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INVESTIGATION OF FRUSTRATION DUE TO COMPETING INTERACTIONS ON A FOUR-SITE SQUARE LATTICE

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Abstract

In this current research work, the effects of frustration arising from competing interactions have been investigated on four-site square lattice within the Ising and Heisenberg models. For the Ising model, the effects of frustration are evident from the multi degeneracies that characterize the ground state. The nondegenerate ground state for the Heisenberg system may be attributed to the presence of quantum spin flip terms in the model. For both models investigated, the presence of frustration gives birth to two competing ground states within the subspace of $S^z_{tot} = 0$***. The competition between the antiferromagnetic and ferromagnetic coupling constants,*** J_1 ***and*** J_2 ***respectively determines the nature of the ground state. For the Ising system, two-fold degenerate pure antiferromagnetic state characterizes the ground state in the regime*** $J_1 / J_2 > 1$***. A cross over from the two-fold degenerate pure antiferromagnetic ground state to four-fold degenerate quasi-antiferromagnetic ground state occurs at the critical point of*** $J_1 / J_2 = 1$***. This is the point at which the degeneracies of the ground state reach its maximum value of six. Beyond this critical point, the ground state is entirely driven by*** J_2 ***and is four-fold degenerate. At this critical point, the ground state of the frustrated Heisenberg system crosses over from a more antiferromagnetic to a less antiferromagnetic state. Beyond this critical point, the ground state is entirely driven by*** J_2***.There is no evidence of phase transition since the cross overs that are observed in this work for both models occur within the subspace of*** $S^z_{tot} = 0$***.***

1. INRTODUCTION

Literally, frustration is the emotional states that occurs when wants, needs, and desire are not readily available or attainable. According to Merriam Webster dictionary, frustration can be defined as a deep chronic sense or state of insecurity and dissatisfaction arising from unresolved problems or unfulfilled needs [1]. The word frustration has been derived from Latin word "*frusta"* meaning to obstruct. Indeed, it is referred to as the blocking behaviour directed toward a goal [2,3]. This is noticed in both living thing and non-living things. There are three important source of frustration which are environmental force, personal inadequacies, and frustration arising from conflict [4,5]. Frustration is not only seen in the human world but also in some areas of Physics. One of the areas where frustration is observed is in the field of quantum magnet, which is the main focus of this research work.

Generally, in Physics, frustration refers to a situation where the contributions to the potential energy of a many body systems cannot be simultaneously minimized. *Magnetic* systems are said to be *frustrated* if a spin cannot arrange its orientation such that it profits from the interaction with its neighbours [6]. Since the degrees of freedom of a spin is two and can't configure itself to fully satisfy all the pairwise interactions with its neighbours, the spin is said to be in a state of frustration. But why can't the possible spin alignments put the system in her minimal energy level? The reasons for this behaviour are due to system geometries and the present of competing interactions.In contrast, unfrustrated system is a situation where all pairwise interactions in a spin lattice are simultaneously satisfied [7]. In other words, the Neel antiferromagnetic spin arrangement in which all nearest neighbour pairs are anti-parallelis a property of unfrustrated system. This behaviour as shown in Fig. 1a is mostly observed in bipartite lattices.

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Geometric frustration arises when lattice structure precludes simultaneous minimization of local interaction energies [8,9]. Geometric frustration in magnetism is best understood in the context of the nearest neighbour Ising antiferromagnetic on a triangular lattice as shown in Fig. 1b. Frustration can also arise as a result of competition between two coupling parameters in a lattice. Frustration of this type can be studied in models with competing nearest neighbour and further neighbour interactions, notably the J_1 -J_2 model on the square lattice [10]. This type of frustration is captured in Fig. 1c.
This current paper will focus on frustration arising from competing interaction. An important advantage of this type of frustrated systems is the possibility of varying the degree of frustration by tuning individual exchange couplings. It thus gives rise to the formation of different ground states within one model and the access to quantum critical points are possible [11]. While models of this kind provide an attractive starting point for theoretical work, there are likely to be difficulties in finding experimental realisations with interaction strengths that place them close to the degeneracy point. A simple four-site system is used in this work to elucidate and project out the inherent properties of frustrated system in the special case of competing interactions. To the best of our knowledge, this kind of elaborate, simplified and detailed treatment of frustration arising from competing interaction has not being carried out. The rest of the paper is organised as follows: Section 2 introduces the Heisenberg and the Ising models; while the Hilbert space and the geometry of the four-site square latticeare presented in section 3; the interactions of the spin on the Ising and Heisenberg models are presented in sections 4 and 5 respectively. Results and discussions are presented in section 6; while conclusion is done in section 7.

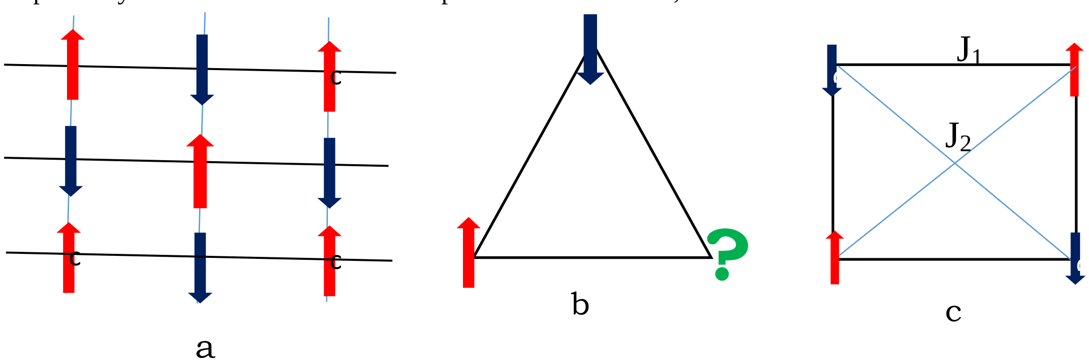

Fig. 1.(a) For the unfrustrated antiferromagnet on the square lattice, each spin can be anti-aligned with all its neighbors. **(b)** On a triangular lattice, such a configuration is impossible: Three neighboring spins cannot be pairwise anti-aligned, and the system is frustrated. **(c)** frustrated four-site 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 neighbour interactions (NNN). The system is frustrated because there is no possible orientation of the spins coupled by J_2 that will anti-align them.

2. THE ISOTROPIC HEISENBERG SPIN AND ISING HAMILTONIANS

The Heisenberg Hamiltonian is a quantum mechanical analogue of the Ising model that describes the pairwise interactions between localized spins.This model is a variant of the Hubbard model at half filling and large onsite Coulomb repulsion U, which enforces the constraint of singly occupied site.The ground state properties of this model has been investigated by several authors [12,13].In particular, Ehika and Idiodi has investigated the effect of finite external fields on the unfrustrated Heisenberg spinsystem[14]. In spite of its simple mathematical form, it has an unimaginable richness, arising from dimensionality and geometrical constraints, competing exchange interaction, the type of spin degrees of freedom, and additional interactions with external magnetic fields or other degrees of freedom such as phonons [13,14]. This model simply reads

$$H = J\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j \qquad (1)$$

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

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

Hence, we have

$$H = \sum_{\langle i,j\rangle} S_i^x S_j^x + S_i^y S_j^y + S_i^z S_i^z \qquad (3)$$

In second quantized form, the spin operators takes the form

$$\left.\begin{aligned} S_i^x &= \frac{1}{2}\left(c_{i\uparrow}^{\dagger}c_{i\downarrow} + c_{i\downarrow}^{\dagger}c_{i\uparrow}\right) \\ S_i^y &= -\frac{i}{2}\left(c_{i\uparrow}^{\dagger}c_{i\downarrow} - c_{i\downarrow}^{\dagger}c_{i\uparrow}\right) \\ S_i^z &= \frac{1}{2}\left(c_{i\uparrow}^{\dagger}c_{i\uparrow} - c_{i\downarrow}^{\dagger}c_{i\downarrow}\right) \end{aligned}\right\} \quad (4)$$

Also, the electron density operator n_i at site i is given by

$$n_i = \sum_{\sigma} n_{i\sigma}\ , \quad (5)$$

where

$$n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma} \quad (6)$$

Hence, in the second quantized form, the Heisenberg Hamiltonian written in terms of annihilation (c_i) and creation operator $(c_i^{\dagger})$ takes the form

$$H = \frac{J}{4}\sum_{\langle i,j\rangle}\left(c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{j\uparrow}^{\dagger}c_{j\uparrow} - c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{j\downarrow}^{\dagger}c_{j\downarrow} - c_{i\downarrow}^{\dagger}c_{i\downarrow}c_{j\uparrow}^{\dagger}c_{j\uparrow} + c_{i\downarrow}^{\dagger}c_{i\downarrow}c_{j\downarrow}^{\dagger}c_{j\downarrow}\right), \quad (7)$$

$$+ \frac{J}{2}\sum_{\langle i,j\rangle}\left(c_{i\uparrow}^{\dagger}c_{i\downarrow}c_{j\downarrow}^{\dagger}c_{j\uparrow} + c_{i\downarrow}^{\dagger}c_{i\uparrow}c_{j\uparrow}^{\dagger}c_{j\downarrow}\right)$$

Introducing the spin raising (lowering) $S_i^{+}\,(S_i^{-})$ operators which effectively flip the spin of the electron residing on ith site, (7) can concisely be written as

$$H = J\sum_{\langle i.j\rangle}\left[S_i^z S_j^z + \frac{1}{2}\left(S_i^{+}S_j^{-} + S_i^{-}S_j^{+}\right)\right] \quad (8)$$

These operators given by

$$\left.\begin{aligned} S_i^{+} &= c_{i\uparrow}^{\dagger}c_{i\downarrow} \\ S_i^{-} &= c_{i\downarrow}^{\dagger}c_{i\uparrow} \end{aligned}\right\} \quad (9)$$

has the following properties:

$$S^{+}\left|\downarrow\right\rangle = \left|\uparrow\right\rangle, S^{-}\left|\uparrow\right\rangle = \left|\downarrow\right\rangle, S^{+}\left|\uparrow\right\rangle = 0, S^{-}\left|\downarrow\right\rangle = 0 \quad (10)$$

The Ising model is obtained by switching off the spin fluctuation term in the Heisenberg model (i.e $S_i^{+}S_j^{-} + S_i^{-}S_j^{+} = 0$). Under this consideration, the Hamiltonian in (8) becomes

$$H_I = J\sum_{\langle i,j\rangle} S_i^z S_j^z \quad (11)$$

This Ising model, though simple looking, has been used to study both quantum and thermal phase transitions in various magnetic systems [15, 16].

3. THE HILBERT SPACE AND GEOMETRY OF FRUSTRATED FOUR-SITE SQUARE LATTICE

The geometry of the four sites square lattice system with competing interaction is shown in Fig.2

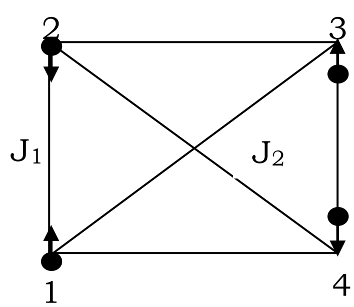

Fig 2. A frustrated four-site system with competing interactions J_1 and J_2. J_1 is coupling strength for nearest neighbour interactions (NN), while J_2 is the coupling strength for next nearest neighbour interactions (NNN).

The Hilbert space is not altered by the geometry of the system. The system is frustrated because there is no possible arrangement of the spins that will anti-aligned the spins coupled with J_2.The electronic states (basis states) arising from the Hilbert space of 2^N, where N is the number of sites are listed below according to the subspaces of S^z_{tot} .

Subspace of S^z_{tot}=0

$|1\rangle = |1100\rangle,\ |2\rangle = |0110\rangle,\ |3\rangle = |0011\rangle,\ |4\rangle = |1001\rangle,\ |5\rangle = |1010\rangle,\ |6\rangle = |0101\rangle$

Subspace of S^z_{tot}=1

$|1\rangle = |1110\rangle,\ |2\rangle = |0111\rangle,\ |3\rangle = |1011\rangle,\ |4\rangle = |1101\rangle$

Subspace of S^z_{tot}=-1

$|1\rangle = |0001\rangle,\ |2\rangle = |1000\rangle, |3\rangle = |0100\rangle,\ |4\rangle = |0010\rangle$

Subspace of S^z_{tot}=2

$|1\rangle = |1111\rangle,$

Subspace of S^z_{tot}= -2

$|1\rangle = |0000\rangle$

Here, the qubit or binary representation is used for the Ising states. In this representation, 1 denotes an up spin (↑), while 0 denotes a down spin (↓). This representation offers the advantage of easy manipulation of spins of electrons.

4 FRUSTRATED SPIN INTERACTION ON THE ISING MODEL

The Ising model for this system is given by

$$H_I = J_1\left(S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z + S_4^z S_1^z\right) + J_2\left(S_1^z S_3^z + S_2^z S_4^z\right) \qquad (12)$$

The actions of (12) on the basis states within the various subspaces of S^z_{tot} are given below

Subspace of S^z_{tot}=0

$$H_I|1\rangle = H_I|1100\rangle = \frac{J_1}{4}|1\rangle - \frac{J_1}{4}|1\rangle + \frac{J_1}{4}|1\rangle - \frac{J_1}{4}|1\rangle - \frac{J_2}{4}|1\rangle - \frac{J_2}{4}|1\rangle = -\frac{J_2}{2}|1\rangle$$

$$H_I|2\rangle = H_I|0110\rangle = -\frac{J_1}{4}|2\rangle + \frac{J_1}{4}|2\rangle - \frac{J_1}{4}|2\rangle + \frac{J_1}{4}|2\rangle - \frac{J_2}{4}|2\rangle - \frac{J_2}{4}|2\rangle = -\frac{J_2}{2}|2\rangle$$

$$H_I|3\rangle = H_I|0011\rangle = \frac{J_1}{4}|3\rangle - \frac{J_1}{4}|3\rangle + \frac{J_1}{4}|3\rangle - \frac{J_1}{4}|3\rangle - \frac{J_2}{4}|3\rangle - \frac{J_2}{4}|3\rangle = -\frac{J_2}{2}|3\rangle$$

$$H_I|4\rangle = H_I|1001\rangle = -\frac{J_1}{4}|4\rangle + \frac{J_1}{4}|4\rangle - \frac{J_1}{4}|4\rangle + \frac{J_1}{4}|4\rangle - \frac{J_2}{4}|4\rangle - \frac{J_2}{4}|4\rangle = -\frac{J_2}{2}|4\rangle$$

$$H_I|5\rangle = H_I|1010\rangle = -\frac{J_1}{4}|5\rangle - \frac{J_1}{4}|5\rangle - \frac{J_1}{4}|5\rangle - \frac{J_1}{4}|5\rangle + \frac{J_2}{4}|5\rangle + \frac{J_2}{4}|5\rangle = -J_1|5\rangle + \frac{J_2}{2}|5\rangle$$

$$H_I|6\rangle = H_I|0101\rangle = -\frac{J_1}{4}|6\rangle - \frac{J_2}{4}|6\rangle - \frac{J_1}{4}|6\rangle - \frac{J_1}{4}|6\rangle + \frac{J_2}{4}|6\rangle + \frac{J_2}{4}|6\rangle = -J_1|6\rangle + \frac{J_2}{2}|6\rangle$$

Subspace of S^z_{tot}=1

$$H_I|1\rangle = H_I|1110\rangle = \frac{J_1}{4}|1\rangle + \frac{J_1}{4}|1\rangle - \frac{J_1}{4}|1\rangle - \frac{J_1}{4}|1\rangle + \frac{J_2}{4}|1\rangle - \frac{J_2}{4}|1\rangle = 0$$

$$H_I|2\rangle = H_I|0111\rangle = -\frac{J_1}{4}|2\rangle + \frac{J_1}{4}|2\rangle + \frac{J_1}{4}|2\rangle - \frac{J_1}{4}|2\rangle - \frac{J_2}{4}|2\rangle + \frac{J_2}{4}|2\rangle = 0$$

$$H_I|3\rangle = H_I|1011\rangle = -\frac{J_1}{4}|3\rangle - \frac{J_1}{4}|3\rangle + \frac{J_1}{4}|3\rangle + \frac{J_1}{4}|3\rangle + \frac{J_2}{4}|3\rangle - \frac{J_2}{4}|3\rangle = 0$$

$$H_I|4\rangle = H_I|1101\rangle = \frac{J_1}{4}|4\rangle - \frac{J_1}{4}|4\rangle + \frac{J_1}{4}|4\rangle + \frac{J_1}{4}|4\rangle - \frac{J_2}{4}|4\rangle + \frac{J_2}{4}|4\rangle = 0$$

Subspace of S^z_{tot}=-1

$$H_I|1\rangle = H_I|0001\rangle = \frac{J_1}{4}|1\rangle + \frac{J_1}{4}|1\rangle - \frac{J_1}{4}|1\rangle - \frac{J_1}{4}|1\rangle + \frac{J_2}{4}|1\rangle - \frac{J_2}{4}|1\rangle = 0$$

$$H_I|2\rangle = H_I|1000\rangle = -\frac{J_1}{4}|2\rangle + \frac{J_1}{4}|2\rangle + \frac{J_1}{4}|2\rangle - \frac{J_1}{4}|2\rangle - \frac{J_2}{4}|2\rangle + \frac{J_2}{4}|2\rangle = 0$$

$$H_I|3\rangle = H_I|0100\rangle = -\frac{J_1}{4}|3\rangle - \frac{J_1}{4}|3\rangle + \frac{J_1}{4}|3\rangle + \frac{J_1}{4}|3\rangle - \frac{J_2}{4}|3\rangle + \frac{J_2}{4}|3\rangle = 0$$

$$H_I|4\rangle = H_I|0010\rangle = \frac{J_1}{4}|4\rangle - \frac{J_2}{4}|4\rangle - \frac{J_1}{4}|4\rangle + \frac{J_1}{4}|4\rangle - \frac{J_2}{4}|4\rangle + \frac{J_2}{4}|4\rangle = 0$$

Subspace of S^z_{tot}=2

$$H_I|1111\rangle = \frac{J_1}{4}|1111\rangle + \frac{J_2}{4}|1111\rangle + \frac{J_1}{4}|1111\rangle + \frac{J_1}{4}|1111\rangle + \frac{J_2}{4}|1111\rangle$$
$$+\frac{J_2}{2}|1111\rangle = \left(J_1 + \frac{J_2}{2}\right)|1111\rangle$$

Subspace of S^z_{tot}=-2

$$H_I|0000\rangle = \frac{J_1}{4}|0000\rangle + \frac{J_2}{4}|0000\rangle + \frac{J_1}{4}|0000\rangle + \frac{J_1}{4}|0000\rangle + \frac{J_2}{4}|0000\rangle$$
$$+\frac{J_2}{2}|0000\rangle = \left(J_1 + \frac{J_2}{2}\right)|0000\rangle$$

Hence, the eigenvalues are:

$$E_1 = \frac{-J_2}{2},\ E_2 = \frac{-J_2}{2},\ E_3 = \frac{-J_2}{2},\ E_4 = \frac{-J_2}{2},\ E_5 = -J_1 + \frac{J_2}{2},\ E_6 = -J_1 + \frac{J_2}{2}$$
$$E_7 = J_1 + \frac{J_2}{2}, E_8 = J_1 + \frac{J_2}{2},\ E_8 = 0,\ E_{10} = 0,\ E_{11} = 0,\ E_{12} = 0,\ E_{13} = 0,\ E_{14} = 0$$
$$E_{15} = 0,\ E_{16} = 0$$

Hence, the presence of frustration gives to two unique competing states within the subspace of S^z_{tot}= 0, namely one of the four quasi-antiferromagnetic states (e.g. $|\psi_\alpha\rangle = |1100\rangle$) with energy $E_\alpha = \frac{-J_2}{2}$, and one of the two pure antiferromagnetic states (e.g. $|\psi_\beta\rangle = |1010\rangle$) with energy $E_\beta = -J_1 + \frac{J_2}{2}$). The effect of variation of J_2 (frustration) on the ground state property of the Ising system will be discussed in section 6.

5. FRUSTRATION IN THE PRESENCE OF QUANTUM FLUCTUATIONS.

In this section, the effect of quantum spin fluctuation is investigated. To achieve this, the isotropic Heisenberg antiferromagnetic modelis employed since it contains the quantum spin flip terms. The Heisenberg model for the frustrated four-site system is expanded to given

$$\begin{aligned} H &= J_1\left(S_1^zS_2^z + S_2^zS_3^z + S_3^zS_4^z + S_4^zS_1^z\right) + J_2\left(S_1^zS_3^z + S_2^zS_4^z\right) \\ &+ J_1\left(S_1^+S_2^- + S_1^-S_2^+ + S_2^+S_3^- + S_2^-S_3^+ + S_3^+S_4^- + S_3^-S_4^+ + S_1^+S_4^- + S_1^-S_4^+\right) \\ &+ J_2\left(S_1^+S_3^- + S_1^-S_3^+ + S_2^+S_4^- + S_2^-S_4^+\right) \end{aligned} \quad (13)$$

Subspace of S^z_{tot}=0

$$H|1\rangle = H|1100\rangle = -\frac{J_2}{2}|1100\rangle + \frac{J_1}{2}|0101\rangle + \frac{J_2}{2}|0110\rangle + \frac{J_1}{2}|1010\rangle + \frac{J_2}{2}|1001\rangle$$
$$= -\frac{J_2}{2}|1\rangle + \frac{J_1}{2}|6\rangle + \frac{J_2}{2}|2\rangle + \frac{J_1}{2}|5\rangle + \frac{J_2}{2}|4\rangle$$
$$H|2\rangle = H|0110\rangle = -\frac{J_2}{2}|0110\rangle + \frac{J_2}{2}|1100\rangle + \frac{J_1}{2}|0101\rangle + \frac{J_2}{2}|0011\rangle + \frac{J_1}{2}|1010\rangle$$
$$= -\frac{J_2}{2}|2\rangle + \frac{J_2}{2}|1\rangle + \frac{J_2}{2}|3\rangle + \frac{J_1}{2}|5\rangle + \frac{J_1}{2}|6\rangle$$
$$H|3\rangle = H|0011\rangle = -\frac{J_2}{2}|3\rangle + \frac{J_2}{2}|1001\rangle + \frac{J_1}{2}|1010\rangle + \frac{J_2}{2}|0110\rangle + \frac{J_1}{2}|0101\rangle$$
$$= -\frac{J_2}{2}|3\rangle + \frac{J_2}{2}|4\rangle + \frac{J_1}{2}|5\rangle + \frac{J_1}{2}|6\rangle + \frac{J_2}{2}|2\rangle$$
$$H|4\rangle = H|1001\rangle = -\frac{J_2}{2}|4\rangle + \frac{J_1}{2}|0101\rangle + \frac{J_2}{2}|0011\rangle + \frac{J_1}{2}|1010\rangle + \frac{J_2}{2}|0011\rangle$$
$$= -\frac{J_2}{2}|4\rangle + \frac{J_1}{2}|6\rangle + \frac{J_2}{2}|3\rangle + \frac{J_1}{2}|5\rangle + \frac{J_2}{2}|1\rangle$$
$$H|5\rangle = H|1010\rangle = -J_1|5\rangle + \frac{J_2}{2}|5\rangle + \frac{J_1}{2}|0110\rangle + \frac{J_1}{2}|0011\rangle + \frac{J_1}{2}|1100\rangle + \frac{J_1}{2}|1001\rangle$$
$$= -J_1|5\rangle + \frac{J_2}{2}|5\rangle + \frac{J_1}{2}|2\rangle + \frac{J_1}{2}|3\rangle + \frac{J_1}{2}|1\rangle + \frac{J_1}{2}|4\rangle$$

$$H\left|6\right\rangle = H\left|0101\right\rangle = -J_1\left|6\right\rangle + \frac{J_2}{2}\left|6\right\rangle + \frac{J_1}{2}\left|0110\right\rangle + \frac{J_1}{2}\left|0011\right\rangle + \frac{J_1}{2}\left|1100\right\rangle + \frac{J_1}{2}\left|1001\right\rangle$$
$$= -J_1\left|6\right\rangle + \frac{J_2}{2}\left|6\right\rangle + \frac{J_1}{2}\left|2\right\rangle + \frac{J_1}{2}\left|3\right\rangle + \frac{J_1}{2}\left|1\right\rangle + \frac{J_1}{2}\left|4\right\rangle$$

Subspace of S^z_{tot}=1

$$H\left|1\right\rangle = H\left|1110\right\rangle = \frac{J_1}{2}\left|0111\right\rangle + \frac{J_2}{2}\left|1011\right\rangle + \frac{J_1}{2}\left|1101\right\rangle = \frac{J_1}{2}\left|2\right\rangle + \frac{J_2}{2}\left|3\right\rangle + \frac{J_1}{2}\left|4\right\rangle$$
$$H\left|2\right\rangle = H\left|0111\right\rangle = \frac{J_1}{2}\left|1011\right\rangle + \frac{J_2}{2}\left|1101\right\rangle + \frac{J_1}{2}\left|1110\right\rangle = \frac{J_1}{2}\left|3\right\rangle + \frac{J_2}{2}\left|4\right\rangle + \frac{J_1}{2}\left|1\right\rangle$$
$$H\left|3\right\rangle = H\left|1011\right\rangle = \frac{J_1}{2}\left|0111\right\rangle + \frac{J_1}{2}\left|1101\right\rangle + \frac{J_2}{2}\left|1110\right\rangle = \frac{J_1}{2}\left|2\right\rangle + \frac{J_1}{2}\left|4\right\rangle + \frac{J_1}{2}\left|1\right\rangle$$
$$H\left|4\right\rangle = H\left|1101\right\rangle = \frac{J_2}{2}\left|0111\right\rangle + \frac{J_1}{2}\left|1011\right\rangle + \frac{J_1}{2}\left|1110\right\rangle = \frac{J_2}{2}\left|2\right\rangle + \frac{J_1}{2}\left|3\right\rangle + \frac{J_1}{2}\left|1\right\rangle$$

Subspace of S^z_{tot}=-1

$$H\left|1\right\rangle = H\left|0001\right\rangle = \frac{J_1}{2}\left|1000\right\rangle + \frac{J_2}{2}\left|0100\right\rangle + \frac{J_1}{2}\left|0010\right\rangle = \frac{J_1}{2}\left|2\right\rangle + \frac{J_2}{2}\left|3\right\rangle + \frac{J_1}{2}\left|4\right\rangle$$
$$H\left|2\right\rangle = H\left|1000\right\rangle = \frac{J_1}{2}\left|1000\right\rangle + \frac{J_2}{2}\left|0010\right\rangle + \frac{J_1}{2}\left|0001\right\rangle = \frac{J_1}{2}\left|3\right\rangle + \frac{J_2}{2}\left|4\right\rangle + \frac{J_1}{2}\left|1\right\rangle$$
$$H\left|3\right\rangle = H\left|0100\right\rangle = \frac{J_1}{2}\left|1000\right\rangle + \frac{J_1}{2}\left|0010\right\rangle + \frac{J_2}{2}\left|0001\right\rangle = \frac{J_1}{2}\left|2\right\rangle + \frac{J_1}{2}\left|4\right\rangle + \frac{J_2}{2}\left|1\right\rangle$$
$$H\left|4\right\rangle = H\left|0010\right\rangle = \frac{J_2}{2}\left|1000\right\rangle + \frac{J_1}{2}\left|0100\right\rangle + \frac{J_1}{2}\left|0001\right\rangle = \frac{J_2}{2}\left|2\right\rangle + \frac{J_1}{2}\left|3\right\rangle + \frac{J_1}{2}\left|1\right\rangle$$

Subspace of S^z_{tot}=2

$$H_I\left|1111\right\rangle = H_I\left|1111\right\rangle = \frac{J_1}{4}\left|1111\right\rangle + \frac{J_2}{4}\left|1111\right\rangle + \frac{J_1}{4}\left|1111\right\rangle + \frac{J_1}{4}\left|1111\right\rangle + \frac{J_2}{4}\left|1111\right\rangle$$
$$+ \frac{J_2}{2}\left|1111\right\rangle = \left(J_1 + \frac{J_2}{2}\right)\left|1111\right\rangle$$

Subspace of S^z_{tot}=-2

$$H_I\left|0000\right\rangle = H_I\left|0000\right\rangle = \frac{J_1}{4}\left|0000\right\rangle + \frac{J_2}{4}\left|0000\right\rangle + \frac{J_1}{4}\left|0000\right\rangle + \frac{J_1}{4}\left|0000\right\rangle + \frac{J_2}{4}\left|0000\right\rangle$$
$$+ \frac{J_2}{2}\left|0000\right\rangle = \left(J_1 + \frac{J_2}{2}\right)\left|0000\right\rangle$$

The Hamiltonian matrix is block diagonalized with respect to the aforementioned subspaces. The subspaces of S^z_{tot}=2 and -2, have the same entry of $J_1 + \frac{J_2}{2}$, which is an eigenvalue. For the Subspace of S^z_{tot}=0, the corresponding Hamiltonian matrix is given by

$$H = \begin{bmatrix} -J_2/2 & J_2/2 & 0 & J_2/2 & J_1/2 & J_1/2 \\ J_2/2 & -J_2/2 & J_2/2 & 0 & J_1/2 & J_1/2 \\ 0 & J_2/2 & -J_2/2 & J_2/2 & J_1/2 & J_1/2 \\ J_2/2 & 0 & J_2/2 & -J_2/2 & J_1/2 & J_1/2 \\ J_1/2 & J_1/2 & J_1/2 & J_1/2 & -J_1 + \frac{J_1}{2} & 0 \\ J_1/2 & J_1/2 & J_1/2 & J_1/2 & 0 & -J_1 + \frac{J_1}{2} \end{bmatrix} \quad (14)$$

The subspaces of S^z_{tot}=1and S^z_{tot}=-1 are symmetric. Hence, the corresponding matrix for any two of these subspaces is

$$H = \begin{bmatrix} 0 & J_1/2 & J_2/2 & J_1/2 \\ J_1/2 & 0 & J_1/2 & J_2/2 \\ J_2/2 & J_1/2 & 0 & J_1/2 \\ J_1/2 & J_2/2 & J_1/2 & 0 \end{bmatrix} \quad (15)$$

The complete diagonalization of these matrices, in addition to the single entries for subspaces of $S^z_{tot}=2$ and $S^z_{tot}=-2$ gives the following eigenvalues.

$$E_1 = J_1 + \frac{J}{2},\ E_2 = J_1 + \frac{J}{2},\ E_3 = \frac{-3J_2}{2},\ E_4 = \frac{-J_2}{2},\ E_5 = \frac{-J_2}{2},\ E_6 = \frac{-J_2}{2},\ E_7 = \frac{-J_2}{2}$$

$$,\ E_8 = \frac{-J_2}{2},\ E_9 = \frac{-J_2}{2},\ E_{10} = \frac{1}{2}[-4J_1 + J_2],\ E_{11} = \frac{1}{2}[-2J_1 + J_2], E_{12} = \frac{1}{2}[-2J_1 + J_2]$$

$$E_{13} = \frac{1}{2}[-2J_1 + J_2],\ E_{14} = \frac{1}{2}[2J_1 + J_2],\ E_{15} = \frac{1}{2}[2J_1 + J_2],\ E_{16} = \frac{1}{2}[2J_1 + J_2]$$

Two competing ground states in the subspace of $S^z_{tot}=0$ can be identified, namely $|\psi_\lambda\rangle$ and $|\psi_\sigma\rangle$. These competing ground states are given by (16) and (17) below.

$$|\psi_\lambda\rangle = \frac{1}{2\sqrt{3}}[2|1010\rangle + 2|0101\rangle - |1100\rangle - |0110\rangle - |0011\rangle - |1001\rangle]$$

$$|\psi_\sigma\rangle = \frac{1}{2}[|0110\rangle - |1100\rangle + |1001\rangle - |0011\rangle]$$

Their corresponding energy will be identified as $E_\lambda = E_{10} = \frac{1}{2}[-4J_1 + J_2]$ and $E_\sigma = E_3 = \frac{-3J_2}{2}$

The effect of frustration on these competing ground states of the four-site Heisenberg system will be presented in section six.

6. RESULTS OF FOUR-SITE FRUSTRATED SYSTEM AT ZERO FIELD

The result for four-site Ising model with competing interaction is presented in Table 1. The presence of frustration gives rise to two competing ground states within the subspace of $S^z_{tot} = 0$, namely the quasi-antiferromagnetic states, $|\psi_\alpha\rangle$ and the pure antiferromagnetic states, $|\psi_\beta\rangle$ with energy E_α and E_β respectively. In the absence of frustration ($J_2 = 0$), the ground state energy gives $E_g = E_\beta = -J_1 = -J$, which is purely antiferromagnetic and two-fold degenerate as shown in Table 1. In the regime $J_1/J_2 > 1$, the ground state is held by $|\psi_\beta\rangle$ with a degeneracy of 2. A cross over from pure antiferromagnetic states to quasi-antiferromagnetic states occurs at the critical point of $J_1/J_2 = 1$. At this critical point, the ground state degeneracy (GDS) reaches its peak value of six. Beyond this level, that is in the regime of $J_1/J_2 < 1$, the ground state is entirely driven by J_2 and is four-fold degenerate.

The ground state energy for the Heisenberg model at $J_2 = 0$ gives $-2J$ as shown in Table 2. Hence, the ground state energy of the isotropic Heisenberg model on four-site chain with periodic boundary conditions is recovered. On switching on the frustration due to competing interaction, the fate of the ground state energy is decided by the competition between J_1 and J_2. In the regime of $J_1/J_2 > 1$, the ground state is held by ψ_λ which is nondegenerate. A cross over from the nondegenerate ground state ψ_λ to the nondegenerate ground state ψ_σ within the subspace of $S^z_{tot} = 0$ occurs at the critical point of $J_1/J_2 = 1$. Beyond this critical point, that is in the regime of $J_1/J_2 < 1$, the ground state is entirely driven by J_2 and is nondegenerate.

Table 1. The effect of frustration on the ground state energy of four-site Ising chain

J_1	J_2	E_α	E_β	GSD
1	0.0	0.00	-1.00	2
1	0.1	-0.05	-0.95	2
1	0.2	-0.10	-0.90	2
1	0.4	-0.20	-0.80	2
1	0.6	-0.30	-0.70	2
1	0.8	-0.60	-0.40	2
1	1.0	-0.50	-0.50	6
1	1.2	-0.60	-0.40	4
1	1.4	-0.70	-0.30	4
1	1,6	-0.80	-0.20	4
1	1.8	-0.10	-0.90	4
1	2.0	-1.00	0.00	4

Table 2. The effect of frustration on the ground state energy of four-site Heisenberg chain

J_1	J_2	E_λ	E_σ	GSD
1	0.0	-2.00	0.00	None
1	0.1	-1.95	-0.15	None
1	0.2	-1.90	-0.30	None
1	0.4	-1.80	-0.60	None
1	0.6	-1.70	-0.90	None
1	0.8	-1.60	-1.20	None
1	1.0	-1.50	-1.50	None
1	1.2	-1.40	-1.80	None
1	1.4	-1.30	-2.10	None
1	1.6	-1.20	-2.40	None
1	1.8	-1.10	-2.70	None
1	2.0	-1.00	-3.00	None

7. CONCLUSION

The effect of frustration due to competing interaction has been investigated on four-site square lattice within the Ising and Heisenberg models. For the Ising model, the presence of frustration gives birth to two competing ground states. The competition between the antiferromagnetic and ferromagnetic coupling constants, J_1 and J_2 respectively determines the nature of the ground state. Hence, in the regime $J_1/J_2 > 1$, two-fold degenerate state, that is $|0101\rangle$ and $|1010\rangle$ characterize the ground state of the system. 2. A cross over from the two-fold degenerate pure antiferromagnetic ground state to four-fold degenerate quasi-antiferromagnetic ground states occurs at the critical point of $J_1/J_2 = 1$. At this critical point, the total number of degeneracies of the ground state reaches its maximum value of six. Beyond this level, that is in the regime of $J_1/J_2 < 1$, the ground state is entirely driven by J_2 and is four-fold degenerate. For the Heisenberg model, the ground state energy remains nondegenerate irrespective of the variation of the coupling ratio J_1/J_2. However, at the critical point $J_1/J_2 = 1$,there is an evidence of a cross over from the ground state ψ_λ, which is more antiferromagnetic to the ground state ψ_σ, which is less antiferromagnetic. Beyond this critical point, the ground state is entirely driven by J_2.

In both models used in this work, the effect of frustration is two folds, namely it introduces competing ground states and multiple ground state degeneracies in the case of the Ising model. These degeneracies are a consequence of the inability of the spins in the four-site square system to anti-aligned with their nearest neighbours. Hence, the system finds it difficult to have a perfect antiferromagnetic ordering that will minimize its energy.The cross overs that are observed in this work as the coupling ratio is varied occur within the subspace of $S^z_{tot} = 0$. Hence, no phase transition is observed for both models investigated in this work. The absence of degenerate ground state in the Heisenberg system may be attributed to the presence of quantum fluctuation term in the model. In order to observe phase transition at zero temperature (that is quantum phase transition) in this frustrated system, it is recommended that the system be subject to finite external fields.

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