The Antiferromagnetic Sawtooth Lattice -
the study of a two spin variant

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by
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ABSTRACT

Generalising recent studies on the sawtooth lattice, a two-spin variant of the model is considered. Numerical studies of the energy spectra and the relevant spin correlations in the problem are presented. Perturbation theory analysis of the model explaining some of the features of the numerical data is put forward and the spin wave spectra of the model corresponding to different phases are investigated.
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Chapter 1

Introduction

There has been a lot of recent interest ([4], [5] to [8]) in one dimensional and quasi-one-dimensional quantum spin systems having two different spins in the unit cell with antiferromagnetic couplings. Depending on the presence or the absence of frustration and its strength when it is present these systems exhibit a rich variety of phases in the ground state. Quantum ferrimagnets for example, are one such class of systems where the system has a finite magnetic moment in the ground state. Chemists have been successful in synthesising families of organo-metallic compounds ([9] to [12]) which provide experimental realisations for some such systems.

In this report we present the study of a mixed spin variant of the Sawtooth Lattice. Recent studies ([1], [2], [3]) on this model have concentrated on systems where all the spins on the lattice are the same. The compound Delafossite (YCuO$_2$.5) provides an experimental realisation of such a model with the copper ions forming a lattice of spin-$\frac{1}{2}$ sites. In an attempt to generalise such studies we considered a two spin variant of the above model and studied it numerically and analytically. In this chapter the model and its Hamiltonian are introduced and some of the classically expected properties of the ground state are discussed. In subsequent chapters the numerical data and the analytical results obtained have been presented.
1.1 The model and its classical ground states

The model under consideration is described by the Hamiltonian,

\[ H = J_1 \sum_n \vec{S}_{1n} \cdot \vec{S}_{1(n+1)} + J_2 \sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)}) \]  \hspace{1cm} (1.1)

Or equivalently,

\[ H = \delta \sum_n \vec{S}_{1n} \cdot \vec{S}_{1(n+1)} + \sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)}) \]  \hspace{1cm} (1.2)

where \( \delta \equiv J_1 / J_2 \) and \( J_2 \) has been set to 1. Thus all energies in the problem are measured in units of \( J_2 \). Here \( S_{1i} \) denotes a spin-1 site and \( S_{2i} \) denotes a spin-\( \frac{1}{2} \).

Schematically the model looks like,

Classically, the ground state of this system is characterised by a planar or a collinear arrangement of spin vectors. Which of these arrangements is the ground state depends on the relative strengths of the two couplings \( J_1 \) and \( J_2 \).

When \( J_2 S_2 > 2J_1 S_1 \) the classical ground state is characterised by a collinear arrangement of spins and this phase is called the **ferrimagnetic state**. Schematically the ferrimagnetic phase looks as follows:
When $J_2S_2 < 2J_1S_1$, the classical ground state is characterised by a planar arrangement of spins in each triangle and this phase is called the **spiral/canted** phase. Schematically this phase looks as follows:

\[
\theta \theta \theta \theta \theta \theta \theta \theta
\]

where $\cos \theta \equiv J_2S_2/2J_1S_1$. Because of the freedom of choosing the direction of spins even when the spin vectors in each triangle are constrained to be on a plane, the classical spiral/canted phase has an infinite amount of degeneracy. We note that because of the above reason though the spin vectors in a particular triangle have to be in a plane, all the spin vectors need not lie in the same plane.

For our simulations and the analytical results that follow, the parameter in the problem is $\delta$. Numerically we have studied the energy spectra and the spin correlations as a function of $\delta$. These results are presented in the next chapter. And perturbation theory calculations to compute the effective Hamiltonian between the spin-$\frac{1}{2}$'s in the large $\delta$ limit and the spin wave spectra obtained for the above two phases are presented in chapters 3 and 4 respectively.
Chapter 2

Exact Diagonalization and related results

Numerical studies of the model have been done using the Exact Diagonalisation method. By calculating the required eigenvalues and eigenvectors using the Lanczos algorithm the following quantities were calculated:

- The variation of the ground state and the first excited state energies with $\delta$.
- The correlations between the spins in the ground state.
- The effective Hamiltonian governing the spin-$\frac{1}{2}$’s when the coupling between the spin-1’s is much stronger than $J_2$, the spin-1 - spin-$\frac{1}{2}$ coupling.

In this chapter we begin with a brief introduction to the Lanczos algorithm and the version of it which has been used. Following that the numerical results of the first two categories above are presented. The effective Hamiltonian calculations, being semi-analytical in nature are presented in a subsequent chapter.
2.1 The Lanczos Algorithm

The **Lanczos Algorithm** is a widely used method for finding a few eigenvalues of a large symmetric matrix. Since the matrices that one deals with in quantum spin systems are usually symmetric (or Hermitian, whose eigenvalue problem can be formulated as one of a symmetric matrix double the size), this method is commonly used to find the lowest few eigenvalues and eigenvectors corresponding to the ground state and the lowest excited states.

The basic content of the version of the Lanczos procedure used for our simulations is the following recursion relation.

\[
\beta_{i+1}v_{i+1} = Av_i - \alpha_i v_i - \beta_i v_{i-1}
\]  

(2.1)

for \(i=1,2,\ldots\)

where \(A\) is the matrix whose eigenvalues we want to calculate and \(\alpha_i \equiv v_i^TAv_i\) and \(\beta_{i+1} \equiv v_{i+1}^TAv_i\). \(\beta_1\) is taken to be 0 and \(v_1\) is chosen to be a random vector normalised to unity. For any \(i = m\) the a symmetric tridiagonal matrix \(T_m\) is defined whose diagonal elements are \(\alpha_i\) and the off-diagonal elements are \(\beta_j\) \((j=2,m)\). It can be proved (for infinite precision arithmetic) that if \(\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \lambda_m\) are eigenvalues of \(T_m\) and \(\Lambda_1 \geq \Lambda_2 \geq \Lambda_3 \geq \ldots \Lambda_m\) are the \(m\) largest eigenvalues of \(A\), then the sequence of \(\lambda_i\)'s converges to the sequence of \(\Lambda_i\)'s as \(m\) is incremented.

Again, let \(V_m\) be the \(n \times m\) (where \(n\) is the order of \(A\)) whose \(i\)th column is \(v_i\). Then if \(x_i\) is the eigenvector of \(\lambda_i\) and \(X_i\) is the eigenvector of \(\Lambda_i\) then \(V_mx_i \longrightarrow X_i\) as \(m\) is incremented. The vectors \(V_mx_i\) are called **Ritz vectors**.

The Lanczos vectors \(v_i\) which are generated by the above recursion are an orthonormal set. The proof of the two claims made above hinges on this orthonormality of the Lanczos vectors. In reality when these vectors are generated numerically, finite precision effects enter and the set of vectors generated are not strictly orthogonal. The loss of orthogonality of the Lanczos vectors affects the computations primarily in two ways. Eigenvalues which are simple appear as multiple eigenvalues of the system and more im-
portantly spurious eigenvalues which are not eigenvalues of $A$ at all appear as eigenvalues of $T_m$.

Various methods have been devised to overcome the difficulties posed by this loss of orthogonality. One way is to resort to reorthogonalisation of the Lanczos vectors. We don’t use this method in our computations. We instead use the identification test developed by Cullum and Willoughby ([14]) to explicitly identify the eigenvalues which are spurious and discard them as they are detected.

As already mentioned in finite precision calculation the appearance of an eigenvalue as a multiple eigenvalue of the tridiagonal matrix $T_m$ is no guarantee of that eigenvalue being a true multiple eigenvalue of $A$. But this difficulty can be overcome by looking at the corresponding Ritz vectors. If Ritz vectors are calculated for a large enough $T_m$ for which a particular eigenvalue is duplicate then for a true multiple eigenvalue two linearly independent Ritz vectors can be generated using appropriate $T_m$’s of different sizes. But if the eigenvalue is simple any two Ritz vectors of the same eigenvalue will essentially be the same (upto a sign). In this way we can determine the degeneracy of eigenvalues by computing more and more Ritz vectors and checking for linear independence. In our program we employ this method to determine the degeneracy of an eigenvalue.

2.2 Results of Exact Diagonalisation

All the computations have been done by generating the Hamiltonian in the total $S_z$ basis. The variation of various energies and correlations with the ratio of interaction strength $\delta = J_1/J_2$ has been studied. In all the results reported $\delta$ varies from 0.1 to 2. The correlations have been calculated for a system size of 10 triangles and all the other graphs are for a system size of 8 triangles. All through the computations periodic boundary conditions have been used (the spin-1’s are joined in a ring). For all the reported data the accuracy measured by $| (A X - \Lambda X)^T (A X - \Lambda X) |$ for an eigenvalue $\Lambda$ and its corresponding eigenvector $X$ (normalised to unity) is $\sim 10^{-12}$ or less.
2.2.1 Variation of ground state energy and first excited state energy with $\delta$
2.2.2 Variation of total spin of the ground and first excited states with $\delta$

Variation of total spin of ground state with $\delta$

Variation of total spin of first excited state with $\delta$
2.2.3 Variation of energy gap to the 1st excited state with $\delta$

Significant aspects of the above results are the following:

- For a small $\delta$ this sawtooth lattice can be approximated by an alternating spin-$\frac{1}{2}$/spin-$\frac{1}{2}$ chain. This system has a ferrimagnetic ground state of total spin $N(S_1-S_2)$ and the first excited state is a state of total spin one less than that of the ground state ([4]). One can see clearly from the figures that for small $\delta$ this is indeed the case for this system.

- There is a sudden change in the total spin of both the ground state and the first excited state at around $\delta = 0.25$. This is the point where we expect the transition from ferrimagnetic to the spiral phase from the classical analysis. We have analysed this particular region closely by studying the total spin behaviour of the ground state at a number of closely spaced points from $\delta = 0.2$ to $\delta = 0.35$. Numerically we have found that for the ground state the spin drops to zero at $\delta = 0.265$. 
• There are two values of $\delta$ where the system seems to be gapless. The first is near $\delta = 0.5$ and the other is near $\delta = 1.0$. This actually divides the phase diagram into three phases as opposed to the two phases that we expected classically. The nature of the two quantum phases other than the ferrimagnetic phase is not clear as of now.

• For any $\delta$ if all the spin-$\frac{1}{2}$ interactions are made zero ($J_2 = 0$) then the ground state energy must essentially be that of a spin-1 Heisenberg antiferromagnet. In the thermodynamic limit this energy per site has been calculated [13] to very good accuracy. Our result ($E_0/N = -1.41712J_1$) for the 8 site cluster agrees with the above value ($E_0/N = -1.40148J_1$) up to finite size effects.

2.3 Spin correlations in the ground state

All the spin correlation calculations have been done with a system size of 10 triangles. In order to check the accuracy of the data the following checks were employed.

• The three correlations $< S_i^z S_j^z >, < S_i^+ S_j^- >, < S_i^- S_j^+ >$ were calculated separately. Then for each case it was checked that the latter two were equal and for $\delta$’s for which the eigenstate was a singlet it was checked that the $< \vec{S}_i, \vec{S}_j >$ (which can be computed from the above three was thrice the $< S_i^z S_j^z >$ correlation as would be expected for a singlet.

• For the singlet states it was verified that $\sum_j < \vec{S}_i, \vec{S}_j >$ where $j$ runs over all the spins for a given $i$ was zero.

In the graphs that follow, the $< S_i^z S_j^z >$ correlations are reported. The numbering scheme for the spins is same as shown in the figure in chapter 1.
2.3.1 Spin-1 - Spin-1 correlations in the ground state

2.3.2 Spin-1 - Spin-1/2 correlations in the ground state
2.3.3 Spin-$\frac{1}{2}$ - Spin-$\frac{1}{2}$ correlations in the ground state

Salient features of the correlation function plots are the following:

- Though for most of the region the correlation functions behave regularly, in the neighbourhood of $\delta = 0.5$ and $\delta = 1.0$ the correlations vary very rapidly with $\delta$. From a preliminary examination of the data it seems that the rate of change of correlations with $\delta$ is divergent at $\delta = 1.0$.

- The spin-1 - spin-1 correlations show the expected behaviour as we go towards the large $\delta$ limit. The spin correlations are alternating in sign as we move from one spin to the next (going farther from the first spin) and also decaying with distance as we would expect for a pure spin-1 system.

- The spin-1 - spin$\frac{1}{2}$ correlations all tend to zero in the large $\delta$ limit as we see from the plot. This is to be expected as in the large $\delta$ limit the system behaves essentially as a spin-1 system which forms a singlet and all the orderings of spin halves are essentially
degenerate as their interaction is much weaker in comparison to the spin-1 - spin-1 interaction. Thus the spin-1’s and spin-$\frac{1}{2}$’s are not strongly correlated and thus the correlations tend to zero.

- The most interesting behaviour in the large $\delta$ limit is shown by the spin-$\frac{1}{2}$ - spin-$\frac{1}{2}$ correlations. The most striking feature in this plot is that the next-nearest-neighbour correlation is larger than all the other correlations, even the nearest neighbour one. This and some of the other features can be explained if we calculate the effective Hamiltonian governing the spin-$\frac{1}{2}$’s in the large $\delta$ limit. This calculation and the results that come forth from that analysis have been presented in chapter 3.
Chapter 3

Perturbation theory and the effective Hamiltonian

The model Hamiltonian we have been concerned with is the following:

\[ H = J_1 \sum_n \vec{S}_{1n} \cdot \vec{S}_{1(n+1)} + J_2 \sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)}) \]  \hspace{1cm} (3.1)

where \( S_1 \)'s are the spin-1 sites and \( S_2 \) are the spin-\( \frac{1}{2} \) sites.

In the regime where the interaction between spin-1’s is much stronger than the interaction between the spin-\( \frac{1}{2} \)'s, we can consider the second term in the above Hamiltonian to be a perturbation to the spin-1 system. By doing perturbation theory calculations we can then find the effective Hamiltonian (for a few low lying states) governing the spin-\( \frac{1}{2} \)'s once the spin-1’s are essentially decoupled from them as a pure spin-1 system.

We have found that to second order in perturbation theory this effective Hamiltonian has a particularly simple form which has only two spin interactions involving terms of the form \( \vec{S}_i \cdot \vec{S}_j \). In this chapter we set up the formalism to find that Hamiltonian and give a proof of the fact that to second order it has the form mentioned above. Then we describe a numerical technique to calculate the various interaction strengths in the problem.
3.1 The calculation of effective Hamiltonian

We calculate the effective Hamiltonian in the following manner:

- The first term of the Hamiltonian in equation 3.1 is treated as the unperturbed Hamiltonian \( H_0 \). And the second term is the perturbation \( V \). Let \( |\psi_i> \) be the eigenstates of \( H_0 \), the spin-1 system. We assume that \( |\psi_i> \) are simultaneous eigenstates of \( H_0 \), the total angular momentum \((\sum_i \vec{S}_1^i)^2\) and the total \( S_z^i(\sum_i S_z^i) \) operators. Such states can always be found as they form a mutually commuting set of operators.

- The ground state of \( H_0 \) is known to be a singlet and furthermore it is non-degenerate. We calculate the "corrections" to this ground state energy using non-degenerate perturbation theory.

- The perturbation term \( V \) contains both spin-1 and spin-\( \frac{1}{2} \) operators. But in calculating the corrections to the ground state energy, the required matrix elements will be evaluated using the spin-1 system eigenstates. Thus we will be left at every order in perturbation theory with spin-\( \frac{1}{2} \) operators and their products. Just as we would have got the perturbative corrections to the unperturbed energy eigenvalues of \( H_0 \) if the above mentioned matrix elements had been numbers, here we get perturbative corrections to the spin-1 Hamiltonian. These corrections order by order will constitute the effective Hamiltonian of the spin-\( \frac{1}{2} \) system. We note here that this effective Hamiltonian can be used to find only the states of the full Hamiltonian which lie close to the singlet ground state. That is because it is calculated by evaluating the effect of the perturbation only on the singlet ground state.

Having set up the formalism we now proceed to calculate the effective Hamiltonian.
3.1.1 The effective Hamiltonian: First order

The effective Hamiltonian to the first order (in $J_2$) is given by,

$$\Delta H_1 = J_2 < 0 | (\sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1n+1})) | 0 >$$

where we denote by $|0> \text{ the singlet ground state of the spin-1 system.}$

Clearly, this is zero. That is because the state $|0> \text{ is a spherically symmetric state}$ and the spin-1 operators occur in the above expression linearly. This can also be argued from Wigner-Eckart theorem. We know that all the spin-1 operators can be expressed as linear combinations of spherical tensors of rank 1. But the state with respect to which the expectation value is being taken is a singlet. Since we cannot add $J_1 = 0$ and $J_2 = 1$ to give $J_{\text{total}} = 0$, the above expression must be zero.

So to first order in $J_2$, the effective Hamiltonian vanishes.

3.1.2 The effective Hamiltonian: Second order

The effective Hamiltonian to second order in $J_2$ is given by,

$$\Delta H_2 = \sum_{k \neq 0} \frac{<0 | J_2 \sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)}) | \psi_k> <\psi_k | J_2 \sum_{n'} (\vec{S}_{2n'} \cdot \vec{S}_{1n'} + \vec{S}_{2n'} \cdot \vec{S}_{1(n'+1)}) | 0>}{E_0 - E_k}$$

where the $k \neq 0$ implies that the sum is taken over all eigenstates except the singlet ground state. $E_i$ is the energy of the state $\psi_i$ and $E_0$ is the energy of the singlet ground state.
Let us consider the matrix element,

\[ <0| (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)})|\psi_k> \]

The state on the left is a singlet \((J = 0)\) and components of both \(\vec{S}_{1n}\) and \(\vec{S}_{1(n+1)}\) can be expressed as spherical tensors of rank 1. Thus Wigner-Eckart theorem guarantees that the only those states \(|\psi_k>\) will contribute which have a value of total angular momentum which when added to \(J = 1\) can give us \(J_{tot} = 0\). But that means that the only allowed value is 1. Thus we come to the conclusion that in Eq. 3.3 we only have to sum over such \(|\psi_k>\) which are spin 1 states. Equipped with this simplification we now look at one particular term in eq 3.3 corresponding to a particular spin 1 state. It will look like,

\[
\sum_i \frac{<0|J_2\sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)})|\psi^k_i><\psi^k_i|J_2\sum_{n'} (\vec{S}_{2n'} \cdot \vec{S}_{1n'} + \vec{S}_{2n'} \cdot \vec{S}_{1(n'+1)})|0>}{E_0-E_k}
\]

where \(k\) labels the particular spin 1 state and the sum is over \(i\) which labels the particular \(S_z\) component \((i=-1, 0, 1)\).

One generic term in the above sum will look like

\[
J_2^2 \sum_i \frac{<0|\vec{S}_{2n} \cdot \vec{S}_{1n}|\psi^k_i><\psi^k_i|\vec{S}_{2n'} \cdot \vec{S}_{1n'}|0>}{E_0-E_k}
\]

We note here the the denominator will be the same for all the \(i\)’s as the states have the same total angular momentum. Furthermore, we as of now don’t make any assumptions as to the relative values of \(n\) and \(n'\). Whatever we derive below will be true whether they are equal or not. In terms of components the numerator of the above expression will look like,

\[
\sum_{\alpha\beta} S_{2n}^{\alpha} S_{2n'}^{\alpha} <S_{1n}^{\alpha}_0 | S_{1n'}^{\beta}_i < S_{1n'}^{\beta}_i >_{0i} < S_{1n}^{\alpha}_i >_{0i}
\]

where \(\alpha, \beta = x, y, z\). And \(<S_{1n}^{\alpha}>_{0i} \equiv <0|S_{1n}^{\alpha} | \psi_i>\) and \(<S_{1n}^{\alpha}>_{i0}\) is the complex conjugate of the same (for now we drop the superscript \(k\) as we will talk about a particular spin-1 state).
We make the following two claims:

\[
\sum_i < S_{1n}^x >_0 < S_{1n'}^x >_{i0} = \sum_i < S_{1n}^y >_0 < S_{1n'}^y >_{i0} = \\
\sum_i < S_{1n}^z >_0 < S_{1n'}^z >_{i0} \quad \text{......... (A)}
\]

\[
\sum_i < S_{1n}^\alpha >_0 < S_{1n'}^\beta >_{i0} = 0 \text{ if } \alpha \neq \beta \quad \text{......... (B)}
\]

Before proceeding to prove the above we define the following:

\[
\sqrt{2} U_{+1} \equiv -S_{1n}^+, \sqrt{2} V_{+1} \equiv -S_{1n'}^+, \sqrt{2} U_{-1} \equiv S_{1n}^-, \sqrt{2} V_{-1} \equiv S_{1n'}^-, U_0 \equiv S_{1n}^z, V_0 \equiv S_{1n'}^z
\]

\[
U_{\pm 1,0} \text{ and } V_{\pm 1,0} \text{ are by definition components of spherical tensors of rank 1 and } S_{1n}^\alpha \text{ and } S_{1n'}^\beta \text{ can be expressed as linear combinations of components of } U \text{ and } V \text{ defined above.}
\]

We now prove the above two assertions:

**Proof of (A)**

We consider the x-x term first.

\[
\sum_i < S_{1n}^x >_0 < S_{1n'}^x >_{i0} = \sum_i < 0 | S_{1n}^x | \psi_i > < \psi_i | S_{1n}^x | 0 > = \\
= \sum_i < 0 | \frac{-U_{i+1}+U_{i-1}}{\sqrt{2}} | \psi_i > < \psi_i | \frac{-V_{i+1}+V_{i-1}}{\sqrt{2}} | 0 > = \\
= < 0 | \frac{-U_{i+1}+U_{i-1}}{\sqrt{2}} | \psi_0 > < \psi_0 | \frac{-V_{i+1}+V_{i-1}}{\sqrt{2}} | 0 > + < 0 | \frac{-U_{i+1}+U_{i-1}}{\sqrt{2}} | \psi_{-1} > < \psi_{-1} | \frac{-V_{i+1}+V_{i-1}}{\sqrt{2}} | 0 > \quad (3.4)
\]

where we have summed over the three values of \( S_{z}^{\text{tot}} \) for the spin-1 state.
We can now use the m-selection rule to eliminate those terms above which are zero. After doing that we see that the above expression reduces to:

\[ \sum_i <S^x_i>_{0i} <S^x_i'>_{i0} = <0|\frac{U_{-1}}{\sqrt{2}}|\psi_1> <\psi_1|\frac{-V_{-1}}{\sqrt{2}}|0> \]

\[ + <0|\frac{-U_{-1}}{\sqrt{2}}|\psi_{-1}> <\psi_{-1}|\frac{V_{-1}}{\sqrt{2}}|0> \]  

(3.5)

In an exactly analogous manner the y-y term reduces to:

\[ \sum_i <S^y_i>_{0i} <S^y_i'>_{i0} = -<0|\frac{U_{-1}}{\sqrt{2}}|\psi_1> <\psi_1|\frac{V_{-1}}{\sqrt{2}}|0> \]

\[ - <0|\frac{-U_{-1}}{\sqrt{2}}|\psi_{-1}> <\psi_{-1}|\frac{-V_{-1}}{\sqrt{2}}|0> \]  

(3.6)

which is the same as the x-x term. Finally the z-z term is given by,

\[ \sum_i <S^z_i>_{0i} <S^z_i'>_{i0} = <0|U_0|\psi_0> <\psi_0|V_0|0> \]  

(3.7)

Once we have proven that the x-x and y-y terms are equal the above has to be equal to the other two by rotational invariance. This can also be seen explicitly by application of the Wigner-Eckart theorem. The arguments are the following:

- The matrix element of the form \(<\psi_i|\hat{O}|0>\) wherever it occurs must have the same value everywhere as all the relevant Clebsch-Gordon coefficients are 1 (we are adding \(J_1 = 0\) and \(J_2 = 1\)) and the other term that we need to evaluate is the same for all such elements as it does not depend on the \(S_z\) values.

- The matrix element of the form \(<0|\hat{O}|\psi_i>\) even though has the same magnitude in all the three equations has the opposite sign in the z-z term, this is because \(<1,1,\pm 1|1,1;0,0>= - <1,0;1,1;0,0>\) (we have used the notation \(<j_1,j_{1z};j_2,j_{2z}|j_1,j_2;j_{tot},j_{z}^{tot}>)\). This negates the sign difference in the right hand sides of Eqs 3.5, 3.6 and 3.7. Moreover the factor of \(\frac{1}{2}\) in the x-x and y-y terms is also accounted for by the fact the the x-x and the y-y terms contain the sum of two terms each of which are equal in magnitude to the z-z term. Thus having proved that the x-x, y-y and the z-z terms are equal we have proved (A).
Proof of (B)

We first consider the x-y term. We have after eliminating terms using the m selection rule,

$$\sum_i <S_i^x>_{>0} <S_i^y>_{>0} = + <0|\frac{U_{1/2}}{\sqrt{2}}|\psi_1><\psi_1|\frac{iV_{1/2}}{\sqrt{2}}|0>$$
$$- <0|\frac{U_{1/2}}{\sqrt{2}}|\psi_{-1}><\psi_{-1}|\frac{iV_{1/2}}{\sqrt{2}}|0>$$

we see that both terms again have the same magnitude (note the point about the relevant C-G coefficients in the proof of (A)) but opposite sign so this term vanishes.

Thus y-z and the x-z term must also vanish by rotational invariance (these can be also be shown explicitly using arguments similar to those used in the proof of (A)). Thus having proved the two assertions we now come to the conclusion that the effective Hamiltonian governing the almost decoupled spin-\(^{1/2}\)'s (close to the ground state) to the second order in perturbation theory is given by two-spin interactions of the form \(S_i \cdot S_j\).

The final form will thus look like,

$$H_{eff} = a + \frac{J_2^2}{J_1}[c_1(S_1 \cdot S_2 + S_2 \cdot S_3...)+c_2(S_1 \cdot S_3 + S_2 \cdot S_4...)+c_3(S_1 \cdot S_4 + S_2 \cdot S_5...)]$$

where \(a \equiv N a_0 J_1 + N \frac{J_2^2}{J_1} b_0\) and \(c_1, c_2, c_3\) etc (upto a factor of \(J_2^2/J_1\)) are the coupling strengths between the nearest neighbours, next-nearest-neighbours and so on. The first term in \(a\) corresponds to the energy of the spin-1 system and the second term comes from spin-\(^{1/2}\) terms of the form \(S_i \cdot S_j\).

We note here that the \(c_i\)’s involve a sum over matrix elements connecting all the spin-1 excited states with the singlet ground state (eq 3.3). Analytically calculating this sum is difficult as we do not have the complete information of all such states in order to calculate the required matrix elements. Thus we calculated the coefficients numerically. The method used is described in the following section.
3.1.3 Calculation of interaction strengths between the spin-$\frac{1}{2}$’s

The computation of the interactions strengths was done using $\delta(\equiv J_1/J_2) = 10$ and for a system size of 8 triangles. This ensures that the perturbative corrections are convergent as the matrix elements calculated in eq 3.3 are of the order $J_2$ and for convergence of the perturbation theory this must be greater than the difference in the energy between the ground state and the first excited state of the spin-1 system. That is known to be of the order $J_1$.

We calculated the interaction strengths $(J_2^2/J_1)c_1$, $(J_2^2/J_1)c_2$ etc as follows:

- We begin by reducing all the bond strengths to the spin-$\frac{1}{2}$s to zero. This will give us the constant $a_0$.
- Now we connect the bonds with strength $J_2$ to only two of the spin-$\frac{1}{2}$ s. We do this successively for nearest neighbours next nearest neighbours and so on.
- There being only two spin-$\frac{1}{2}$ s in the system, the effective Hamiltonian governing them to second order in perturbation will be of the form $A + B \vec{S}_i \cdot \vec{S}_j$.
- $\vec{S}_i$ and $\vec{S}_j$ being spin-$\frac{1}{2}$ s we know that the ground state and the first excited states will have values $A - \frac{3}{4}B$ and $A + \frac{1}{4}B$ or vice versa. Which of these is the ground state depends on the sign of the coupling. If the coupling is ferromagnetic, the ground state will be a triplet and the latter will be the ground state and else the former will be the ground state.
- Thus knowing the ground state and the first excited state and thus $A$ and $B$ we get $b_0$ and the $c_i$ s.

The various coefficients of eq 3.9 calculated using the above method (for a system size of 8 triangles) turn out to be,

$$
\begin{array}{ll}
a_0 = -1.41712, & b_0 = -0.12665 \\
c_1 = 0.0183, & c_2 = 0.1291 \\
c_3 = -0.0108, & c_4 = 0.0942
\end{array}
$$
The important feature that we notice is that the next nearest neighbour coupling $c_2$ is stronger than the nearest neighbour coupling $c_1$. This is the reason why the spin-$\frac{1}{2}$ - spin-$\frac{1}{2}$ correlations between the next-nearest-neighbours is larger than the correlations between the nearest neighbours.

To this order in perturbation theory, the effective Hamiltonian seems to have the pattern AAFA (A → antiferromagnetic, F → Ferromagnetic). One curious thing that we notice in the spin-$\frac{1}{2}$ - spin-$\frac{1}{2}$ correlation plot is that though $c_2$ and $c_4$ are both positive (antiferromagnetic) the relevant correlations seem to be opposite in sign. The reason for this is that though both couplings are antiferromagnetic, $c_2$ larger and thus it exercises greater control over the alignment of $\vec{S}_5$ than $c_4$. That is why though $c_4$ would dictate $\vec{S}_1$ and $\vec{S}_5$ to be oppositely aligned, $c_2$ being larger will win over in trying to align $\vec{S}_1$ and $\vec{S}_5$ in the same direction. This is what results in the correlations of opposite sign.

For a system size of 10 triangles, the spins \{1,3,5,7,9\} and \{2,4,6,8,10\} because of a large $c_2$ will form two distinct frustrated systems and thus the correlations reported for this size will be smaller than for system sizes which have even number of triangles (this has been checked for 8 triangles). The general features of the effective Hamiltonian nevertheless remain unchanged as we can see from the plots.

Higher orders in perturbations theory: It is an interesting question to ask if the higher orders in perturbation theory will contribute in this case ($\delta = 10$). Analytically the effective Hamiltonian will have a more complicated form than just the two-spin interaction and we cannot use the method just described used to calculate $c_i$ numerically. We can try to eliminate the higher order effects by going to a higher $\delta$, say 100. But calculating the eigenvalues corresponding to $\delta = 100$ to compute $c_i$ to required accuracy is difficult. But if we look at the graph we see that even for $\delta = 2$ we already see the features that we have predicted for $\delta = 10$ quite clearly. This gives us an indication of the fact that the higher orders in all probability wont change the general features at $\delta = 10$. 

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Chapter 4

Spin wave analysis

In this chapter we look at the spin wave spectra obtained assuming the classical ground states described in Chapter 1 to be good approximations to the quantum ground states.

4.1 Spin wave spectra in the Ferrimagnetic state

The ferrimagnetic state which is stable for $J_2S_2 > 2J_1S_1$, is characterised by a collinear arrangement of spins with the spin-$\frac{1}{2}$’s and the spin-1’s pointing along opposite directions. Thus the spin-1’s and spin-$\frac{1}{2}$’s belong to two different sublattices having net magnetic moments in opposite directions. We proceed as follows to do the spin wave calculation for this phase,

We write the Hamiltonian in the form,

$$H = H_1 + H_2$$  \hspace{1cm} (4.1)

where $H_1 \equiv J_1 \sum_n \vec{S}_{1n} \cdot \vec{S}_{1(n+1)}$, and $H_2 \equiv J_2 \sum_n (\vec{S}_{2n} \cdot \vec{S}_{1n} + \vec{S}_{2n} \cdot \vec{S}_{1(n+1)})$. 

We now introduce the bosonic variables (we assume that the spin-1’s are pointing along the +z direction),

\[
\begin{align*}
S_{1n}^+ &= \sqrt{2} S_1 a_n, & S_{2n}^+ &= \sqrt{2} S_2 b_n^\dagger \\
S_{1n}^- &= \sqrt{2} S_1 a_n^\dagger, & S_{2n}^- &= \sqrt{2} S_2 b_n \\
S_{1n}^z &= S_1 - a_n^\dagger a_n, & S_{2n}^z &= -S_2 + b_n^\dagger b_n
\end{align*}
\] (4.2)

which are essentially the Holstein-Primakov transformations for the two sublattices truncated to the lowest order (the equations for \(S_z\) though are not approximations). And being bosonic variables \([a_n, a_n^\dagger] = \delta_{n,n'}\) and \([b_n, b_n^\dagger] = \delta_{n,n'}\).

We also introduce the bosonic variables in the reciprocal space,

\[
a_n = \frac{1}{\sqrt{N}} \sum_k a_k e^{i k n}, \quad b_n = \frac{1}{\sqrt{N}} \sum_k b_k e^{-i (n + \frac{1}{2})}
\] (4.3)

We assume unit lattice spacing. Thus the wave vectors \(\{k\}\) go from \(-\pi\) to \(\pi\) in units of \(2\pi/N\) where \(N\) is the number of sites on each sublattice.

Having defined these variables we now write \(H_1\) and \(H_2\) in terms of these bosonic operators assuming the classical configuration of the spins in the ferrimagnetic state to be a good approximation to the quantum ground state. If we look at \(H_1\) we see that the configuration of spin-1s mimics the ferromagnetic ground state of a Heisenberg ferromagnet in one dimension. So we can directly put down the form of \(H_1\) in terms of the bosonic operators taking into account the fact that in the present case \(J_1 > 0\). It will be,

\[
H_1 = NJ_1 S_1^2 - 4J_1 S_1 \sum_k \sin^2(\frac{k}{2}) a_k^\dagger a_k
\] (4.4)

Now using Eqs 4.2 and 4.3 we write \(H_2\) too in terms of the fourier variables. This will have the form,

\[
H_2 = -2N J_2 S_1 S_2 + 2J_2 S_1 \sum_k b_k^\dagger b_k + 2J_2 S_2 \sum_k a_k^\dagger a_k + 2J_2 \sqrt{S_1 S_2} \sum_k (b_k^\dagger a_k^\dagger + b_k a_k) \cos \frac{k n}{2}
\] (4.5)

Finally adding up \(H_1\) and \(H_2\) we get the full Hamiltonian in the fourier variables to be,

\[
H = NJ_1 S_1^2 - 2N J_2 S_1 S_2 + 2J_2 S_1 \sum_k b_k^\dagger b_k + \sum_k (2J_2 S_2 - 4J_1 S_1 \sin^2 \frac{k}{2}) a_k^\dagger a_k + \sum_k (2J_2 \sqrt{S_1 S_2} \cos \frac{k n}{2}) (b_k^\dagger a_k^\dagger + b_k a_k)
\] (4.6)
We note that the first term is the energy of the classical ground state. For convenience of expression we now define,
\[
A_k = 2J_2S_2 - 4J_1S_1 \sin^2 \left( \frac{k}{2} \right), \quad B_k = 2J_2S_1, \quad C_k = 2J_2 \sqrt{S_1S_2} \cos \frac{k}{2}
\] (4.7)

\(B_k\) is \(2J_2S_1\) for all \(k\). Thus we have,
\[
H = NJ_1S_2^1 - 2NJ_2S_1S_2 + \sum_k A_k a_k^\dagger a_k + \sum_k B_k b_k^\dagger b_k + \sum_k C_k (b_k^\dagger a_k^\dagger + b_k a_k)
\] (4.8)

We now use the Bogoliubov transformation to bring the above Hamiltonian to a more conveniently diagonalisable form. They are,
\[
a_k = u_k \cosh \theta_k - v_k^\dagger \sinh \theta_k \\
b_k = v_k \cosh \theta_k - u_k^\dagger \sinh \theta_k
\] (4.9)

\(u_k\) and \(v_k\) satisfy the same bosonic commutation relations as \(a\) and \(b\). We for now leave \(\theta_k\) as undetermined. Writing the Hamiltonian (4.8) in terms of the new variables \(u_k\) and \(v_k\),
\[
H = -J_1NS_1^2 - NJ_2S_1S_2 - \sum_k C_k \sinh 2\theta_k + \sum(A_k + B_k) \sinh^2 \theta_k \\
+ \sum(A_k \cosh^2 \theta_k + B_k \sinh^2 \theta_k - C_k \sinh 2\theta_k)u_k^\dagger u_k \\
+ \sum(A_k \sinh^2 \theta_k + B_k \cosh^2 \theta_k - C_k \sinh 2\theta_k)v_k^\dagger v_k \\
+ \sum[-\left(\frac{A_k}{2} + \frac{B_k}{2}\right) \sinh 2\theta_k + C_k \cosh 2\theta_k](u_k v_k + u_k^\dagger v_k^\dagger)
\] (4.10)

The last term suggests that we choose \(\theta_k\) according to the following definition:
\[
\tanh 2\theta_k = \frac{2C_k}{A_k + B_k}
\] (4.11)

This reduces the Hamiltonian apart from constant numbers (which we can ignore by setting the zero of energy appropriately) to a form in which all the operators are of the form \(\hat{O}^\dagger \hat{O}\).

Thus the Hamiltonian finally looks like,
\[
H = \sum_k (A_k \cosh^2 \theta_k + B_k \sinh^2 \theta_k - C_k \sinh 2\theta_k)u_k^\dagger u_k \\
+ \sum_k (A_k \sinh^2 \theta_k + B_k \cosh^2 \theta_k - C_k \sinh 2\theta_k)v_k^\dagger v_k
\] (4.12)
where we have dropped the constants. So we have two modes given by,

\[ \omega^- = A_k \cosh^2 \theta_k + B_k \sinh^2 \theta_k - C_k \sinh 2\theta_k, \]
\[ \omega^+ = A_k \sinh^2 \theta_k + B_k \cosh^2 \theta_k - C_k \sinh 2\theta_k \]

(4.13)

The mode \( \omega^- \) is gapless as \( k \to 0 \) and is also dispersionless when \( J_2 S_2 = 2J_1 S_1 \). The mode \( \omega^+ \) is always gapped as shown in the figure below:

---

### 4.2 Spin wave spectra in the Spiral state

We now investigate the spin wave spectra in the spiral state. This phase is stable for \( J_2 S_2 < 2J_1 S_1 \). We assume a coplanar configuration of spins in the system as the classical ground state as shown in the figure of the same in Chapter 1. The basic unit of this ground state (which keeps repeating) schematically looks as follows:
where \( \cos \theta \equiv \frac{J_2 S_2}{2 J_1 S_1} \) and \( S_1^1 \) and \( S_2^2 \) denote spin-1’s and spin-\( \frac{1}{2} \)'s respectively and the subscripts are the site indices. In order to do valid spin-wave calculations with this classical configuration, for the spin-1s on the baseline we must choose (for each spin-1 separately) the +z direction to be along (or opposite to) the classically expected direction of the spin vector. In doing so, we obtain the following transformation equations for the components of spin vectors (and thus for the corresponding operators) corresponding to the spin-1s,

\[
\begin{align*}
S_{2m}^{1x} &= S_{2m}^{1x'} \cos \theta - S_{2m}^{1z'} \sin \theta, \\
S_{2m-1}^{1x} &= S_{2m-1}^{1x'} \cos \theta + S_{2m-1}^{1z'} \sin \theta, \\
S_{2m}^{1z} &= S_{2m}^{1z'} \sin \theta + S_{2m}^{1x'} \cos \theta, \\
S_{2m-1}^{1z} &= -S_{2m-1}^{1z'} \sin \theta + S_{2m-1}^{1x'} \cos \theta, \\
S_{2m}^{1y} &= S_{2m}^{1y'}, \\
S_{2m-1}^{1y} &= S_{2m-1}^{1y'}.
\end{align*}
\] (4.14)

Here we have chosen the direction in which spin-\( \frac{1}{2} \)'s are aligned to be the +z direction and the +y direction is into the page. The primed coordinates are obtained by rotation about the \( y \)-axis by an angle \( \theta \). Because of the different classical orientations of the spin-1’s on the even and odd numbered sites we see that the transformation equations for them are different (\( \theta \) has changed sign). We also note that the classical spin-1 vectors are along the \( -z' \) directions at each site. We can now proceed with the spin wave calculation as the approximation used (that the deviation of \( S_z \) from \( S_1 \) is small) is valid if we use the primed coordinates for the spin-1’s.
As opposed to the ferrimagnetic case here we have to define three categories of bosonic variables. They are

\[
\begin{align*}
S_{2m}^{1+} &= \sqrt{2} S_1 b_{2m}, & S_{2m-1}^{1+} &= \sqrt{2} S_1 d_{2m-1}, & S_{n}^{2+} &= \sqrt{2} S_2^c \cr
S_{2m}^{1-} &= \sqrt{2} S_1 b_{2m}^{\dagger}, & S_{2m-1}^{1-} &= \sqrt{2} S_1 d_{2m-1}^{\dagger}, & S_{n}^{2-} &= \sqrt{2} S_2^d \cr
S_{2m}^{z'} &= -S_1 + b_{2m} b_{2m}, & S_{2m-1}^{z'} &= -S_1 + d_{2m-1} d_{2m-1}, & S_{n}^{z} &= S_2 - c_{n}^{\dagger} c_{n}
\end{align*}
\]

(4.15)

Where the b’s d’s are the bosonic variables for the spin-1’s at the even and the odd numbered sites respectively (in the above expressions, \(S_{2m}^{1+}\) etc have been defined in terms of the primed components). The index \(n\) runs over all the spin-\(\frac{1}{2}\) sites. From here the calculation proceeds in the following stages:

1. We use Eq. 4.14 and Eq. 4.15 to write the Hamiltonian (4.1) in terms of the three bosonic variables in the unprimed coordinates.

2. The first order terms in \(b_{2m}\)’s, \(d_{2m-1}\)’s and \(c_n\)’s vanish. We thus keep the terms to the second order in the above variables as the approximation to the Hamiltonian.

3. At this point the Hamiltonian doesn’t have a simple form which can be diagonalised using the Bogoliubov transformation used in the ferrimagnetic case. We use another method to find the spectrum here. We define a new set of canonically conjugate variables using the following equations,

\[
\begin{align*}
\sqrt{2} b_{2m} &= q_{b2m} + i p_{b2m}, & \sqrt{2} b_{2m}^{\dagger} &= q_{b2m} - i p_{b2m} \\
\sqrt{2} d_{2m-1} &= q_{d(2m-1)} + i p_{d(2m-1)}, & \sqrt{2} d_{2m-1}^{\dagger} &= q_{d(2m-1)} - i p_{d(2m-1)} \\
\sqrt{2} c_{n} &= q_{cn} + i p_{cn}, & \sqrt{2} c_{n}^{\dagger} &= q_{cn} - i p_{cn}
\end{align*}
\]

(4.16)

4. Now we write the Hamiltonian obtained in step 2 in terms of these operators. In terms of these operators we find a couple of properties of the Hamiltonian. The q’s and the p’s don’t couple in any of the terms. Secondly \(q_{b2m}\)’s and \(q_{d(2m-1)}\)’s and the corresponding momenta occur completely symmetrically in the Hamiltonian. There
is no way to choose one over the other. So instead of having two different variables for the odd and even numbered spin-1 sites we can express the Hamiltonian using just one set of variables for all spin-1’s. We call that set $Q_1$ and $P_1$ where $n$ runs over all spin-1’s. For convenience of expression we now call $q_{cn}$, $p_{cn}$ $Q_2$ and $P_2$ respectively and $n$ here runs over all spin-$\frac{1}{2}$’s.

5. After all the above simplifications the Hamiltonian finally looks like (omitting the constant term),

$$H = \sum_n A(Q_{1n}^2 + P_{1n}^2) + \sum_n B(Q_{2n}^2 + P_{2n}^2) + \sum_n C \cos 2\theta Q_{1n}Q_{1(n+1)} + \sum_n D \cos \theta Q_{2n}(Q_{1n} + Q_{1(n+1)}) + \sum_n C P_{1n}P_{1(n+1)} - \sum_n D P_{2n}(P_{1n} + P_{1(n+1)})$$

(4.17)

where, $A = J_2S_2\cos \theta - J_1S_1\cos 2\theta = J_1S_1$ (using the definition of $\cos \theta$), $B = J_2S_1\cos \theta$, $C = J_1S_1$ and $D = J_2\sqrt{S_1S_2}$.

Clearly this is the Hamiltonian for coupled linear harmonic oscillators with nearest neighbour and next-to-nearest neighbour interactions. This tells us that for the purpose of finding the eigenfrequencies we can use the classical equations of motion. This is because the eigenfrequencies of any such system on quantisation turn out to be the same as the classical ones. Thus using the Hamilton’s equations of motion and the trial solutions,

$$Q_{1n} = \epsilon_{1q}\exp i(kn - \omega t), \quad P_{1n} = \epsilon_{1p}\exp i(kn - \omega t)$$

$$Q_{2n} = \epsilon_{2q}\exp i(kn - \omega t), \quad P_{2n} = \epsilon_{2p}\exp i(kn - \omega t)$$

(4.18)

(where $k \in \{-\pi, \pi\}$) we get the following matrix equations,

$$\dot{P}_n = -A'Q_n$$

$$\dot{Q}_n = B'P_n$$

(4.19)

where,

$$P_n = \begin{bmatrix} P_{1n} \\ P_{2n} \end{bmatrix} \quad \text{and} \quad Q_n = \begin{bmatrix} Q_{1n} \\ Q_{2n} \end{bmatrix}$$

$A'$ and $B'$ are calculated to be,
\[
A' = \begin{pmatrix}
2A + 2C \cos 2\theta \cos k & 2De^{-\frac{ik}{2}} \cos \theta \cos \frac{k}{2} \\
2De^{\frac{ik}{2}} \cos \theta \cos \frac{k}{2} & 2B
\end{pmatrix}
\]
\[
B' = \begin{pmatrix}
2A + 2C \cos k & 2De^{-\frac{ik}{2}} \cos \frac{k}{2} \\
2De^{\frac{ik}{2}} \cos \frac{k}{2} & 2B
\end{pmatrix}
\]

Clearly the eigenvalues of the matrix \(B'A'\) will give us the squares of the eigenfrequencies. The following can be easily shown using the definitions of \(A, B\) etc.

\[\text{Det} B' = 0, \quad \text{Det} A' \neq 0\] (4.20)

Both of these together clearly imply that one of the eigenvalues of \(B'A'\) will be 0. Since the trace of \(B'A'\) will be the sum of its eigenvalues, the other mode can be calculated by calculating the trace of \(B'A'\) as one of the eigenvalues has already been determined to be 0. After taking the trace of \(B'A'\), we find the other mode to be given by

\[
\omega^2 = 4J_2^2 \left[ (S_1 \cos \theta - S_2 \cos^2 \left(\frac{k}{2}\right))^2 + \left(\frac{S_2}{4}\right) \tan^2 \theta \sin^2 k \right].
\] (4.21)

The above mode has a minimum at \(k = 0\) (\(\omega(k = 0) = 2J_2S_2\left|1-\frac{J_1}{J_2}\right|\)) which vanishes at \(\frac{J_2}{J_1} = 2\). At this point the nonvanishing mode looks as shown in the figure:
Thus the spiral state spin wave spectra consists of two modes one of which is dispersionless and gapless and the other gapped with the gap vanishing at $\delta = 0.5$. Notably $\delta = 0.5$ is indeed one of the points where the system has been observed to be gapless numerically. Spin wave analysis doesn’t give an indication of the point $\delta = 1.0$ being gapless.

### 4.3 Conclusions

To conclude, we have studied numerically and analytically, a two-spin (1 and 1/2) variant of the antiferromagnetic sawtooth lattice. Interesting features brought to light by this study are the following:

- The system seems to be gapless at two points in the phase diagram. Thus there seem to be more than the two expected phases from the classical analysis. Moreover none of these points correspond to the classically expected point for the transition from the ferrimagnetic to the spiral phase. Spin wave analysis does give some indication of the point $\delta = 0.25$ being gapless but the points which are actually found to be gapless are $\delta = 0.5$ and $\delta = 1.0$. This may be due to the small values of spins because of which spin wave analysis may not be very accurate. The properties of the system at $\delta = 0.5$ and $\delta = 1.0$ are unclear as of now.

- In the large $\delta$ limit, though the other correlations behave as expected, the correlations between the spin-$\frac{1}{2}$’s have the curious feature that the strongest coupled spins are the next-nearest-neighbours. This we have been able to explain using perturbation theory analysis of the model.

The study of the nature of the quantum phases at the points $\delta = 0.5$ and $\delta = 1.0$ is an interesting direction in which further work on this model can proceed. Numerically one can try to go the larger system sizes using DMRG to eliminate the finite size effects and thus better approximate the thermodynamic limit. The aspect of the problem we haven’t touched on at all is the effect of a magnetic field and the thermodynamics of the system. This is a another direction of study which can lead to a better understanding of this model.
Bibliography

[1] D. Sen, B. S. Shastry, R. E. Walstedt and R. Cava, Phys. Rev. B 53, 6401 (1996)
[2] S. A. Blundell and M. D. Nunez-Regueiro, cond-mat/0204405
[3] I. Rudra, D. Sen and S. Ramashesha, cond-mat/0210122
[4] Swapan. K. Pati, S. Ramasesha and D. Sen, Phys. Rev. B 55, 8894 (1997)
[5] N. B. Ivanov and J. Richter, Phys. Rev. B 63, 144429 (2001)
[6] N. B. Ivanov, Phys. Rev. B 62, 3271 (2000)
[7] J. Richter, U. Schollwöck and N. B. Ivanov, Physica B 281 & 282, 845 (2000)
[8] N. B. Ivanov, J. Richter and U. Schollwöck, Phys. Rev. B 58, 456 (1998)
[9] O. Kahn, Y. Pei and Y. Journax, Inorganic Materials, John Wiley & Sons Ltd, New York, 59-114 (1992)
[10] O. Kahn, Molecular Magnetism, VCH, New York (1993).
[11] Y. Pei, M. Verdaguer, O. Kahn, J. Sletten and J. P. Renard, Inorg. Chem. 26, 138 (1987)
[12] A. Gleizes and M. Verdaguer, J. Am. Chem. Soc. 106, 3727 (1984)
[13] S. R. White and D. K. Huse, Phys. Rev. B 48, 3844 (1993)
[14] J. K. Cullum and R. A. Willoughby, Lanczos Algorithms for Large Symmetric Eigenvalue Computations, Birkhäuser (1985)