ISOTROPIC PHENOMENA OF THE THREE – SITE CLUSTER HEISENBERG MODEL

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ABSTRACT

The linear and triangular 3-site Cluster of the spin – ½ Heisenberg antiferromagnet was studied and its magnetic properties are analyze via Exact Diagonalization technique. The results of the ground state energies were used to determine the magnetic phase diagram of the system. It was found that the transition points for both the linear and triangular lattice system are the same irrespective of having different ground state energies and geometries.

KEYWORDS: - Ground state energy, Antiferromagnetic phase, Ferromagnetic phase, Transition point.

1.0 INTRODUCTION

In the past several decades, there has been increasing interest in spin structure of several frustrated spin system where non-collinear spin configurations appear due to competition of interaction. The structure symmetry of the non-collinear structures causes various types of interesting ordering processes.[1]

Triangular antiferromagnets occupy a special niche in studies of quantum magnetism. The Ising antiferromagnet on a triangular lattice has a finite zero-temperature entropy, which reflect an extensive degeneracy of the ground-state manifold.[2] Most experimental results confirmed the universality hypothesis which states that critical behavior depends only on the dimensionality of the system (D) and on the degree of freedom of the order parameter (n). For instance, antiferromegnetic materials, provided that only short-range interactions are relevant, can be described by a Heisenberg model.[3] A magnetic system with Heisenberg spins that sit on the vertices of triangular lattice of corner sharing tetrahedral and interact among themselves via nearest-neighbour antiferromagnetic exchange interactions is highly geometrically frustrated. Such a system is theoretically predicted not to develop conventional magnetic long range order at finite temperature for either classical or quantum spins.[4] The classical Heisenberg model on a triangular lattice represents the textbook example of the full SU(2) symmetry-breaking and noncollinear spiral spin ordering in the ground state.[2] For a quantum S = - ½ antiferromagnet on a triangular lattice, Anderson proposed back in 1973 the disordered resonating valence bond (RVB) ground state. This suggestion stimulated extensive research for over 25 years. A RVB ground state on a triangular lattice has been found recently, albert for a quantum dimer model. It was also established by large-*N* and gauge theory approaches, that a disordered ground-state of a triangular antiferromagnet must possess unconfirmed massive spin on excitations.

The ideas about the disordered ground state of unconfirmed spinons, however, could not be immediately applied to the most studied Heisenberg model of quantum S = - ½ spins as a triangular lattice, as both perturbative $^1/_S$ and numerical calculations show that the classical, 120^0 spin structure survives quantum fluctuations[2].

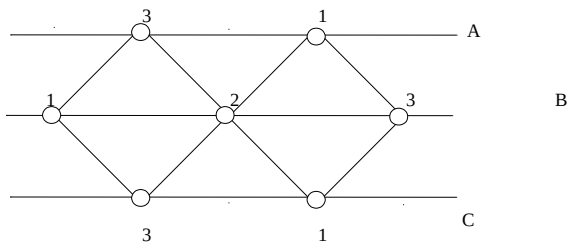

Figure 1: Exchange interactions in the Heisenberg Model on Triangular and Linear lattices.

In Fig. 1, Sites 1, 2 and 3 of line B can be considered as a linear lattices while Sites 1, 2 and 3 of Line AB or BC can be used for the Triangular Lattices.

The rest of the paper is organized as follows: After introducing the spin – ½ Heisenberg Hamiltonian in section 2, the problem of 3-site Cluster under this Hamiltonian is solved in section 3, we present our results and discussion in section 4, and we offered concluding remark and select other works in section 5.

2.0 MODEL AND METHODOLOGY

We consider an antiferromagnetic S = - ½ Heisenberg model on a linear and triangular lattice. More precisely we will analyze a two parameter Hamiltonian of this type, given by [5,6,7]

$$H=\sum_{i,j} J_{ij}\vec{S}_i.\vec{S}_j-\vec{h}\sum_i \vec{S}_i \qquad (1)$$

here S_i are spin – ½ operators. The first sum is over nearest neighbor connected by horizontal bonds (see Figure 1), J_{ij} are exchange integrals between spins at site *i* and *j*. *h* represents an applied external magnetic field. We suppose that *S* is the total spin of each atom, and classify the spin state of the i^{th} atom by the eigenstate of S_i^z, the *z*-component of the spin.[8] Thus

$$S_i^Z|m\rangle_i=m|m\rangle_i,-s\le m\le s \qquad (2)$$

For a state with spin component *m* in the *z*-direction. It may be shown that for J > 0, the ground state of the Hamiltonian (1) is the totally aligned state.

$$|\psi_G\rangle=|S\rangle_1|S\rangle_2.....|S\rangle_N \qquad (3)$$

in which S^z has its maximum value S at each lattice site.[7] It is easy to show that this state is an exact eigenstate of H. We define the spin deviation operators by

$$S_j^{(+)} = S_j^{(x)} + iS_j^{(y)}, S_j^{(-)} = S_j^{(x)} - iS_j^{(y)} \tag{4}$$

These are such that, for any lattice site

$$S^{(+)}|m\rangle = |m+1\rangle, S^{(-)}|m\rangle = |m-1\rangle \quad , \quad S^{+}|s\rangle = 0, S^{-}|-s\rangle = 0 \tag{5}$$

and the Hamiltonian equation for the H_{linear} and $H_{triangular}$ lattice may be written as (6) and (7) respectively.

$$H_{linear} = J\left\{S_1^z S_2^z + S_2^z S_3^z + \frac{1}{2}\left(S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+\right)\right\} - h\left(S_1^z + S_2^z + S_3^z\right) \tag{6}$$

$$H_{triangular} = J\left\{S_1^z S_2^z + S_2^z S_3^z + S_3^z S_1^z + \frac{1}{2}\left(S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+ + S_3^+ S_1^- + S_3^- S_1^+\right)\right\}$$

$$-h\left(S_1^z + S_2^z + S_3^z\right) \tag{7}$$

Clearly when H operates on $|\psi_G\rangle$, only the z-components of the spin contribute, and the ordered state (3) is thus an eigenstate of the Hamiltonian. Other spin configurations can be shown to have higher energies by evaluating matrix elements of H. Since the Heisenberg interaction (1) is isotropic, the direction of the spin alignment in the groundstate is arbitrary and the state (3) is in fact (N+1) – fold degenerate. [6,7] Classical bits, used for computation, are often denoted as "1" and "0" they can be represented by an effective spin – ½ degree of freedom, where "1" corresponds to the spin pointing up, and "0" represents a spin pointing down. To solve a complex many-body problem such as determining the ground state of a Heisenberg Hamiltonian requires 2^N classical bits or Hilbert space for a system, with N sites.[6] Hence $N=3$ is the 3-sites Cluster or dimer corresponding to 8 basis electronic states.

3.0 THREE-SITE CLUSTER

Considering three-site spin - ½ Heisenberg Clusters. For this case, there are two possible distinct geometries. A three-site open chain and a closed triangle with exchange interaction (Figure 1); Open sites chain correspond to the linear lattice system while the closed site chain corresponds to triangular lattice system. The Hilbert space does not depend on the geometry. It has $2^3 = 8$ states. In the same Ising basis used for the previous two-sites [5,6]; this leads to the basis electronic states given below

$$|1\rangle=|111\rangle,|2\rangle=|110\rangle,|3\rangle=|101\rangle,|4\rangle=|011\rangle,|5\rangle=|001\rangle,|6\rangle=|010\rangle,|7\rangle=|100\rangle,|8\rangle=|000\rangle$$
(8)

The two geometries shall be considered in parallel.

3.1 LINEAR CLUSTER

Using the Hamiltonian (6) to act on the basis electronic states (8) leads to the matrix representation

$$H_{ij}=\begin{bmatrix} \frac{J-3h}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-h}{2} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{J}{2} & \frac{-J-h}{2} & \frac{J}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{J}{2} & \frac{-h}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{h}{2} & \frac{J}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{J}{2} & \frac{-J+h}{2} & \frac{J}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & \frac{h}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{J+3h}{2} \end{bmatrix}$$
(9)

and the eigenvalues are given by

$$\frac{-h}{2},\quad \frac{h}{2},\quad \frac{1}{2}(-h-2J),\quad \frac{1}{2}(h-2J),\quad \frac{J-3h}{2},\quad \frac{J-h}{2},\quad \frac{J+h}{2} \text{ and } \frac{J+3h}{2}$$
(10)

3.2 TRIANGULAR CLUSTER

Using the Hamiltonian (2.8) to acts on the states (3.5) leads to the matrix representation

$$H_{ij}=\begin{vmatrix} \frac{3J-6h}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-(J+2h)}{4} & \frac{J}{2} & \frac{J}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{J}{2} & \frac{-(J+2h)}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{J}{2} & \frac{J}{2} & \frac{-(J+2h)}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{-(J+2h)}{4} & \frac{J}{2} & \frac{J}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{J}{2} & \frac{-(J+2h)}{4} & \frac{J}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{J}{2} & \frac{J}{2} & \frac{-J+2h}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3J+6h}{4} \end{vmatrix} \quad (11)$$

and the eigenvalues are given below

$$\frac{-h}{2},\quad \frac{h}{2},\quad \frac{1}{2}(-h-2J),\quad \frac{1}{2}(h-2J),\quad \frac{J-3h}{2},\quad \frac{J-h}{2},\quad \frac{J+h}{2} \text{ and } \frac{J+3h}{2} \quad (12)$$

4. 0 RESULTS AND DISCUSSION.

4.1 RESULTS

The linear Heisenberg results are presented in Table 1 and 2 with their corresponding graph Figure 1 and 2. For the triangular Heisenberg results, Table 3 and 4 with their corresponding graphs Figure 3 and 4 are used to illustrate the phase diagram

Table 4.1 Singlet (E_s) and triplet (E_t) state energies as *h* increases, while *J* remains constant for the Linear lattice system.

J (Exchange integral)	***h*** (External magnetic field)	$\mathbf{E_s}$ (Singlet state energies)	$\mathbf{E_s}$ (Triplet state energies)
2.00	0.00	-3.00	-1.00
2.00	2.00	-2.00	-3.00
2.00	4.00	-1.00	-5.00
2.00	6.00	0.00	-7.00

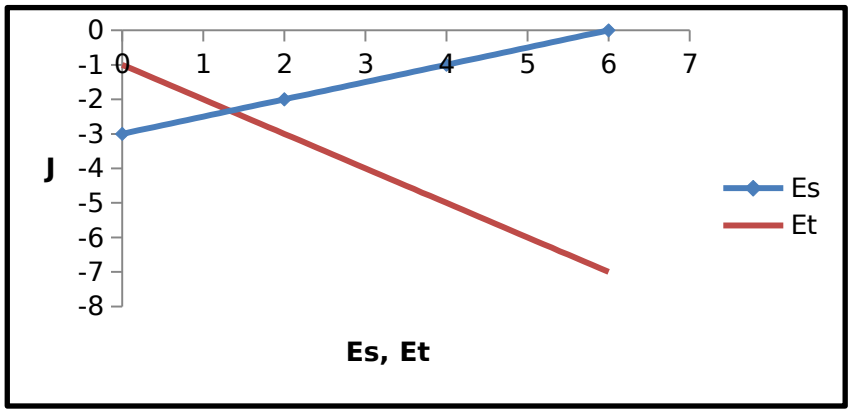

Figure 4.1: Graph of Singlet (E_s) and Triplet state energies (E_t) energies plotted against *h* for the Linear lattice system.

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Table 4.2: Singlet (E_s) and triplet (E_t) state energies as *J* increases, while *h* remains constant for the Linear lattice system.

h (External magnetic field)	***J*** (Exchange integral)	**E_s** (Singlet state energies)	**E_t** (Triplet state energies)
2.00	0.00	1.00	-2.00
2.00	2.00	-2.00	-3.00
2.00	4.00	-5.00	-4.00
2.00	6.00	-8.00	-5.00

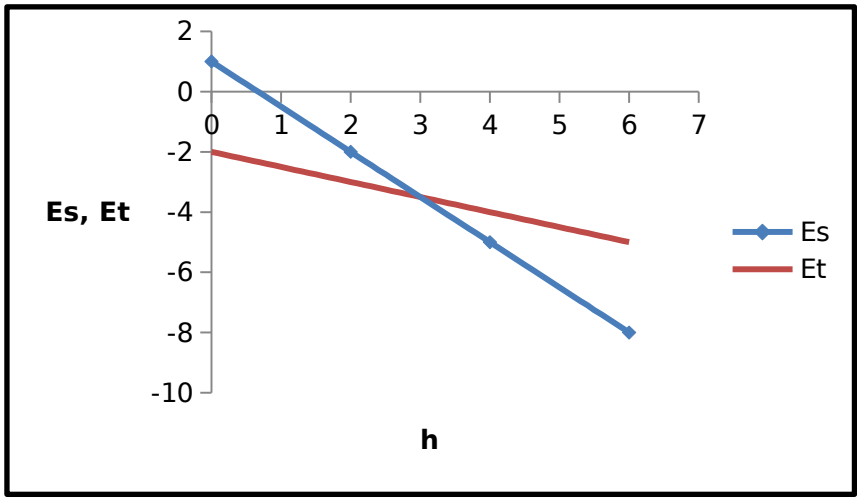

Figure 4.2: Graph of Singlet (E_s) and Triplet state energies (E_t) energies plotted against *J*.

Table 4.3 : Singlet (E_s) and triplet (E_t) state energies as *h* increases, while *J* remains constant for the triangular lattice.

J (Exchange integral)	***h*** (External magnetic field)	**E_s** (Singlet state energies)	**E_t** (Triplet state energies)
2.00	0.00	-3.00	-1.00
2.00	2.00	-1.50	-2.50
2.00	4.00	0.00	-4.00

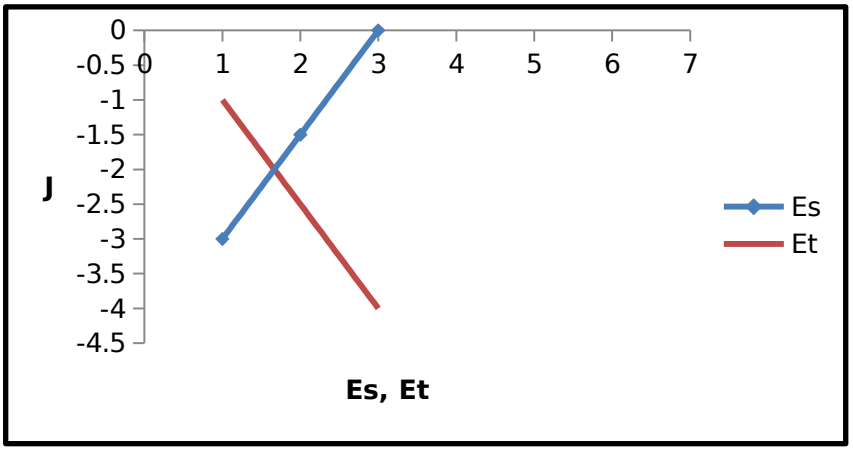

Fig. 4.3 Graph of Singlet (E_s) and Triplet state energies (E_t) energies plotted against *h* for the triangular lattice.

Table 4.4 :Singlet (E_s) and triplet (E_t) state energies as *J* increases, while *h* remains constant for the triangular lattice.

h (External magnetic field)	***J*** (Exchange integral)	E_s (Singlet state energies)	E_t (Triplet state energies)
2.00	0.00	1.50	-1.50
2.00	1.00	0.00	-2.00
2.00	2.00	-1.50	-2.50
2.00	3.00	-3.00	-3.00
2.00	4.00	-4.50	-3.50
2.00	5.00	-6.00	-4.00

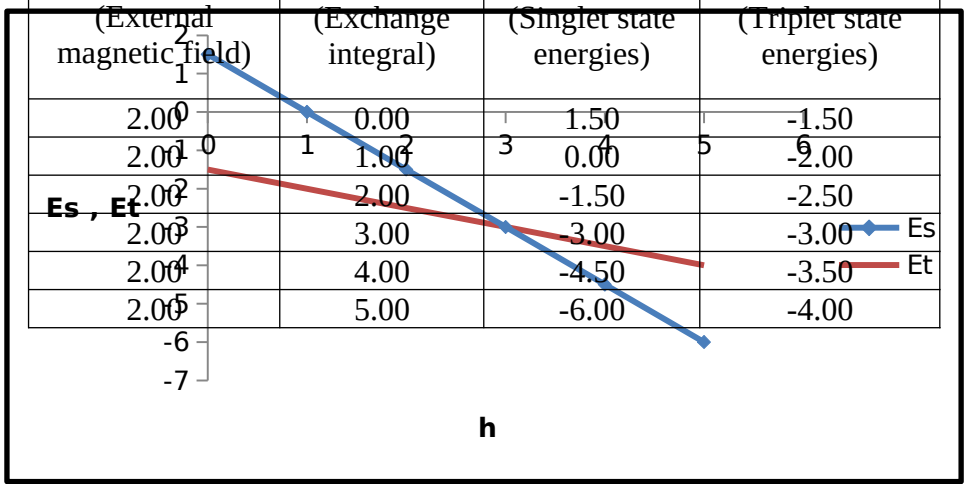

Figure 4.4: Graph of Singlet (E_s) and Triplet state energies (E_t) energies plotted against *J* for the triangular lattice.

4.2 DISCUSSION

Usually, the eigenvalue solution of the matrix form of the Hamiltonian will yield the total energy which is the energy spectrum of the system and the lowest of them is the ground state energy of the system.

The condition to produce a ferromagnetic phase is that the lowest state energy of the triplet state, E_t must be smaller than that of the singlet state, E_s, i.e $E_t < E_s$.[9] If the singlet states provides the lowest energy, then the system will be Antiferromagnetic (AFM), while it will be ferromagnetic (FM) if the triplet state provides the ground state energy.

The value at which $E_t = E_s$ gives rise to a transition from antiferromagnetic phase to the ferromagnetic phase or vice-versa. This point is called the transition point, T_p.[9]

From Table 1 and 3 and their corresponding graphs Figure 1 and 3 show that, as the value of the exchange integral, *J* increases, the ground-state continue to increase to a transition point T_p, where $E_s=E_t$ and as the values are further increased beyond T_p, where $E_s > E_t$ the system becomes Ferromagnetic (FM). The physical implication is that the electronic correlations favouring AFM gets weaker while that of FM gets stronger as the values of the exchange integral, *J* increases. This continue on till the electronic correlation favouring ferromagnetism begins to dominate (i.e. there is cross-over to ferromagnetism) and this domination is enhanced as *J* increases. Hence, this direct exchange interaction provides a natural way for stabilizing ferromagnetic states.[11]

From the computation of Table 2 and 4 with their corresponding Figure 2 and 4, we see that as the external magnetic field, *h* increases, for example from 0 to 2.99, the lattice system is still FM. At *h* = 3.00MeV, which is the transition point, T_p a cross over from FM phase to an AFM phase was observed. Within this section, the energy relation becomes $E_s<E_t$, which is the condition for ferromagnetism.

On the whole the first excited state is a triplet and the ground state energy of the lattice system is a spin singlet respectively for both the linear and Triangular Heisenberg antiferromagnet.

The triangle has multiple degeneracy[6], which are not split by the external magnetic field, whereas in the chain case all degeneracies at zero field are split at finite fields. The critical point at which the ground state crosses over from $S^z_{tot}=\frac{1}{2}$ to $S^z_{tot}=\frac{3}{2}$ is different for two cases: $h_c=\frac{3J}{2}$ for the chain and $h_c=3J$ for the triangular, indicating that the triangular geometry protects zero-field $S^z_{tot}=\frac{1}{2}$ ground state more efficiently. At the zero magnetic field, there is a degenerate ground state, similar to an isolated spin -½ particle which has degenerate up-spin and down-spin configuration. The degenerate is removed by infinitesimal applied field. For the three site clusters this means that strictly at *h=0* the magnetization is zero, then it jumps to ½ at infinitesimal fields, and then it jumps to $^3/_2$ at critical magnetic field. Similar to the two site cluster,[9] the low temperature behavior depends on the specific magnetic field that is applied, whereas the high temperature is Curie-like as usual.[6]

5.0 CONCLUSION

In this paper the power of direct exact Diagonalization technique is apply to Heisenberg Model to study the effect of three interacting electrons on linear and triangular lattices. We elucidate the nature of the ground state and determine the tendency to ferromagnetism. Attention was focused on the parameter region where a transition from AFM to FM occurs.

Consideration of the four site cluster is highly desirable which a subject for further studies.

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