



FRUSTRATED MAGNETISM: A CASE STUDY OF GEOMETRIC FRUSTRATION

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ABSTRACT: *In this research work, frustrations arising from the geometries of triangular lattices have been studied with the aid of Ising and Heisenberg models. The study reveals that geometrical frustrations can generate multiple degeneracies in the ground state. The quantum spin flip terms in the Heisenberg model are observed to play a vital role in the partial lifting up of these degeneracies. Hence, multiple degeneracies as consequence of frustrations are more pronounced for the Ising systems, which are devoid of quantum fluctuations. The observed six- and four-fold ground state degeneracies at zero field for three spins Ising and Heisenberg systems respectively are broken down to half at finite longitudinal fields. For this three-spin system, quantum phase transitions (QPT) are observed at critical longitudinal fields of J and $1.5J$ respectively for the Ising and Heisenberg models. At these critical fields, the ground states are observed to shift from quasi-antiferromagnet to ferromagnet. However, for the Heisenberg three-spin system in the presence of a transverse field, no transition is observed.*

KEYWORDS: Frustrated Magnetism, Geometric Frustration, Heisenberg Models, Quantum Phase Transitions (QPT)

INTRODUCTION

Background to the Study

Generally, frustration in solid state Physics refers to a situation where the contributions to the potential energy of a many-body system cannot be simultaneously minimized. Magnetic systems are frustrated if a spin cannot arrange its orientation such that it profits from the interaction with its neighbors. (Huse & Rutenberg, 1992; Diep, 2016). Since the degrees of freedom of a spin is two and cannot configure itself to fully satisfy all the pairwise interactions with its neighbors, the spin is said to be “confused and unhappy”. The question we need to address is this: why is it that the possible spin alignment cannot put the system in its minimal energy level? The reasons for this behavior are due to system geometries and the presence of competing interactions.

In order to have an insight and a deep perception of frustrated systems, it will be worthwhile to recall the behavior of an unfrustrated system. To be definite, consider the Ising model spins ($\sigma = \pm 1$) on a square lattice with nearest neighbor (NN) coupling $J > 0$ as shown in Fig. 1a. When $J > 0$ (antiferromagnetic ground state), one may naively expect that the ground state would correspond to all NN pairs being antiparallel. However, in contrast to a ferromagnet, such an antiferromagnetic state may not exist for a given lattice. The existence of such a state in a lattice, with all pairwise interactions satisfied, is possible only when the lattice sites can be divided into two disjoint subsets (or sub-lattices) such that all neighbors of a site in one set belong to the other set (Tiwari, 2013). This is a geometric property of the lattice, and when it is satisfied we call the lattice bipartite. The nearest neighbors of a given site in such a lattice are not themselves nearest neighbors of each other. Therefore, a spin arrangement exists in which all NN pairs are anti-parallel. This state is the Neel antiferromagnet and it is a property of unfrustrated system. It can occur, for example, on a square lattice (Fig. 1a), and simple cubic lattices. A contrast is provided by the triangular lattice (Fig. 1b), where the nearest neighbors of a given site are also themselves nearest neighbors.

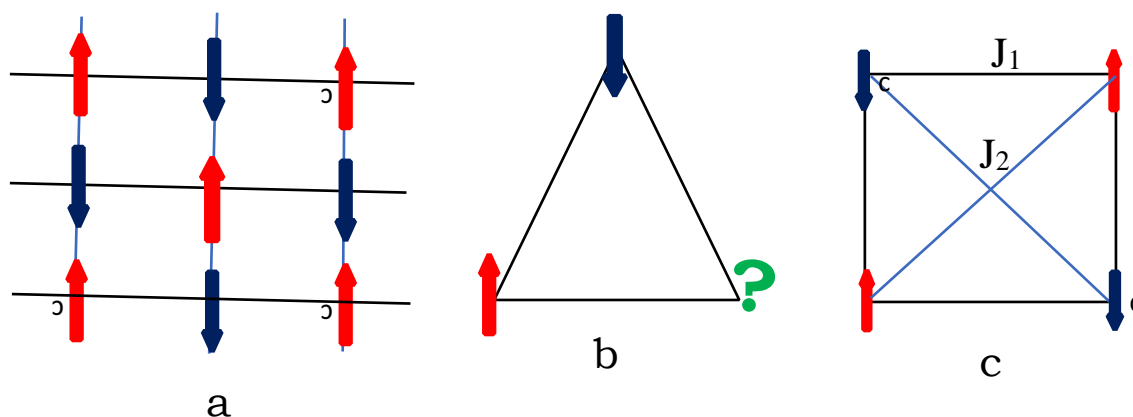


Fig. 1(a) In the unfrustrated antiferromagnet on the square lattice, each spin can be anti-aligned with all its neighbors. **(b)** On a triangular lattice, such a configuration is impossible: Three neighboring spins cannot be pair wise anti aligned, and the system is frustrated. **(c)** Frustrated four-site system with competing interactions J_1 and J_2 . J_1 is coupling strength for nearest neighbour interactions (NN), while J_2 is the coupling strength for next nearest neighbor interactions (NNN). The system is frustrated because there is no possible orientation of the spins coupled by J_2 that will anti-align them.



Geometric frustration arises when lattice structure precludes simultaneous minimization of local interaction energies (Han et al., 2008; Moessner & Ramirez, 2006). Geometric frustration in magnetism is best understood in the context of the nearest neighbor Ising antiferromagnetic on a triangular lattice as shown in Fig. 1b. Variants of this, involving triangular motifs in higher dimensions, quantum spins, and more complex interactions, define this well explored field. All these systems are 'insulators', with no relevant charge degrees of freedom, and the nature of spin-spin interaction is predefined (otherwise the concept of frustration itself becomes ambiguous). In this frustrated triangular system, if two neighboring spins can minimize their energy by aligning in opposite directions, the third spin becomes frustrated. This is because no possible configuration of the third spin can simultaneously give an antiferromagnetic alignment with the two neighboring spins. The antiferromagnetic triangle is the simplest case in which a conflict arises between the geometry of the space inhabited by a set of degrees of freedom and the local correlations favored by their interactions. This phenomenon is one aspect of a powerful paradigm for discovery over the past few decades—namely, our ability to experimentally manipulate the space in which magnetic, charge, or vibrational degrees of freedom interact. A central reason for the interest in geometrically frustrated magnets is that they hold out the possibility of evading Neel order. Other examples of lattices with geometric frustration include Face-centered cubic (FCC), Kagome, checkerboard, and pyrochlore lattices.

Frustration can also arise as a result of competition between two coupling parameters in a lattice. Frustration of this type has been studied extensively in models with competing nearest neighbor and further neighbor interactions, notably the J_1 - J_2 model on the square lattice (Chandra & Doucot, 1988). The classical ground state of this model depends on the ratio J_1/J_2 . Depending on the system being studied, in some regime, say, $J_2 > J_1$, neighbouring spins are antiparallel, enforcing ferromagnetic alignment of second neighbors and frustration of the interaction J_2 . This type of frustration is captured in Fig. 1c. An important advantage of this type of frustrated system is the possibility of varying the degree of frustration by tuning individual exchange couplings. Hence, the formation of different ground states within one model and the access to quantum critical points are possible (Nath et al., 2008). While models of this kind provide an attractive starting point for theoretical work, there are likely to be difficulties in finding experimental realizations with interaction strengths that place them close to the degeneracy point. Nevertheless, a number of frustrated chain systems with $J_2/J_1=0$ have been studied, and even the vicinity of the quantum critical point at $J_2/J_1=-0.25$ was accessed experimentally (Drechsler et al., 2007).

Objectives of the Study

The overall aim of this work is to investigate the effects of frustration induced by geometry. The objectives of this research work are:

- a) to study both Ising and Heisenberg models on one dimensional and quasi-two dimensional triangular geometries and compare and contrast the nature of multiple degeneracies in the Ising and Heisenberg models;
- b) to study the effect of quantum spin fluctuation in the isotropic Heisenberg model on frustrated triangular systems;
- c) to use the exact diagonalization method to reproduce the dominant results as obtained by other theoretical and experimental results; and
- d) to account for the phenomenon of quantum phase transition in these frustrated systems.



RESEARCH METHODS

In this research work, the following two models, namely the Ising and Heisenberg models will be used to study triangular frustrated spin systems.

i. THE HEISENBERG MODEL

This model simply reads

$$H_H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \tag{1}$$

where J is the super exchange coupling parameter between spins on site i and j which decay rapidly with the distance between these sites and \vec{S}_i are the spin operators. The symbol $\langle i,j \rangle$ means that the interaction is restricted to nearest neighbors. In vector notation, the spin operator is given by

$$\vec{S}_i = \hat{x}S_i^x + \hat{y}S_i^y + \hat{z}S_i^z \tag{2}$$

The Heisenberg model will be used to stimulate the dynamics of the electron's spin in the frustrated triangular systems. Due to the presence of quantum flip terms in this model, it can initiate quantum spin fluctuation between nearest antiferromagnetically aligned spins. In second quantized form, the spin operators take the form

$$\left. \begin{aligned} S_i^x &= \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}) \\ S_i^y &= -\frac{i}{2}(c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow}) \\ S_i^z &= \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) \end{aligned} \right\} \tag{3}$$

Where (c_i) is the annihilation operator, (c_i^\dagger) is the creator operator.

$$\begin{aligned} H &= \frac{J}{4} \sum_{\langle i,j \rangle} (c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\uparrow}^\dagger c_{j\uparrow} - c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow} - c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\downarrow}) \\ &+ \frac{J}{2} \sum_{\langle i,j \rangle} (c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{i\uparrow} c_{j\uparrow}^\dagger c_{j\downarrow}) \end{aligned} \tag{4}$$

At this juncture, S_i^+ (S_i^-), the spin raising (lowering) operators which effectively flip the spin of the electron residing on i th site are introduced. These operators are given by

$$\left. \begin{aligned} S_i^+ &= c_{i\uparrow}^\dagger c_{i\downarrow} \\ S_i^- &= c_{i\downarrow}^\dagger c_{i\uparrow} \end{aligned} \right\} \tag{5}$$



In terms of the spin lowering and raising operators the Heisenberg model in a more compact form gives

$$H_H = J \sum_{\langle i,j \rangle} \left[S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right] \tag{6}$$

ii. ISING MODEL

This model is achieved by switching off the spin of fluctuation term in the Heisenberg model (i.e. $S_i^+ S_j^- + S_i^- S_j^+ = 0$). Under this consideration, the Ising model gives

$$H_I = J \sum_{i=1}^N S_i^z S_{i+1}^z \tag{7}$$

The ising model allows the classical treatment of dynamics of the spins, since it is devoid of quantum spin fluctuations. In otherwords, only diagonal spin interactions are considered. This model makes it possible to observe the enhancement or otherwise of the multiple degeneracies in the ground state.

In second quantized form it gives

$$H_I = \frac{J}{4} \sum_{\langle i,j \rangle} (c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\uparrow}^\dagger c_{j\uparrow} - c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow} - c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\downarrow}) \tag{8}$$

iii. These models will be used to operate on the electronic states or (Hilbert space) of the frustrated system.

iv. The Hamiltonian matrix arising from these operations takes the form

$$H_{ij} = \begin{bmatrix} \langle 1|H|1 \rangle & \cdot & \cdot & \cdot & \langle 1|H|n \rangle \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \langle n|H|1 \rangle & \cdot & \cdot & \cdot & \langle n|H|n \rangle \end{bmatrix} \tag{9}$$

Subject to the condition

$$\langle i|H|j \rangle = \delta_{ij} \tag{10}$$

v. This Hamiltonian matrix in (9) be diagonalized using the eigenvalue equation

$$(H - \lambda I) = 0 \tag{11}$$

Where λ is the eigenvalue.

vi. Finally, quantum phase transition (QPT) induced by frustration will be investigated by perturbing the system with the external magnetic field given by

$$H_h = -h_z \sum S_i^z - h_x \sum S_i^x \tag{12}$$

The first term and second term on the right hand side of (12) will henceforth be denoted by H_z and H_x respectively. The symbols S_i^z and S_i^x are the diagonal and off diagonal spin operators respectively. These operators act in the reduced Hilbert space of no doubly occupied sites. The longitudinal and transverse fields are respectively denoted by h_z and h_x .

PRESENTATION AND DISCUSSION OF RESULTS

This section presents and discusses the results obtained in three site triangular systems

FRUSTRATED ISING THREE-SITE TRIANGULAR GEOMETRY AT ZERO FIELD

Exact diagonalization of the three-site triangular geometry at zero field using the Ising model gives six-fold degenerate ground states with energy $-J/4$, and only two-fold degeneracy in the excited state, with energy $3J/4$. The schematic diagram for these six-fold degeneracies in the ground state is shown in Fig.1. These multiple degeneracies in the ground state are due to the presence of a frustrated spin in these systems.

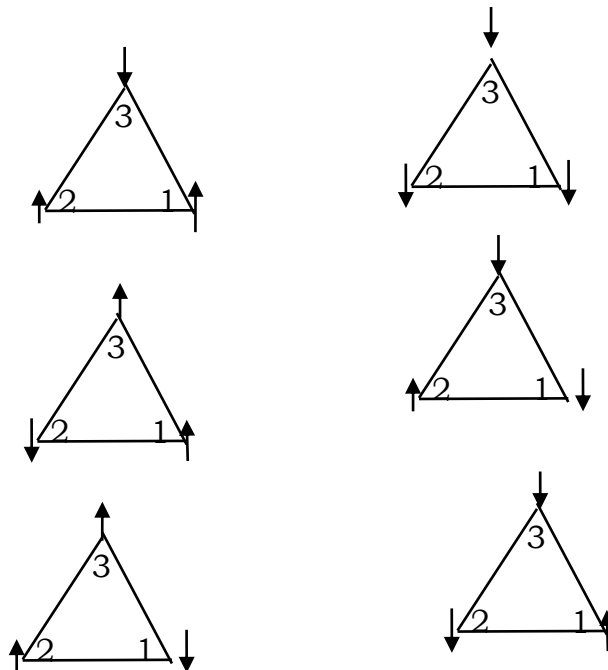


Figure 2: Six possible representations of the spin configuration in the ground state. Each of this representation has the same energy of $-J/4$

FRUSTRATED THREE-SITE ISING TRIANGULAR GEOMETRY AT FINITE LONGITUDINAL FIELD AND THE EMERGENCE OF QPT

In the presence of a finite longitudinal field, the six-fold degenerate ground state splits into 3 folds as shown in Table 1. This implies that the longitudinal field could not effectively lift up all the degeneracies caused by frustration. These three degenerate states begin to compete with other states for the ground state of the system. These competing states are depicted schematically in Figure 2.

Table 1: Eigenvalues and eigenvectors of the 3-site triangular Ising system at zero temperature and finite longitudinal fields

Eigenvectors	Eigenvectors at h=0	Eigenvalues at h=0	S^z_{tot}
$ 111\rangle$	$3J/4$	$\frac{3J}{4} - \frac{3h_z}{2}$	$3/2$
$ 110\rangle$	$-J/4$	$-\frac{J}{4} - \frac{h_z}{2}$	$1/2$
$ 101\rangle$	$-J/4$	$-\frac{J}{4} - \frac{h_z}{2}$	$1/2$
$ 011\rangle$	$-J/4$	$-\frac{J}{4} - \frac{h_z}{2}$	$1/2$
$ 010\rangle$	$-J/4$	$-\frac{J}{4} + \frac{h_z}{2}$	$-1/2$
$ 001\rangle$	$-J/4$	$-\frac{J}{4} + \frac{h_z}{2}$	$-1/2$
$ 100\rangle$	$-J/4$	$-\frac{J}{4} + \frac{h_z}{2}$	$-1/2$
$ 000\rangle$	$3J/4$	$\frac{3J}{4} + \frac{3h_z}{2}$	$-3/2$

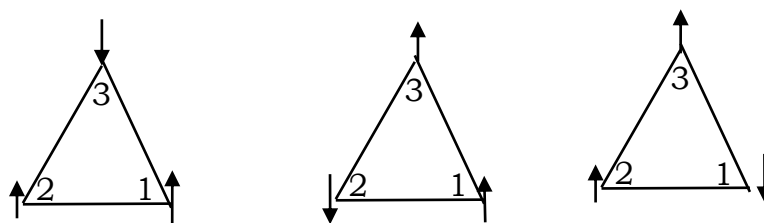


Figure 2: Three possible representations of the spin configuration in the ground state. Each of this representation has the same energy of $-\frac{J}{4} - \frac{h_z}{2}$.



In order to investigate the presence of QPT, and hence the emergence of a new ground state in this system, we shall vary the external longitudinal field across the entire energy spectrum. The response of the competing states and the other energy spectrum to these variations are shown in Table 2. As the field is varied, a critical field of $h_{zc} = J$ is reached at which the system makes a transition from $S_{tot}^z = 1/2$ to $S_{tot}^z = 3/2$. Hence, the system undergoes a QPT from a quasi-antiferromagnetic state (insulator) to a ferromagnetic state (metallic). This crossover in energy level from E_4 to E_1 at $h_{zc} / J = 1$.

Table 2: Investigation of quantum Phase transition in the 3-site triangular Ising system in the presence of longitudinal field

h_z/J	E_1/J	E_2/J	E_3/J	E_4/J	E_5/J	E_6/J	E_7/J	E_8/J
0	0.75	-0.25	-0.25	-0.25	-0.25	-0.25	-0.25	0.75
0.25	0.375	-0.375	-0.375	-0.375	-0.125	-0.125	-0.125	1.125
0.5	0	-0.5	-0.5	-0.5	0	0	0	1.5
0.75	-0.375	-0.625	-0.625	-0.625	0.125	0.125	0.125	1.875
1.0	-0.75	-0.75	-0.75	-0.75	0.25	0.25	0.25	2.25
1.25	-1.125	-0.875	-0.875	-0.875	0.375	0.375	0.375	2.625
1.5	-1.5	-1	-1	-1	0.5	0.5	0.5	3

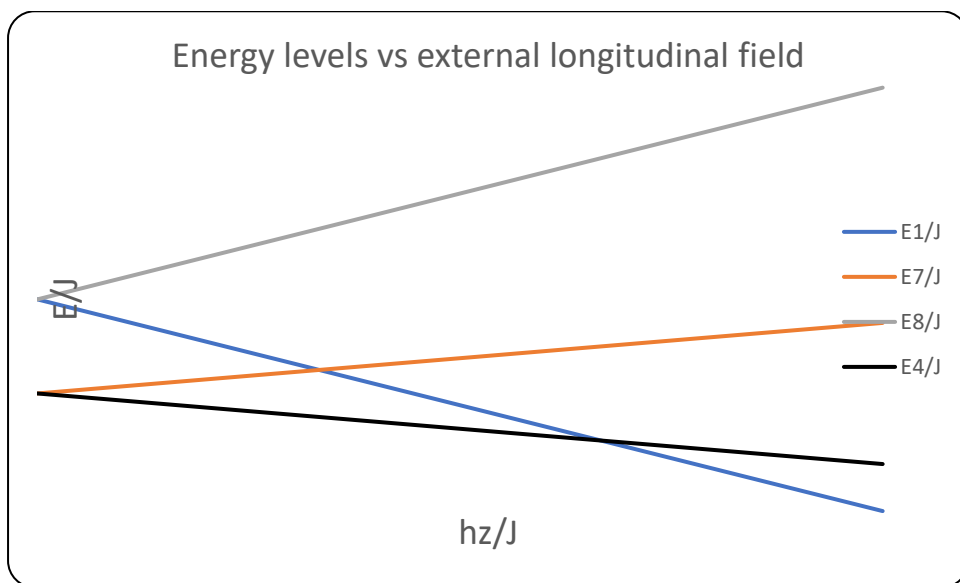


Figure 3: A crossover in ground state configuration from $S_{tot}^z = 1/2$ to $S_{tot}^z = 3/2$ at $h_{zc} / J = 1$



1@FRUSTRATED THREE-SITE ISING TRIANGULAR GEOMETRY AT FINITE TRANSVERSE FIELD AND THE EMERGENCE OF QPT

An investigation of the effect of the transverse field with the entire spectrum of this system is presented in Table 3. The six-fold degenerate ground state observed at zero field is now broken down to two-fold degenerate competing ground states. As the transverse field is varied, a sharp QPT is observed at an infinitesimal field. Hence, there is a transition from quasi-antiferromagnetic state to quasi-ferromagnetic state. For instance, at $h_x/J=1$, the new ground state with energy E_7/J is given by,

$$|\psi_g\rangle = \frac{1}{\sqrt{2+3p_1^2+3p_2^2}} [p_1|110\rangle + p_1|101\rangle + p_1|011\rangle + p_2|010\rangle + p_2|001\rangle + p_2|100\rangle + |000\rangle - |010\rangle]$$

where the symbol p_1 and p_2 are given by

$$p_1 = -\frac{1}{2} + \frac{1}{6}(3 + 2\sqrt{3})$$

$$p_2 = \frac{1}{2} + \frac{1}{6}(-3 - 2\sqrt{3})$$

The other two degenerate competing quasi-antiferromagnetic ground states with energy $\frac{1}{4}[-2h_x - J]$ is given by

$$|\psi_1\rangle = \frac{1}{2} [|101\rangle - |011\rangle - |010\rangle + |100\rangle]$$

$$|\psi_2\rangle = \frac{1}{2} [|101\rangle - |110\rangle - |010\rangle + |001\rangle]$$

The quantum phase transition from either $|\psi_1\rangle$ or $|\psi_2\rangle$ to $|\psi_g\rangle$ was spontaneous, and hence the actual critical field could not be detected. Fig.4 also shows the spontaneous quantum phase transition from E_1 to E_7 .



Table 3: Investigation of quantum Phase transition in the 3-site triangular Ising system in the presence of transverse field

h_x/J	E_1/J	E_2/J	E_3/J	E_4/J	E_5/J	E_6/J	E_7/J	E_8/J
0.0	-0.25000	-0.25000	-0.25000	-0.25000	-0.25000	0.75000	-0.25000	0.75000
0.1	-0.30000	-0.30000	-0.20000	-0.20000	-0.15826	0.75826	-0.35678	0.75678
0.2	-0.35000	-0.35000	-0.15000	-0.15000	-0.08589	0.78589	-0.47450	0.77450
0.3	-0.40000	-0.40000	-0.10000	-0.10000	-0.03589	0.83589	-0.60000	0.80000
0.4	-0.45000	-0.45000	-0.05000	-0.05000	-0.00826	0.90825 8	-0.73106	0.83103
0.5	-0.50000	-0.50000	0.00000	0.00000	0.00000	1.00000	-0.86603	0.86603
0.6	-0.55000	-0.55000	0.05000	0.05000	-0.00678	1.10678	-1.00374	0.90394
0.7	-0.60000	-0.60000	0.10000	0.10000	-0.02500	1.22450	-1.14403	0.94403
0.8	-0.65000	-0.65000	0.15000	0.15000	-0.05000	1.35000	-1.28578	0.98578
1.0	-0.75000	-0.75000	0.25000	0.25000	-0.11603	1.61603	-1.57288	1.07288

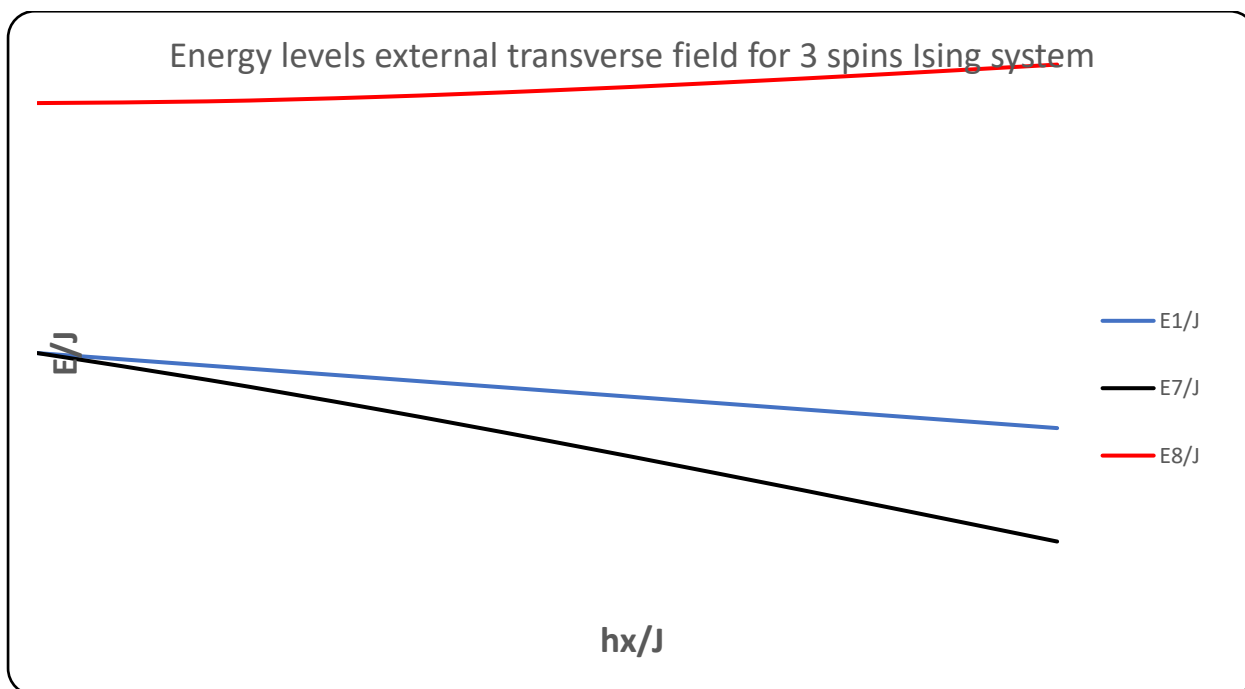


Figure 4: Spontaneous quantum phase transition from E_1 to E_7

FRUSTRATED HEISENBERG THREE-SITE TRIANGULAR GEOMETRY AT ZERO FIELD

Exact diagonalization of the three-site triangular geometry using the Heisenberg model gives four-fold degenerate ground states with energy $-3J/4$ and four-fold degeneracy in the excited state, with energy $3J/4$ which is due to the presence of a frustrated spin in the three-site frustrated triangle. Despite the presence of quantum fluctuations in the Heisenberg model, it is surprising to observe that multiple degeneracies still persist in both the ground and excited states.

FRUSTRATED HEISENBERG THREE-SITE TRIANGULAR GEOMETRY AT FINITE LONGITUDINAL FIELD AND THE EMERGENCE OF QPT

In the presence of a finite longitudinal field, the four-fold degenerate ground state at zero field splits into two-fold degenerate states with energy $1/4(-2h_z - 3J)$ and two-fold excited degenerate states with energy $1/4(2h_z - 3J)$ as shown in Table 4. This implies that the longitudinal field could not effectively remove all the degeneracies caused by frustration. These degenerate states begin to compete with other states for the ground state of the system as h_z is varied. At critical field of $h_{zc} = 3J/2$ as shown in Table 5, the system is observed to quantum transit from a quasi-antiferromagnetic state to ferromagnetic state. Hence, the competing states $1/\sqrt{2}[|011\rangle - |110\rangle]$ and $1/\sqrt{2}[|101\rangle - |110\rangle]$ with energy $1/4(-2h_z - 3J)$ loses the ground state



to $|111\rangle$ with energy $1/4(-6h_z + 3J)$. Hence, there is a cross over from $S_{tot}^z = 1/2$ to $S_{tot}^z = 3/2$. This indicates that the triangular geometry protects the zero-field $S_{tot}^z = 1/2$ ground state more efficiently.

Table 4: Eigenvalues and eigenvectors of the 3-site triangular Heisenberg system at zero and finite longitudinal fields

Eigenvectors at $h \neq 0$	Eigenvalues at $h=0$	Eigenvalues at $h \neq 0$	S_{tot}^z
$\frac{1}{\sqrt{2}}[011\rangle - 110\rangle]$	-3J/4	$\frac{1}{4}(-2h - 3J)$	1/2
$\frac{1}{\sqrt{2}}[101\rangle - 110\rangle]$	-3J/4	$\frac{1}{4}(-2h - 3J)$	1/2
$\frac{1}{\sqrt{2}}[100\rangle - 010\rangle]$	-3J/4	$\frac{1}{4}(2h - 3J)$	-1/2
$\frac{1}{\sqrt{2}}[001\rangle - 010\rangle]$	-3J/4	$\frac{1}{4}(2h - 3J)$	-1/2
$ 111\rangle$	3J/4	$\frac{1}{4}(-6h + 3J)$	3/2
$ 000\rangle$	3J/4	$\frac{1}{4}(6h + 3J)$	-3/2
$\frac{1}{\sqrt{3}}[110\rangle + 101\rangle + 011\rangle]$	3J/4	$\frac{1}{4}(-2h + 3J)$	1/2
$\frac{1}{\sqrt{3}}[010\rangle + 001\rangle + 100\rangle]$	3J/4	$\frac{1}{4}(2h + 3J)$	-1/2

Table 5: Investigation of quantum Phase transition in the 3-site triangular Heisenberg system in the presence of a longitudinal field

h_x/J	E_1/J	E_2/J	E_3/J	E_4/J	E_5/J	E_6/J	E_7/J	E_8/J
0.0	-0.750	-0.750	-0.750	-0.750	0.7500	0.750	0.750	0.750
0.1	-0.800	-0.800	-0.700	-0.700	0.600	0.900	0.700	0.800
0.5	-1.000	-1.000	-0.500	-0.500	0.000	1.500	0.500	1.000
1.5	-1.500	-1.500	0.000	0.000	-1.500	3.000	0.000	1.500
2.0	-1.750	-1.750	0.250	0.250	-2.250	3.750	-0.250	1.750
2.5	-2.000	-2.000	0.500	0.500	-3.000	4.500	-0.500	2.000
3.0	-2.250	-2.250	0.750	0.750	-3.750	5.250	-0.750	2.250
3.5	-2.500	-2.500	1.000	1.000	-4.500	6.000	-1.000	2.500
4	-2.750	-2.750	1.250	1.250	-5.250	6.75	-1.250	-1.250



FRUSTRATED HEISENBERG THREE-SITE TRIANGULAR GEOMETRY AT FINITE TRANSVERSE FIELD AND THE EMERGENCE OF QPT

In the presence of a finite transverse field, the four-fold degenerate ground state at zero field splits into two-fold degenerate states with energy $1/4(-2h_x - 3J)$ and two-fold excited degenerate states with energy $1/4(2h_x - 3J)$ as shown from the exact diagonalization result. This implies that the transverse field could not effectively remove all the degeneracies caused by frustration. These degenerate states begin to compete with other states for the ground state of the system as h_z is varied. However, as shown in Table 6 below, no visible phase transition occurred as h_x/J is varied across the energy spectrum. The two-fold degenerate states that survive the fluctuating transverse field finally emerge as the two-fold degenerate ground states with energy $1/4(-2h_x - 3J)$. These states are given by the following equation

$$\psi_{g1} = \frac{1}{2} [|101\rangle - |011\rangle - |010\rangle + |100\rangle]$$

$$\psi_{g2} = \frac{1}{2} [|101\rangle - |110\rangle - |010\rangle + |001\rangle]$$

The ground states are linear combination of states from $S_{tot}^z = 1/2$ and $S_{tot}^z = -1/2$. This indicates that the triangular geometry could not protect the zero-field $S_{tot}^z = 1/2$ or $S_{tot}^z = -1/2$ ground states efficiently.

Table 6: Investigation of quantum Phase transition in the three-site triangular Heisenberg system in the presence of a transverse field

h_x/J	E_1/J	E_2/J	E_3/J	E_4/J	E_5/J	E_6/J	E_7/J	E_8/J
0.0	-0.750	-0.750	-0.750	-0.750	0.7500	0.750	0.750	0.750
0.1	-0.800	-0.800	-0.700	-0.700	-0.600	0.900	0.700	0.800
0.5	-1.000	-1.000	-0.500	-0.500	0.000	1.500	0.500	1.000
1.5	-1.500	-1.500	0.000	0.000	1.500	3.000	0.000	1.500
2.0	-1.750	-1.750	0.250	0.250	2.250	3.750	-0.250	1.750
2.5	-2.000	-2.000	0.500	0.500	3.000	4.500	-0.500	2.000
3.0	-2.250	-2.250	0.750	0.750	3.750	5.250	-0.750	2.250
3.5	-2.500	-2.500	1.000	1.000	4.500	6.000	-1.000	2.500
4.0	-2.750	-2.750	1.250	1.250	5.250	6.750	-1.250	2.75
4.5	-3.000	-3.000	1.500	1.500	6.000	7.500	-1.500	3.000



SUMMARY, FINDINGS AND CONCLUSION

SUMMARY

In this work, frustration arising from geometry of a system has been studied. The study reveals that geometrical frustration can generate multiple degeneracies in the ground state energy. These degeneracies are a consequence of the inability of the spins in a triangular geometry system to anti-align with their nearest neighbors. Hence, the system finds it difficult to have a perfect antiferromagnetic ordering that will minimize its energy.

These multiple degeneracies are more pronounced in the Ising model than the Heisenberg model. This is because of the presence of the quantum spin fluctuations in the Heisenberg model which are not present in the Ising model. For example, for the case of the three-site system studied in this work, a six-fold degeneracy in the ground state energy is observed for the Ising model, whereas it is four-degenerate for the Heisenberg model. However, this quantum spin fluctuation present in the Heisenberg model is not able to remove all degeneracies arising from geometrical frustration in the ground state.

FINDINGS

The following findings are made from this research work:

- a) The eight-fold degenerate ground state observed at zero field for three Ising spins is partially broken down to three-fold and two-fold degenerate states in the presence of longitudinal and transverse fields respectively.
- b) The four-fold degenerate ground state observed at zero field for three Heisenberg spins is partially broken down to two-fold degenerate state in the presence of both longitudinal and transverse fields.
- c) Quantum phase transition from quasi antiferromagnetic to ferromagnetic state is observed at a critical longitudinal field of $h_{zc} = J$ and $h_{zc} = J$ for Ising systems of three site spins.
- d) Quantum phase transition from quasi antiferromagnetic to ferromagnetic state is observed at a critical longitudinal field of $h_{zc} = 3J/2$ and $h_{zc} = 5J/2$ for Heisenberg of three site spin.
- e) A sharp and spontaneous quantum phase transition from quasi-antiferromagnet to ferromagnetic is observed at infinitesimal field for the Ising three spin systems.
- f) Quantum phase transition from quasi antiferromagnetic to ferromagnetic state for Ising three spins is observed at a critical longitudinal field of $h_{zc} = J$.
- g) In the presence of varying transverse fields, the two degenerate states for the three Heisenberg spins emerge as the ground states, hence no QPT occurs.



CONTRIBUTION TO KNOWLEDGE

This research contributed to knowledge in the following areas:

- a) This study has been able to establish a firm correlation between multiple degeneracies in the ground state and system topology or geometry.
- b) This study has shown that multiple degeneracies in ground state of any system can be partially lifted by quantum spin fluctuations present in the Heisenberg model.
- c) This study has also shown that the exact diagonalization method is able to reproduce the dominant result obtained by theoretical and experimental methods.
- d) This current work has been able to show in a very robust way that quantum phase transition is enhanced by frustration.

RECOMMENDATION AND CONCLUSION

The introductory field into the system has shown us how degenerate ground states split, the presence of competing states, crossing over of energies level from one point to another, system transit from quasi-antiferromagnet to ferromagnet, tables shows how quantum phase transition is observed. Further research can be done to determine how fields can induce ising and Heisenberg six and seven site geometry. This work is recommended for researchers who are currently working in this area.

REFERENCES

- Aharoni, Amikam (2000). *Introduction to the theory of ferromagnetism (2nd Ed.)*. Oxford: Oxford University Press. [ISBN 9780198508090](https://doi.org/10.1017/CBO9780511528090)
- Aminov, T.G., Shabunina, G.G. and Novotortsev, V.M.. (2014): Spin glasses in CdCr₂S₄-ZnCr₂S₄ solid solutions Russ. J. Inorg. Chem. Vol.59, pp647-657.
- Anderson, P. W. (1973): *Resonating valence bonds: A new kind of insulator?*. *Mater. Res. Bull.* **8** (2): 153–160.
- Anderson P.W. (1987). The resonating valence bond state in La²CuO⁴ and superconductivity. *Science*, 235, pp1196-1198.
- Anderson, P. W. (1990). *Spin Glass VII: Spin Glass as Paradigm*. *Physics Today*. 43(3):9
- Balakirev F. F., Betts J. B., Migliori A., Tsukada I., Ando Y., and Boebinger G. S.(2009). Quantum Phase Transition in the Magnetic-Field-Induced Normal State of Optimum-Doped High-*T_c* Cuprate Superconductors at Low Temperatures. *Phys. Rev. Lett.* 102, pp017004-017007.
- Berciu M. (2009). Challenging a hole to move through an ordered insulator. *Physics* 2, 55, pp.1-3.
- Bode M., Vedmedenko E. Y., von Bergmann K., Kubetzka A., Ferriani P., Heinze S. and Wiesendanger R. (2006). Atomic spin structure of antiferromagnetic domain walls. *Nature Materials*. 5, pp477 – 481.
- Bramwell, S. T. and Gingras, M.J. P. (2001): Spin Ice State in Frustrated Magnetic Pyrochlore *Materials Science* Vol. 294, Issue 5546, pp. 1495-1501



- Burnell F. J. and Sondhi S. L. (2009). *Monopole flux state on the pyrochlore lattice* *Phys.Rev. B* 79, 144432
- Chandra, P., Doucot, B. (1988): Possible spin-liquid state at large S for the frustrated square Heisenberg lattice. *Phys. Rev. B* 38, 9335.
- Chandra, P., Lonzarich, G.G., Rowley, S.E., and Scott, J.F. (2017). Prospects and applications near ferroelectric quantum phase transitions. *Reports on Progress in Physics*, 80, 112502. DOI:[10.1088/1361-6633/aa82d2](https://doi.org/10.1088/1361-6633/aa82d2)
- Chubukov, A. V. and Jolicoeur, T.H. (1992): Order-from-disorder phenomena in Heisenberg antiferromagnets on a triangular lattice. *Phys. Rev. B* 46, 11137
- Coldea,R.,Tennant,D. A, Habicht,K., Smeibidl,P., Wolters,C., and Tylczynski,Z., (2002): Direct Measurement of the Spin Hamiltonian and Observation of Condensation of Magnons in the 2D Frustrated Quantum Magnet Cs₂CuCl₄. *Phys. Rev. Lett.* 88, 137203
- Coldea,R.,Tennant, D.A., Wheeler, E.M., Wawrzynska, E., Prabhakaran, D., Telling M., Habicht, K., Smeibidl, P. and Kiefer, K.(2010): Quantum criticality in an Ising chain: Experimental evidence for the emergent E₈ symmetry. *Science*, 327, 177- 180.
- Coleman P. and Schofield A. J. (2005). Quantum criticality. *Nature* vol. 433, 226-229.
- Cullity, B.D., & Graham, C.D. (2011). "Ferrimagnetism". *Introduction to Magnetic Materials*. John Wiley & Sons. [ISBN 9781118211496](https://doi.org/10.1002/9781118211496).
- Dagotto E., Moreo A., Alcaraz F. C. and Gagliano E. R. (1986). Correlation functions of the antiferromagnetic Heisenberg model using a modified Lanczos method. *Phys. Rev. B* 34, pp1677-1682.
- Dagotto E., Moreo A., Joynt R., Bacci S., and Gagliano E. (1990). Dynamics of one hole in the $t - J$ model. *Phys. Rev. B* 41, pp2585-2588.
- Diep, H. T. (2016): Theoretical methods for understanding advanced magnetic materials: the case of frustrated thin films. *Journal of Science: Advanced Materials and Devices (JSAMD) Vol1 (1)*, 31-44
- Drechsler, S.-L., Tristan, N., Klingeler, R., Büchner, B., Richter, J., Málek, J., Volkova O., Vasiliev, A., Schmitt, M., Ormeci, A., Loison, C., Schnelle, W., and Rosner, H. (2007): Helimagnetism and weak ferromagnetism in NaCu₂O₂ and related frustrated chain cuprates. *J. Phys.: Condens. Matter* 19, 145230
- Duo, Lamberto, Marco Finazzi, Franco Ciccacci. (2010). *Magnetic Properties of Antiferromagnetic Oxide Materials*. KGA, Weinheim: Wiley-VCH Verlag GmbH & Co.
- Ehika S., Ataman O. J. and Idioidi J.O.A. (2012). Symmetry Considerations in the Exact Diagonalization of Heisenberg Spin Chains. *Journal of NAMP Vol. 22*, pp 9-20.
- Ehika, S., Ataman, O. J., Iyayi S.E. (2017). Quantum and Thermal Fluctuations in the Ising Chains: A Case Study of Spin-Two System. *IOSR-JAP Vol. 9*, pp. 32-42.
- Ehika S., Idioidi, J.O.A. (2012): Quantum Phase Transition in the Heisenberg Model: A Case Study of a Two-Spin System. *Journal of NAMP Vol. 21*, pp 11-20.
- Ehika S. and Idioidi J.O.A. (2012). The Dynamics of a Hole in Two Dimensional Mott Insulators. *Journal of NAMP Vol. 21*, pp 1-10.
- Ehika S. and Idioidi J.O.A. (2015). Single Hole Dynamics in One Dimensional Quantum Antiferromagnet. *Trans. of NAMP Vol. 1*, pp 21-32.
- Ehika S., Iyoha, A. and Okanigbuan, O.R. (2009): The Magnetic Behaviour of an Isolated Paramagnetic Spin-1 and Spin-1/2 Degree of Freedom.



- Greedan, J. E., Sato, M., Yan Xu, Razavi, F. S (1986): Spin-glass-like behavior in $Y_2Mo_2O_7$, a concentrated, crystalline system with negligible apparent disorder. *Solid State Commun.* Vol.59, pp 895-897.
- Han, Y., Shokef, Y., Alsayed, A. M., Yunker, P., Lubensky, T. C. and Yodh, A. G. (2008): Geometric frustration in buckled colloidal monolayers. *Nature* vol.456, pp 898–903
- Haijiao Ji, Haiwen Liu, Hua Jiang and Xie, X.C. (2021): Disorder effects on quantum transport and quantum phase transition in low-dimensional superconduction and topological systems; vol. 6, No. 1, 1884133
- Harris, M., & Zinkin, M. P. (1996). Frustration in the pyrochlore antiferromagnets. *Modern Physics Letters B*, (10), 417-438.
- Houtappel, R. M. F. (1950) Order-disorder in hexagonal lattices.
- Huse, D. A. and Rutenberg, A. D. (1992): Classical antiferromagnets on the Kagomé lattice *Phys. Rev. B* 45, 7536.
- Jolicoeur, Th., Dagotto, E., Gagliano, E., and Bacci, S. (1990): Ground-state properties of the $S=1/2$ Heisenberg antiferromagnet on a triangular lattice. *Phys. Rev. B* 42, 4800(R)
- Kandpal, H. C., Opahle, I., Zhang, Y.-Z., Jeschke, H. O., and Valenti, R. (2009): Revision of Model Parameters for κ -Type Charge Transfer Salts: An *Ab Initio* Study *Phys. Rev. Lett.* 103, 06700.
- Kawamura, H. and Taniguchi, T. (2015): Chapter 1 - Spin Glasses. *Handbook of Magnetic Materials*, Volume 24, pp 1-137
- Keren A., Mendels P., Horvatic M., Ferrer F., Uemura Y. J. (1998): $^{69,71}\text{Ga}$ NMR in the kagomé lattice compound $\text{SrCr}_{9-x}\text{Ga}_{3+x}\text{O}_{19}$ *Phys. Rev. B* 57, 10745.
- Lecheminant P., Bernu, B., Lhuillier, C., and Pierre, L. (1995): J_1 - J_2 quantum Heisenberg antiferromagnet on the triangular lattice: A group-symmetry analysis of order by disorder *Phys. Rev. B* 52, 6647.
- Luo, Nannan and Xiaolong Zou. (2021). Two-dimensional magnetic materials: structures, properties and external controls. *Nanoscale*. 2021 Jan 28; 13(3):1398-1424 Doi: 10.1039/d0nr06813f.
- Mengxing, Y. and Andrey, V. C. (2017): Quantum phase transitions in the Heisenberg J_1 - J_2 triangular antiferromagnet in a magnetic field. *Phys. Rev. B* 95, 014425
- Moessner, R. and Ramirez, A. P. (2006): Geometrical frustration, *Physics Today* 59, 2, 24
- Munoz, C., Gaeta, M., Gomez, R., and Klimov, A.B. (2019). Picturing quantum phase transitions. *Physics Letters A*, Volume 383, Issues 2–3, Pages 141-147
- Nath, R., Tsirlin, A. A., Kaul, E. E., Baenitz, M., Büttgen, N., Geibel, C., and Rosner, H. (2008): Strong frustration due to competing ferromagnetic and antiferromagnetic interactions: Magnetic properties of $M(\text{VO})_2(\text{PO}_4)_2$ ($M=\text{Ca}$ and Sr). *PHY. REV. B* 78, 024418