging, however. The system is critical in the extended s-wave channel. Recently, we considered the same simplified model with electron-phonon (e-ph) interaction. We find that the s-wave projection together with e-ph interaction can lead to an ordering in the non-local pairing channels, the extended s-wave channel in the present case. This (projection + e-ph interaction) may be a useful way towards the understanding of superconductivity in systems with strong local correlation such as cuprates. We also present a new sum-rule for these models.

We have also considered the implication of the idea of order by projection in a model of two level atoms interacting with a single mode quantized radiation field. We find that it leads to some kind of anti-superradiant cooperative behaviour in the atom-field system, which otherwise would have shown superradiance.

\(^1\)The true LRO in extended s-wave would mean \( \langle A^\dagger A \rangle \sim O(L^2) \)
Chapter 1 Introduction
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Chapter 2

Frustrated quantum spin models

The spin-1/2, quantum antiferromagnetic chains with linearly decreasing exchange coupling are constructed. The exchange coupling beyond a separation \((R - 1)\) is zero, where \(R\) is a positive integer. For odd values of \(R\), the ground state of all the Hamiltonians consists of two degenerate singlet dimer configurations. These models have low-lying kink excitations with an energy gap. The Majumdar-Ghosh model is the first member of the odd family. The models with even values of \(R\) are qualitatively different from the ones with odd values, and admit an exact dimer ground state only in the asymptotic limit when \(R\) is infinitely large. The scheme of construction is applied in two and three dimensions, to construct quantum spin models with exact dimer ground states. The Shastry-Sutherland model in two dimensions is a well known example which fits in our general scheme. Many of these models have finite entropy density in their ground states. An interesting property of superstability is pointed out for the dimer ground states of these models.

The subject of frustrated antiferromagnets is an old and interesting one. Magnetism is what we know as the study of magnetic properties of the matter. The frustrating geometry or the competing exchange interactions can give rise to exotic magnetic phases which otherwise, in a simpler magnetic system, would not be possible. There has been a great resurgence of interest in this area recently, mainly because of many real materials that one has been able to synthesize. The borate compound, \(\text{SrCu}_2(\text{BO}_3)_2\), is a good recent example of a material with frustrated magnetism [1]. Interestingly, this compound happens to be a material realization of the Shastry-Sutherland model of frustrated quantum antiferromagnet in two dimensions [2].

In the present chapter, our interest lies in studies of frustrated quantum spin models.
The frustrated quantum antiferromagnets can have interesting low temperature properties [3]. Generally, they are found to have spin liquid ground states where the spin correlations are rapidly decaying functions of the separation. In most cases, we don’t have an exact understanding of the nature of their ground state and excitation spectrum. A well-studied example of a frustrated quantum antiferromagnet is the Majumdar-Ghosh model. It is a one dimensional (1D) model with nearest and next nearest exchange couplings. The fact that it admits an exact ground state solution for a certain ratio of the two couplings, makes it a special model. Inspired by the exact solution of this model, we discovered a general scheme for constructing quantum spin models with exact singlet dimer (or simply dimer) ground states, which forms the subject matter of the present chapter.

The plan of the chapter is the following. In Section 2.1, first we discuss in sufficient detail the exact ground state solution of the Majumdar-Ghosh model, then we describe the idea of a general construction. In later sections, this idea is used in 1D to construct the quantum models with exact dimer ground states, and also applied to higher dimensions. An interesting class of models that we construct in 1D, happens to have a linearly decreasing exchange coupling. So, we call them as the linear exchange spin models.

Section 2.2 describes the construction of the linear exchange models. First, we introduce the idea of completely connected spin blocks, and then describe the construction of the linear exchange models. These blocks are fundamental to our scheme of construction. The family of linear exchange models has two subfamilies: odd and even. The odd family is constructed using odd sized blocks, and the even sized blocks make even family. The size of the building blocks also decides the range of the exchange interaction, and acts as a parameter to label the members in the family. Interestingly, odd family models have exact dimer ground states, whereas even family admits exact dimer ground state only in the asymptotic limit when the range of exchange coupling is infinitely large, in a thermodynamically large system.

In Section 2.3, we present the exact solution for the ground state of the odd family of the linear exchange models. We rigorously prove that the ground state consists of two degenerate dimer configurations. We give a proof by mathematical induction, and also emphasize upon the superstability property of the ground state. Then, we discuss the nature of the elementary excitations in these models. We propose that the propagating domain wall or kink excitations form a good variational choice for the low-lying excited states, and show that they are gapped.

The even family of the linear exchange models is qualitatively different from the odd family. In Section 2.4, we discuss the possible nature of the ground state in these models for the finite range of exchange interaction. We also prove that in the asymptotic limit,
the apparent disparity between the odd and the even family disappears, and the model has an exact dimer ground state with two-fold degeneracy.

Section 2.5 highlights the apparent connection between the linear exchange spin models and the 1D Coulomb problem. In Section 2.6, we discuss a few models in 1D whose ground state degeneracy is exponential in the system size. Section 2.7 describes the application of the idea of to higher dimensions with some interesting examples. This chapter is mainly based on our Reference [4], except for the discussion on the even family models in Section 2.4 which is newly added. Incidentally, the work in Reference [5] has some overlap with our present work. Though there are interesting similarities, the approach and the emphases in the two are different.

2.1 Majumdar-Ghosh model

Majumdar and Ghosh studied a spin-1/2, one dimensional quantum antiferromagnet with nearest and next nearest neighbour exchange interactions [6, 7]. The model that they studied, is known as the Majumdar-Ghosh (MG) model. The Hamiltonian for the MG model is written as:

\[ H_{MG} = J \sum_{i=1}^{L} (2S_i \cdot S_{i+1} + \alpha S_i \cdot S_{i+2}) \]  (2.1)

where \( J \) and \( \alpha \) are positive, and \( L \) is the number of sites on the 1D lattice with periodic boundary condition (PBC).

The presence of a non-zero second neighbour antiferromagnetic coupling brings frustration into this model. This is an interesting model which shows quantum phase transition from magnetically ordered phase to disordered spin-liquid like phase as \( \alpha \) is increased. The numerical studies of MG model for \( S=1/2 \) have shown that for \( \alpha > 0.482 \), the ground state is a spin liquid [8]. At \( \alpha = 0 \), the MG model is same as the nearest neighbour Heisenberg chain which is an integrable spin model with Néel like, but algebraically decreasing spin-spin correlations. For arbitrary values of \( \alpha \), the MG model is not exactly soluble. But \( \alpha = 1 \) happens to be a special point where the ground state of the MG model is exactly known. In all the discussions regarding MG model, we will be interested only in the case of \( \alpha = 1 \).

It was found that for even number of lattice sites, the bond-singlet (or dimer, as we often refer to it) configurations form an exact two-fold degenerate ground state. Let \( |l, m\rangle = (|\uparrow_l \downarrow_m\rangle - |\downarrow_l \uparrow_m\rangle)\sqrt{2} \) denote the singlet state of a pair of spins at sites \( l \) and \( m \), representing a double bond in the chemical sense. The ground state configurations of the
MG model, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, can be written as:

$$|\psi_{g1}\rangle = [1, 2] \otimes [3, 4] \otimes [5, 6] \otimes \cdots \otimes [L - 1, L] \quad (2.2)$$

$$|\psi_{g2}\rangle = [2, 3] \otimes [4, 5] \otimes [6, 7] \otimes \cdots \otimes [L, 1] \quad (2.3)$$

These dimer states are pictorially represented in Figure 2.1. The ground state energy, in units of the nearest neighbour exchange $(2J)$, is $-(3/8)L$. The nature of the low energy excitations above the dimer ground state is also reasonably well understood. Shastry and Sutherland argued that the propagating domain boundaries or kinks form a good variational choice for the low lying elementary excitations, and calculated their dispersion relation [10]. These excitations have an energy gap above the ground state. Later, it was proved rigorously that the excitation spectrum of the MG model is gapped [11]. In the following subsection, we discuss the exact ground state solution of the MG model in detail, and see what we learn from it.

2.1.1 Exact ground state solution

For $\alpha = 1$, on a closed chain, the MG Hamiltonian can be re-written as:

$$H_{MG} = J \sum_{i=1}^{L} (S_i \cdot S_{i+1} + S_i \cdot S_{i+2} + S_{i+1} \cdot S_{i+2}) = J \sum_{i=1}^{L} h_i \quad (2.4)$$

The little Hamiltonian, $h_i = S_i \cdot S_{i+1} + S_i \cdot S_{i+2} + S_{i+1} \cdot S_{i+2}$, is that of a block of three spins, the $i^{th}$ spin and its next two neighbours, coupled to each other identically. Let us refer to these blocks as $\mathcal{B}_3$ where $\mathcal{B}$ stands for a block of completely connected spins, and the subscript, 3, refers to the number of spins in a block. Spins within a
2.1 Majumdar-Ghosh model

block are understood to be identically coupled, unless specified. The minimum eigenvalue of \( h_i \) is \( e_{i \text{min}} = -3/4 \), for \( S = 1/2 \). This is easy to see if we re-write \( h_i \) as

\[
\frac{1}{2} \left[ (S_i + S_{i+1} + S_{i+2})^2 - S_i^2 - S_{i+1}^2 - S_{i+2}^2 \right].
\]

The lowest eigenvalue of \( h_i \) will correspond to the lowest value of total spin, \( (S_i + S_{i+1} + S_{i+2}) \). For three \( S=1/2 \) spins, the minimum total spin is 1/2. Therefore, the lowest eigen-energy of the block is \(-3/4\), and the minimum energy spin configuration for \( B_3 \) has one free spin and the rest two spins forming a singlet. For example, \([i, i+1] \otimes \langle \uparrow_{i+2} \rangle\) is one such eigen-configuration. There are two linearly independent ways of forming such configurations for which the total spin of \( B_3 \) is 1/2.

Since the MG chain is made up of \( B_3 \) units, the ground state of the MG chain can be constructed in such a way that it is also the lowest energy eigen-configuration of each of the \( B_3 \) units of the chain. This is not possible in general. Interestingly, this is possible for MG chain because the minimum energy configuration of \( B_3 \) has strictly one dimer and a free spin. This “free” spin is free in the sense that it can bond with the “outside” world, and the new composite configuration will still be the eigen configuration of the block-Hamiltonian with energy, \(-3/4\), provided other two spins of \( B_3 \) form a singlet. Since every spin on the MG chain has identical exchange connectivity, the above considerations imply that the ground state configuration of \( H_{MG} \) is the one where every three neighbouring spins share exactly one dimer. This gives rise to the ground state dimer configurations shown in Figure 2.1.

The statements made above, regarding the ground state of the MG model, can be proved formally in the following way. The first step is to prove that the dimer states, \( |\psi_{g1}\rangle \) and \( |\psi_{g2}\rangle \), are the eigenstates of \( H_{MG} \). This is proved by making use of the identities given below.

\[
S_k \cdot (S_l + S_m)[l, m] = 0 \ \forall \ k \neq l \text{ and } m \quad (2.5)
\]

\[
S_l \cdot S_m[l, m] = -S(S+1)[l, m] \quad (2.6)
\]

This straightforwardly gives us, \( h_i |\psi_{g1,2}\rangle = -3/4 |\psi_{g1,2}\rangle \), for all values of the site index \( i \). Here, \( |\psi_{g1,2}\rangle \) refers to states \( |\psi_{g1}\rangle \) and \( |\psi_{g2}\rangle \). Thus, we find that \( H_{MG} |\psi_{g1}\rangle = -(3J/4)L |\psi_{g1,2}\rangle \). This proves that states \( |\psi_{g1}\rangle \) and \( |\psi_{g2}\rangle \) are the eigenstates of the MG Hamiltonian with energy \(-3J/4\). The second step in the proof is to show that these eigenstates are also the lowest energy states of the MG Hamiltonian. This can be shown by making use of the following inequality. For a given eigenstate, \( |\psi_i\rangle \), of a Hamiltonian, \( H \), with energy eigenvalue, \( E \), the following inequality always holds, provided the Hamiltonian can be written as a sum of \( N \) block Hamiltonians, \( H_i \), with the lowest eigenvalue,
This inequality implies that $|\psi\rangle$ is also a ground state of $H$, if the upper bound of the inequality is same as the lower bound. Clearly, from Equation 2.4, we know that $H_{MG}$ has the desired block structure for the applicability of Inequality 2.7, and therefore one can check whether $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ are also the ground state configurations of $H_{MG}$ or not. We have already shown that $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ are the eigenstates of $H_{MG}$ with eigen energy $E = -(3J/4)L$. And, we also know that $\mathcal{E}_{i}^{min} = -3J/4$ (since $H_{i} = J h_{i}(B_{3})$ and $N = L$ for $H_{MG}$), therefore, the lower bound of the Inequality 2.7 for $H_{MG}$ is $-(3J/4)L$. Since, the upper bound is same as the lower bound, we have proved that the dimer configurations, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ as given in Equations 2.2 and 2.3, form the exact ground state of the MG model.

### 2.1.2 The lesson and the idea

Now let us reflect upon what was the key to the exact ground state solution of the MG model. We might say that being able to write in an appropriate block structure was at the core of finding the exact ground state. But this is only partially correct. This can be seen easily by considering the nearest neighbour Heisenberg antiferromagnetic chain. There also, we can write the full Hamiltonian as a sum of the block Hamiltonians of two (neighbouring) spins. That is, $H = J \sum_{i=1}^{L} h_{i}$ where $h_{i} = S_{i} \cdot S_{i+1}$. We may call such blocks as $B_{2}$, keeping in line with our convention. But we know that we can not find the exact ground of the nearest neighbour Heisenberg chain with the above set of steps, as we had used for $H_{MG}$ knowing its block structure. In fact, unlike the MG model, the ground state of the nearest neighbour Heisenberg antiferromagnetic chain is not the ground state of an individual block, $B_{2}$. This is a serious qualitative difference between the two. We will elaborate upon this point later in this chapter. Thus, block decomposition is an important step in the exact ground state solution of the MG model, but it is not the most decisive feature which makes the exact solution possible.

The key observations that deserve serious attention are the following facts that we came across while doing the exercise for the MG model.

1. The fundamental block, $B_{3}$, has odd number of spins, that is three.

2. Spins within a block are completely and identically connected, that is every spin is coupled to every other spin in a block with the same strength of exchange interaction. The eigen energies of such a block depend only upon the total spin of the block.
3. Since we are interested in the antiferromagnetic exchange, the block’s minimum energy corresponds to the total spin being $1/2$. Thus the minimum energy configuration of a fundamental block contains exactly one free spin while rest forming a singlet.

4. The successive blocks, in forming the MG spin chain, share an even number of common spins. This is important because only an even number of $S=1/2$ spins can form a singlet.

The lesson we learn from these facts is that the number of spins being odd, and the complete and identical connectedness of exchange interaction in a fundamental block are the most important features. Otherwise, such a simple ground state solution would not have existed for the MG model. It is these features that make sure that there is a free spin in each block’s minimum energy configuration which acts as a link to the neighbouring blocks while preserving its own singlet. Thus, it becomes possible for the MG model to have an exact ground state.

These considerations provoke a general thought that instead of three spins per block, we can have blocks of bigger size, but with odd number of spins. For example, we can have $B_5$ block of spins at sites $i$ through $(i+4)$ on a chain. We can easily check that for bigger blocks with odd number of spins, second and third of the aforementioned points will go through. And a translationally invariant chain made up of bigger fundamental blocks will automatically satisfy the fourth point. Thus, one may hope that the consideration of the ground state of such spin models will not be very different from what we know for the MG model.

In the following section, we will construct a new family of quantum spin chains along these lines of thought, and will prove rigorously that the dimer states which form an exact ground state of the MG model are, also the exact ground state configurations for the whole family. As we will see, the exchange coupling in these models vary linearly with separation between the coupled spins. Therefore, we call them as the linear exchange spin chains.

## 2.2 Linear exchange quantum spin chains

First, we discuss the fundamental spin blocks. Next, we will illustrate how these blocks give rise to a new family of translationally invariant quantum spin models in one dimension. We will, then, study this family of models.
2.2.1 Fundamental spin blocks

We denote a fundamental spin block as $\mathcal{B}_R$. Symbol $\mathcal{B}$ stands for a block of completely and identically connected spins. $R$ refers to the number of spins in the block, and can take any positive integer value $\geq 2$. Here connectivity between spins means the exchange interaction. The notation $\mathcal{B}_R$ for the spin blocks will have only the above stated meaning, unless the variations upon the current definition are explicitly mentioned. For the present discussion, we strictly stick to the present definition of the fundamental block. Later in the chapter, we may, for example, relax the condition of identical connectedness. But wherever there is any change in the convention, it will be explicitly mentioned.

\[ R = 3 : \quad (1D) \equiv (2D) \]

\[ R = 4 : \quad (1D) \equiv (2D) \quad (3D) \]

\[ R = 5 : \quad (1D) \equiv (2D) \quad (3D) \]

Figure 2.2: The $\mathcal{B}_R$ blocks for $R = 3, 4$ and 5, in 1D, 2D and 3D. The filled circles (●) represent the spins and a line represents the exchange interaction.

The simplest block that one can construct is for $R = 2$, that is $\mathcal{B}_2$. The corresponding block Hamiltonian is $h[\mathcal{B}_2] = S_1 \cdot S_2$, where $S_1$ and $S_2$ are the spins of $\mathcal{B}_2$. The exchange interaction within the block is taken to be unity. As we have mentioned earlier, the spin chain made up of $\mathcal{B}_2$ units is the nearest neighbour Heisenberg model. The next block is $\mathcal{B}_3$ which is the building block for the solvable MG model. Figure 2.2 shows pictorial representation of many such fundamental spin blocks in one, two and three spatial dimensions. Here, we wish to stress upon a point. Any pairwise exchange coupled spin model is obviously made up on $\mathcal{B}_2$ units. Therefore, even the MG model is made up
of $\mathcal{B}_2$ at some level. But we still say that $\mathcal{B}_3$ is its fundamental spin block, because it is the largest completely connected block possible for the MG model. Just to illustrate the point, consider the Heisenberg model on the pyrochlore lattice. Then, according to our convention, the fundamental block for this model is $\mathcal{B}_4$. The block Hamiltonian for $\mathcal{B}_4$ can be written as:

$$h[\mathcal{B}_4] = S_1 \cdot (S_2 + S_3 + S_4) + S_2 \cdot (S_3 + S_4) + S_3 \cdot S_4$$

The Hamiltonian for a general fundamental block, $\mathcal{B}_R$, is given below.

$$h[\mathcal{B}_R] = S_1 \cdot (S_2 + S_3 + \cdots + S_R) + S_2 \cdot (S_3 + \cdots + S_R) + \cdots + S_{R-1} \cdot S_R \quad (2.8)$$

The Hamiltonian, $h[\mathcal{B}_R]$, can also be re-written as:

$$h[\mathcal{B}_R] = \frac{1}{2} \{(S_1 + S_2 + \cdots + S_R)^2 - (S_1^2 + S_2^2 + \cdots + S_R^2)\} \quad (2.9)$$

It is evident from Equation 2.9 that the lowest eigen energy of the block corresponds to the minimum total spin of the block. Let $R$ be an odd integer, that is $R = 2\nu + 1$, where $\nu$ is a positive integer. Since we are dealing with spin-1/2 objects, the minimum total spin is also 1/2 for $\mathcal{B}_{2\nu+1}$, and the minimum energy is, $e^{min}[\mathcal{B}_{2\nu+1}] = -3\nu/4$. If $R = 2\nu$, then the total minimum spin of the block is zero, and the lowest energy is, $e^{min}[\mathcal{B}_{2\nu}] = -3\nu/4$. The minimum energy spin configuration for $\mathcal{B}_{2\nu+1}$ is the one where any $2\nu$ spins form a singlet, and there is one free spin.

The block singlet configurations which arise here are degenerate and non-orthogonal. For example, the minimum total spin state of $\mathcal{B}_3$ has one dimer and one free spin which can be written as: $[1,2] \otimes |\sigma_3\rangle$ or $|\sigma_1\rangle \otimes [2,3]$, where $\sigma_1$ and $\sigma_3$ can be $\uparrow$ or $\downarrow$. It can be easily checked that the configuration where $S_2$ is free, that is $|\sigma_2\rangle \otimes [3,1]$, can be described as a linear combination of the previous configurations. The same thing is graphically shown in Figure 2.3 below. Similarly, the block singlet made up of four spin-

![Figure 2.3](image_url)

Figure 2.3: The graphical representation of the equation, $[1,2] \otimes |\uparrow_3\rangle + |\uparrow_1\rangle \otimes [2,3] = |\uparrow_2\rangle \otimes [3,1]$. 

1/2, has two degenerate dimer configurations. Let $[1,2,3,4]$ represent the block-singlet state of $\mathcal{B}_4$. The two independent dimer representations of $[1,2,3,4]$ are $[1,2] \otimes [3,4]$ and $[2,3]$.
The other singlet configurations of $B_4$ can be written as the linear combination of these configurations. Figure 2.4 shows an example of $B_4$ singlet states. We will denote a general block-singlet state of $2\nu$ spins as $[1, 2, 3, \ldots, 2\nu]$. A singlet state of $2\nu$ spins can be represented by many linearly independent dimer configurations. Having discussed the structure of the fundamental spin blocks in sufficient detail, now let us construct the spin models using these blocks.

![Diagram](image.png)

Figure 2.4: The graphical representation of the equation, $[1,2] \otimes [3,4] - [2,3] \otimes [4,1] = [1,3] \otimes [2,4]$.

### 2.2.2 The Hamiltonian

Consider a fundamental block, $B_R$, consisting of spins at sites $i$ to $i + R - 1$, on a 1D lattice with PBC. The corresponding block Hamiltonian, $h_i[B_R]$, is written as:

$$h_i[B_R] = \{ S_i \cdot (S_{i+1} + \cdots + S_{i+R-1}) + S_{i+1} \cdot (S_{i+2} + \cdots + S_{i+R-1}) + \cdots + S_{i+R-3} \cdot (S_{i+R-2} + S_{i+R-1}) + S_{i+R-2} \cdot S_{i+R-1} \}$$

(2.10)

The Hamiltonian, $H[B_R]$, of the spin chain made up of $B_R$ units is the sum of all block Hamiltonians associated with each site. Thus, $H[B_R] = J \sum_{i=1}^L h_i[B_R]$, where $J$ is taken to be positive. For simplicity, we will denote $H[B_R]$ by $H_R$. Since there are exactly $(R-1)$ number of first neighbour (nearest neighbour) pairs, $(R-2)$ number of second neighbour pairs and so on, within each $B_R$ unit, the Hamiltonian of $B_R$ spin chain can be written the following form.

$$H_R = J \sum_{i=1}^L \{ (R - 1) S_i \cdot S_{i+1} + (R - 2) S_i \cdot S_{i+2} + \cdots + 2 S_i \cdot S_{i+R-2} + S_i \cdot S_{i+R-1} \}$$

$$= J \sum_{i=1}^L \sum_{n=1}^{R-1} (R - n) S_i \cdot S_{i+n}$$

(2.11)
2.3 Models with exact dimer ground states

Clearly, $\mathcal{R}$ acts as a family parameter which generates different Hamiltonians. It also signifies the range of the exchange interaction in the model. Thus, on a $\mathfrak{B}_\mathcal{R}$ spin chain, $i^{th}$ spin is coupled only with next $(\mathcal{R} - 1)$ neighbours. As is evident from Equation 2.11, the strength of the exchange interaction decreases linearly with the separation between coupled spins. Therefore, we call this class of 1D quantum spin models as the linear exchange spin models. Note that the Hamiltonian corresponding to $\mathcal{R} = 2$, that is $H_2$, is the nearest neighbour Heisenberg model. The MG model with exact dimer ground state corresponds to the case of $\mathcal{R} = 3$.

Earlier, we had argued that the Hamiltonians with odd integer values of $\mathcal{R}$, that is $\mathcal{R} = 2\nu + 1$, may admit an exact solution for their ground states, like the MG model. In the following discussion, we will see that this indeed turns out to be true. In fact the two dimer states of Equations 2.2 and 2.3 form the exact ground states of the linear exchange Hamiltonians, for all odd integer values of parameter $\mathcal{R}$. We will also discuss the case when $\mathcal{R}$ is an even integer, that is $\mathcal{R} = 2\nu$. We will point out the qualitative difference between these two subclasses of the linear exchange 1D spin models. We will refer to them as the odd and the even family of linear exchange models, or simply, the odd and even family.

### 2.3 Odd family : models with exact dimer ground states

The topic of discussion in this section is the odd sub-family of the linear exchange spin chains. The Hamiltonian, $H_{2\nu+1}$, of the odd-family is:

$$H_{2\nu+1} = J \sum_{i=1}^{L} \left\{ 2\nu \mathbf{S}_i \cdot \mathbf{S}_{i+1} + (2\nu - 1) \mathbf{S}_i \cdot \mathbf{S}_{i+2} + \cdots + 2 \mathbf{S}_i \cdot \mathbf{S}_{i+2\nu-1} + \mathbf{S}_i \cdot \mathbf{S}_{i+2\nu} \right\}$$

$$= J \sum_{i=1}^{L} \sum_{n=1}^{2\nu} (2\nu + 1 - n) \mathbf{S}_i \cdot \mathbf{S}_{i+n}$$

(2.12)

where $\nu$ is a positive integer. This is $H_\mathcal{R}$ for $\mathcal{R} = 2\nu + 1$. We will now find its exact ground state, and also study its elementary excitations in some detail.

#### 2.3.1 The ground state

In order to find the ground state energy and the corresponding eigen-configurations of $H_{2\nu+1}$, consider the minimum energy configurations for a $\mathfrak{B}_{2\nu+1}$ unit. Re-writing $h_{i[\mathfrak{B}_{2\nu+1}]}$ as $\frac{1}{2} \left[ (\mathbf{S}_i + \mathbf{S}_{i+1} + \cdots + \mathbf{S}_{i+2\nu})^2 - (\mathbf{S}_i^2 + \mathbf{S}_{i+1}^2 + \cdots + \mathbf{S}_{i+2\nu}^2) \right]$ tells us that the total spin,
\[\sum_{n=0}^{2\nu} S_{i+n},\] being minimum corresponds to the lowest energy of the block. For \(S = 1/2\), the minimum energy is \(-3\nu/4\), and the corresponding spin configurations are such that there is exactly one free spin while rest \(2\nu\) spins forming a block-singlet. A block-singlet can be described in terms of the bond-singlets (dimers or valence bonds, as we often call them so). Since there are many, independent ways of doing that, a block-singlet has an intrinsic degeneracy of dimer configurations. All this has been discussed sufficiently in the previous section. Now let us see how these things help us in finding the exact ground state of \(H_{2\nu+1}\).

If we can find a configuration where every block of successive \((2\nu + 1)\) spins has exactly one block-singlet of \(2\nu\) spins, then it is the ground state configuration of \(H_{2\nu+1}\). The meaning of this statement can be understood as follows. Every spin \(S_i\) together with its next \(2\nu\) neighbours makes a \(\mathcal{B}_{2\nu+1}\) block. The minimum energy configuration of \(\mathcal{B}_{2\nu+1}\) consists of a block singlet of \(2\nu\) spins and a free spin. If for a given spin configuration of the full chain, every \(\mathcal{B}_{2\nu+1}\) unit on the spin chain is simultaneously able to achieve its lowest energy eigenstate, then the given configuration is necessarily the ground state of \(H_{2\nu+1}\). This is ensured by Inequality 2.7, since the energy of such a state (if one is able to find) will be same as the lower bound to the ground state energy, that is \(-(3J\nu/4)L\). Let us try to construct such a configuration for \(\mathcal{B}_{2\nu+1}\) spin chain.

Consider a \(\mathcal{B}_5\) chain for explicitness. One can easily check that the dimer configurations of Figure 2.1 satisfy the criterion as stated above for a possible ground state configuration. Since every block of successive five spins contains exactly two dimers, each \(\mathcal{B}_5\) is able to satisfy its minimum energy configuration. Therefore, dimer states \(|\psi_{g1}\rangle\) and \(|\psi_{g2}\rangle\), as given in Equation 2.2 and 2.3, are also the exact ground state configurations of \(H_5\). But at the level of an individual unit, there are other dimer configurations which are allowed for the lowest energy state of the block. Consider spins sitting at sites 1 to 5. The state \([1,2]\otimes[3,4]\otimes|\uparrow_5\rangle\) is one configuration. One of the other configurations is \([1,[2,3],4]\otimes|\uparrow_5\rangle\), where \([1,[2,3],4]\) stands for \([2,3]\otimes[4,1]\). The problem arises when the configurations of latter type are part of the full chain configurations. One such state is shown.
in Figure 2.5 where block of spins at sites 5 to 9 does not have two complete dimers. The block is not able to achieve its minimum energy state. Therefore, state in Figure 2.5 does not qualify for being the ground state of $H_5$. In fact one can check that it is not even an eigen state.

The above considerations go through for all $H_{2^\nu+1}$, and are not specific to $H_5$. Since the fundamental blocks of bigger size have higher degeneracy of dimer representation, one might think that it may give rise to more number of ground state configurations for $H_{2^\nu+1}$. But the fact that we have successive blocks with maximal overlap (one can not have successive block any nearer than being nearest neighbours) suppresses other choices of dimer configurations. The one shown in Figure 2.5 is a typical example of this type.

The two dimer state, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, are the only ones which qualify as the exact ground state of $H_{2^\nu+1}$ for all positive integer values of $\nu$. Thus, we have:

$$H_{2^\nu+1} \left\{ |\psi_{g1}\rangle \langle \psi_{g1}| + |\psi_{g2}\rangle \langle \psi_{g2}| \right\} = -\frac{3J\nu}{4L}$$

(2.13)

The following identities are straight forward generalization of the identities given in Equations 2.5 and 2.6, and are used in proving that $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ form the exact ground state of $H_{2^\nu+1}$.

$$(S_{i_1} + \cdots + S_{i_{2\nu}}) \cdot S_{i_{2^\nu+1}} [i_1, i_2, \ldots, i_{2\nu}] = 0$$

(2.14)

$$\sum_{j_1=1}^{2\nu-1} \sum_{j_2>j_1}^{2\nu} S_{i_{j_1}} \cdot S_{i_{j_2}} [i_1, i_2, \ldots, i_{2\nu}] = -\frac{3\nu}{4}$$

(2.15)

where $[i_1, i_2, \ldots, i_{2\nu}]$ denotes a block singlet of $2\nu$ spins, and all the site indices are distinct. In the Equation 2.14, $i_{2\nu+1} \notin \{i_1, i_2, \ldots, i_{2\nu}\}$.

In the following subsection, we give another proof of $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ being the ground state configurations of $H_{2^\nu+1}$ for all values of $\nu$, despite the fact that we have already shown it. The proof is based on the principle of mathematical induction. This approach also reveals an interesting property of superstability [9] of the ground state dimer configurations. The idea of superstability is like this. An eigen state, $|\phi\rangle$, of some Hamiltonian, $H$, is called superstable if it is also the eigen state of the operator $H + V$, for a certain operator $V$ where the commutator, $[H, V] \neq 0$. To make a definitive statement about the superstability, we should clearly understand the relationship between successive Hamiltonians in the family. The proof by induction is based on the understanding of such relationships, and hence illustrates the superstability of the dimer configurations as the ground state of our family of Hamiltonians, in a rigorous way.
2.3.2 Proof by induction

The Hamiltonian, \( H_{2\nu+1} \), has an integer index \( \nu \). For \( \nu = 1 \), the Hamiltonian is \( H_3 = H_{MG} \). It is known that the dimer states \(|\psi_{g1}\rangle\) and \(|\psi_{g2}\rangle\) are the exact ground state configurations of \( H_{MG} \). Hence, we have:

\[
H_3 \left\{ \begin{array}{c}
|\psi_{g1}\rangle \\
|\psi_{g2}\rangle
\end{array} \right\} = -\frac{3J}{4} L \left\{ \begin{array}{c}
|\psi_{g1}\rangle \\
|\psi_{g2}\rangle
\end{array} \right\} \quad (2.16)
\]

Assume that \(|\psi_{g1}\rangle\) and \(|\psi_{g2}\rangle\) are also the eigenstates of \((\nu - 1)^{th}\) member in the family, with eigen energy \( E_{2\nu-1} \) (for the sake of this proof ignore the fact that we have already proved it!). That is,

\[
H_{2\nu-1} \left\{ \begin{array}{c}
|\psi_{g1}\rangle \\
|\psi_{g2}\rangle
\end{array} \right\} = E_{2\nu-1} \left\{ \begin{array}{c}
|\psi_{g1}\rangle \\
|\psi_{g2}\rangle
\end{array} \right\} \quad (2.17)
\]

Now, we consider the \( \nu^{th} \) Hamiltonian \( H_{2\nu+1} \), which for \( \nu > 1 \), can be re-written in the following way.

\[
H_{2\nu+1} = J \sum_{i=1}^{L} \sum_{n=1}^{2\nu} (2\nu + 1 - n) S_i \cdot S_{i+n}
\]

\[
= H_{2\nu-1} + J \sum_{i=1}^{L} \left\{ S_i \cdot S_{i+2\nu} + 2 \sum_{n=1}^{2\nu-1} S_i \cdot S_{i+n} \right\}
\]

\[
= H_{2\nu-1} + H_3 + J \sum_{i=1}^{L} \{ S_i \cdot S_{i+2} + 2S_i \cdot (S_{i+3} + \cdots + S_{i+2\nu-1}) + S_i \cdot S_{i+2\nu} \}
\]

\[
= H_{2\nu-1} + H_3 + J \sum_{i=1}^{L} (S_i + S_{i+1}) \cdot (S_{i+3} + \cdots + S_{i+2\nu}) \quad (2.18)
\]

One can easily show that

\[
\sum_{i=1}^{L} (S_i + S_{i+1}) \cdot (S_{i+3} + \cdots + S_{i+2\nu}) \left\{ \begin{array}{c}
|\psi_{g1}\rangle \\
|\psi_{g2}\rangle
\end{array} \right\} = 0 \quad (2.19)
\]

Clearly, from Equations 2.18 and 2.19, \( H_{2\nu+1} |\psi_{g1,2}\rangle = (E_{2\nu-1} - (3J/4) L) |\psi_{g1,2}\rangle \). This proves that \(|\psi_{g1}\rangle\) and \(|\psi_{g2}\rangle\) are also the eigen configurations of \( H_{2\nu+1} \), and we get the following relation for the energy eigenvalue, \( E_{2\nu+1} \).

\[
E_{2\nu+1} = E_{2\nu-1} - (3J/4) L \quad (2.20)
\]

Since, \( E_1 = -(3J/4) L \), this gives \( E_{2\nu+1} = -(3\nu J/4) L \). The value of \( E_{2\nu+1} \) that we get here is same as the lower bound of the Inequality 2.7, therefore the states \(|\psi_{g1}\rangle\) and \(|\psi_{g2}\rangle\) are
2.3 Models with exact dimer ground states

also the ground states. Thus, we have been able to prove that the dimer configurations, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, form a superstable, two-fold degenerate ground subspace of the whole family of $H_{2\nu+1}$, parameterized by a positive integer $\nu$, on a one dimensional lattice with PBC.

The summary of our findings for the odd family of linear exchange spin chains is the following:

- A family of spin models with exact dimer ground state is constructed. The ground subspace is two-fold degenerate.

- The general Hamiltonian of the family is: $H_{2\nu+1} = J\sum_{i=1}^{L}\sum_{j=1}^{2\nu}(2\nu + 1 - j)S_i \cdot S_{i+j}$. Here, $J > 0$, $\nu$ is a positive integer and $\mathcal{B}_{2\nu+1}$ refers to the fundamental building blocks for different members of the family. Note that the Hamiltonian has translational invariance, the exchange coupling decrease linearly with distance between the coupled neighbours, and for a given $\nu$, every spin is coupled only up to $2\nu^{th}$ neighbour, starting from the nearest one.

- The ground state energy, in units of the strongest exchange coupling (the nearest neighbour coupling, $2\nu J$), is $-\frac{3}{8}L$, for all members of the family.

- The dimer states, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, are superstable ground state configurations with respect to all members of the family.

Having described in detail the construction, and the exact ground state of this family of one dimensional spin models, let us discuss the nature of their elementary excitations.

2.3.3 Low energy elementary excitations

The question of the low lying elementary excitations in the MG model was first addressed by Shastry and Sutherland [10]. They proposed an elegant and simple physical construction for the low energy excited states. The idea is that two degenerate ground state configurations will always admit a domain boundary defect. And these domain walls or kinks may have dispersion. In the case of the MG model, a dangling spin will act as the kink between two degenerate ground state configurations, and can hop from one site to another, thus acquiring a finite dispersion. These kink states are the low-lying elementary excitations proposed and studied variationally by Shastry and Sutherland. Figure 2.6 shows a domain boundary state for the MG model. The set of all such kink states, $\{|2r\rangle\}$, is not a complete set under the action of $H_{MG}$, and hence only a variational choice. Nevertheless, it is a good physical choice. They also found an energy gap in the
excitation spectrum with respect to the dimer ground state. Later, the existence of the energy gap in the spectrum of the MG model was proved exactly by Affleck, Kennedy, Lieb and Tasaki [11].

![Diagram of a defect configuration](image)

Figure 2.6: This is one of the defect configurations with dangling spin being ↑, at site 2r. The polarization of the dangling spin can be ↓ as well, without affecting the dispersion relation.

We have calculated the dispersion relation for propagating kink states, variationally, for \( B_3 \), \( B_5 \) and \( B_7 \) chains, following the procedure given by Shastry and Sutherland. In fact the calculation for \( B_3 \) is already given in Reference [10], and we re-did it to learn it. The procedure of calculation is same for all members of the family since they all have the same ground state. From these dispersion relations, we find that the energy gap towards such kink excitations exists for each of these members of the family, and seems to increase monotonically for higher members in the family. We have not done a general calculation, covering all members of the family. We only chose to do the calculations for first three members, in order to get an idea of the nature of elementary excitations. In our calculation, we just study the case of a free kink, and don’t consider the situations where there can be bound states of two or more kinks. We know from the work of Shastry and Sutherland that the bound pairs of kink excitations are higher in energy, and lie well above the gap.

The dispersion relation of a kink excitation for \( B_3 \) is \( E_3(k) = \frac{5}{4} + \cos(2k) \). This is already known from Reference [10]. The lattice parameter, \( a \), is taken to be unity, and \(-\pi/2 \leq k \leq \pi/2\). The excitation energies of a domain wall for the next two members of the family, that is \( B_5 \) and \( B_7 \), are the following.

\[
E_5(k) = 2 + \frac{3}{4} \cos(2k) - \frac{1}{2} \cos(4k)
\]

\[
E_7(k) = \frac{11}{4} + \frac{3}{4} \cos(2k) - \frac{3}{8} \cos(4k) + \frac{1}{4} \cos(6k)
\]

The excitation energy, \( E_{2\nu+1}(k) \), is defined as

\[
E_{2\nu+1}(k) = \frac{\langle k | H_{2\nu+1} | k \rangle - E_\nu}{\langle k | k \rangle}
\]

where \( E_\nu = -\frac{3}{4} \nu N \); \( N \) is the total number of \( B_{2\nu+1} \) units forming a finite chain of \( L \) sites. \( N = L \) for a chain with PBC, and \( N = L - 2\nu \) for an open chain. Actually, in our
2.3 Models with exact dimer ground states

calculation, we consider an open spin chain with odd number of sites, \( L = 4M + 1 \), and take the limit \( M \to \infty \). The ket, \( |k\rangle \) is defined as,

\[
|k\rangle = \frac{1}{\sqrt{2M+1}} \sum_{r=-M}^{M} e^{ikr} |2r\rangle
\]  
(2.24)

The ket, \( |2r\rangle \), as shown in Figure 2.6, is a configuration where there is a dangling spin at \( 2r^{th} \) site, and the rest forming the dimer configuration of \( |\psi_{g1}\rangle \) type on one side of the dangling spin and of \( |\psi_{g2}\rangle \) type on the other side. The dangling spin can have either \( \uparrow \) polarization or \( \downarrow \) polarization without affecting the dispersion relation of the defect. These defect configurations are non-orthogonal. Since \( \{ |2r\rangle \} \) do not form a complete set of states, the defect “Bloch” state, \( |k\rangle \), is only a variational choice. Let us briefly discuss why \( \{ |2r\rangle \} \) is not a complete set.

Consider, for example, the calculation for \( H_3 \). The ket, \( |2r\rangle \), is such that it does not satisfy \( \mathfrak{B}_3 \) unit consisting of spins at sites \((2r-1), 2r \) and \((2r + 1)\). The action of this unhappy block is to disperse the kink. This can be understood by operating on \( |2r\rangle \) by operators, \((2S_{2r-1} \cdot S_{2r} - \frac{1}{2})\), \((2S_{2r} \cdot S_{2r+1} - \frac{1}{2})\) and \((2S_{2r-1} \cdot S_{2r+1} - \frac{1}{2})\). These operators, put together appropriately, make \( h_{2r-1} \mathfrak{B}_3 \). It is convenient to use them, since their action on \( |2r\rangle \) is simply expressed, as given below.

\[
\left(2S_{2r-1} \cdot S_{2r} - \frac{1}{2}\right) |2r\rangle = |2r - 2\rangle
\]  
(2.25)

\[
\left(2S_{2r} \cdot S_{2r+1} - \frac{1}{2}\right) |2r\rangle = |2r + 2\rangle
\]  
(2.26)

\[
\left(2S_{2r-1} \cdot S_{2r+1} - \frac{1}{2}\right) |2r\rangle = |2r\rangle^\ast
\]  
(2.27)

The ket \( |2r\rangle^\ast \) is different from \( |2r\rangle \) in the following sense. The singlet bonds, \( |2r-2, 2r-1\rangle \) and \( |2r+1, 2r+2\rangle \) on either sides of the dangling spin at \( 2r \) in the ket \( |2r\rangle \), are re-adjusted to form two new singlet bonds, \( |2r-2,2r+2\rangle \) and \( |2r-1,2r+1\rangle \) under the action of operator, \( (2S_{2r-1} \cdot S_{2r+1} - \frac{1}{2}) \). This new configuration, with dangling spin still at site \( 2r \), is the ket \( |2r\rangle^\ast \). This state can be decomposed into the states belonging to set \( \{ |2r\rangle \} \) and states which are not in this set of the domain boundary states. Figure 2.7 illustrates the same fact graphically. It is due to this reason that the kink states do not form a complete set under the action of \( H_3 \). The same is true for other Hamiltonians in the family. In fact higher members generate more complicated configurations, and thus enhancing the complexity of the calculation.

From the dispersion relation of the kink excitation, we find that there is an energy gap. At the Brillouin zone boundary, \( k = \pm \pi/2 \), the energy of the excitation is minimum,
but not zero, as can be seen from the Equations 2.21 and 2.22 which give the dispersion relations for $B_5$ and $B_7$ chains respectively. The energy gap, in units of the nearest neighbour exchange interaction, for $B_3$, $B_5$ and $B_7$ spin chains, is $1/8$, $3/16$ and $11/48$, respectively. Presently, we have not been able to identify any simple relation between the members of the odd family and the corresponding energy gaps, nonetheless we see that there is a gap, and it seems to be increasing as we go up in the hierarchy. With this, we close our discussion on the nature of the elementary excitations in odd sub-family of the linear exchange models of spin-1/2 objects.

\[
|2r\rangle^* = \begin{array}{c}
|2r\rangle^* = \\
= \\
+ \\
+ \\
+ \\
\end{array}
\]

\[
\begin{array}{c}
2r-2 & 2r-1 & 2r & 2r+1 & 2r+2 \\
2r-2 & 2r & 2r-2 & 2r & 2r+2 \\
2r & 2r+2 \\
2r & 2r+2 \\
\end{array}
\]

Figure 2.7: Linear superposition of $|2r\rangle^*$ in terms of the kink states of set $\{|2r\}\}$, and other states with a dangling spin.

### 2.4 Even family of the linear exchange models

Having discussed the exact ground state of the odd family Hamiltonians in great detail, an obvious question that one can ask is what about the even family. As we will see, the
nature of the ground state of even family models is apparently qualitatively different from
the odd family models. Although we have no exact ground state solution for this class
of models, we will try to convince ourselves of the qualitative differences by some simple
observations. But the dimer ground state of the odd family also becomes the exact ground
state of the even family in the asymptotic limit, when the range parameter $R$ is infinitely
large in a thermodynamically large spin chain. Thus, the odd-even disparity disappears
when the exchange coupling becomes thermodynamically long ranged. There is not much
that we can say in exact terms about this family, nevertheless we will present all that we
find interesting.

First, let us write the Hamiltonian of the family. It is $H_R$ with $R = 2\nu$ where as usual,$\nu$ is a positive integer. The Hamiltonian is:

\[ H_{2\nu} = J \sum_{i=1}^{L} h_i [B_{2\nu}] \]
\[ = J \sum_{i=1}^{L} \sum_{n=1}^{2\nu-1} (2\nu - n) S_i \cdot S_{i+n} \]  

(2.28)

We will consider two cases. One where $2\nu$ is a finite number, and two, when $2\nu$ is of
the order of system size ($\sim L/2$), with $L \to \infty$. In the first case, we will present some
simple observations and arguments in relation to the nature of the ground state in these
models. For the second case, we will present a rigorous proof of the fact that the dimer
configurations, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, also form the exact ground state of the even family.

### 2.4.1 Finite range

Consider $\nu = 1$, the first members of both the even and the odd families of the linear
exchange models. For odd family, it is the MG model, described by the Hamiltonian, $H_3$.
For even family, the first member is the well known nearest neighbour Heisenberg antifer-
romagnet, $H_{nn}$. We have $H_{nn} = H_2$ in our notation. $H_2$ is an integrable model, whose exact
solution by Bethe ansatz is a landmark in the history of mathematical physics [12, 13].
Let us compare the nature of the ground state and the elementary excitations of $H_2$ and
$H_3$.

The ground state of spin-1/2, antiferromagnetic $H_2$ Hamiltonian has algebraically
declining, but long ranged correlations. The ground state of $H_3$, on the other hand, has
ultra-short ranged spin correlations. Only the nearest neighbouring spins are correlated
in the ground state configurations of $H_3$. Both $H_2$ and $H_3$ have low-lying, spin-1/2, spinon
excitations above their antiferromagnetic ground states. But the elementary excitations
of \(H_2\) are gap-less whereas that of the \(H_3\) are gapped. So, we know how the first members of the odd and the even families differ. Now let us discuss the higher members. All the higher members of the odd family have same ground state as \(H_3\), and the nature of elementary excitations is also the same. Let us look at the even family members in the block Hamiltonian way, and see what happens there.

In \(H_2\), we have the nearest neighbouring pairs of spins forming \(B_2\). The minimum energy configuration for the (antiferromagnetic) \(B_2\) is the singlet state of the pair. Since, the successive blocks share one common spin, it is not possible to achieve the singlet state for each block. And therefore, what we have as the ground state of \(H_2\), is a highly non-trivial combination of various spin configurations. The ground state is exactly known by Bethe ansatz, and has power law antiferromagnetic spin correlation. Qualitatively speaking, each block in the chain, is unable to satisfy its lowest energy configuration simultaneously. And therefore, they settle to a state where all of them are “partially” happy.

If we look at the higher members of the even family, i.e. \(H_4\), \(H_6\) etc., then we realize that these Hamiltonians also can not have a simple dimer ground state. For any two successive blocks, there is an odd number of spins that are common. This rules out the possibility of sharing a common dimer. In fact the situation here is like \(H_2\). And hence, the ground state of the even family Hamiltonians can not be simply determined like that of the odd family. We expect that some signatures of a ground state property, like the power law spin correlation in \(H_2\), will carry over to higher members. In order to see this, we consider a simpler situation of Ising model on linear exchange chains. This is the classical version of the spin-1/2 quantum chains. We study the ground state configurations of the linear exchange Ising models. We will find below some interesting difference between the odd and the even Ising families, which may have some bearing upon the different nature of the ground state spin correlations in the fully quantum mechanical models of this chapter.

The rule for finding the Ising ground state configurations is the same. The sum of all \(\sigma\)’s (the Ising variables) within a block should be minimum. For odd sized blocks, the minimum total \(\sigma\) is either \(\uparrow\) or \(\downarrow\). For even blocks, it is zero. All we have to do is to find out the appropriate Ising configurations for a given member of the linear exchange Ising chains such that all blocks simultaneously minimize their total Ising spin. We denote the Ising ground state of the \(R^{th}\) member by \(|I_R\rangle\). Given below are the Ising ground states for a few members of the Ising linear exchange family. We express the states in terms of the Ising variable \(\sigma\), and \(\bar{\sigma}\) denotes the opposite of \(\sigma\). In our notation, successive \(\sigma\)’s correspond to the value of Ising variables on the successive sites. For example, \(|\sigma\sigma\rangle\)
denotes both sites having same value of the Ising spin, that is either $|↑↑⟩$ or $|↓↓⟩$.

$$|I_2⟩ = |σσσσσ...⟩$$  \hspace{1cm} (2.29)

$$|I_3⟩ = |σσσσσσ...⟩$$  \hspace{1cm} (2.30)

It is clear that $|I_2⟩$ has Néel order. In $|I_3⟩$, $σ^1$, $σ^2$ etc. are all independent of the value of each other, and therefore, the ground state is $3 \times 2 \times 2^{L/3}$ fold degenerate. The quantum mechanical ground state of $H_2$ seems to retain partially the character of the Ising ground state $|I_2⟩$. The exponentially degenerate $|I_3⟩$ state, however, turns into a dimer state with ultra-short ranged spin liquid character in the fully quantum mechanical case. The Ising ground state $|I_4⟩$ can be written in the following two ways.

$$|I_4⟩ = |σσσσσ...⟩$$  \hspace{1cm} (2.31)

or

$$= |σσσσσσσσσ...⟩$$  \hspace{1cm} (2.32)

Let us denote the zero spin Ising configurations for $B_4$, $σσσσ$ and $σσσσ$, as $Σ_4$. In general, $Σ_{2ν}$ denotes all zero spin Ising configurations for $B_{2ν}$. There are total $2^νC_ν$ number of distinct such configurations for a $B_{2ν}$ block. With this notation, we can, for example, denote $|I_5⟩$, $|I_6⟩$ and $|I_7⟩$ in the following ways.

$$|I_5⟩ = |Σ_4σ_1Σ_4σ_2Σ_4σ_3Σ_4...⟩$$  \hspace{1cm} (2.33)

$$|I_6⟩ = |Σ_6Σ_6Σ_6Σ_6Σ_6Σ_6...⟩$$  \hspace{1cm} (2.34)

$$|I_7⟩ = |Σ_6σ_1Σ_6σ_2Σ_6σ_3Σ_6...⟩$$  \hspace{1cm} (2.35)

The most important thing to note is that the degeneracy of the even Ising ground states is considerably low as compared with that of the odd Ising ground states. The state $|I_{2ν}⟩$ is $2^νC_ν$ fold degenerate, whereas the state $|I_{2ν+1}⟩$ has a degeneracy of $(2ν + 1) \times 2^νC_ν \times 2^{L/(2ν+1)}$ Ising configurations. The former is independent of $L$, whereas the latter is exponential in $L$. This is a serious difference. Even at the Ising level of description, the effect of frustration, in terms of degeneracy, is less severe for the even family than the odd family. Thus, for the even family of finite ranged linear exchange quantum spin models, we expect the ground state to have power law spin correlations. In the asymptotic limit however, when $R \sim L/2$ and $L$ is infinitely large, the degeneracies of the ground state Ising configurations in the even and the odd families, become comparable (with same entropy density $\sim \frac{1}{2} \ln 2$). That is to say that the distinction between odd and even families of the linear exchange models seems to vanish in the asymptotic limit. And therefore in this limit, one may expect the ground state to be same in both the cases for the quantum models as well. Later, we will rigorously prove that this is indeed the case.
Before moving onto the proof of exact dimer ground state in the asymptotic limit, we also present a few numerical exact diagonalization calculations. These are shown in Figure 2.8. It is clear from the ground state energy and the correlation function plots that the finite range even and odd models have different ground states, but the difference seems to disappear in the asymptotic limit. Two things which should be noticed about the nature of the ground state spin correlation are the following. One, the nearest neighbour correlation approaches the value of 0.125 (the dimer ground state spin correlation value) as $R$ increases while the farther distance correlations are vanishing faster. This is as we had anticipated. And two, a reasonable revival of the spin correlation at the distance of $R$. In the $B_4$ chain, for example, there is a slight rise in the value of $\langle S_i^zS_j^z \rangle$ when $|i - j| = 4$. For a $B_6$ chain the same thing happens for $|i - j| = 6$, and so on. We can understand this phenomenon by looking at the Ising states $|I_4\rangle$, $|I_6\rangle$ etc. There, a spin at site $i$ strictly decides the spin value at site $i + R$. But for the intermediate separations, it is not so due to degeneracy. Since the degeneracy of the block Ising configurations is not large for small $R$, it appears as if the quantum fluctuations have not fully diluted the spin correlation. One would in principle see similar, but weaker, revivals in spin correlations for distances, $2R$, $3R$ and higher integer multiples of $R$. We can not see them here since the chain lengths can not be very large, due to limitations of the numerical computation [14].

Figure 2.8: The exact diagonalization results for the linear exchange spin chains of length, $L = 20$. (a) The ground state energy, $E_g$, of the even and the odd family models, in units of their nearest neighbour couplings. (b) The spin correlation function for different members of the even family.
2.4 Even family

2.4.2 Infinite range

We, now, consider the case of $\nu$ being infinitely large. We expect that the dimer configurations of Equations 2.2 and 2.3, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, will form the exact ground state of $H_{2\nu}$ in the asymptotic limit. In order to check whether it is so or not, we do the following things.

1. Find the expectation value of $H_{2\nu}$ in the dimer states $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, for finite $\nu$ and $L$. This gives us the energy expectation, $E_{2\nu}(L)$, of the even family Hamiltonians with finite range exchange interaction on finite length spin chains.

2. Find the fluctuation, $\Delta E_{2\nu}(L)$, in the energy around the expectation value, $E_{2\nu}(L)$, in the dimer states.

3. Let $2\nu \sim O(L)$, say $L/2$. Rescale the exchange coupling, $J$ as $J/(2\nu - 1)$, such that the energy remains extensive. Take the limit $L \to \infty$, and see how $\Delta E_{2\nu}(L)$ behaves in this limit.

Step 3 is the most important of all for deciding whether the dimer configurations form the exact eigenstate of the Hamiltonian or not. If $\Delta E_{2\nu}(L)$ goes to zero in the asymptotic limit, then it proves that the dimer states, $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ are indeed the exact eigenstates. To check whether they also form the ground state in the asymptotic limit, we will once again consider the Inequality 2.7. If $\Delta E_{2\nu}(L)$ is non zero, then clearly the dimer states are not the exact eigenstates of the system.

Any even family Hamiltonian $H_{2\nu+2}$ can be written as: $H_{2\nu+2} = H_{2\nu+1} + V_{2\nu+1}$, where

$$V_{2\nu+1} = J \sum_{i=1}^{L} S_i \cdot [S_{i+1} + S_{i+2} + \cdots + S_{i+2\nu+1}]$$

(2.36)

Since the dimer states are the ground states of $H_{2\nu+1}$, all the variance in the expectation value of $H_{2\nu+2}$ in the dimer states, comes from $V_{2\nu+1}$. The energy expectation value, $E_{2\nu+2}(L) = -(3\nu J/4)L + \langle V_{2\nu+1} \rangle$, where $\langle V_{2\nu+1} \rangle$ denotes the expectation value of $V_{2\nu+1}$ in the states $|\psi_{g1}\rangle$ or $|\psi_{g2}\rangle$. The energy fluctuation, $\Delta E_{2\nu+2}(L)$, in the dimer states can be written as:

$$\Delta E_{2\nu+2}(L) = \sqrt{\langle V_{2\nu+1}^2 \rangle - \langle V_{2\nu+1} \rangle^2}$$

(2.37)

Both for $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$, we find that

$$\langle V_{2\nu+1} \rangle = -\frac{3J}{8}L \quad \text{(2.38)}$$

and

$$\langle V_{2\nu+1}^2 \rangle = \frac{9J^2}{64}L^2 + \frac{3J^2}{32}L$$

(2.39)
Therefore, the energy expectation value and the energy fluctuation of $H_{2\nu+2}$ in the dimer states are

$$E_{2\nu+2}(L) = -\frac{3}{8}(2\nu + 1)JL \quad (2.40)$$

$$\Delta E_{2\nu+2}(L) = \frac{J}{2} \sqrt{\frac{3L}{2}} \quad (2.41)$$

Since the energy scales as $(2\nu + 1)$, it will become super-extensive for $\nu \sim \mathcal{O}(L)$. In order to make the energy extensive, we rescale $J$ as $J/(2\nu + 1)$. Now, take $(2\nu + 2) = L/2$. In the asymptotic limit $L \to \infty$, the energy fluctuation $\Delta E_{2\nu+2}(L) \to 0$. This proves that the dimer states $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ are exact eigenstates of the even family models in the asymptotic limit. As to the question of their also being the ground state, consider the energy density,

$$E_{2\nu+2}(L)/L = -\frac{3}{8} \cdot \frac{(2\nu + 2)}{(2\nu + 1)}JL.$$ 

It clearly shows that in the asymptotic limit, the lower bound to the ground state energy density is also $-3J/8$. This proves that the dimer states $|\psi_{g1}\rangle$ and $|\psi_{g2}\rangle$ are the exact ground states of the even family in the asymptotic limit.

### 2.5 Connection with the 1D Coulomb problem

In one dimensional space, the Coulomb potential, $v(x)$, at a point $|x|$ distance away from the point charge $Q$, is given as

$$v(x) = -\frac{Q}{2} |x| \quad (2.42)$$

Therefore, the Coulomb interaction energy in one dimension between two point charges $Q$ and $Q'$, placed at positions given by $x$ and $x'$, is $-QQ'|x - x'|/2$. The one dimensional Coulomb potential as given in Equation 2.42, can easily be derived by taking the Fourier transformation of $1/k^2$, where $k$ is the variable reciprocal to $x$, and $1/k^2$ comes from the Poisson equation for a point source charge. The classical statistical mechanics of one dimensional many particle Coulomb system was studied exactly by Lenard and Baxter long ago [16, 17, 18]. Lenard considered the case where there are equal number of positively and negatively charged particles of same mass. The main results of their studies in the thermodynamic limit are: (1) in the high temperature limit, the plasma behaves like an ideal gas of $2N$ particles, where $N$ is the number of each type of particles, and (2) in the low temperature limit, the system behaves like an ideal gas of $N$ (and not $2N$) particles. Lenard was able to explain it by supposing that in this limit particles exist in tightly bound pairs, each pair having net zero charge. Thus, the system essentially acts like an ideal gas of $N$ neutral molecules at low temperatures.
2.5 Connection with 1D Coulomb problem

It is interesting to observe that in the linear exchange models that we constructed in the previous sections, the exchange coupling, $J_{ij} \propto (R - |i - j|)$, is exactly like the Coulomb interaction in one dimension, albeit with a range $R$ [15]. Spins separated by $R$ or more sites have no exchange interaction, and $R$ can be any positive integer greater than or equal to 2, as discussed earlier. Hence, what we have found, essentially, is a quantum spin analogue of the one dimensional Coulomb problem. It is an interesting and unexpected connection. In fact the connection appears more interesting when we compare the low temperature thermodynamic state of the Coulomb problem and the ground state of the linear exchange quantum antiferromagnets. At low temperatures, the 1D Coulomb system goes into a state where oppositely charged particles tend to form bound pairs, and very much similar to the bound pair Coulomb state, the ground state of the spin models has spin dimers. For odd subfamily this is true for any $R$. For even subfamily, this is rigorously shown to be true only for $R$ being infinitely large in the thermodynamic limit. Analogous to the Coulomb problem, one would also expect plasmon like gapped excitations in a spin model with infinitely long ranged, linear exchange coupling. For antiferromagnetic exchange coupling, that we discussed in the previous sections, there exists an energy gap. But the analogy has interesting consequences for the spin models with ferromagnetic linear exchange coupling.

The Hamiltonian for the ferromagnetic case can be obtained simply by replacing $J$ by $-J$ in Equation 2.11. This is written as: $H = -J \sum_{i=1}^{L} \sum_{m=1}^{R-1} (R - m) S_i \cdot S_{i+m}$, where $J > 0$ and $R$ can be any positive integer (with no distinction between odd or even) greater than or equal to two. The ground state energy for a general spin $S$ is, $E_g = -JS^2R(R - 1)L/2$. And the exact one magnon dispersion with respect to the ground state energy is:

$$E(k) = JS \left\{ R^2 - \frac{1 - \cos(Rk)}{1 - \cos(k)} \right\}$$

(2.43)

for $k = 2n\pi/L$, where is $n$ is an integer. The wavenumber, $k$, takes values between $-\pi$ and $\pi$. For any finite $R$, $E(k) \to 0$ quadratically, as $k \to 0$. Hence, the excitations are gap-less. In order to consider the analogue of Coulomb problem, $R$ should of the order of $L$, and let $L$ go to infinity. We put $R = L/2$, and rescale $J$ to $J/R^2$ (as the ground state as well as the magnon excitation energy goes as $R^2$ for large $R$). We get the rescaled magnon dispersion, $E(k) = JS \left\{ 1 - \frac{4}{L^2} \frac{1 - \cos(k)^n}{1 - \cos(k)} \right\}$. This tells us that, in the thermodynamic limit, the magnon excitation has a gap of value $JS$, and a totally flat dispersion. Hence, a ferromagnetic chain with infinite ranged linear exchange coupling is gapped. It is nice to see that two somewhat evidently disconnected systems have surprising connections. The exact nature of things may not be same in the two, nevertheless the similarities are fairly
noticeable.

So far, we have discussed the case of linear exchange quantum antiferromagnets. Since the fundamental blocks making these spin chains are maximally overlapping, we only had a two fold degeneracy in the dimer ground state. It was, though, mentioned earlier that the fundamental blocks have intrinsic degeneracy of the dimer configurations in their singlet states. Therefore in the next section, we discuss other types of one dimensional spin models where the ground state consists of exponentially large number of dimer configurations.

### 2.6 Exponential degeneracy in the ground state

The block-singlets made up of four or more spins always have degenerate valence bond representations. For example, four spin-1/2 objects can make a singlet state in two linearly independent ways. Similarly, six spin-1/2 objects will make a singlet state in five linearly independent ways. These five ways, as shown in Figure 2.9, are in fact the famous valence bond configurations of a Benzene ring [19]. In general, there are total $(2N)!/(N+1)!N!$ number of linearly independent valence bond (singlet) configurations for $2N$ spin-1/2 objects. These are essentially the non-crossing valence bonds configurations as introduced by Linus Pauling.

![Figure 2.9: Five linearly independent, non-crossing valence bond configurations for the singlet state of six spin-1/2 objects.](image)

The degeneracy in the valence bond or dimer configurations of a block-singlet, however, could not be greatly exploited in our previous construction which led to the class of linear exchange spin models on a chain. The dimer ground state of this class of models is only two-fold degenerate. In the present section, we will construct another type of one dimensional spin models whose ground state has exponential degeneracy of dimer configurations. By exponential, we mean that the degeneracy of the ground state is
2.6 Exponential degeneracy in the ground state

exponential in the number of lattice sites, \( L \). In higher dimensions also, we will encounter models with exact ground states having such exponentially large degeneracy of valence bond configurations. To illustrate this class of models in one dimension, we describe below a particular construction using \( \mathcal{B}_5 \) units on a closed chain. It can be done for open chains as well. One can do the same for other blocks or even a combination of blocks of different sizes. Our purpose here is just to illustrate the idea.

Consider a closed chain with even number of sites. Connect spins at 1\( ^{st} \), 2\( ^{nd} \), 3\( ^{rd} \) and 4\( ^{th} \) sites identically among themselves with exchange coupling \( \alpha J \). Then connect each of these four spins to the spin at 5\( ^{th} \) site, as shown in Figure 2.10, with an exchange coupling of strength \( J \). Again, connect spins from 5\( ^{th} \) to 8\( ^{th} \) site identically with coupling \( \alpha J \), and then connect these four spins to the spin at 9\( ^{th} \) site with coupling \( J \). Repeat this procedure for further spins, starting with 13\( ^{th} \) site, 17\( ^{th} \) and so on. Thus we construct a spin chain of \( \mathcal{B}_5 \) units. These \( \mathcal{B}_5 \) units are slightly different from the ones that we used earlier. Here we have two exchange couplings \( J \) and \( \alpha J \), and for \( \alpha = 1 \) the present \( \mathcal{B}_5 \) units become identical with the earlier ones. The Hamiltonian for this new type of spin chain can be written as:

\[
H = J \sum_{i=1}^{L/4} h'_{u-3}[\mathcal{B}_5], \quad \text{with } J > 0.
\]

The block Hamiltonian,

\[
h'_{u-3}[\mathcal{B}_5] = \alpha \{ S_{u-3} \cdot (S_{u-2} + S_{u-1} + S_u) + S_{u-2} \cdot (S_{u-1} + S_u) + S_{u-1} \cdot S_u \} + S_{u+1} \cdot (S_{u-3} + S_{u-2} + S_{u-1} + S_u)
\]

(2.44)

is a slightly generalized version of the previously defined \( \mathcal{B}_5 \) block Hamiltonian, \( h[\mathcal{B}_5] \).

For \( \alpha > 1 \), the minimum energy of \( h'_{u-3}[\mathcal{B}_5] \) is equal to \(-3\alpha/2\) for \( S = 1/2 \). Spins, \( S_{u-3}, S_{u-2}, S_{u-1} \) and \( S_u \) form a two-fold degenerate block-singlet corresponding to the block Hamiltonian’s lowest eigen energy, and spin \( S_{u+1} \) remains “free” to become a part of the next block-singlet. Therefore, the ground state energy of this spin model is \(-3\alpha J L/8\), and the ground state configurations can be written as:

\[
|\psi_g\rangle = [1, 2, 3, 4] \otimes [5, 6, 7, 8] \otimes \cdots \otimes [L - 3, L - 2, L - 1, L]
\]

(2.45)
Since each of these four spin block-singlet, \([4l - 3, 4l - 2, 4l - 1, 4l]\), has two dimer representations, \(|\psi_g\rangle\) represents \(2^{L/4}\) degenerate, dimer configurations forming the ground subspace.

For \(\alpha = 1\), the ground state energy is still given by the above expression, but the degeneracy of the ground state is \(2(2^{L/4})\). This is so because, for \(\alpha = 1\), any four spins of a \(B_5\) block can form singlet in the minimum energy configuration. This allows following configurations, together with \(|\psi_g\rangle\), in the ground state.

\[
|\psi'_g\rangle = [2, 3, 4, 5] \otimes [6, 7, 8, 9] \otimes \cdots \otimes [L - 2, L - 1, L, 1] \tag{2.46}
\]

And hence, the degeneracy is doubled. The procedure, described here in detail, can be directly applied to construct models using bigger spin blocks. In fact, an appropriate combined construction using both even and odd blocks can give rise to models with exact dimer ground states of similar kind. But we will not go into more examples of this type. There is an interesting thing to note here. The ground state of the models discussed in the present section, is exactly known for \(\alpha \geq 1\), unlike the linear exchange models where \(\alpha\) is strictly one. Or, in other words, the dimer configurations are superstable for all values of \(\alpha\) greater than or equal to one. We will come across the models with similar ground state features once more in the following section while considering the higher dimensional application of our scheme.

### 2.7 Models in higher dimensions

Though the models discussed in the previous sections are exclusively one dimensional, the idea of construction using fundamental blocks is not special to one dimension. In fact, as shown in Figure 2.2, all these blocks can be readily visualized as two or three dimensional objects. For example, \(B_3\) unit is certainly a triangle. Similarly \(B_5\) can be seen as a square pyramid, or a \(B_4\) block can be seen a tetragonal unit. The bigger blocks may have more complicated geometrical correspondence in higher dimensions. The important thing about these fundamental blocks is their exchange connectivity, and not the fact as to which space we place them in. This encourages us to construct quantum spin models with exact dimer ground states, in two and three spatial dimensions.

Interestingly, the Shastry-Sutherland (SS) model had already set a precedent for us in this direction, and we just followed it. It was constructed and studied by Shastry and Sutherland almost two decades ago \([2]\). It is a frustrated quantum antiferromagnet on a square lattice with the usual nearest neighbour exchange coupling, and a certain choice of the frustrating next nearest neighbour coupling. Figure 2.11 shows the exchange
connectivity of the SS model. We will call this as the SS lattice. For $S=1/2$, the model has an exact ground state consisting of dimers along the diagonal bonds, when $\alpha \geq 1$. The parameter $2\alpha$ is the ratio of the diagonal exchange coupling to the nearest neighbour coupling. The SS model, like the MG model, is made up of (generalized) $B_3$ units. It can be thought of as an implementation of the idea of the solvable MG model, in 2D.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{ss_model.png}
\caption{The Shastry-Sutherland model}
\end{figure}

In the present section, we construct quantum spin models in two and three dimensions with exact dimer ground states. We describe a set of rules below, which gives us a general idea of how various models can be constructed. Let us mention some important things right at the outset. In two and three dimensions, the possibilities of satisfying the singlet configurations of each fundamental block may be met in many different ways, therefore, one can make different kinds of models with exact dimer ground states. Also, the disparity between odd and even blocks is not striking. We will show this by constructing some models using even blocks which have exact dimer ground states. Therefore, the rules below should only be taken in an empirical spirit. These are sufficiently general to guide one’s construction, but these are not mathematical theorems. What remains most important, no matter what one does with the blocks, is that each block should be simultaneously “happy” in order to make the exact ground state solution possible. In the following, we state the rules for odd blocks. For even blocks, we will just illustrate the idea with a few examples. The rules are:

1. For an odd block, $B_{2\nu+1}$, pick one of the spin as free. Let rest $2\nu$ spins form a block-singlet.

2. Each of the $2\nu$ spins of the singlet forming block can act as the “free” spin for the
neighbouring blocks. And any given block-singlet can be fully or partially shared by other “free” spins. This allows us to extend the network in higher dimensions.

3. The Hamiltonian for any such model is just the sum of all the block-Hamiltonians. Only those dimer configurations which satisfy each building block’s minimum energy configuration, form the exact ground state.

Since the singlet forming block can be thought of as a separate group of spins, fully connected with the free spin, we can have a generalized $B_{2\nu+1}$ unit similar to the ones considered in Section 2.6. In a generalized $B_{2\nu+1}$ unit that we consider here, a group of $2\nu$ spins is completely connected within itself by an exchange coupling $\alpha J$, and the remaining one spin is connected to the rest by an exchange coupling $J$. The minimum energy configuration, for $\alpha > 1$, of this block is such that the spins coupled via an exchange of strength $\alpha J$, will form a block-singlet, and the remaining spin remains free. For $\alpha = 1$, however, any $2\nu$ spins will form a block singlet, leaving any one spin free. The minimum energy, for $\alpha \geq 1$, of the block Hamiltonian is $-\alpha \nu 3/4$. There can be more general forms of a $B_{2\nu+1}$ block, but we are not interested in them. Now let us discuss a few concrete examples.

First, we will describe models in two dimensions. The SS model is already a well known example of $B_3$ units. Therefore, we will discuss models, made up of $B_5$ units. Figure 2.2 shows a two dimensional way of visualizing $B_5$ unit, where there is a square block of spins and a “lone” spin. In the generalized version of the block, spins within the square are connected with coupling $\alpha$ (in units of J), and the lone spin is coupled with the rest by an exchange coupling of unit strength.

![Figure 2.2: The ladder made up of $B_5$ blocks. The exchange couplings are: thin solid line $\equiv J$, dashed line $\equiv 2J$, and thick solid line $\equiv 4\alpha J$.](image)

Following the rules stated above, a spin-1/2 ladder model, as shown in Figure 2.12, is constructed with $B_5$ unit. Each square, drawn with thick lines in the figure, is shared by its four neighbouring spins, two of which come from the left of the square and the other two from the right. Thus we essentially have four $B_5$ units sharing a common square, in the ladder. The final strength of various exchange couplings are discussed in the figure.
caption. Now let us see what the ground state will be for this ladder. The Hamiltonian for this ladder model can be simply written as a sum of $L$ blocks Hamiltonians, $h'[\mathfrak{B}_5]$, each one corresponding to a site on the ladder, where $L$ is the total number of sites. Assume a ribbon like geometry for the ladder, just for simplicity (to avoid free ends).

The solution for the ground state is rather simple. For $\alpha \geq 1$, each of the thick line squares will form a singlet. And each square-singlet is two-fold degenerate, therefore, the ground state of the ladder is $2^{L/4}$ degenerate. Figure 2.13 shows the ground state of the ladder model. The ground state energy (in units of the strongest exchange coupling of the ladder, that is, $4\alpha J$) is $E_g = -3L/8$.

![Figure 2.13: The ground state configuration of the ladder model. Each of the square block is a singlet which has two linearly independent dimer representations as shown by vertical and horizontal dimers.](image)

These ladders properly arranged on a plane, give rise to a certain 2D spin model as shown in Figure 2.14. What has been done here is just an appropriate stacking of the previously discussed ladder both horizontally as well vertically, so that each thick square of a ladder overlaps completely with that of the other ladders. The Hamiltonian is again simply written as the sum of two $h'[\mathfrak{B}_5]$ corresponding to each site, one for the vertical ladder and the other for the horizontal. Thus there are total $2L$ number of $\mathfrak{B}_5$ units.

For the 2D model, the final strength of the exchange couplings within the squares is doubled, that is $8\alpha J$. This is because each square is common to one horizontal ladder and one vertical ladder. The other couplings remains the same. The ground state is also simple. Assuming a toroidal geometry for the 2D model, we find that the exact ground state is such that each square forms a block-singlet. Again there is degeneracy of $2^{L/4}$ dimer configurations in the ground subspace. The ground state energy, for $\alpha \geq 1$, of the 2D model is $-3\alpha JL$, respectively. In units of the strongest coupling, $8\alpha J$, $E_g = -3L/8$.

A few things are worth observing in these exact ground state solutions. First, the finite entropy density in the ground state. The two-fold intrinsic degeneracy of each block-singlet gives rise to $2^{L/4}$-fold degeneracy in the ground state. The system is able to
exploit this intrinsic degeneracy because the singlet forming blocks are *spatially disjoint*. The ground state entropy is \(\frac{1}{4}\log(2)\), just one fourth of that of a paramagnet. Secondly, the ground subspace consists of \(2^{L/4}\) distinct valence bond configurations. For example, two of these configurations are the columnar dimer states which are the exact ground states of a certain model constructed by Bose and Mitra [21]. There are many different kinds of them. Thus, what we have as the ground state is essentially a huge subset of the short range valence bond configurations that are possible on a square lattice. And lastly, the ground state of models discussed here is a spin-liquid as well as a dimer-liquid. The spin correlation exists only within each dimer, thus it is ultra short ranged. And the dimers are correlated only within a square block, thus making it a dimer liquid as well. One can easily construct certain other models, using same rules, whose ground states are dimer solids, though we will not discuss them explicitly. These models will essentially have overlapping blocks of singlets, which allows only a certain dimer configurations.

Before going into three dimensional models, let us discuss a few simple models made up of even blocks, which admit exact dimer ground state. These are constructed in such a way that each of the building block shares at least one bond. First, we consider a spin-1/2 ladder made up of \(B_4\) units. This ladder models is shown in Figure 2.15. It is constructed by putting one completely connected square after the other such that the neighbouring squares share one common bond. These common bonds are the rungs of the ladder, and the exact ground state consists of the dimers along the rungs. There is however another
2.7 Models in higher dimensions

Figure 2.15: A ladder of $\mathcal{B}_4$ units. The thick lines are represents an exchange interaction of $2J$, and the dashed lines have exchange interaction of strength $J$.

way of making the same ladder using the triangles ($\mathcal{B}_3$ blocks). In the construction using triangles, each rung is shared by two triangles where the third spin for each of these triangles come from the previous rung. Here, we can also have a slight generalization where the rung exchange interaction is $2\alpha J$. For $\alpha \geq 1$, the ground state is made up of dimers along the rungs of the ladder.

Figure 2.16: The two dimensional model of bond-sharing $\mathcal{B}_6$ units. Thick lines denote an exchange coupling of $2J$ whereas the thin ones have an exchange strength of $J$.

Next, we describe a two dimensional model of $\mathcal{B}_6$ units. A $\mathcal{B}_6$ block can be thought of as a hexagon of spins, and each spin in the hexagon is coupled with every other spin in the block with an exchange coupling $J$. Since $J > 0$, the block-singlet is the ground state of the block. Figure 2.9 shows all the five independent dimer configurations that forms the singlet state of six spin-1/2 objects. The model that we construct using $\mathcal{B}_6$ is shown in Figure 2.16, and the corresponding ground state, as shown in Figure 2.17, is a rather interesting looking arrangement of the dimers on the hexagonal lattice.
Chapter 2  Frustrated quantum spin models

Figure 2.17: The exact dimer ground state of the model given in Figure 2.16. Thick lines stand for the dimers.

Now let us discuss the construction of the models in 3D. Generalizations of the SS model, considered in Reference [20], provide good examples of the higher dimensional models made up of $\mathcal{B}_3$ units. So, we will consider the next block, that is, $\mathcal{B}_5$. In Figure 2.2, the three dimensional $\mathcal{B}_5$ block is shown as a square pyramid. One may find many ways of constructing 3D models using $\mathcal{B}_5$ pyramids. We consider a particular case where two such pyramids share the basal plane to form an octahedron. For $\alpha \geq 1$, the four spins of the common basal plane form a block-singlet. A layer of these corner-sharing octahedra will have the ground state shown in Figure 2.18, where each of the thick line is actually denoting a singlet state of four spin-1/2 objects. The singlet forming basal planes in this layer are all perpendicular the plane of the layer. The spins of the singlet can act as the apex for the pyramids in the neighbouring layers. Thus, appropriate stacking of different layers of the corner-sharing octahedra will make 3D model with exact dimer ground state. The ground state again has an exponential degeneracy in the valence bond configurations. This is all due to the fact that each singlet-forming is spatially disjoint, and thus free to exploit its intrinsic degeneracy. The topology of arrangement of the block-singlet in this model is same as the arrangement of dimers in the exact ground state of 2D SS model.

One last thing before we end our discussion on quantum spin models with exact dimer ground states. We have been talking so far exclusively for the case of $S = 1/2$. The exact
2.7 Models in higher dimensions

Figure 2.18: This is a projection on x-y plane, of the ground state configuration of a layer of the corner sharing octahedra made out of square pyramids (the $\mathcal{B}_5$ units in 3D). Thick lines, here, represent the common basal plane of two $\mathcal{B}_5$ pyramids making an octahedra. In the ground state, four spins lying on the common basal plane form a two-fold degenerate block-singlet. These block-singlets lie in x-z or y-z planes. It is interesting to observe the topological equivalence of the arrangement of block-singlets on orthogonal planes, here, to that of the dimers in the exact ground state of the SS model.

dimer ground state of the linear exchange models in 1D is possible only for spin-1/2. The situation, however, is not so exclusive to $S = 1/2$, when the singlet forming blocks are arranged in spatially disjoint way. This, for example, is the case for various models in 2D and 3D, and also for the 1D models of Section 2.6. In these models, the exact singlet dimer ground states can be possible for higher spin quantum numbers as well. However, the condition on parameter $\alpha$, for this to be possible, is different from $\alpha \geq 1$. For a generalized $\mathcal{B}_{2\nu+1}$ block, the Hamiltonian is:

\[ h'[\mathcal{B}_{2\nu+1}] = \alpha \sum_{i=1}^{2\nu-1} \sum_{j>i}^{2\nu} S_i \cdot S_j + S_{2\nu+1} \cdot \sum_{i=1}^{2\nu} S_i \]  

(2.47)

When spin quantum number $S$ is greater than 1/2, the following condition on $\alpha$, needs to be satisfied for $h'[\mathcal{B}_{2\nu+1}]$ to have the ground state where spins $S_1$ to $S_{2\nu}$ form a block singlet. The general condition on $\alpha$, for $S \geq 1$, is

\[ \alpha \geq 1 + S \]  

(2.48)
2.8 Summary

The possibilities for constructing such models are enormous, and therefore cannot be exhausted in one place. But one thing must be emphasized upon. The basis for constructing models with exact dimer ground states, as discussed in the present chapter, is very general. The model Hamiltonians that can be constructed with these rules, may be of some importance in understanding the physics of the frustrated quantum antiferromagnets.

We summarize the main results before moving on to the next chapter. We have come up with a general idea of constructing quantum antiferromagnetic models with exact dimer ground states. The most fundamental objects in our scheme are the completely connected blocks. We used this idea to construct an interesting family of 1D spin models with linear exchange interaction. These models have two fold degenerate exact dimer ground state for odd family. The even family also admits the same ground state in the asymptotic limit. The kink excitations form a good choice for low-lying elementary excitation. But they are only a variational choice. They have a finite energy gap. We have also constructed 1D models with exact dimer ground state having extensive entropy. This scheme of construction is then applied in higher dimensions. We have illustrated the construction of models in 2D and 3D with the help of a few explicit examples. Many of these models have extensive entropy in their exact ground states. The ground subspace in these models is a huge set of the valence bond configurations on a given lattice. An interesting property of these dimer states is that they superstable. We find many Hamiltonians with same dimer ground state. The two fold degenerate dimer ground state in 1D, is a very good example of a superstable ground state.

Though we have not looked at the quantum phase transition related questions in these models, various competing exchange interactions present in all of these models evidently provide a scope for studying the quantum phase transitions in these frustrated antiferromagnets. The building-block way of constructing the models, is closer to the spirit of synthetic chemistry. It might be possible to make materials which are realizations of this kind of spin models.
Bibliography


[14] We used H. Nishimori’s TITPACK for numerical computation.

[15] Prof. B. Sriram Shastry brought this point to my attention.


Chapter 3

Resonating valence bond mean field theory of the Shastry-Sutherland and triangular lattice t-J models

The question of superconductivity in doped SrCu$_2$(BO$_3$)$_2$ and Na$_x$CoO$_2$ · yH$_2$O, is addressed within the framework of t-J model RVB mean field theory on respective two dimensional lattices. In SrCu$_2$(BO$_3$)$_2$, the Shastry-Sutherland lattice is the underlying lattice, whereas cobalt ions in a CoO$_2$ layer of Na$_x$CoO$_2$ form the triangular lattice. Of the two compounds, former is where we propose to search for superconductivity, and for the latter, an attempt is made to understand the observed superconducting state. In both cases, the regions of superconducting phases are found, and the symmetry of the order parameter is identified, within the RVB mean field calculation. The question of gap in the quasi-particle spectrum is also addressed. An important prediction of the high frequency Hall constant growing linearly with temperature on triangular lattice, at high temperatures, is made.

The discovery of SrCu$_2$(BO$_3$)$_2$ as a material realization of the Shastry-Sutherland (SS) model was an interesting event in the area of frustrated magnetism [1]. The SS model preceded this discovery almost by two decades [2]. Exact solvability, for the ground state, of the SS model under a simple condition, makes it a special model. Ever since this discovery was made, both the material and the model have become the subjects of extensive research. Variety of experiments have been carried out on this material which give us good understanding of its physical properties. Finding the quantum phase diagram of the SS model with proper identification of various phases, and the consistent
understanding of the magnetization plateaus in the presence of external magnetic field, have been some of the main topics of current theoretical interest. Here in this chapter, we wish to initiate a new objective for research in this material and the model, that is of the search for superconductivity in doped SrCu$_2$(BO$_3$)$_2$. It is encouraging to know that the exact ground state of the (undoped) SS model is a simple configuration of the spin singlets. As we believe, this makes its doped variant a good candidate to search for the resonating valence bond (RVB) state of superconductivity [3].

The recent discovery of superconductivity at low temperatures in CoO$_2$ layered compounds [4] is an exciting event, since it may be the long sought low temperature RVB superconductor, on a lattice which was at the basis of Anderson’s original ideas on a possible quantum spin liquid state [6]. Although the spin-1/2 triangular lattice appears to have better states with three sublattice magnetic order, it is possible that the RVB state is attained for sufficiently high doping, and it seems to be both useful and worthwhile to explicitly state the detailed results of the RVB ideas applied to this lattice so as to serve as a reference point for further experiments that are surely forthcoming shortly. Motivated by this discovery of superconductivity in two dimensional CoO$_2$ layers, we present some possibly useful results of the RVB mean field theory applied to the triangular lattice. The high frequency Hall constant in this system is potentially interesting, since it is pointed out to increase linearly with temperature without saturation for $T > T_{\text{degeneracy}}$.

The present chapter consists of two parts, one concerning the question of superconductivity in doped SrCu$_2$(BO$_3$)$_2$ and the other related with the CoO$_2$ layered compounds. In Sections 3.1 to 3.4, we describe the physical properties of SrCu$_2$(BO$_3$)$_2$ briefly, and perform the RVB mean field calculation on the SS lattice t-J model. The results of the mean field calculations are carefully interpreted, and useful predictions are made regarding the superconducting order parameter and the quasi-particle excitation spectrum in SrCu$_2$(BO$_3$)$_2$ under doping. Similar mean field calculations are performed on the triangular lattice t-J model, and predictions are made for the CoO$_2$ layered superconductors in Sections 3.5 to 3.7 of this chapter.

### 3.1 SrCu$_2$(BO$_3$)$_2$

The strontium di-copper di-borate, SrCu$_2$(BO$_3$)$_2$, was synthesized in 1991 by Smith and Keszler [7]. The motivation behind their synthesis of this new orthoborate$^1$ was to be able

---

$^1$The *orthoborates* are the compounds made up of BO$_3$ coordination group such that the ratio of the number of O atoms to the number of B atoms is 3 and there are no oxygen atoms shared between two such groups. This is a standard convention of nomenclature in the oxygen chemistry of boron [8]. For example, there are metaborates where the ratio O:B is 2 and each BO$_3$ group shares two O atoms with
to produce finely granular copper for the purpose of catalysis. The fact that this material is a realization of the Shastry-Sutherland (SS) model of a two dimensional quantum antiferromagnet was discovered only later in 1999, by the experimental investigations carried out by Kageyama and collaborators [1]. It is nice a piece of historical development to note that the SS model was put forward in 1981 by Shastry and Sutherland. A decade after that a material was synthesized with no interest in its magnetic properties. And surprisingly after another eight years, it was realized that the material is a quasi two-dimensional manifestation of the SS model.

3.1.1 Structure

The structure of SrCu$_2$(BO$_3$)$_2$ was also determined by Smith and Keszler [7]. It is a simple structure exhibiting layers of interconnected planar BO$_3$ and rectangular planar CuO$_4$ groups. Figure 3.1 shows the arrangement of CuO$_4$ and BO$_3$ units in a–b plane. The layers are stalked along c–axis, and separated by heavy Sr$^{2+}$ ions. At room temperature, the material has a tetragonal unit cell with the cell constant values of $a = b = 8.995$ Å and $c = 6.649$ Å. It shows structural phase transition at 395 K, but the intra-planar structure remains essentially the same.

Figure 3.1: The structure of a layer of interconnected CuO$_4$ and BO$_3$ groups in the a-b plane of SrCu$_2$(BO$_3$)$_2$.

One unit cell of the material contains four Cu$^{2+}$ ions, and all copper ions occupy crystallographically equivalent sites in the lattice. Since the electronic configuration of Cu$^{2+}$ is [Ar]3d$^9$, each copper ion contributes a localized spin-1/2 to the material. The other BO$_3$ groups.
material is an insulator. The other species in the material have closed shell configurations in their respective ionic states, therefore do not contribute the low temperature electronic properties of the material. Let us consider the lattice of the copper (spin) sites only. As evident from Figure 3.1, the copper spins have two kinds of superexchange routes for the spin-spin interaction. One is the oxygen-only mediated superexchange between the nearest neighbour copper spins. The second superexchange is established via the borate ligand, \((\text{BO}_3)^3^-\), which couples the spins coming from two neighbouring pairs of coppers. Figure 3.2 shows the “spin” lattice of a layer of \(\text{SrCu}_2(\text{BO}_3)_2\), with the intervening ligands replaced by the effective exchange couplings. Thus, we have an effective 2D model of a spin-1/2 antiferromagnet with two competing exchange interactions. The nearest neighbour Cu-Cu distance is 2.905 Å, and the next nearest neighbour separation between copper ions is 5.132Å. These distances, together with the ligand bond angles, decide the strength of the exchange interactions.

\[
\begin{matrix}
& J & \\
\hline
J' & & \\
\end{matrix}
\]

Figure 3.2: Comparing the Shastry-Sutherland lattice (left) with the Cu lattice of \(\text{SrCu}_2(\text{BO}_3)_2\) (right). They are topologically equivalent.

### 3.1.2 Physical properties

A variety of experiments have been done on \(\text{SrCu}_2(\text{BO}_3)_2\) in order to understand its physical properties. Here, we present a summary of some important experimental findings. This gives us a general background of the physics of the material. Various physical properties of \(\text{SrCu}_2(\text{BO}_3)_2\) are reviewed in detail in the Ph.D. thesis of Miyahara [14]. We will briefly describe two very important features of this material. These are the spin gap and the magnetization plateaus.

**Spin gap**: An important feature of this material is the spin-gap, that is an energy gap to spin excitations. In the measurement of the temperature dependence of magnetic
susceptibility $\chi$, Kageyama et al. [1] found that the susceptibility drops sharply as temperature is lowered below 20 K. They also observed the activated temperature dependence of $1/T_1$, the NQR relaxation rate. This suggested the existence of an energy gap to spin excitations.

The low temperature split of the Cu NQR signal into two component points towards the nuclear spin-spin interaction in a Cu-dimer, and thus also strongly suggesting the existence of spin dimers at low temperature. The NMR experiments also give direct evidence of the spin dimers at low temperatures [16]. From Cu NQR relaxation rate measurement, the spin gap was estimated to be around 30 K. The values of spin gap measured by different experiment are in good agreement with each other. Miyahara has neatly tabulated the estimated spin gap from different experiments in his thesis [14]. Since it is an important piece of information, we reproduce it here in Table 3.1.

<table>
<thead>
<tr>
<th>Experimental method</th>
<th>Spin gap</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic susceptibility [10]</td>
<td>34 K</td>
</tr>
<tr>
<td>Cu NQR-T$_1$ [1]</td>
<td>30 K</td>
</tr>
<tr>
<td>ESR [19]</td>
<td>34.7 K</td>
</tr>
<tr>
<td>Neutron scattering [12]</td>
<td>35 K</td>
</tr>
<tr>
<td>Raman scattering [20]</td>
<td>35.2 K</td>
</tr>
<tr>
<td>Far infrared spectroscopy [21]</td>
<td>34.8 K</td>
</tr>
</tbody>
</table>

Table 3.1: Spin gap estimated from various experiments.

With the realization of the fact that spin dimers seem to govern the low temperature physics of the material, and knowing the structure of the copper lattice, Kageyama et al. proposed a model for SrCu$_2$(BO$_3$)$_2$ as shown in the right hand side picture of Figure 3.2 [1], which was soon realized to be same as the SS model. The estimated values of the exchange couplings are: $J' \approx 100$ K and $J \approx 68$ K [13].

**Magnetization plateaus**: Another striking physical property of SrCu$_2$(BO$_3$)$_2$ is the appearance of the quantized magnetization plateaus at high magnetic fields. This is claimed to be the first observation of magnetization plateaus in a real quasi 2D spin system [1, 10, 15]. High field magnetization measurements upto 57T have been performed on SrCu$_2$(BO$_3$)$_2$ at sufficiently low temperature (around 1 K) on the single crystal samples.
Three plateaus at the magnetization values of 1/8, 1/4 and 1/3 of the saturation magnetization are observed at the field strengths greater than 20T, below which the magnetization is zero.

Just to give an idea of the width and the position of the plateaus, we mention the experimental observations for the magnetic field parallel to the $c-$axis from Reference [15]. The lower and the upper critical fields for the 1/8-plateau are $H_{cL}^{1/8} = 26.9T$ and $H_{cU}^{1/8} = 28.2T$. Similarly for 1/4-plateau, the critical fields are $H_{cL}^{1/4} = 34.1T$ and $H_{cU}^{1/4} = 39.1T$. The lower critical field for which the 1/3-plateau sets in is same as $H_{cU}^{1/4}$, but the upper critical field is not decided since the plateau continues till the highest available field, that is 57T. And therefore, one could not be sure of the upper critical field for the 1/3-plateau.

The theoretical understanding of the physics of magnetization plateaus in SrCu$_2$(BO$_3$)$_2$ is an interesting problem. It was realized quite early that due to geometrical reasons, the triplets excitations are extremely weakly dispersed [13]. And therefore, the different plateaus are explained to arise from the localized triplet dimers, arranged in different crystalline superstructures. In fact, the 1/3-plateau was observed after the prediction of these calculations [15]. Experimental investigations are being carried out in order to understand the nature of these magnetic superstructures at the plateaus [17]. The other approach, based on ideas in parallel with the quantum Hall effect, has also been applied to understand the magnetization plateaus [18]. But the triplet superstructure picture appears to be more direct and perhaps correct. However, what decides the width of the plateaus, and the nature of evolution of the system from one plateau to the next, are some of the things which are not yet clear.

### 3.2 Shastry-Sutherland model

Having described the material properties, now we discuss the Shastry-Sutherland (or simply the SS) model. The SS model is an antiferromagnetic model of spins on the SS lattice (the left hand side picture in Figure 3.2) with the following Hamiltonian.

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle i,j \rangle}^' \mathbf{S}_i \cdot \mathbf{S}_j$$  \hspace{1cm} (3.1)

The first term in the Hamiltonian corresponds to the spin-spin interaction over all the nearest neighbour bonds of the SS lattice. The second term with primed summation describes the spin-spin interaction over all the diagonal bonds of the SS lattice, as shown in Figure 3.2 by the dashed lines. Both $J$ and $J'$ are positive. In a more general formulation, the exchange interaction can be anisotropic, and there can be an external magnetic
field present. In fact, both of these were considered in the original paper by Shastry and Sutherland [2]. Here, we will not consider these two extra ingredients. The most interesting feature of the SS model is that it has an exact ground state for $J' \geq 2J$ (for spin-1/2).

The exact ground state consists of singlets along the diagonal bonds of the SS lattice. Another interesting feature of this model is the quantum phase transition due to the competition between two exchange interactions. In the following, we will briefly discuss the quantum phase diagram of the SS model. We will not discuss the exact ground state solution of the SS model, since it has been described in the previous chapter (Section 2.7).

**Quantum phase diagram**: The SS model has two competing exchange interactions, $J$ and $J'$. For $J' = 0$, the system is in the antiferromagnetically ordered (AF) phase, whereas for $J' \geq 2J$ the dimer state is the exact ground state. Therefore, it is natural to ask, what all phases could possibly arise, as the parameter $\lambda = J'/J$ is varied. ‘How far does the dimer phase persist as $\lambda$ is lowered below 2 ?’, is an important question. It has become more so, ever since the discovery of SrCu$_2$(BO$_3$)$_2$. The value $\lambda \approx 1.47$ in this material is less than 2. And yet, the observations confirm the presence of dimer-singlets at very low temperatures. This has given rise to serious theoretical investigations of the quantum phase transition in the SS model.

![Quantum Phase Diagram of the SS Model](image)

Figure 3.3: The quantum phase diagram of the SS model. Region-I denotes the AF ordered phase. Region-III denotes the dimer-singlet phase. Region-II denotes an exotic spin-liquid phase which is believed to be a plaquette-singlet phase.

The quantum phase diagram of the SS model, as shown in Figure 3.3, is inferred from different theoretical investigations. Since there is only one parameter $\lambda$, the quantum phase diagram is just a line. There are three different line segments denoting three distinct phases [22]. The segment I denotes the AF ordered phase. It extends from $\lambda = 0$ to 1.16 roughly. For $\lambda \geq 1.48$, the system goes into a dimer-singlet phase which is shown as segment III in the phase diagram. The intermediate region of the parameter, denoted as segment II, is a complex one, and not yet completely understood. However, there are evidences of a non-trivial spin-liquid phase in this little window of $\lambda$. The nature of this phase and the bounds on $\lambda$ for region-II, are not yet fully settled. Nevertheless, there seems more favour to the observation that the spin-liquid state in region-II is adiabatically
derived from a state of independent plaquette singlets [22, 23, 24], against the other proposals like the helically ordered phase [25]. The phases II and III are gapped. The spin gap jumps discontinuously from phase-III to phase-II, and goes down continuously to zero across the transition from phase-II to phase-I [22]. The finer estimates of $\lambda$ for SrCu$_2$(BO$_3$)$_2$ give values greater than 1.48, roughly around 1.57 or so. It clearly indicates that the material exists in the critical regime, and towards the dimer side in the phase diagram.

### 3.3 Superconductivity in doped SrCu$_2$(BO$_3$)$_2$?

In the present section, we address the question of superconductivity in SrCu$_2$(BO$_3$)$_2$ under doping. The ground state of the SS model, which consists of the singlet pairs of electrons, is like the Cooper pairs in real space, frozen independently in a certain spatial configuration. What we intend to do is to discuss the possibility of doping the dimer state of SrCu$_2$(BO$_3$)$_2$, and to see if one may expect superconductivity from it. The question mark in the section heading also stands for the fact that superconductivity has not been explored experimentally in this system. Therefore, the discussion and the calculations, that will be presented in this section, address this question at a formal, predictive level.

We consider our point of view of the material as a Mott insulator. The parent ground state, then, is a Mott insulating spin-liquid, and deriving superconductivity from such a parent state by doping is a popular scenario. A scenario which originated in the context of superconductivity in cuprates, in the form of Anderson’s idea of resonating valence bond (RVB) superconductivity [3]. We believe that the experimental search for superconductivity in doped SrCu$_2$(BO$_3$)$_2$ may prove fruitful in understanding and testifying such an important idea.

#### 3.3.1 SrCu$_2$(BO$_3$)$_2$ : a Mott insulator

Firstly we remark that the insulating dimerized ground state of SrCu$_2$(BO$_3$)$_2$ may usefully be considered as a Mott insulating state of an underlying Hubbard model. To see this consider the Hubbard model on the SS lattice with

$$
H = -t \sum_{<i,j>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - t' \sum_{<i,j>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}
$$

(3.2)

where the first and the second terms denote the hopping along the nearest neighbour and the diagonal bonds on the SS lattice, respectively. Let the diagonal hopping, $t'$, be $\alpha t$, where $\alpha$ is a dimensionless parameter. $U$ is the Hubbard interaction energy. Clearly
the superexchange argument fixes $\alpha$ in terms of the ratio of the exchange parameters via $\alpha^2 = \lambda = J'/J$, and we note that $\alpha \approx \pm 1.25$ using the insulating state estimates, with the sign undetermined.

In the non-interacting limit the band structure is interesting. We have four subbands, with the extrema of two of them touching quadratically at the zone centre. A brief description of the tight-binding band structure on SS lattice is presented in the following subsection. At half filling, one has four electrons per unit cell and the system is a semi-metal with a finite density of states, and thus a linear specific heat etc. This situation is reminiscent of the semi-metallicity of graphite with two electrons per unit cell and also of a fiduciary MgB$_2$ with well separated planes. In the case of graphite where one has a “Dirac like” linear spectrum, the density of states near the “Fermi point”, i.e. the contact point goes to zero.

This semi-metal becomes an insulator at large enough $U$, undergoing a transition to the dimerized state that does not break rotation invariance nor the lattice translation symmetry, and may be called a Mott transition in the same sense as that of the 1D Hubbard model at half filling at infinitesimal $U$. Since the large $U$ behaviour is exactly known, namely the dimer ground state, further terms in the $t/U$ expansion beyond superexchange should be useful in elucidating the nature of the Mott transition here. This transition has not yet been studied in literature. Starting from the semi-metal and turning on $U$, one may either have a level crossing transition to the gapped insulator, or more interestingly a continuous opening of the charge gap. In the gapped insulating phase, there occurs a weak symmetry breaking, namely the four spin correlation function pertaining to dimer order $<S_aS_bS_cS_d><S_aS_b><S_cS_d>$, and thus there is ODLRO in this correlation function. With this distinction, without necessarily a major difference, we may refer to SrCu$_2$(BO$_3$)$_2$ as a Mott insulator.

Having this realization of the Mott insulator, we naturally enquire if the philosophy of the RVB theory of Superconductivity due to Anderson applies here. This theory is built upon the idea that repulsive interactions of the Hubbard type lead to superconductivity via the intermediate step of superexchange, or Heisenberg interactions in the insulating state. The superexchange leads to singlet pairing between electrons of opposite spin, and these pairs are analogous to the Cooper pairs, but are localized due to the Mott-Hubbard gap. Under doping the Mott Hubbard gap collapses, these preexisting pairs propagate freely, and lead to superconductivity. In the present case, the Cooper pairs at half filling should be viewed as the dimer-singlets, which on doping should move around by the same logic, and lead to superconductivity. Since the values of exchange are smaller by an order of magnitude from those in high-$T_C$ systems, we expect lower $T_C$’s, say tens of degrees K, but accompanied by the characteristic signature of singlet pairing and also of
definite phase relations of Cooper pairs on the bonds, analogous to the d-wave pairing. While this theory is remarkably effective in providing a comprehensive viewpoint, it still lacks unambiguous experimental support or a rigorous mathematical foundation, and one would welcome other supports to its validity or otherwise. In this context we work out in this section the mean field theory of a fiducial doped SrCu$_2$(BO$_3$)$_2$, and calculate some characteristics of the *proposed* superconducting compound.

Before doing so, let us note that doping can be of either chemical type, as in say Sr$_{1-x}$M$_x$Cu$_2$(BO$_3$)$_2$ with a monovalent alkali M or a trivalent lanthanide. However, one interesting possibility is suggested by the comparison of MgB$_2$ with graphite. One learns that MgB$_2$ is isoelectronic with graphite, but avoids being a semimetal by dispersing the bands in the direction transverse to the two dimensional sheets, it self dopes by decreasing the transverse lattice constant. It is possible that a divalent element like Mg in place of Sr with a smaller ionic radius could decrease the transverse lattice constant of SrCu$_2$(BO$_3$)$_2$ sufficiently so that it would have substantial transverse dispersion. We should clarify that unlike MgB$_2$ which appears to be a case of phonon mediated superconductivity [26], we are examining the case for a non phononic mechanism, the RVB mechanism for doped SrCu$_2$(BO$_3$)$_2$. We now turn to the calculation proper.

### 3.3.2 Tight binding band structure on SS lattice

![SS lattice diagram](image)

Figure 3.4: The SS lattice with an appropriate labelling of the sites in a unit cell. Here, $t' = \alpha t$ and from the superexchange argument, we have $J' = \alpha^2 J$.

It is useful to understand the band structure of non-interacting electrons on the SS lattice. Figure 3.4 shows the labelling of different sites in a unit cell of the SS lattice, and also the strength of hopping and exchange interaction along various directions. We will be using the same convention in the rest of the chapter.
3.3 Superconductivity in doped SrCu$_2$(BO$_3$)$_2$?

The SS lattice has a periodicity of 2$a_0$, both along $\hat{x}$ as well as $\hat{y}$ directions, where $a_0$ is the lattice constant of the underlying square lattice. With each site contributing just one relevant orbital, the tight-binding model on the SS lattice is described by a four band Hamiltonian given below.

$$H_t = \sum_{k,\sigma} \begin{bmatrix} c_0^\dagger(k) & c_1^\dagger(k) & c_2^\dagger(k) & c_3^\dagger(k) \end{bmatrix} \begin{bmatrix} c_0(k) \\ c_1(k) \\ c_2(k) \\ c_3(k) \end{bmatrix}_\sigma T(k)$$

(3.3)

Here, $\sigma = \uparrow$ or $\downarrow$, and the wave-vector, $k = (k_x, k_y)$, is such that $\frac{-\pi}{2a_0} \leq k_x, k_y \leq \frac{\pi}{2a_0}$. The subscripts, 0, 1, 2, 3, refer to four different sites within a unit cell. The dispersion matrix, $T(k)$, is a $4 \times 4$ hermitian matrix as given below.

$$T(k) = -t \begin{bmatrix} 0 & 2\cos(k_xa_0) & 2\cos(k_ya_0) & \alpha e^{i(k_x-k_y)a_0} \\ 2\cos(k_xa_0) & 0 & \alpha e^{i(k_x+k_y)a_0} & 2\cos(k_ya_0) \\ 2\cos(k_ya_0) & \alpha e^{-i(k_x+k_y)a_0} & 0 & 2\cos(k_xa_0) \\ \alpha e^{-i(k_x-k_y)a_0} & 2\cos(k_ya_0) & 2\cos(k_xa_0) & 0 \end{bmatrix}$$

(3.4)

The band-structure for $|\alpha| = 1.25$ is shown in Figure 3.5. This value of $\alpha$ is taken from the studies on SrCu$_2$(BO$_3$)$_2$. What is known from the experiments is $\alpha^2$, and not $\alpha$. This leaves us with the ambiguity of sign of $\alpha$. Therefore, we consider both positive as well negative values of $\alpha$.

![Figure 3.5: The tight binding band-structure on the SS lattice. The wave vectors are written in units of $\frac{1}{a_0}$. Notice that the band-structure is odd with respect to $\alpha$.](image)

Let us make a few essential observations regarding the band-structure. Firstly, the system is a semi-metal at half filling, since the middle two bands touch each other at the
zone centre. Secondly, there is a band which is flat along the $X\Gamma$ symmetry direction in the Brillouin Zone. This band gives rise to a severe van Hove singularity at $\alpha$. Thirdly, the values of band energies at zone centre are $(-4 - \alpha)$, $\alpha$, $\alpha$ and $(4 - \alpha)$. For $|\alpha| > 2$, the middle two bands no more touch each other, and there is a finite band gap which makes it a band insulator at half filling. We consider only $\alpha = 1.25$, since this is roughly the value of $\alpha$ for $\text{SrCu}_2(\text{BO}_3)_2$.

Figure 3.6 shows the non-interacting single particle density of states on the SS lattice for both negative as well positive values of $\alpha$. When we hole dope the system to take it away from half filling, it is expected to behave differently for positive and negative $\alpha$, since the density of states is asymmetric for $\alpha$ going to $-\alpha$ (due to the frustrated geometry of the SS lattice).

![Figure 3.6: The non-interacting single-particle density of states on the SS lattice.](image)

### 3.4 RVB calculation on the SS lattice

The physics of the large $U$ Hubbard model can be described by an effective $t - J$ model with projected hopping. We now consider the same on the SS lattice, and do the valence bond mean field calculation, very much in the spirit of the RVB mean field theories on square lattice, in the context of the high-$T_c$ superconductivity [37, 29].
3.4 RVB calculation on the SS lattice

3.4.1 Mean field Hamiltonian and equations

The mean field Hamiltonian: The \( t-J \) Hamiltonian on the SS lattice can be written as:

\[
\tilde{H} = \mathcal{P}H_t\mathcal{P} + H_J - t\mu \sum_{k,\sigma} \sum_{p=0}^{3} c_{p,\sigma}^{\dagger}(k)c_{p,\sigma}(k)
\] (3.5)

The first term in \( \tilde{H} \) accounts for the projected hopping. It is essentially \( H_t \) as given in Equation 3.3, but with projection operator \( \mathcal{P} \) which suppresses the double occupancy of any site (due to large Hubbard \( U \)). At a simple level, the effect of \( \mathcal{P} \) can be brought in by replacing \( t \) by \( \delta t \). Here, \( \delta = 1 - n \), is the number of holes per site, and \( n \) is the electron filling per site. The last term is the chemical potential, \( \mu t \), times the total number of electrons. Here, \( p \) is the site (or the orbital) label within a unit cell. The second term in Equation 3.5, \( H_J \), which accounts for the interaction among electrons, can be written as:

\[
H_J = J \left\{ \sum_{n.n.} + \alpha^2 \sum_{\text{diagonal}} \right\} \left( S(r) \cdot S(r') - \frac{\hat{n}(r)\hat{n}(r')}{4} \right)
\] (3.6)

Here, \( r \) and \( r' \) are the site labels, and \( \hat{n}(r) \) denotes the number operator at site \( r \). The summation is pairwise in \( r, r' \) on the SS lattice. The operator, \( (S(r) \cdot S(r') - \hat{n}(r)\hat{n}(r')/4) \), can also be written as \( -\frac{1}{2} b^\dagger(r, r')b(r, r') \), which provides the basis for mean field decoupling of \( H_J \) in the off-diagonal channel. The operator, \( b(r, r') = c_{\uparrow}(r)c_{\downarrow}(r') - c_{\downarrow}(r)c_{\uparrow}(r') \), is the singlet bond operator.

Let us define an off-diagonal or the pairing mean field, \( \langle b(r, r') \rangle \), in the following way.

\[
\langle b(r, r') \rangle = \begin{cases} 
\Delta e^{i\theta_x} & \text{for } r - r' = \pm a\hat{x} \\
\Delta e^{i\theta_y} & \text{for } r - r' = \pm a\hat{y} \\
\Delta' e^{i\theta_{x+y}} & \text{for } r - r' = \pm a(\hat{x} + \hat{y}) \\
\Delta' e^{i\theta_{x-y}} & \text{for } r - r' = \pm a(\hat{x} - \hat{y}) 
\end{cases}
\] (3.7)

The internal phases, \( \theta_x, \theta_y, \theta_{x+y} \) and \( \theta_{x-y} \), as well as the amplitudes, \( \Delta \) and \( \Delta' \), are all independent of the coordinates. We are considering a uniform case. With this choice of the order parameter, we decouple \( H_J \). The corresponding mean field Hamiltonian can be written as:

\[
\tilde{H}^{MF} = \tilde{H}_t + H_J^{MF} + L(4J\Delta^2 + J'\Delta'^2)
\] (3.8)

where \( L \) is the number of unit cells. In order to write \( \tilde{H}_t \) and \( H_J^{MF} \) conveniently, we introduce a notation. Let us define the Nambu operators, \( \Psi_{C\uparrow}(k) \) and \( \Psi_{R\downarrow}(-k) \) in the
following way.

\[ \Psi_{C\uparrow}(k) = \begin{bmatrix} c_{0\uparrow}(k) \\ c_{1\uparrow}(k) \\ c_{2\uparrow}(k) \\ c_{3\uparrow}(k) \end{bmatrix} \]  

\[ \Psi_{R\uparrow}(-k) = \begin{bmatrix} c_{0\downarrow}(-k) \\ c_{1\downarrow}(-k) \\ c_{2\downarrow}(-k) \\ c_{3\downarrow}(-k) \end{bmatrix} \]  

(3.9)  

(3.10)  

The subscripts, \( C \) and \( R \), indicate that \( \Psi_{C\uparrow}(k) \) is a column vector and \( \Psi_{R\uparrow}(-k) \) is a row vector. In this notation, \( \tilde{H}_t \) can be written as:

\[ \tilde{H}_t = \sum_k \left\{ \text{tr} \left\{ \tilde{T}(-k) \right\} + \left[ \Psi_{C\uparrow}^\dagger(k) \right. \left. \Psi_{R\uparrow}(-k) \right] \begin{bmatrix} \tilde{T}(k) & 0 \\ 0 & -\tilde{T}(k) \end{bmatrix} \begin{bmatrix} \Psi_{C\uparrow}(k) \\ \Psi_{R\uparrow}^\dagger(-k) \end{bmatrix} \right\} \]  

(3.11)  

Here, \( \tilde{T}(k) \) is essentially same as the dispersion matrix, \( T(k) \), except that the chemical potential forms its diagonal elements, and all the off-diagonal entries have a factor of hole doping, \( \delta \), in order to account for the projection.

\[ \tilde{T}(k) = -t \begin{bmatrix} \mu & 2\delta \cos(k_xa_0) & 2\delta \cos(k_ya_0) & \delta \alpha e^{i(k_x-k_y)a_0} \\ 2\delta \cos(k_xa_0) & \mu & \delta \alpha e^{-i(k_x+k_y)a_0} & 2\delta \cos(k_ya_0) \\ 2\delta \cos(k_ya_0) & \delta \alpha e^{-i(k_x+k_y)a_0} & \mu & 2\delta \cos(k_xa_0) \\ \delta \alpha e^{i(k_x-k_y)a_0} & 2\delta \cos(k_ya_0) & 2\delta \cos(k_xa_0) & \mu \end{bmatrix} \]  

(3.12)  

With the same notation, \( H_j^{MF} \) can be written as:

\[ H_j^{MF} = \begin{bmatrix} \Psi_{C\uparrow}^\dagger(k) & \Psi_{R\uparrow}(-k) \end{bmatrix} \begin{bmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{bmatrix} \begin{bmatrix} \Psi_{C\uparrow}(k) \\ \Psi_{R\uparrow}^\dagger(-k) \end{bmatrix} \]  

(3.13)  

where \( D(k) \) is a non-hermitian \( 4 \times 4 \) matrix as given below.

\[ D(k) = -J \begin{bmatrix} 0 & J \Delta e^{i\theta_x} \cos(k_xa_0) \\ J \Delta e^{i\theta_x} \cos(k_xa_0) & 0 \\ J \Delta e^{i\theta_y} \cos(k_ya_0) & J \Delta e^{i\theta_y} \cos(k_ya_0) \\ J \Delta e^{i\theta_y} \cos(k_ya_0) & J \Delta e^{i\theta_y} \cos(k_ya_0) \\ J \Delta e^{i\theta_x} \cos(k_xa_0) & J \Delta e^{i\theta_x} \cos(k_xa_0) \\ J \Delta e^{i\theta_x} \cos(k_xa_0) & J \Delta e^{i\theta_x} \cos(k_xa_0) \\ J \Delta e^{i\theta_x} \cos(k_xa_0) & J \Delta e^{i\theta_x} \cos(k_xa_0) \\ J \Delta e^{i\theta_x} \cos(k_xa_0) & J \Delta e^{i\theta_x} \cos(k_xa_0) \end{bmatrix} \]  

(3.14)  

Finally, we write the \( \tilde{H}^{MF} \) as:

\[ \tilde{H}^{MF} = \sum_k \left[ \Psi_{C\uparrow}^\dagger(k) \right. \left. \Psi_{R\uparrow}(-k) \right] \begin{bmatrix} \tilde{T}(k) & D(k) \\ D^\dagger(k) & -\tilde{T}(k) \end{bmatrix} \begin{bmatrix} \Psi_{C\uparrow}(k) \\ \Psi_{R\uparrow}^\dagger(-k) \end{bmatrix} + L \left( 4J\Delta^2 + J'\Delta'^2 - 4t\mu \right) \]  

(3.15)
Let us denote the matrix \[
\begin{bmatrix}
\tilde{T}(k) & D(k) \\
D^\dagger(k) & -\tilde{T}(k)
\end{bmatrix}
\] by \(A(k)\). It is an \(8 \times 8\) symplectic, hermitian matrix whose eigenvalues are real and occur in pairs. That is, an eigenvalue’s negative is also an eigenvalue.

The mean field free energy and the self-consistent equations: The grand canonical free energy, \(\Phi\), at a given temperature, \(T\), for the mean field Hamiltonian described above is,

\[
\Phi = 4L \left( J\Delta^2 + \frac{J'\Delta'^2}{4} - t\mu \right) - \sum_{k} \sum_{j=1}^{4} \left\{ E_j^+(k) + \frac{2}{\beta} \log \left( 1 + e^{-\beta E_j^+(k)} \right) \right\} 
\]  

Here, \(\beta = 1/k_B T\), and \(\{E_j^+(k), j = 1, 4\}\) are the positive eigenvalues of \(A(k)\). Let us put \(t = 1\). Now, all the energies are in the units of \(t\). We find the self-consistent equations for \(\Delta\) and \(\Delta'\) by minimizing \(\Phi\) with respect to \(\Delta\) and \(\Delta'\). These are as follows.

\[
\Delta = \frac{1}{2J} \frac{1}{4L} \sum_k \sum_{j=1}^{4} \frac{\partial E_j^+(k)}{\partial \Delta} \tanh \left( \frac{\beta E_j^+(k)}{2} \right) 
\]  

\[
\Delta' = \frac{2}{J'} \frac{1}{4L} \sum_k \sum_{j=1}^{4} \frac{\partial E_j^+(k)}{\partial \Delta'} \tanh \left( \frac{\beta E_j^+(k)}{2} \right) 
\]

Since \(\partial \Phi / \partial \mu = -N\), where \(N\) is the total number of electrons, we get the following equation for the chemical potential.

\[
\delta = -\frac{1}{4L} \sum_k \sum_{j=1}^{4} \frac{\partial E_j^+(k)}{\partial \mu} \tanh \left( \frac{\beta E_j^+(k)}{2} \right) 
\]

The hole doping, \(\delta = 1 - N/4L\). Solving these sets of equations self-consistently gives us \(\Delta\), \(\Delta'\) and \(\mu\) as a function of \(\delta\), for given values of \(\alpha\), \(J\), \(\beta\) and the phase angles \(\theta_x\) etc.

3.4.2 Order parameter and quasi-particle spectrum

We solve Equations 3.17, 3.18 and 3.19 self-consistently for different values of \(\delta\). We consider only the hole doping for both positive and negative values of \(\alpha\), since it is clear from the band structure that the hole doping for \(\alpha\) is same as the electron doping for \(-\alpha\).

The values of various parameters used for computation are: \(t = 1\) and \(|\alpha| = 1.25\). The value of \(J\) for \(\text{SrCu}_2(\text{BO}_3)_2\) is roughly 700K, but the value of \(t\) is not known. Therefore, the ratio of \(J\) to \(t\) is only tentative.
Chapter 3 RVB mean field theory

Figure 3.7: The mean field order parameters, $\Delta$ and $\Delta'$, as a function of the hole doping $\delta$, in the ground state for $J = 0.3t$. For higher values of $t/J$, the value of the mean field order parameter is even smaller, and drops faster towards zero as the doping is increased (though we have not shown it here). For $\alpha = -1.25$, $\Delta$ is not shown, since it is identically zero.

Though there are four different phases, $\theta_x, \theta_y, \theta_{x+y}$ and $\theta_{x-y}$, only three relative phases are required since one of the phases can be gauged away. Therefore, we fix $\theta_x = 0$. By solving the mean field equations, we try to find out those values of phases for which the free energy is minimized, and see how the mean field order parameters, $\Delta$ and $\Delta'$, evolve as a function of the hole concentration, $\delta$.

First we consider the zero temperature ($\beta \rightarrow \infty$) case. For $\alpha = -1.25$, the minimum of free energy occurs for $\theta_{x+y} - \theta_{x-y} = \pi$ regardless of the values of $\theta_x$ and $\theta_y$, and $\Delta$ is identically zero. It is like d-wave pairing along the diagonal bonds. For $\alpha = 1.25$, the minimum of free energy corresponds to $\theta_x = 0$, $\theta_y = \pi$, $\theta_{x+y} = 0$ and $\theta_{x-y} = \pi$. It is a weak minimum as many other choices of the phases have similar values of the free energy. Nevertheless, this choice of phases appears to be the minimum.

We do rest of the computations for $\theta_x = 0$, $\theta_y = \pi$, $\theta_{x+y} = 0$ and $\theta_{x-y} = \pi$, i.e. with d-wave symmetry for both kinds of pairs. Figure 3.7 shows the variation of $\Delta$ and $\Delta'$ with respect to $\delta$, for $\alpha = -1.25$ and 1.25 at zero temperature. It is interesting to note that for $\delta = 0$, the diagonal bond order parameter, $\Delta'$, is one and $\Delta$ is zero (and is independent of the phases $\theta_x, \theta_y, \theta_{x+y}$ and $\theta_{x-y}$). Thus, the valence bond mean field theory at half filling exactly reproduces the known dimer ground state of the SS model.

Figure 3.8 shows the quasi-particle dispersion in the mean field theory. The quasi-
3.4 RVB calculation on the SS lattice

Figure 3.8: The quasi-particle dispersion from the RVB mean field calculation. Very close to half filling, excitation spectrum is gapped (left), and for higher doping, it becomes gap-less (right).

particle spectrum is gapped very close to half filling (and at half filling), as it should be (due to the persistence of spin-gap phase). However, the gap collapses rather quickly as doping is increased, and the RVB state becomes gap-less. For example, at $\delta = 0.2$ for $\alpha = -1.25$, the RVB solution is gap-less. The situation is same for positive value of $\alpha$, but the range of doping for which the RVB solution exists is small. This is an important point which comes out this RVB calculation. The negative $\alpha$ with hole doping provides a robust case for the RVB superconducting state, whereas the positive $\alpha$ with hole doping is a weaker case. Remember that $t$ is taken to be positive in the calculation. For $t < 0$, the same conclusion will follow through, but for electron doping in place of the hole doping.

3.4.3 Phase diagram

Having non-zero value of the mean field pairing order parameter does not necessarily imply superconductivity. For example, we know for sure that at half filling the system has insulating ground state consisting of singlet dimers. In order to describe superconductivity in our mean field theory, we define a physical order parameter, $\Delta_{SC} = F_B \Delta_{MF}$. Here, $\Delta_{MF}$ is the mean-field order parameter ($\Delta$ or $\Delta'$ whichever is larger for a given doping), and $F_B$ is a bosonic mean field. Such an order parameter can be understood in the framework of slave boson approach [38]. Here the physical electron operator $c_{\sigma}^\dagger = f_{\sigma}^\dagger b$, where $f_{\sigma}^\dagger$ is a neutral fermion field and $b$ is a charged boson field. The double occupancy projection is built into this transformation.

In this representation, the off-diagonal order parameter of the physical electrons,
\[ \langle c^+_i c^+_j \rangle \text{ is described as} \langle b_i b_j f^+_i f^+_j \rangle. \] In a mean field decoupled theory, this is like \( \langle b_i b_j \rangle \langle f^+_i f^+_j \rangle \equiv F_B \Delta_{MF}. \) Thus, in our mean field theory we have been essentially calculating the singlet spin pairing order parameter. In order to correctly identify the superconducting region in phase diagram, we need Bose condensation which comes from factor \( F_B. \) The superconducting state is one where both \( F_B \) and \( \Delta_{MF} \) both are simultaneously non-zero. The superconducting transition temperature, \( T_{SC} \), is the temperature where either \( \Delta_{MF} \) or \( F_B \) vanishes first while increasing the temperature. For low doping, \( \Delta_{MF} \) is large. Therefore, \( T_{SC} \) is same as the Bose condensation temperature \( T_{BC} \), for which the bosonic field \( F_B \) vanishes.

**Bose condensation temperature, \( T_{BC} \):** Estimating \( T_{BC} \) requires some care. There is a way of estimating \( T_{BC} \) [38], but we briefly discuss our alternative (equivalent) approach for the same. At the simplest level of mean field description, one can think of boson field as non-interacting. Then the bosons will have essentially the same dispersion as the tight binding model on the SS lattice. Since the non-interacting bosons can not condense in two dimensions, we consider a three dimensional anisotropic dispersion. The Bose condensation temperature \( T_{BC} \) that we estimate, therefore, is a three dimensional Bose condensation temperature (with large c-axis anisotropy).

We consider an approximate dispersion of the form, \( c^*(k_x^2 + k_y^2 + \frac{1}{\gamma} k_z^2) \), with the c-axis anisotropy \( \gamma \), around the (quadratic) extrema of one of the two middle tight binding bands (see Figure 3.5). Assuming that most of the action happens in the middle bands (since that is where the chemical potential is for close to half filling), we call that temperature as the Bose condensation temperature where the boson chemical potential, \( \mu^*_b \), takes the value of middle band extrema (essentially the point where two bands touch). This is just a choice. In fact, this prescription might seem very simplistic or even vague, but then all we want here is an order of magnitude estimate for the superconducting transition temperature. As we will see, it is not too badly off the anticipated temperature scales.

At the Bose condensation temperature,

\[
\delta = \frac{1}{4L} \sum_{k,j} \frac{1}{\exp(\epsilon_{k,j} - \mu^*_b)/T_{BC} - 1}
\approx \frac{T_{BC}}{c^* \pi} \left[ 2 + \log(\gamma/\pi) \right] \quad \text{for} \quad \gamma \gg \pi
\]

(3.20)

The band curvature, \( c^* \approx 1/(\pi \rho^*) \) where \( \rho^* \) is the non-interacting density of states (on two dimensional SS lattice) at the band extrema (as mentioned above). Finally, we get
the following expression for the Bose condensation temperature.

\[ T_{BC} \approx \frac{\delta}{\rho^*} \frac{1}{2 + \log(\gamma/\pi)} \]  

We have \( \rho^* \approx 0.1 \) and taking \( \gamma \approx 100 \), we get \( T_{BC} \approx 1.83 \delta \). Since the anisotropy parameter \( \gamma \) affects the \( T_{BC} \) only logarithmically, we can take some reasonable large value (like 100) for \( \gamma \), as we are interested in a (quasi) two dimensional situation.

**Phase diagram** : The phase diagram in the temperature-doping plane, as estimated from the RVB mean field calculation, is shown in Figure 3.9.

![Phase Diagram](image)

Figure 3.9: The phase diagram for the negative as well positive values of \( \alpha \). Notice that the range of the hole doping for the RVB superconducting phase is very small for \( \alpha > 0 \) as compared with the same for \( \alpha < 0 \).

Typically there are four distinct regions that one can identify, in the RVB mean field theory phase diagram. These are :

- spin-gapped : \( \Delta_{MF} \neq 0 \) and \( F_B = 0 \),
- RVB superconductor : \( \Delta_{MF} \neq 0 \) and \( F_B \neq 0 \),
- normal Fermi metal : \( \Delta_{MF} = 0 \) and \( F_B \neq 0 \), and
- strange metal : \( \Delta_{MF} = F_B = 0 \)
The temperature \( T_{MF} \) is the transition temperature calculated in the mean field theory where \( \Delta_{MF} \) vanishes. The estimated \( T_{BC} \), and the computed \( T_{MF} \) are plotted as a function of the hole concentration. The common region under these two curves, in Figure 3.9, is the RVB superconducting phase. Among the remaining three regions of T-\( \delta \) phase diagram, the low doping region below \( T_{MF} \) and above \( T_{BC} \) is the spin gap phase. Similarly, the high doping region is the normal Fermi liquid, and then there is a region which is usually referred to as the strange metal phase. The phase diagram is similar for both positive as well negative values of \( \alpha \), but the range of hole concentration for which the mean field solution exists is very small for \( \alpha > 0 \) and the mean field transition temperature drops very fast. This indicates that \( \alpha < 0 \) and hole doping (or \( \alpha > 0 \) and electron doping) favour the RVB superconductivity more than the other case. Though the Bose condensation line makes the superconducting region start from arbitrarily close to the half filling, we would expect it to start from some small but finite doping. And, the spin-gap phase will persist close to half filling at zero temperature, before the system goes superconducting.

As can be seen in Figure 3.9, the typical temperature scale involving superconducting phase is of the order of a few tens of Kelvin, which is what we had expected. In order to estimate the optimal \( T_C \) for the RVB superconducting phase, we consider the case when \( t/J = 10 \). This seems to be a reasonable choice of parameters (the estimates of \( t \) are somehow not available). Since \( J \sim 70K, t \sim 700K \) which is roughly 58 meV, not too badly off the typical values of \( t \) in strongly correlated systems, though it could be even higher. For the higher values of \( t \), the RVB mean field temperatures will become still smaller. For \( J = 0.1t \), the optimal \( T_C \) for both positive and negative \( \alpha \) is roughly 15 K around 0.05 doping. Though the optimal \( T_C \) are similar in both cases, the region of superconducting phase is very small in \( \alpha > 0 \). Thus, \( \alpha < 0 \) under hole doping provides a better choice for the RVB superconductivity.

One comment should be made regarding the interpretation of the result \( \Delta = 0 \) and \( \Delta' \neq 0 \) (for \( \alpha < 0 \)). While at half filling this implied the dimerized insulating state, away from half filling it must be interpreted as superconductivity. The BCS type wavefunction implies the fermion pairing in real space,

\[
\langle c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger \rangle \sim \sum_k e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \frac{\Delta_{k}}{\sqrt{\Delta_{k}^2 + (\epsilon_{k} - \mu)^2}} ,
\]

and it extends over a range of lattice constants (due to the non-trivial \( \mathbf{k} \) dependence of \( \epsilon_{k} \) away from \( \delta = 0 \)), despite the mean field Hamiltonian having \textit{n.n.} pairing only. A similar remark holds for the four Fermi operator that determines the superconducting ODLRO of Yang, namely \( \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j'\downarrow} c_{i'\uparrow} \rangle \neq 0 \) for \( |\mathbf{r}_i - \mathbf{r}_j| >> 1 \).
3.5 Superconducting Na$_x$CoO$_2$ · $y$H$_2$O

3.4.4 Summary

In the following, we summarize the main predictions, as deduced from the RVB mean field calculations on the SS lattice t-J model.

- The case of ‘$\alpha < 0$ and hole doping’ (or equivalently, $\alpha > 0$ and electron doping) is robust for the RVB superconducting phase.

- The pairing order parameter has d-wave symmetry. The quasi-particle excitation spectrum is gap-less in the superconducting phase, though close to half filling it is gapped (spin-gapped phase).

- The typical superconducting transition temperature is of the order of 10 K.

3.5 Na$_x$CoO$_2$ · $y$H$_2$O : a new superconductor

Recently, a cobalt oxide layered compound, Na$_x$CoO$_2$ · $y$H$_2$O is reported to exhibit superconductivity at around 5 K [4], where $x \approx 0.35$ and $y \approx 1.3$. This is an exciting new addition to the family of oxide superconductors, with similar quasi two dimensionality as in cuprates. This material is a derivative of a general family of compounds, Na$_x$CoO$_2$ (0.5 ≤ $x$ ≤ 1), which are reasonably good metals with large thermopower [27]. The discovery of superconductivity in the hydrated cobaltate has also been confirmed by other groups [5].

3.5.1 Structure

The structure of Na$_x$CoO$_2$ consists of CoO$_2$ layers and sodium mono-layers, as shown in Figure 3.10, stalked alternately along c-axis. The layered structure of the cobaltates is similar to that of the cuprates. However, in the CoO$_2$ layers the cobalt ions make a triangular lattice whereas in cuprates the copper ions form a square lattice. The superconducting cobalt oxide, Na$_x$CoO$_2$ · $y$H$_2$O, has the same structure except the presence of water layers between sodium and CoO$_2$ layers. The hydration increases the c-axis separation, and makes the system more two dimensional. The role of water is not very clear, though some recent studies indicate its importance for superconductivity in cobaltates [5]. The lattice parameters of the superconducting cobaltate, Na$_{0.35}$CoO$_2$ · 1.3H$_2$O, are : $a = 2.823\text\AA$ and $c = 19.6207\text\AA$ [4].
Figure 3.10: (A) Schematic diagram; (B) A cobalt oxide layer with cobalt ions forming a triangular lattice. Each cobalt ion is surrounded by six oxygens forming an edge-sharing octahedral arrangement.

### 3.5.2 An effective physical model

The valency of cobalt in CoO$_2$ layers is 4+, and it is in the octahedral environment of oxygen ions. The electronic configuration of Co$^{4+}$ is [Ar]3d$^5$. Due to the large crystal field splitting, Co$^{4+}$ favours a low spin configuration, that is S=1/2. Therefore, a cobalt oxide layer in Na$_x$CoO$_2$ can be modelled as a spin-1/2 triangular lattice, and acts as a half filled reference system (in an effective one band picture). The sodium atoms in the compound donate their single valence electrons to the CoO$_2$ layers, thereby electron-doping the triangular lattice, and changing a fraction of the Co$^{4+}$ ions to Co$^{3+}$ with S=0. To start with, a one band t-J model on the triangular lattice is a good physical model for this cobaltate.

In the present work, we perform what seems to be a consistent and simple version of RVB theory, one which yields d-wave order for the square lattice [29] and also for the other interesting case of SrCu$_2$(BO$_3$)$_2$ [9]. In a similar spirit to ours, earlier there have been done some calculations. The calculation in Reference [28] is confined to half filling. And a recent preprint by Baskaran [30] makes some qualitative points that are common to our calculations. Within this version, we evaluate the case of positive as well as negative hopping since these are so very different in their physical content. Using the particle-hole transformation for fermions, we may define two broad cases of interest:

- Case A: here we have either
  
  (i) $t > 0$ and electron doping, or
3.5 Superconducting $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$

(ii) $t < 0$ with hole doping, and

- Case B: where we have either
  (i) $t > 0$ and hole doping, or
  (ii) $t < 0$ and electron doping.

Here we note that the Hamiltonian of the t-J model is written in the standard form:

$$H = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P} c_{i\sigma}^\dagger c_{j\sigma} \mathcal{P} + J \sum_{\langle i,j \rangle} (S_i \cdot S_j - \frac{n_i n_j}{4})$$

(3.22)

where $\mathcal{P}$ stands for the Gutzwiller projection due to large U, and the summation is over nearest neighbours. The notation of hole and electron filling is relative to half filling in the effective one band model for this system, and as usual, $\delta = |1 - n|$, where $n$ is the electron concentration.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{density_of_states.png}
\caption{The density of states for the triangular lattice tight binding Hamiltonian, and locations of various systems.}
\end{figure}

A first step in the direction of identifying an effective one band model is in the work of Singh [31], whose LDA calculation of the band structure shows that the Fermi energy for the case of $\text{Na}_{0.5}\text{CoO}_2$ is in a tight binding like set of states of $t_{2g}$ symmetry, in the close proximity of and slightly above a sharp peak in the electronic density of state. We interpret this as an example of Case A(i) above, since the Fermi surface for triangular lattice tight binding band structure, $\epsilon(k) = -2t(\cos(k_x) + 2 \cos(k_x/2) \cos(\sqrt{3}k_y/2)$, gives a density of states (DOS) (see Figure 3.11) with a prominent peak near the Fermi level.
for Na$_{0.5}$CoO$_2$ as well as the extremity of the band, and to the extent that the low energy structures are irrelevant, this matches the LDA DOS[32].

3.6 Remarks on ferromagnetism and Hall constant in the triangular lattice

Before describing the RVB calculation, we recount a few remarkable features of the triangular lattice Hubbard model physics, that may be useful in future studies.

3.6.1 Ferromagnetism

Singh has noted that the LDA calculations of Na$_{0.5}$CoO$_2$ show an instability of the paramagnetic state towards a ferromagnetic state. Indeed this is exactly what one expects from the Nagaoka physics on the triangular lattice as shown by Shastry, Krishnamurthy and Anderson [33], who pointed out that while Case B above is highly detrimental to ferromagnetism in the infinite U limit, Case A highly favours the ferromagnetic state. This follows from a stability analysis of the low energy excitations of the state, and is presumably the fate of the t-J model at J = 0, and also in the high electron density limit of Case A(i) (where J becomes irrelevant) since in the limit of an almost filled band, with the Fermi energy near a peak in the DOS (as in transition metal ferromagnetism) the work of Kanamori and Galitskii predicts ferromagnetism. Thus notwithstanding the results of the RVB state, we must expect metallic ferromagnetism in the case when the electron doping is high in Case A(i).

3.6.2 High frequency Hall effect

A fascinating property of the triangular lattice was noted in Reference [34]. The high frequency Hall constant $R_H^*$ is amenable to a lattice walk expansion, and a simple calculation leads to

$$R_H^* = \frac{v}{8e} \frac{k_B T}{t} \frac{1 + \delta}{\delta(1 - \delta)}$$  \hspace{1cm} (3.23)

Here $e$ is the electronic charge (negative in sign) and $v$ is the physical (three dimensional) unit cell volume containing one cobalt ion$^2$, which from Reference [4] may be estimated to be $67.71 \times 10^{-24}$ cm$^3$. We remark that this result is computed in the case of hole doping.

$^2$The physical cell volume containing one cobalt ion, $v = \frac{1}{2} \sqrt[3]{a^2 c}$. The factor of 1/2 is there because each crystallographic unit cell of Na$_x$CoO$_2 \cdot y$H$_2$O contains two CoO$_2$ layers, each contributing one cobalt ion.
3.7 RVB calculation on the triangular lattice

3.7.1 Mean field equations

The ‘J’ term in Equation 3.22 can be re-written as \(-J\sum_{i,j} b_{ij}^\dagger b_{ij}\), where the bond operator, \(b_{ij}^\dagger = (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger)/\sqrt{2}\), is a singlet pair creation operator acting on a pair of sites \(i\) and \(j\).

The RVB mean field calculations are carried out by defining a complex order parameter, \(\Delta_{ij} = \langle b_{ij}^\dagger \rangle\). On the triangular lattice, we have three different nearest neighbor bonds, one along say x-direction and the other two at an angle of \(\pi/3\) and \(2\pi/3\) with x-axis.

We consider a simple situation where the \(|\Delta_{ij}| = \Delta\) along all bonds, but three different phases are allowed along three different bonds. Since one of the phases can be gauged away, only two (relative) phases are sufficient. We assign zero phase along the x-direction, \(\theta\) and \(\phi\) along the \(\pi/3\) and \(2\pi/3\) directions, respectively. In momentum space, this choice of mean field order parameter leads to the following k-space function, \(D(\mathbf{k})\), which carries the order parameter symmetry information.

\[
D(\mathbf{k}) = \cos(k_x) + e^{i\theta} \cos(k_x/2 + \sqrt{3}k_y/2) + e^{i\phi} \cos(k_x/2 - \sqrt{3}k_y/2) \tag{3.25}
\]

The effect of projection of double occupancy on hopping is accounted for by a simple approximation where \(t\) is replaced by \(t\delta\), with \(\delta\) being the hole concentration. Our calculations have been done only for hole doping case, but for both \(t > 0\) as well as \(t < 0\) (Cases

\[3\text{Very recently, the non-saturating linear behaviour at high temperatures for the transport Hall coefficient has been reported in Reference [39].}\]
B(i) and A(ii)). The case of electron doping can easily be related to these calculations by particle-hole transformation, as described earlier.

We get two mean field equations, one for $\Delta$ and the other for $\mu$, the chemical potential. These are:

$$\Delta = \frac{1}{6JL} \sum_k \frac{\partial E(k)}{\partial \Delta} \tanh \left( \frac{\beta E(k)}{2} \right)$$

(3.26)

$$\delta = -\frac{1}{L} \sum_k \frac{\partial E(k)}{\partial \mu} \tanh \left( \frac{\beta E(k)}{2} \right)$$

(3.27)

Here, $E(k) = \sqrt{(\epsilon(k) - \mu)^2 + 2J^2 \Delta^2 |D(k)|^2}$, $D(k)$ is given in Equation 3.25.

### 3.7.2 Order parameter and quasi-particle spectrum

We solve Equations 3.26 and 3.27 self-consistently for given values of $\delta$ and $t$, and for different choices of $\theta$ and $\phi$. All energies are measured in units of J. First, we perform the computation at $T=0$, and find the values of $\theta$ and $\phi$, at different hole concentrations, for which the ground state energy is minimum. This fixes the symmetry of the mean field order parameter.

![Figure 3.12](image)

Figure 3.12: The mean field energy density surface as a function of the internal phases, $\theta$ and $\phi$ (in units of $\pi$) of the order parameter. The minima occur at six corner points of the Brillouin zone.

At $\delta = 0$, the ground state energy is lowest for $(\theta, \phi) = (0, \pm \pi/2)$ and $(\theta, \phi) = (\pm \pi/2, 0)$, in contrast to the case of $(\theta, \phi) = (2\pi/3, 4\pi/3)$ of Reference [28] which has
slightly higher energy. At half filling, the RVB ground state has a lower symmetry of cubic type rather than the six-fold rotational symmetry of the triangular lattice.

Away from half filling, the ground state energy is lowest at \((\theta, \phi) = (2\pi/3, 4\pi/3), (4\pi/3, 2\pi/3)\) and \((2\pi/3, -2\pi/3)\). Three other phase-points, which are related to these via inversion with respect to origin, are equivalent, and together these six minimum energy phase-points reflect the symmetry of the Brillouin zone. Figure 3.12 shows the mean field energy density plotted as a function of \(\theta\) and \(\phi\). In rest of the calculations, we just choose one of these points to perform the computation.

At \(\theta = 2\pi/3\) and \(\phi = 4\pi/3\), for various values of \(t\), the mean field \(\Delta\) is computed as a function of hole concentration, as shown in Figure 3.13. \(\Delta\) decreases more rapidly for \(t > 0\) than for \(t < 0\), as the hole concentration is increased. It suggests that Case A, that is “\(t < 0\) and hole doping” or “\(t > 0\) and electron doping”, presents a robust case for the RVB state of superconductivity.

![Figure 3.13: The mean field \(\Delta\) as a function of the hole concentration, \(\delta\), for both positive and negative \(t\) in units of J.](image)

Next we present the quasi-particle dispersion and the quasi-particle density of states from our mean field calculations. These calculation are done for a physically relevant value of \(\delta \sim 0.35\) at which superconductivity is observed in \(\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}\) [4]. The cobalt oxide layer alone acts as a half filled system in the effective one band picture, therefore the carrier concentration in excess to the half filled case is just \(x\).

Both the quasi-particle dispersion and the density of states, in Figures 3.14 and 3.15
Figure 3.14: The quasi-particle dispersion, $E(k)$. The coordinates of $\Gamma$, $M$ and $K$ symmetry points in the Brillouin zone are given in units of $\pi$. The coordinates $(k_1,k_2)$ given here are such that $k_1 = k_x$ and $k_2 = (k_x + \sqrt{3}k_y)/2$, where $k_x$ and $k_y$ are the usual k-space variables along $x$ and $y$ directions.

Figure 3.15: The quasi-particle density of states.
respectively, show an energy gap in the spectrum. The reason lies in the fact that function $D(k)$ is complex. For $(\theta, \phi) = (2\pi/3, 4\pi/3)$, the function $D(k) = d_1 - id_2$, where $d_1 = \cos(k_x) - \cos(k_x/2)\cos(\sqrt{3}k_y/2)$ and $d_2 = \sqrt{3}\sin(k_x/2)\sin(\sqrt{3}k_y/2)$. Thus our results are akin to the $d_{x^2-y^2} + id_{xy}$ symmetry case in the cuprates.

The modulus of $D(k)$ is non-zero at all points in the Brillouin zone, except at six zone corner points, that is $(2\pi/3, -2\pi/3)$, $(2\pi/3, 4\pi/3)$ etc and the origin. Though $\epsilon(k) - \mu$ has contour of zeros within the Brillouin zone, the chance of six corner points lying exactly on this contour is almost zero. This point is clear in Figure 3.16, where $|D(k)|$ and $\epsilon(k) - \mu$ are plotted along three symmetry directions of the Brillouin zone. The gap for $t = -1$ and $-2$ is approximately 0.2J and 0.1J, respectively. The gap ($\sim |\Delta|$) decreases with increasing $|t|$ as already noted. We mention that the quasi-particle spectrum is gapped for $t > 0$ as well, but the gap is very small around the doping of our interest. In fact for higher values of $t$ (say, 3) it is zero at $\delta = 0.35$, precisely because $\Delta = 0$. Thus, Case B does not favour RVB solution for large values of $t$ and $\delta$.

We have also calculated the temperature at which the mean field order parameter $\Delta$ vanishes for different values of $\delta$. It helps us understand the broad nature of thermodynamic phase diagram in $T$-$\delta$ plane. Figure 3.17 shows the transition temperatures for different hole concentrations for which $\Delta$ vanishes.

The question of RVB superconductivity needs a little more care than what we have given so far. The mean field $\Delta$, though a pairing order parameter, doesn’t by itself imply superconductivity. For example at half filling $\Delta$ is non-zero, but it is insulating. The identification of the superconducting phase in $T$-$\delta$ diagram can, however, be done within
the framework of the slave boson approach. This approach has been quite popular in the RVB theories of t-J model on square lattice \[38\]. Here the physical electron operator, 
\[ c_{\sigma}^\dagger = f_{\sigma}^\dagger b, \]
where \( f \) is the spin-1/2 neutral fermion, and \( b \) is the spin-0 charged boson, and the projection of double occupancy is in-built into the construction.

\[ T \text{ is in units of } J. \text{ The case with } t > 0 \text{ for } \delta \sim 0.35 \text{ is not very robust for the RVB mean field theory whereas } t < 0 \text{ is favourable.} \]

The superconducting order parameter \( \langle c^\dagger c \rangle \) is like \( \langle bb \rangle \langle f^\dagger f^\dagger \rangle \), a product of spin pair ing order parameter and a Bose condensation factor. What we have got from the mean field calculation is essentially the spin-pairing order parameter. The true superconducting order parameter is \( \Delta_{SC} \sim F_B \Delta \), where \( \Delta \) is the mean field order parameter. The Bose condensation temperature for \( b \) bosons (for \( F_B \) to be non-zero) needs to be estimated separately. That region of \( T-\delta \) diagram, where both \( F_B \) as well \( \Delta \) are non-zero, can be interpreted as the RVB superconducting phase. There are three more typical regions according to this interpretation: (1) Spin-gap: \( \Delta \neq 0 \) and \( F_B = 0 \), (2) Strange metal: \( \Delta = F_B = 0 \), and (3) Normal Metal: \( \Delta = 0 \) and \( F_B \neq 0 \). With this qualitative picture in mind, we will present a rough phase diagram for the cobalt oxide superconductors.

The Bose condensation temperature \( T_{BC} \) can be estimated in the similar way as prescribed earlier in the SS lattice mean field calculation. Around the band’s bottom, the energy dispersion can be approximated as \( c^* (k^2 + k_z^2/\gamma) \). The curvature, \( c^* \), is related to the two dimensional density of states at the band edge, \( \rho^* \) as: \( c^* \approx \frac{1}{4\pi \rho^*} \). Now, using the fact that free boson can condense in three dimensions, and doing some simplification for
3.7 RVB calculation on the triangular lattice

\( \gamma \gg \pi/4 \), we get

\[
T_{BC} \approx \frac{\delta}{\rho} \frac{1}{2 + \log(4\gamma/\pi)}
\]

Since the anisotropy affects only logarithmically, we can safely take some large value for \( \gamma \sim 100 \), especially when the real system is a good quasi two dimensional system.

3.7.3 Phase Diagram

Here, we propose a rough phase diagram for triangular lattice, layered cobalt oxide materials over a wide range of doping calculated in the scheme of Case A(ii). It is shown in Figure 3.18. The phase diagram for Case A(ii) seems to encompass a number of interesting phases, including the recently observed superconducting phase. We will briefly describe each of the labelled region in Figure 3.18. We also present, in Figure 3.19, the mean field phase diagram for Case B(i). Though Case B presents a weak case, it can still achieve the RVB superconducting phase for small values of \( t \) (\( \sim J \) or smaller; see Figure 3.17). Since the value of \( |t| \) in these cobaltates is believed to be rather low, it is quite appropriate to mention the results for Case B also.

![Figure 3.18: The mean field phase diagram for \( t = -3J \) and \( (\theta, \phi) = (2\pi/3, 4\pi/3) \).](image)

The exchange coupling \( J \) is estimated from the high temperature susceptibility data for \( \text{Na}_{0.5}\text{CoO}_2 \) [36]. Its Curie temperature\(^4\) is approximately \(-118\)K which gives \( J \sim 79\)K. For

\^4The Curie temperature for the superconducting cobaltate \( \text{Na}_{0.35}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O} \) has not been reported
doping $\delta = 0.35$, the $T_C$ for transition into an RVB superconducting state is approximately 10K, which is not too far from the measured $T_C \sim 5$K [4]. An important prediction for the superconducting phase is the existence of an energy gap in the quasi-particle spectrum. And it is explained to be there because the superconducting order parameter is complex, with relative internal phases being $2\pi/3$ and $4\pi/3$. In order to achieve higher superconducting $T_C$, the one should attempt to lower the electron concentration of the material, the optimal doping seems to be around 0.15.

On the higher side of the doping $\delta \gtrsim 0.5$ in Figure 3.18, we expect the RVB superconducting state to become unstable in favour of a ferromagnetic metallic state where the Nagaoka-Kanamori ferromagnetism plays the dominant role. We call $\delta = 0.5$ (electron concentration, $n = 1.5$) as the Nagaoka-Kanamori line. At sufficiently high temperatures, we expect ferro-metal to para-metal transition across the Nagaoka-Kanamori line.

![Figure 3.19: The mean field phase diagram for $t = J$ and $(\theta, \phi)=(2\pi/3, 4\pi/3)$.](image)

Apart from the above mentioned important phases, one may expect spin-gapped phase in the low doping, low temperature regime, since that is where exchange interaction will play more decisive role. The antiferromagnetic phase is likely to persist for small doping. We also expect a strange metallic phase to exist at moderate doping, but only at higher temperatures. The phase diagram for Case B(i), as shown in Figure 3.19, is just the standard RVB mean field phase diagram. The possibility of a ferromagnetic phase does not arise in this case.
3.7.4 Summary

To summarize the work presented here, we have performed an RVB mean field theory on the triangular lattice inspired by the recent discovery of superconductivity in a cobalt oxide layered material. Several detailed results are presented. We find the symmetry of the superconducting order parameter, and predict the existence of an energy gap. We argue that the real material corresponds to an effective one band case with $t > 0$ and electron doping. We also present an approximate phase diagram for the cobalt oxide superconductor in the $T$-$\delta$ plane. We propose that the low temperature RVB superconducting phase will give way to a ferromagnetic metal at higher doping $\gtrsim 0.5$ where we believe that the Nagaoka-Kanamori physics will dominate over the RVB physics.

For high temperatures ($k_B T \gg |t|$), the high frequency Hall constant is predicted to grow linearly with temperature. This is a special property of the triangular lattice. One major assumption in this work is that the scale of $t$ is not too different from $J$ which is estimated to be around 79K. This estimate is at odds with the LDA estimate of the band width by two orders of magnitude, and thus we cannot claim to have “explained” the low degeneracy temperature scale, we have merely assumed it and worked out the consequences for other properties.
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Bibliography


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[30] G. Baskaran, cond-mat/0303649, here the assignment of the sign of the hopping element "t" seems to be the opposite to ours, namely to Case B(ii).

Our assignment of the sign of “t” leads to an electron like Fermi surface surrounding the Γ point, which might be ascribable to the electron like band in Figure 1 of Reference [31] having a minimum at the Γ point. This is reasonable if remember that the electron count for the superconducting samples $x = 0.35$ forces the Fermi level to dip below the value for the $x = 0.5$ case reported in Reference [31] which has a hole like Fermi surface surrounding the Γ point.


[34] With an absolute scale measurement of $R^*_H$, it should be possible to obtain not only the sign of “t”, but also its magnitude. Optical Hall constant measurements may be roughly guessed at from the transport measurements.


[38] Y. Wang, N. S. Rogado, R. J. Cava and N. P. Ong, cond-mat/0305455
Chapter 4

Order by projection in the models of interacting electrons

A few model calculations exhibiting the phenomenon of order by projection are presented. A possible usefulness of the fusion of electron-phonon interaction and order by projection is pointed out. Its significance is discussed particularly in relation with the question of superconductivity in correlated systems. Implications of order by projection are also discussed in a model of two level atoms interacting with a single mode quantized radiation field.

There is considerable recent interest in models exhibiting superconductivity starting from repulsion. While popular models such as the t-J and Hubbard model display superconducting phases within approximate treatments, such as slave boson mean field theories and variational wavefunction approach, these remains somewhat unconvincing due to the uncontrolled nature of the schemes employed. One may in fact argue that apart from the Kohn-Luttinger [1] result for repulsive continuum electronic systems, there is no other compelling result for superconductivity from repulsion. In particular, electrons on a lattice have an extra property of being “commensurate” at certain fillings, and it is widely expected, but never quite proven that this particular feature is of great significance, especially for high-\(T_C\) cuprates which are interesting near half filling. It is therefore quite important to develop new non-perturbative methods and tools to investigate cooperative behaviour of lattice fermions. In this context, a general idea termed Order by Projection has been introduced recently [2, 3].

The models introduced in References [2, 3] contain pairing terms, as in the BCS reduced Hamiltonian, but with large and repulsive interactions. In the Wannier basis, the
added term corresponds to an infinite ranged hopping of pairs of particles in real space. Such pair hopping terms certainly occur in the lattice representation of the Coulomb interaction, but are of finite range. The theoretical models are thus in the spirit of mean field models, the hope being that some features of the solutions are of a general nature that transcend the limitations of the starting models. In summary, it is found that the lattice Fermi system attains enhanced extended s-wave superconducting fluctuations $A$ in the proximity of half filling in reaction to the suppression of on-site s-wave fluctuations $B$ (defined in following section; also see Equations 1.5 and 1.6). The uncertainty principle plays a crucial role in this since the s-wave and the extended s-wave ordering operators are recognized to be conjugates. Half filling plays a special role in this enhancement, since it is only in its proximity can one suppress both $< B^\dagger B >$ and $< BB^\dagger >$.

The above works have used a combination of techniques including rigorous inequalities and variational methods, on a class of models that are typified by either the Hubbard model, or the kinetic energy, to which we add a pure repulsive BCS like interaction. The rigorous methods tell us that the extended s-wave correlation function is bounded from below by $\text{const}/(1 - \rho)$, where $\rho$ is the filling, and hence there is a large “Gutzwiller” type enhancement. This has been briefly described in Section 1.3.

While the above work gives us an interesting and novel direction, several questions concerning the models and their behaviour remain poorly understood. At precisely half filling, the rigorous inequalities do not give us any guidance with reference to the question of whether the correlation function has actual long ranged order (LRO), or if it is only critical, i.e. $\propto L^{1+\eta} \ (1 > \eta > 0)$. We discover here that the solutions do not have a true LRO, and are superconducting only in the sense that the (normalized) correlations function $\langle A^\dagger A \rangle / L$ diverge in the thermodynamic limit. Also it is not clear if the ground state energy density is affected at half filling. There is also the issue of energy balance away from half filling, we know from the inequalities that the interaction does not change the energy density, and yet one expects non-extensive energy corrections both for the potential and the kinetic energies. Can one say a little more about these?

Most of the explicit results obtained so far concern the repulsive BCS model with a large repulsive coupling constant, for which the variational calculations [3] bear out rather well the expectations arising from the general method of inequalities [2]. Barring the degeneracies of single particle levels, the latter model actually maps on to a spin model in 1-dimension, where energy plays the role of the single dimension. The model, described more fully later in this work, turns out to be difficult to solve explicitly, and was analyzed numerically in Reference [2] by means of exact diagonalization for rather short chains, with a view to answer the above questions. In this work we extend the numerical results further to bigger systems and obtain more robust results.
In this work we introduce and solve explicitly and exactly a rather simple model that is inspired by the above spin model. This spin model consists of a large number of two level systems, these interact via a spin flip coupling that has the same form as in the above spin model, and the simplification consists of replacing a gradual variation of energies in the Zeeman part (representing the filled Fermi sea in the first instance) by just a pair of energies. The model contains many elements of the more general models, but not all. The great advantage however, is that the usual semi-classical methods, such as Holstein-Primakoff transformation, help us solve this simplified model exactly in the thermodynamic limit, and also give an estimation of the finite size corrections. Variations of this model also arise in the study of two level systems in Quantum Optics, and we explore the connections in this work.

We find that a variant of the Feynman-Hellman coupling constant integration theorem can be utilized to formulate a rather remarkable sum rule in the models considered here. The sum rule equates an extensive expectation value to a weighted coupling constant integral of the kinetic energy shift, the latter is not extensive, and yet adds up due to the weight factor to an extensive result. While this sum rule is true quite generally for this class of models, the above simplified model gives us an explicit example of the rule at work, and provides a “feel” for the nature of finite size corrections.

The organization of the chapter is as follows. In Section 4.1, we define the general Hamiltonian with s-wave projection and derive the sum rule. We next present numerical results for the spin model with linear dispersion relation at half filling, and discuss their implications for the behaviour of correlations and energy at half filling in the general models. In Sections 4.2 and 4.3, we present the simplified spin Hamiltonian and proceed with its solution by different methods. We first present some calculations on the spin model with interaction being negative and of the order of inverse system size, as in the usual BCS model. We then discuss the case of repulsion in great detail. In Section 4.4, we discuss order by projection in the presence of electron-phonon interaction. Our hope is that the effective attraction due to phonons may help the system to attain true LRO in A channel under the projection of s-wave pairing. In Section 4.5, we consider the question whether the idea of order by projection can be useful for the two level atoms interacting with the radiation field. Finally in Section 4.6, we present a summary of the results.

4.1 Models and Sum Rule

We collect together in this section, the various models treated in this chapter. To start with, the general Hamiltonian for the interacting electrons with s-wave projection, as
introduced in Reference [2], is the following.

\[ \mathcal{H} = \sum_{i,j} \sum_{\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + U_s B^\dagger B \]  
(Model-I)  
(4.1)

The first two terms in Equation 4.1 with \( U > 0 \) give the Hubbard model, and the third term is new, and represents the on site s-wave projection term for \( U_s > 0 \) and of \( O(1) \).

Here, the operator \( B = \sum_i c_i \downarrow c_i \uparrow \) is the on-site s-wave pairing operator. We refer to this as Model-I. This new added term is of particular interest for the present work, since it leads to an enhancement in the extended s-wave correlations. For completeness note that the extended s-wave pairing operator is defined as \( A = -2 \Sigma_k \epsilon_k c_{k\uparrow} c_{-k\downarrow} \), where \( \epsilon_k = -2t(\cos(k_x) + \cos(k_y)) \), on a square lattice, with \( k \) the momentum label and \( t \) the nearest neighbour hopping amplitude.

The second model considered here corresponds to setting \( U = 0 \) in the Model-I, whereby it reduces to the repulsive version of the reduced Hamiltonian of BCS, with a “large” coupling constant \( U_s \) (since the latter is written for attractive interactions with a coupling constant of \( O(1/L) \) so that the energy is extensive in the ordered state). It is possible to write it in spin notation using the Anderson mapping of the BCS pairing operators to pseudo spins \( s_i^+ = c_{k\uparrow}^\dagger c_{-k\downarrow} \) and \( s_i^z = \frac{1}{2}(n_{k\uparrow} + n_{-k\downarrow} - 1) \) [4]. We find the following spin-1/2 Hamiltonian.

\[ \mathcal{H} = \sum_i \epsilon_i (2s_i^z + 1) + U_s \sum_{i,j} s_i^+ s_j^- \]  
(Model-II).  
(4.2)

We refer to this as Model-II in the sequel. Note that index \( i \), here, corresponds to the \( i^{th} \) \( k \) mode in the momentum space, and the transformation is meaningful only in the subspace where pairs \( (k\uparrow, -k\downarrow) \) are either absent or present. The electrons that are not parts of a ‘Cooper pair’ are thus unaffected by the interaction and are ignored. In the literal mapping of the BCS model, we would find each energy level \( \epsilon_i \) having a large degeneracy, corresponding to the degeneracies of the cosine bands, but in the effective model treated here, we simply consider each energy level as non degenerate. The energies are assumed to have a linear dispersion \( \epsilon_i = -\frac{1}{2} + \frac{i-1}{L-1} \). The linear “ramp” of energies thus represents the fermionic energy levels filled up to a certain level, and the number of electrons is given by \( N = \sum_j (1 + 2s_j^z) \), which also is twice the number of Cooper pairs. Half filling clearly corresponds to the sector \( s_{\text{total}}^z = 0 \).

We finally indicate the simplified model that is obtained by further approximating the above Model-II. We restrict the energies \( \epsilon_i \) to be \(-1 \) \((+1)\) for \( i < L/2 \) \((i > L/2)\) and find

\[ \mathcal{H} = -\sum_{i}^{L/2} 2(s_i^z - s_{i+L/2}^z) + U_s \sum_{i,j} s_i^+ s_j^- \]  
(Model-III).  
(4.3)
In Section 4.2, we rewrite Model-III in a more convenient way, and present detailed calculations.

### 4.1.1 Sum rule

We now present an important sum rule for the general Hamiltonian (Model-I in Equation 4.1) which relates the non-extensive change in the expectation value of the Hubbard part of the Hamiltonian due to $U_s$, to the expectation value of $B^\dagger B$ in the ground state with $U_s = 0$. For convenience, let’s write Model-I as $\mathcal{H} = T + U_s V$ where $T$ stands for the Hubbard part and $V$ stands for $B^\dagger B$. For $U = 0$, $T$ is simply the kinetic energy of the electrons. The expectation values of operators $T$ and $V$ in the ground state, for a particular value of $U_s$, are denoted by $T(U_s)$ and $V(U_s)$, respectively.

Let $E(U_s)$ be the ground state energy of Model-I for a particular value of $U_s$. The Feynman-Hellman theorem states that $\Delta E(U_s) = E(U_s) - E(0) = \int_0^{U_s} d\lambda V(\lambda)$. From the general arguments of Reference [2], we know that

$$\Delta E(U_s) = \int_0^{U_s} d\lambda V(\lambda) \sim o(L) \quad (4.4)$$

Here, $L$ stands for the system size and $o(L)$ implies that the quantity is non-extensive, unlike $O(L)$ which says that the quantity goes like $L$. Thus Equation 4.4 implies that $\Delta E(U_s)/L \to 0$ as $L \to \infty$. The energy shift is non extensive. Using the relation $\lambda V(\lambda) = \Delta E(\lambda) - \Delta T(\lambda)$, and manipulating a bit, we derive the following relation for the change in the ground state energy, in the presence of the s-wave projection term [5].

$$\Delta E(U_s) = U_s \left( V(0) - \int_0^{U_s} \frac{d\lambda}{\lambda^2} \Delta T(\lambda) \right) \quad (4.5)$$

where $\Delta T(\lambda) = T(\lambda) - T(0)$. Equation 4.5 is true in general whereas Equation 4.4, is true only for Model-I. These two together imply the following sum rule:

$$V(0) = \int_0^{U_s} \frac{d\lambda}{\lambda^2} \Delta T(\lambda) + o(L) \quad (4.6)$$

This is quite remarkable as an extensive quantity, $V(0)$, is equated by integration over an intensive quantity, $\Delta T(\lambda)$, in the thermodynamic limit. In Section 4.3.3, we will see explicitly how two sides of Equation 4.6 equate each other, in the thermodynamic limit (see Equations 4.30 and 4.31), from the calculations of Model-III.
4.1.2 Numerical results for Model-II

Here, we present extended numerical results for the Model-II. As mentioned earlier, this model was studied in Reference [2] and a preliminary numerical investigation of short chains, with $L$ up to 14 was presented for somewhat large values of $U_s$. In Reference [2] the numerics was interpreted to be consistent with $\langle A^\dagger A \rangle \sim L^2$. However the analytical results of Reference [3] give $\langle A^\dagger A \rangle \sim L^{3/2}$. In order to resolve this issue we have computed these correlation functions for longer chains.

We computed ground state energy, $E_g$, $\langle A^\dagger A \rangle$ and $\langle B^\dagger B \rangle$ numerically as a function of system size $L$, at half filling upto $L = 22$, for $U_s = 0.5, 1.0, 1.5$ and $2.0$ [6]. The results of these numerical calculations are shown below. In Figure 4.1, we see that the data goes fairly linearly when plotted against $L^{3/2}$ as compared to when plotted against $L^2$, especially for small $U_s$. This favours the theoretical understanding that $\langle A^\dagger A \rangle \sim L^{3/2}$. In Figure 4.2, we have drawn a comparison between two possible behaviours for the ground state energy shift as a function of the system size, $L$. If the system has true LRO then one expects the shift to be linear in $L$, whereas with critical correlations [3], the shift should be $\propto L^{1/2}$, and hence non extensive. We see that the data is more consistent with $\Delta E_g$ going as $L^{1/2}$. We next examine the coefficients of the leading terms of $\langle A^\dagger A \rangle$ and

Figure 4.1: The extended s-wave correlation function, $\langle A^\dagger A \rangle$, at half filling is plotted against (a) $L^{3/2}$, and (b) $L^2$ for chains of length upto 22.
4.1 Models and a sum rule

Figure 4.2: The ground state energy shift, \( \Delta E_g \), at half filling is plotted against (a) \( L^{1/2} \), and (b) \( L \) for chains up to \( L = 22 \).

\[
\frac{E_g}{L} \approx e_{\text{non}} + 2\sqrt{U_s\alpha(0)} \frac{1}{\sqrt{\mu_1 L}} \\
\alpha \approx 12 \sqrt{\alpha(0)\mu_1 U_s L^{1/2}}
\] (4.7) (4.8)

Here, \( \alpha = \langle A^\dagger A \rangle/(4L) \) and \( \mu_1 = \frac{1}{L} \sum_k \epsilon_k (2f_k - 1) \). The \( \alpha(0) \) is the value of \( \alpha \) for \( U_s = 0 \). For linear dispersion,

\[
\alpha(0) = \frac{1}{24} \frac{L + 1}{L - 1} \quad \text{and} \quad \mu_1 = -\frac{1}{4} \frac{L}{L - 1}
\]

Therefore, from Equations 4.7 and 4.8, one finds that \( \langle A^\dagger A \rangle \approx \sqrt{U_s/24L^{3/2}} \) and \( (E_g - E_g^0) \approx \sqrt{2U_s/3L^{1/2}} \), in the thermodynamic limit. We also have a heuristic result for \( \langle A^\dagger A \rangle \) and \( \Delta E_g \) in terms of \( \mu_1 \), \( \Delta E_g \sim \sqrt{2U_s|\mu_1|L} \) and \( \alpha = \frac{1}{2\sqrt{2}} \sqrt{U_s|\mu_1| L} \) at half filling, obtained from a functional integral approach. These are equivalent to replacing \( \alpha(0) \) by \( |\mu_1|^2/2 \) in the variational results.

In Figure 4.3, the numerical estimates of the coefficients of the leading order term of \( \langle A^\dagger A \rangle \) and \( \Delta E_g \) in \( L \) are shown together with the variational and the heuristic results. The latter is closer to the numerical value. We thus see that the theoretical estimates and the exact numerics for relatively short chains are qualitatively in consonance in suggesting critical order rather than true LRO at half filling. Detailed examination shows that there
are some discrepancies in the coefficients of the leading behaviour, these seem to become larger for modestly large values of $U_s$, implying that the values of $U_s$ in Reference [2] were much too large. It seems that further finites size studies on longer systems may be needed to be completely sure of the final coefficients.

4.2 Model-III : a simplified spin model

For a fairly simple choice of the dispersion relation, as mentioned earlier, Model-III is derived from Model-II. Let’s label the group of spins with $\epsilon = -1$ as $a$ and with $\epsilon = 1$ as $b$. Then Model-III can be rewritten in the following convenient form.

$$
\mathcal{H} = 2(-S^z_a + S^z_b) + U_s(S^+_a + S^+_b)(S^-_a + S^-_b)
$$

(4.9)

Here, $S_a = \Sigma_{L/2}^1 s_i$ and $S_b = \Sigma_{L+1}^L s_i$. This turns out to be a problem of two large spins $S_a$ and $S_b$ coupled to each other antiferromagnetically. The analog of s-wave and extended s-wave pairing operators for this spin problem are $B = S^-_a + S^-_b$ and $A = 2(S^-_a - S^-_b)$.

4.2.1 Attractive case : $U_s = -\gamma / \bar{L}$

Before considering the repulsive case ($U_s > 0$ and $\sim \mathcal{O}(1)$) for Model-III (as given in Equation 4.9), we briefly discuss the attractive case with $U_s = -\gamma / L$, where $\gamma \sim \mathcal{O}(1)$ and positive. It is clearly the case of conventional BCS type superconductivity.
At half filling ($\rho = 1$), Model-III with attractive interaction shows a first order phase transition from normal to superconducting ground state as $\gamma$ is varied. In the thermodynamic limit, $\Delta E_g = E_g(\gamma) - E_g(0)$ is

$$\Delta E_g = \begin{cases} -2 + \sqrt{2(2 - \gamma)} & , \gamma < 2 \\ -L(\gamma/4) (1 - 2/\gamma)^2 & , \gamma \geq 2 \end{cases} \tag{4.10}$$

We also calculate $\langle B^\dagger B \rangle$ correlation function, in the thermodynamic limit. To the leading order in $L$, at $\rho = 1$,

$$\langle B^\dagger B \rangle = \begin{cases} L/\sqrt{2(2 - \gamma)} & , \gamma < 2 \\ (L/2)^2 [1 - (2/\gamma)^2] & , \gamma \geq 2 \end{cases} \tag{4.11}$$

We define an order parameter $\Omega = \sqrt{\langle B^\dagger B \rangle}/L$ (in analogy with usual mean field theory). Here, we see that in the thermodynamic limit, there is true LRO in $\langle B^\dagger B \rangle$, and $\Delta E_g$ is extensive. Figure 4.4 shows the exact diagonalization and the semiclassical results for the change in the ground state energy in Equation 4.10. Figure 4.5 shows $\Omega$ as a function of $L$ and $\gamma$. We see that for large enough $L$, the ground state is superconducting for $\gamma > 2$ and normal for $\gamma < 2$. Here, at $\rho = 1$, $\gamma = 2$ is special because the interaction can make one spin flip only if it gains an energy of amount 2 at least (which is the band width). For smaller systems, $\Omega$ is significantly non-zero for $\gamma < 2$, and also deviates from its thermodynamic behaviour in the region $\gamma > 2$.

It is worth mentioning that the reduced BCS model for studying superconductivity in the ultra-small metal particles [11, 12, 13] can easily be mapped to the Model-II with
Chapter 4  Order by Projection

$U_s = -\gamma / L$, and can further be approximated by the simpler Model-III studied here. The results obtained here are in the qualitative agreement with the experimental observations [10]. Firstly, the finite size order parameter is always greater than its thermodynamic value. Secondly, the system is superconducting for average level spacing, $2/L$, less than interaction, $\gamma / L$. Issues like cross-over from bulk behaviour to small size behaviour can not be studied rigorously here, because of the simple structure of the Hamiltonian, i.e. the density of states is structureless and independent of $L$. As $S_a$ and $S_b$ are large spins, the quantum fluctuations are also insignificant.

![Figure 4.5](image)

Figure 4.5: $\Omega$ as a function of $\gamma$. Plot (b) shows the deviation in $\Omega$ from its thermodynamic behaviour for small system size.

### 4.3 Repulsive case of Model-III

Now, we consider the repulsive case of Model-III where $U_s > 0$ and $\sim \mathcal{O}(1)$. This corresponds to the projection of s-wave pairing. In the following subsections, we discuss this case in detail.

#### 4.3.1 Exact diagonalization

We now proceed to solve this model through exact diagonalization. Let’s note that the operators $S^z_a$ and $S^z_b$ commute with the operators $S^{\pm,z}_{a,b}$ and therefore, commute with the spin Hamiltonian. The operator $S^z = S^z_a + S^z_b$ also commutes with the same. Thus, we have three conserved quantities $s_a$ and $s_b$, the quantum numbers associated with
4.3 Repulsive case: $U_s > 0$ and $\sim O(1)$

spins $S_a$ and $S_b$, and $n$, the quantum number associated with total $S^z$. For the exact diagonalization of Model-III, we choose the basis states to be the product states of the two spins $S_a$ and $S_b$. We write the basis states as $\ket{n, s_a; s_b; m} = \ket{s_a, m} \ket{s_b, n - m}$. For a given filling $\rho = N/L$, where $N$ is the number of electrons on a lattice with $L$ number of sites, the allowed values of quantum numbers are

$$n = -\frac{L}{2}(1 - \rho), \quad s_{\text{min}} \leq s_a \leq \frac{L}{4} \quad \text{and} \quad \max(s_{\text{min}}, |n| - s_a) \leq s_b \leq \min\left(\frac{L}{2} - s_a, \frac{L}{4}\right)$$

(4.12)

where $s_{\text{min}}$ is 0 for even value of $L/2$, and 1/2 for odd $L/2$. Only those values of $s_a$ are acceptable for which the $\max(s_{\text{min}}, |n| - s_a) \leq \min(L/2 - s_a, L/4)$. Given the values of $n$, $s_a$ and $s_b$, the running index $m$ in the basis states is such that $\max(n - s_b, -s_a) \leq m \leq \min(n + s_b, s_a)$. We diagonalize the Hamiltonian matrix for fixed values of $n$, $s_a$ and $s_b$. The minimum eigenvalue corresponds to $s_b = L/4$ and $s_a = L|2\rho - 1|/4$. This we identify as the ground state energy and the corresponding eigenvector as the ground state of the system. Fillings $\rho \leq 1/2$ are not interesting as the operators $A$ and $B$ annihilate the ground state of the Hamiltonian. We confine our calculations close to half filling ($\rho = 1$) as this is where one expects large enhancement in the extended s-wave pairing correlations.

4.3.2 Calculations using Holstein-Primakoff transformation

As we noticed above, the quantum numbers $s_a$ and $s_b$ for the ground state are proportional to system size, $L$. More precisely, the ground state for $\rho > 1/2$ corresponds to $s_a = L(2\rho - 1)/4$ and $s_b = L/4$. Therefore, in the thermodynamic limit, we use the Holstein-Primakoff (HP) transformation. This semiclassical approximation enables us to get analytical expressions for various quantities like $E_g$, $\langle A\dagger A \rangle$ etc. to the leading order in the system size.

Let $a$ and $b$ be canonical Bose operators. According to the HP transformation, the spin operators $S_a$ and $S_b$ are defined in the following way.

$$
\begin{align*}
S^+_a &= \sqrt{2s_a - a\dagger a} a \\
S^-_a &= a\dagger \sqrt{2s_a - a\dagger a} \\
S^z_a &= s_a - a\dagger a \\
S^+_b &= b\dagger \sqrt{2s_b - b\dagger b} \\
S^-_b &= \sqrt{2s_b - b\dagger b} b \\
S^z_b &= -s_b + b\dagger b
\end{align*}
$$

(4.13)

For large $L$, we expand square roots appearing in the Equation 4.13 only upto first order in $a\dagger a/2s_a$ and $b\dagger b/2s_b$. This transforms the spin Hamiltonian Equation 4.9 into the following bosonic Hamiltonian:


\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4 + \mathcal{O}(1/L) \] (4.14)

where

\begin{align*}
\mathcal{H}_0 &= -2 (s_a + s_b + 1) + 2 U_s (s_a - s_b) \\
\mathcal{H}_2 &= 2 \left[ (1 + s_a U_s) a^{\dagger} a + U_s \sqrt{s_a s_b} (ab + b^\dagger a^\dagger) + (1 + s_b U_s) bb^\dagger \right] \\
\mathcal{H}_4 &= -U_s \left( a^{\dagger} a a a^{\dagger} + b^\dagger b^\dagger b b \right) \\
&\quad - \frac{U_s}{2} \sqrt{s_a s_b} \left[ \frac{(a^{\dagger} a a b + b^\dagger a^\dagger a^\dagger a)}{s_a} + \frac{(b^\dagger b b a + a^\dagger b^\dagger b^\dagger b)}{s_b} \right] (4.15)
\end{align*}

\( \mathcal{H}_4 \) is of \( \mathcal{O}(1) \) (because \( U_s \sim \mathcal{O}(1) \)) and \( \mathcal{H}_0 + \mathcal{H}_2 \) is of order \( L \). Therefore, \( \mathcal{H}_4 \) can be treated as a small perturbation to the \( \mathcal{H}_0 + \mathcal{H}_2 \) in the thermodynamic limit and is used to find out the higher order corrections, and it is not important to consider \( \mathcal{H}_4 \) for the leading order calculation.

The quadratic Hamiltonian, \( \mathcal{H}_2 \), is diagonalized by the canonical transformation of \((a, b)\) to a new set of Bose operators \((\eta, \gamma)\) defined as

\[ a = \cosh(\theta) \eta - \sinh(\theta) \gamma^\dagger \quad \text{and} \quad b^\dagger = -\sinh(\theta) \eta + \cosh(\theta) \gamma^\dagger. \]

The quadratic Hamiltonian, \( \mathcal{H}_2 \), is diagonal in the operators \((\eta, \gamma)\) for the following value of \( \theta \).

\[ \theta = \frac{1}{2} \ln \left[ \frac{4 + U_s L \rho + U_s \sqrt{2 \rho - 1}}{\sqrt{16 + 8 U_s L \rho + U_s^2 L^2 (1 - \rho)^2}} \right] (4.16) \]

It is interesting to note that \( \theta \) is singular at \( \rho = 1 \) in the thermodynamic limit, and this singularity is carried over to other quantities of interest through \( \theta \).

\[ \theta_\infty = \frac{1}{2} \ln \left( \frac{\rho + \sqrt{2 \rho - 1}}{1 - \rho} \right) (4.17) \]

This indicates that \( \rho = 1 \) is a special filling where system is expected to undergo some kind of a transition. Let \( E_g \) be the ground state energy and define two other quantities, \( \alpha \) and \( \beta \) related to the operators \( A \) and \( B \), respectively such that

\[ \alpha = \frac{\langle A^{\dagger} A \rangle_{U_s}}{4L}, \quad \beta = \frac{\langle B^{\dagger} B \rangle_{U_s}}{L} \] (4.18)

In the limit of large \( L \) and \( \rho \) close to 1,

\[ \frac{E_g}{L} \approx -\rho + \frac{2}{L} \left( \frac{2 \rho - 1}{1 - \rho} \right) + \mathcal{O}(1/L^2) \] (4.19)
4.3 Repulsive case: $U_s > 0$ and $\sim O(1)$

\[
\alpha \approx \frac{2\rho - 1}{1 - \rho} + O(1/L) \tag{4.20}
\]

\[
\beta \approx 0 \tag{4.21}
\]

At $\rho = 1$,

\[
\frac{E_g}{L} = -1 + \sqrt{2U_s/L} - \frac{4 + U_s}{2L} + O(1/L^{3/2}) \tag{4.22}
\]

\[
\alpha = \frac{1}{2} \left( \sqrt{\frac{U_s}{2}} - \frac{U_s}{2\sqrt{L}} + \frac{1 + 2U_s}{\sqrt{2U_s}L} \right) L^{1/2} + O(1/L) \tag{4.23}
\]

\[
\beta = \frac{1}{\sqrt{2U_s L}} - \frac{1}{2L} + O(1/L^2) \tag{4.24}
\]

Equation 4.20 is consistent with enhancement expected from Inequality 1.8. Equation 4.23 implies that correlation function $\langle A^\dagger A \rangle$ goes as $L^{3/2}$ and thus affirms that there exists only a quasi LRO in the pairing correlation of extended s-wave type at a half filling.

Another important point to notice is that both at and away from half filling, the ground state energy density is the same as for the case without the projection term, that is, $\lim_{L \to \infty} (E_g/L) = \langle T \rangle_{U_s=0}/L = -\rho$. However the leading order finite size correction to the energy per site changes from $1/L$ in Equation 4.19 with a coefficient that diverges near $\rho = 1$, to $1/\sqrt{L}$ at $\rho = 1$ as in Equation 4.22.

Let’s compare above results with that of variational calculation on Model-I with $U = 0$, as given in Reference [3]. There, at $\rho = 1$, $E_g/L \approx e_{\text{non}} + 2\sqrt{\alpha(0)U_s}/|\mu_1|L$ and $\langle A^\dagger A \rangle / L \approx 2\sqrt{U_s\alpha(0)/|\mu_1|L}$ where $\alpha = \langle A^\dagger A \rangle / 4L$ and $\mu_n = \sum_k \epsilon_k^0(2f_k - 1)/L$. Here, $e_{\text{non}}$ is the non-interacting energy density, and $\alpha(0)$ is the value of $\alpha$ at $U_s = 0$. For the present choice of dispersion relation, that is $\epsilon_i = -1(+1)$ for $i \leq L/2(> L/2)$, $\alpha(0) = \rho/2$ and $\mu_1 = -\rho$. At $\rho = 1$, we obtain $2\alpha \approx \sqrt{U_s}/2L^{1/2}$ and $E_g/L \approx -1 + \sqrt{2U_s}/L$ which is same as given above. The heuristic results are also the same in this case. In terms of $\mu_1$, away from half filling, the lower bound on $\langle A^\dagger A \rangle$ given by enhancement inequality [2] is $\sim 2\mu_1^2L/(1 - \rho)$. We find that the exact result is twice the value of the lower bound. Thus close to half filling, $\alpha \sim 1/(1 - \rho)$ which is consistent with Equation 4.20.

Figure 4.6 compares the results of exact diagonalization with the semiclassical analytical calculations. One can see a good agreement between the equations of the best fit curves for the exact diagonalization data and the semiclassical leading order expressions for $E_g$ and $\langle A^\dagger A \rangle$.

4.3.3 Variational calculation

We next perform a variational calculation for the bosonized Hamiltonian given in Equation 4.14. The motivation for the variational approach is that while yielding finally the
Figure 4.6: The continuous lines are the best fit lines and the points are the exact diagonalization results. (b) and (d) are at half filling whereas (a) and (c) are at $\rho = 0.9$ and 0.8 respectively.
same result as in the exact diagonalization, it gives an additional picture of the competing energies. In the thermodynamic limit, we neglect $\mathcal{H}_4$ and all higher terms. As we are interested in the ground state, we put $s_a = L(2\rho - 1)/4$ and $s_b = L/4$. Then the kinetic energy part of the spin Hamiltonian Equation 4.9, viz. $T = 2(-S_{a}^{z} + S_{b}^{z})$, becomes $T = -L\rho + 2(a^\dagger a + b^\dagger b)$, under the HP transformation and the potential energy term, $U_s(S_{a}^{+} + S_{b}^{+})(S_{a}^{-} + S_{b}^{-})$, becomes $V = (U_s L/2)(\sqrt{2\rho - 1}a + b^\dagger)(\sqrt{2\rho - 1}a^\dagger + b)$. We use $|\psi_v\rangle = e^{-\theta(a^\dagger a - b^\dagger b)}|0\rangle$ as the variational ansatz for the ground state wavefunction. Here $|0\rangle$ is the vacuum of operators $a$ and $b$. The prefactor in the variational wavefunction generates several Cooper particle and Cooper hole pairs in the ground state $|0\rangle$. The expectation values of operators $T$ and $V$ in this variational wavefunction are:

$$T_v(\theta) = -L\rho + 4\sinh^2\theta$$

$$V_v(\theta) = \frac{U_s L}{2}(\sqrt{2\rho - 1}\cosh\theta - \sinh\theta)^2$$

Minimizing the variational energy, $E_v(\theta) = T_v(\theta) + V_v(\theta)$, with respect to $\theta$ gives us the same value of parameter $\theta$ as given in Equation 4.16. We see that as long as $\theta$ is of $\mathcal{O}(1)$, the kinetic energy shift, $\sinh^2\theta$ is non-extensive. Away from $\rho = 1$, we can thus make $V_v(\theta)$ vanish by choosing $\theta = \ln \left(\frac{1+\sqrt{2\rho - 1}}{\sqrt{2(1-\rho)}}\right)$. At $\rho = 1$, we are pushed to a diverging $\theta \sim \mathcal{O}(\ln L)$, since $V_v(\theta) = U_s L e^{-\theta}/2$. This necessarily costs more kinetic energy shift, but fortunately $\sinh^2\theta \sim \mathcal{O}((\sqrt{L})$ so the shift is not extensive. One can see that in the thermodynamic limit, for $\rho < 1$:

$$E_g = -L\rho + \frac{2(2\rho - 1)}{1-\rho} , \quad \alpha = \frac{2\rho - 1}{1-\rho} , \quad \beta = 0$$

Similarly, for $\rho = 1$, minimizing $E_v(\theta)$ we get $\theta = \frac{1}{4}\ln \left(\frac{U_s L}{2}\right)$ and so

$$E_g = -L + \sqrt{2U_s L}$$

$$\alpha = \frac{1}{2}\sqrt{U_s L/2} , \quad \beta = 1/\sqrt{2U_s L}$$

It is nice to see that this simple spin model explicitly verifies the assertions, based on general physical arguments, made in Reference [2], namely, in the thermodynamic limit, (i) the presence of the s-wave projection term makes no difference to the ground

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1 A more general variational wavefunction, viz., $|\psi_v\rangle = \exp\{-\frac{\theta}{2\pi} [T, B^\dagger B]\} |\phi\rangle$ has been discussed for models exhibiting order by projection in Reference [3] where $|\phi\rangle$ is the ground state of the Hamiltonian without projection. The variational wavefunction used in the present work is a special form of the more general one.
state energy per site, and (ii) it leads to the enhancement in the extended s-wave pairing correlation function near half filling. It also clarifies the situation at half filling that there is only quasi LRO in the extended s-wave pairing correlation.

As we have explicit expressions for $T(U_s)$ and $V(U_s)$ in this simple model, we take this opportunity to see how the sum rule stated in the Equation 4.6 is satisfied in the thermodynamic limit. Putting $\theta$ as given in Equation 4.16 into Equations 4.26 and 4.27 (and writing $U_s$ as $\lambda$), we get:

$$T(\lambda) = -L\rho - 2 + \frac{2(4 + \lambda L\rho)}{\sqrt{16 + 8\lambda L\rho + \lambda^2 L^2(1 - \rho)^2}}$$  \hspace{1cm} (4.30)

$$V(\lambda) = \frac{L}{2} \left[ \frac{4\rho + \lambda L(1 - \rho)^2}{\sqrt{16 + 8\lambda L\rho + \lambda^2 L^2(1 - \rho)^2}} - (1 - \rho) \right]$$  \hspace{1cm} (4.31)

Integrating $\Delta T(\lambda)/\lambda^2$ from $\lambda = 0$ to $U_s$, and taking limit $L \to \infty$ gives $V(0)$ both for $\rho < 1$ and $\rho = 1$. The reason why the integral of a non-extensive quantity, $\Delta T(\lambda)$, equals the extensive quantity $V(0)$, in the thermodynamic limit, is that a very large contribution arises for $\lambda \sim \mathcal{O}(1/L)$ where the weight factor $1/\lambda^2$ becomes large. This becomes very clear when one re-scales $\lambda$ as $\lambda/L$ in the integral $\int_0^{U_s} d\lambda (\Delta T(\lambda)/\lambda^2)$ to bring out a factor of $L$ outside the integral. The remaining integral is a number in the thermodynamic limit which is precisely $V(0)$. Thus, we see that the sum rule is saturated for the $\lambda \sim \mathcal{O}(1/L)$.

### 4.4 Electron-phonon interaction and order by projection

We saw in the previous sections that s-wave projection alone could not give rise to the true LRO in extended s-wave pairing channel. In the present section, we consider a situation where the projection acts in conjunction with the attractive interaction due to phonon mediation. Under these circumstances, we think, what was just a critical order may turn into a true superconducting order in the extended s-wave channel. With this aim, here we perform another toy model calculation.

The Holstein model is a description of electrons coupled with the Einstein phonons. The model Hamiltonian for the Holstein problem is written below.

$$\mathcal{H} = \sum_i \left[ \frac{p_i^2}{2M} + \frac{1}{2}\kappa x_i^2 \right] + \sum_{k,\sigma} \epsilon_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + \lambda \sum_i x_i \left( c_{i,\uparrow}^\dagger c_{i,\downarrow} + c_{i,\downarrow}^\dagger c_{i,\uparrow} \right)$$  \hspace{1cm} (4.32)

$$= \sum_{k,\sigma} \epsilon_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + w_E \sum_q a_q^\dagger a_q + \frac{g}{\sqrt{L}} \sum_q \sum_{k,\sigma} \left( a_q + a_{-q}^\dagger \right) c_{k+q,\sigma}^\dagger c_{k,\sigma}$$  \hspace{1cm} (4.33)
where \( w_E = (\kappa/M)^{1/2} \) is the phonon energy, and \( g = \lambda/(2Mw_E)^{1/2} \). The operators, \( a_q \) and \( c_{k\sigma} \), are the annihilation operators of phonon and electrons, respectively.

In the case of the step function dispersion for electrons (Model-III), the Holstein model suggests the following two-spin model coupled with a single mode phonon field.

\[
\mathcal{H} = -W (S_1^z - S_2^z) + w_E a^\dagger a + \frac{g}{L^{3/2}} (a + a^\dagger) (S_1^+ S_2^- + S_1^- S_2^+) \tag{4.34}
\]

Here, we are interested in the case of half filling only. At half filling, the spin quantum numbers, \( S_1 = S_2 = L/4 \) (with slight change in the notation: \( S_1 \equiv S_a \) and \( S_2 \equiv S_b \); \( W = 2 \) in the previous sections). The spin variables in our model can be treated as classical spins in thermodynamic limit. The corresponding classical spins are

\[
\vec{S}_1^1 = S_1 (\sin \theta_1 \cos \phi_1, \sin \theta_1 \sin \phi_1, \cos \theta_1) \\
\vec{S}_2^2 = S_2 (\sin \theta_2 \cos \phi_2, \sin \theta_2 \sin \phi_2, -\cos \theta_2)
\]

Notice that \( S_1^z = \frac{L}{4} \cos \theta_1 \) and \( S_2^z = -\frac{L}{4} \cos \theta_2 \).

\[
S_1^+ S_2^- + S_1^- S_2^+ = 2 (S_1^z S_2^z + S_1^y S_2^y) = 2S_1 S_2 \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2) \tag{4.35}
\]

The corresponding spin-only problem can described in terms of the following spin-only Hamiltonian. In fact it is only a classical energy function, and not a quantum mechanical operator.

\[
E = -W (S_1 \cos \theta_1 + S_2 \cos \theta_2) - 4 \frac{g^2}{L^3w_E} S_1^z S_2^z \sin^2 \theta_1 \sin^2 \theta_2 \cos^2(\phi_1 - \phi_2) \tag{4.36}
\]

We will consider the minimum energy state of Equation 4.36 at half filling, where \( S_1 = S_2 = L/4 \). Then we will consider the case of Equation 4.36 with projection. At half filling, Equation 4.36 takes the following form.

\[
E = -\frac{WL}{4} (\cos \theta_1 + \cos \theta_2) - \frac{g^2L}{64w_E} \sin^2 \theta_1 \sin^2 \theta_2 \cos^2(\phi_1 - \phi_2) \tag{4.37}
\]

The angles, \( \theta' \)s and \( \phi' \)s are such that \( 0 \leq \theta_{1,2} \leq \pi \) and \( 0 \leq \phi_{1,2} \leq 2\pi \). The minimum of energy, \( E \) as given in Equation 4.37, with respect to \( \phi_1 \) and \( \phi_2 \) occurs when \( \phi_1 - \phi_2 = 0 \) or \( \pi \). Let us call \( \cos \theta_1 = x \) and \( \cos \theta_2 = y \), and define a dimensionless parameter, \( \zeta = g^2/(8w_EW) \). Minimizing \( E \) with respect to \( x \) and \( y \) while \( \cos^2(\phi_1 - \phi_2) = 1 \) gives

\[
x(1 - y^2) = \frac{1}{\zeta} \quad \text{and} \quad y(1 - x^2) = \frac{1}{\zeta} \tag{4.38}
\]
Let \( x^* \) and \( y^* \) be the desired solutions. Equation 4.38 has two things to say regarding the minimum energy solution. First, \( x^* = y^* \). It has to be so also because the total number of particles are fixed. And half filling means \( S_1^x + S_2^x = 0 \) which implies that \( x = y \). Secondly, \( x^* \) and \( y^* \) are positive. It is so because \(|x|, |y| \leq 1\) and \( \zeta \) is a positive quantity. And thirdly, the solution is possible only when \( \zeta > 1 \), since the left hand side of the equalities are less than one. This puts a condition on the electron-phonon coupling, \( g \), such that \( g \geq \sqrt{8w_E \lambda} \). When this condition is not satisfied, \( x^* = y^* = 1 \) would remain the trivial minimum energy solution for Equation 4.37. The meaning of having a non-trivial solution for Equation 4.38 is that spins, \( \vec{S}_1 \) and \( \vec{S}_2 \) will have non-zero component in the direction transverse to \( z \)-direction. In order to appreciate it physical meaning, let us calculate the superconducting correlations of \( B \) as well \( A \) type.

The expectation value of operator \( B^\dagger B \) gives the s-wave superconducting correlation, and that of operator \( A^\dagger A \) gives extended s-wave correlation.

\[
B^\dagger B = (S_1^+ + S_2^+) (S_1^- + S_2^-) \\
= S_1^2 + S_2^2 + (S_1^x + S_2^x) - ((S_1^x)^2 + (S_2^x)^2) + 2 (S_1^x S_2^x + S_1^y S_2^y) \\
= S_1^2 + S_2^2 - ((S_1^x)^2 + (S_2^x)^2) + 2 (S_1^x S_2^x + S_1^y S_2^y) \quad \text{(classical)} \quad (4.39)
\]

\[
A^\dagger A = (S_1^+ - S_2^+) (S_1^- - S_2^-) \\
= S_1^2 + S_2^2 + (S_1^x + S_2^x) - ((S_1^x)^2 + (S_2^x)^2) - 2 (S_1^x S_2^x + S_1^y S_2^y) \\
= S_1^2 + S_2^2 - ((S_1^x)^2 + (S_2^x)^2) - 2 (S_1^x S_2^x + S_1^y S_2^y) \quad \text{(classical)} \quad (4.40)
\]

In terms of \( \theta \)'s and \( \phi \)’s, Equations 4.39 and 4.40 at half filling can be rewritten as:

\[
B^\dagger B = \frac{L^2}{16} \left( \sin^2 \theta_1 + \sin^2 \theta_2 + 2 \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2) \right) \quad (4.41)
\]

\[
A^\dagger A = \frac{L^2}{16} \left( \sin^2 \theta_1 + \sin^2 \theta_2 - 2 \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2) \right) \quad (4.42)
\]

Thus, in the ground state of the toy model, we have either

\[ B^\dagger B \neq 0 \quad \text{and} \quad A^\dagger A = 0 \quad \text{for} \quad \phi_1 - \phi_2 = 0 \]

or

\[ B^\dagger B = 0 \quad \text{and} \quad A^\dagger A \neq 0 \quad \text{for} \quad \phi_1 - \phi_2 = \pi \]

The conclusion that one may derive from above simple calculation is that for sufficiently strong electron-phonon coupling (e-ph), \( g \), the model has superconducting ground state either in s-wave channel or in extended s-wave channel, depending upon whether \( \phi_1 - \phi_2 = 0 \) or \( \pi \), respectively. Thus an e-ph coupled system is susceptible to both the superconducting channel in this simple model. Now let us study the effect of projection on such a model system.
The s-wave projection can be put in effect by adding $U_s B^\dagger B$ to the Hamiltonian in Equation 4.34, where $U_s > 0$. Since $B^\dagger B$ is proportional to $L^2$, this term must be zero for positive $U_s$. Thus, s-wave pairing channel is killed, and this we have for $\phi_1 - \phi_2 = \pi$ with the same solution for $\theta_1$ and $\theta_2$ as we have derived earlier. This, in turn, selects superconducting ground state with extended s-wave pairing channel. Thus, projecting out s-wave channel leads to superconductivity in extended s-wave channel, in a model which is susceptible to superconductivity in extended s-wave channel. This statement is important in the sense that if the term proportional to $g^2$ were zero, then projecting out s-wave alone would not have lead to a non-zero extended s-wave pairing in the ground state. This is the most important point of our calculation. Thus, the projection of s-wave pairing and attraction both together are able to attain superconducting ground state in the extended s-wave pairing channel.

The e-ph interaction term, $(a^\dagger + a)(S_1^+ S_2^+ + S_1^- S_2^-)$, can also be rewritten as $(a^\dagger + a)(B^\dagger B - A^\dagger A)/2$. This is a rather direct way of understanding the previous results (without projection). It says that systems gains same energy by choosing any one of the two channels. And only one of them will be chosen since the two exist only disjointly as seen from Equations 4.41 and 4.42. Now let us consider a situation where there is a bias in the choice. We take the electron-phonon interaction to be, $(a^\dagger + a)(B^\dagger B - \gamma A^\dagger A)/2$. The energy of the classical spin problem can be re-written in the following way.

$$E = -W (S_1 \cos \theta_1 + S_2 \cos \theta_2) - \frac{g^2}{4wEL^3} (1 - \gamma)^2 \left(S_1^2 \sin^2 \theta_1 + S_2^2 \sin^2 \theta_2\right)^2 - \frac{g^2}{wEL^3} (1 + \gamma^2) S_1 S_2 \sin \theta_1 \sin \theta_2 \cos^2(\phi_1 - \phi_2) - \frac{g^2}{wEL^3} (1 - \gamma^2) S_1 S_2 \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2) \left[S_1^2 \sin^2 \theta_1 + S_2^2 \sin^2 \theta_2\right]$$

From the last term in the above equation, it is clear that for $\gamma < 1$, $\phi_1 - \phi_2 = 0$ would lower the energy. Thus s-wave superconducting correlation $B^\dagger B$ would be non-zero at half filling, and the extended s-wave pairing correlation will be zero. This is clearly a biased model which prefers s-wave pairing over the other when $\gamma < 1$. However under the s-wave projection, $\phi_1 - \phi_2 = \pi$. Then we have non-zero extended s-wave pairing correlations even when $\gamma < 1$. This is a very interesting result. It suggests that projection helps in attaining non-local superconducting order even when the electron-phonon interaction strength in these channels is not strong enough to establish superconductivity. Associating electron-phonon interaction strength roughly with the superconducting transition temperature suggests the possibility of attaining superconductivity at higher temperatures than the ones given by purely electron-phonon mechanism.
It appears to us, from the simple calculations presented above, that the \textit{s-wave projection + electron-phonon interaction} may give rise to superconducting phases with \textit{non-local order parameter} at \textit{higher transition temperatures}. One comment regarding the electron filling, $\rho$. We have dealt with the case of half filling for the reason that the model 
\[
\mathcal{H} = -W(S_1^z - S_2^z) + U_s B^\dagger B
\]
has quasi long range order in channel $A$ only at half filling, and close to half filling $A^\dagger A \sim 1/(1 - \rho)$. From Equation 4.36, we can have long range order both in $B$ and $A$ channels at fillings away from half. This is so because $S_1 \neq S_2$, and hence the exact cancellations of terms in either $B^\dagger B$ or $A^\dagger A$ is not possible. But the projection will still have the same effect, that is, killing the s-wave pairing. It is therefore not very important at the level of this simple problem to worry about filling. The important message to take from the present calculation, is that s-wave projection + electron-phonon interaction can be a way to high temperature superconductivity in non-local pairing channels. The role of filling may become clear only in a full quantum many body problem on a lattice.

### 4.5 Order by projection and antisupeerradiance

In this section, we study a system of two-level atoms coupled to a single mode radiation field, and interacting among themselves. The aim is to discuss the implications of order by projection in quantum optics. The model Hamiltonian that we study here, is given below. It is essentially a Dicke model of two species of atoms with an extra ‘exchange’ interaction among the atoms.

\[
\mathcal{H}_{DJ} = a^\dagger a + \epsilon_1 S_1^z + \epsilon_2 S_2^z + \frac{\gamma}{\sqrt{L}} \left[ (S_1^+ + S_2^+)a + a^\dagger (S_1^- + S_2^-) \right] + \frac{J}{L} S_1 S_2
\]

(4.44)

Here $J \sim O(1)$ and positive, $\epsilon_1$ and $\epsilon_2$ are the transition energies of the two species of the two-level atoms and $L$ is the total number of atoms (of both type). The energy is measured in the units of photon energy. The coupling of the atoms of different types to the field is assumed to be the same, \textit{i.e.}, $\gamma$ which is an intensive number proportional to the $\sqrt{L/V}$, where $V$ is the volume of the cavity. The operators $S_{1,2}^\pm$ are known as the population inversion operators in quantum optics. The operators $S_{1,2}^+$ and $S_{1,2}^-$ are such that the total electric dipole operator of the atomic subsystems is proportional to $(S^+ + S^-)_{1,2}$ where the magnitude of the atomic dipole matrix element is the proportionality constant (phase factor included in the definition of $S^\pm$). In terms of the Pauli matrices, $S_i^+ = \sum_i \sigma_i^+$ and $S_i^z = \sum_i \sigma_i^z/2$, where index $i$ runs over the atoms of type-1. The operator $\sigma_i^+$ causes the transition of $i^{th}$ atom from its ground state to its excited state. Similarly, one can
write corresponding operators for atoms of type-2. These operators follow the angular momentum algebra, and behave like the spin operators.

\[ \langle S_x^2 + S_y^2 \rangle = 0 \]

\[ S = N/2 \]

\[ 0 < S < N/2 \]

\[ \langle a \rangle \sim \sqrt{L} \]

\[ \langle S_x^2 + S_y^2 \rangle \sim L^2 \]

\[ J / 2 \]

\[ S_z \]

\[ \text{Anti-superradiance} \]

\[ \gamma \]

\[ \varepsilon \]

\[ J = 20. \]

(a) $\epsilon_1 = \epsilon_2$, (b) $\epsilon_2 >> \epsilon_1$. In the plot where $\epsilon_1 \neq \epsilon_2$, there is an anti-superradiant phase with total $S_z = 0$.

The inclusion of exchange interaction, $\frac{i}{L} S_1.S_2$, in the Hamiltonian is purely mathematical with no clear idea of how such an interaction can be realized in real experiments. For $J = 0$, this is the Dicke model of superradiance [7, 8] for two species of atoms. It has a superradiant ground state with $\langle a \rangle \sim \sqrt{L}$ and $\langle S_x^2 + S_y^2 \rangle \sim L^2$. Here, $S_{x,y}$ are the $x, y$ components of the total 'spin' $S_1 + S_2$. Thus, 'superradiant phase' is a thermodynamic phase with large number of atoms in their excited states, in cooperation with the photons unlike a 'normal' phase where all atoms are in their ground sates. It is a phase where photons condense and two atomic subsystems develop in-phase macroscopic dipoles. Superradiance is attained below a certain temperature, $T_c$, for $\gamma^2 > \epsilon$ where $\epsilon^{-1} = (\epsilon_1^{-1} + \epsilon_2^{-1})/2$. For $\gamma^2 < \epsilon$, system is normal. For $J > 0$, the exchange interaction tends to break the cooperation between the field and atoms. For suitable strength of $J$, it drives the systems to a new ground state where two atomic subsystems develop out of phase dipoles and photons don’t condense. Thus, $\langle S_x^2 + S_y^2 \rangle = 0$ and $\langle a \rangle = 0$. We identify it as the anti-superradiant state (this term is borrowed from Mandel and Wolf [14]). This is in analogy with the states identified with extremely weak decay which have been observed experimentally [9] for a system of low density excited molecules enclosed between metallic mirrors. The Hamiltonian in Equation 4.44 is studied by mean-field methods and by using the Holstein-Primakoff transformation. The phase diagram obtained is shown in Figure 4.7.
The coupling of atoms to the radiation can be viewed as an effective interaction, $-(\gamma^2/L)(S_1^+ + S_2^+)(S_1^- + S_2^-)$, among atoms. This is same as what we studied for the case of superconductivity in the metallic grains in subsection 4.2.1. Extending this analogy further, projecting out s-wave cooper pairing can be taken as projecting out superradiance in the atom-field system. Under this projection, ordering occurs in the operator, $A = \epsilon_1 S_1^+ + \epsilon_2 S_2^+$, due to anti-parallel transverse fluctuations for $\epsilon_1 \neq \epsilon_2$ and total $S^z = 0$. Adding exchange term to Dicke model has a similar effect of suppressing superradiance, though it does not project out superradiance. Thus, it is clear that anti-superradiance does not necessarily imply order in $A$, but the anti-superradiant phase in Figure 4.7-b is a region where one can look for the phenomenon of order by projection.

4.6 Summary

In the present chapter we have explored the phenomenon of “order by projection” within a simple solvable model (Model-III) in detail. We derived a sum rule for the lattice Fermi systems with s-wave projection which relates the intensive change in the kinetic energy to the extensive interaction energy. We solved the simple spin model both exactly and semiclassically. It is shown explicitly that away from half filling $\langle A^\dagger A \rangle \sim 1/(1 - \rho)$ and that the energy shift $\Delta E_g$ is intensive. At $\rho = 1$, $\langle A^\dagger A \rangle \sim L^{3/2}$ and $\Delta E_g \sim L^{1/2}$. Thus the energy density is unchanged and there is quasi LRO in $A$ at half filling. The numerical results for $\langle A^\dagger A \rangle$ and $\Delta E_g$ are presented for Model-II with linear dispersion. They are in agreement with the above behaviour of the correlation function and the ground state energy. We briefly discuss the attractive case of the Model-III which is equivalent to the reduced BCS model of superconductivity.

We also discuss a possible scenario, supported by a simple model calculation, where both the e-ph interaction and the s-wave projection act simultaneously. We find that what was only a critical order without e-ph interaction, now becomes a true LRO in the extended s-wave channel. This, we believe, may provide a new direction to the understanding of superconductivity in strongly correlated electronic systems.

Finally, we discussed the possible relevance of order by projection in quantum optics. We discussed anti-superradiance, and found a region in phase diagram where one may hope to look for the phenomena analogous to order by projection.
Bibliography

[6] We used H. Nishimori’s TITPACK for numerical computation.