

Ordering Due to Disorder in Frustrated Quantum Magnetic Systems

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Abstract

The phenomenon of *order by disorder* in frustrated magnetic systems is reviewed. Disorder (thermal or quantum fluctuations) may sometimes give rise to long range ordering in systems with frustration, where one must often consider the selection among classically degenerate ground states which are not equivalent by any symmetry. The lowest order effects of quantum fluctuations in such frustrated systems usually resolves the continuous degeneracy of the ground state manifold into discrete Ising-type degeneracy. A unique ground state selection out of this Ising degenerate manifold then occurs due to higher order effects of quantum fluctuations. For systems such as face-centered cubic and body-centered tetragonal antiferromagnets where the number of Ising parameters to describe the ground state manifold is not macroscopic, we show that quantum fluctuations choose a unique ground state at the first order in $1/S$. However for kagomé antiferromagnet where the ground state manifold is macroscopic, a unique ground state selection can only occur at high orders in $1/S$. We show that the main effect of the zero-point fluctuations is at small wavevector and can be well modeled by an effective biquadratic interaction of the form

$$\Delta E_Q^{\text{eff}} = -\frac{1}{2}Q \sum_{i,j} (\mathbf{S}_i \cdot \mathbf{S}_j)^2 / S^3$$

This interaction opens a quantum spin gap by splitting the classical zero-energy modes into one zero-energy Goldstone mode and nonzero energy modes. We calculate this quantum gap at relative order $1/S$ using the standard Hartree decoupling of the higher order interaction terms.

1. Introduction

Interest in frustrated magnetic systems and quantum fluctuation effects in such systems have greatly increased in the last few years.[1, 2] Disorder, antiferromagnetic interactions of competing strength, and certain lattice symmetries often lead to situations,

where the energy of the spin bonds in the system can not be minimized simultaneously, the phenomenon known as “frustration”. In such systems, a degenerate ground-state manifold often results. Probably the simplest example is the Ising antiferromagnet on a triangle lattice as shown in Figure 1. Considering a single triangle of spins, one sees that after fixing the direction of one spin to remove the global up-down degeneracy, a two fold degeneracy remains. Thus a ground state degeneracy arises as the system is unable to simultaneously satisfy the minimum energy condition for all bonds in the system. This is the principle effect of the frustration. It assures that the classical ground state manifold is of higher symmetry than the underlying Hamiltonian. In such systems, fluctuations (which can be thermal or quantum) play a special role because they may partially or completely lift the degeneracy and make the system more ordered.

There are now many examples of systems which classically exhibit an accidental degeneracy which is removed by quantum mechanics. As we will discuss, this phenomenon occurs frequently in the context of the Heisenberg model of antiferromagnetism, for which the Hamiltonian is

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \quad (1)$$

where $\langle ij \rangle$ indicates a sum over pairs of nearest neighbors. The Heisenberg antiferromagnet (AF) on a square lattice with random ferromagnetic (F) defect bonds as illustrated in Figure 1 is one example of a frustrated quantum spin system. Models of this type were proposed in connection with magnetic properties of CuO_2 -plane in high- T_c cuprates, where hole doping in the oxygen site causes the adjacent interaction between nearest neighbor Cu-spins ($S=1/2$) to be ferromagnetic (F) and therefore leads to frustration. This type of frustration caused by site disorder is common to most of the spin glasses and therefore called *spin glass frustration*[2]

Another example, one in which the frustration is geometrical (i. e. it does not require adjustment of the magnitude of the coupling constants), is that studied by Shender[4] in which spins on a BCC lattice have strong second neighbor antiferromagnetic interactions and weaker first neighbor interactions as shown in Figure 2. In that case, the geometrical arrangement guaranteed that the classical exchange field at any site on one sublattice due to the spins in the other sublattice was zero. One therefore has two simple cubic antiferromagnetic sublattices which are decoupled in the mean field sense.

So, for such a classical system, the energy is independent of the value of the angle θ between the two sublattices. The ”optical” mode wherein one sublattice precesses relative to the other one thus accidentally has zero energy (*phason mode*). However, as Shender showed[4] and was verified by inelastic neutron scattering[18], this optical mode develops a nonzero energy when quantum fluctuations are included. Perhaps the easiest way to see this is to calculate the quantum zero-point energy as a function of θ . Simple arguments[17], which we will repeat below, show that the zero point energy is minimized by collinear spin arrangement (i.e. $\cos(\theta)^2 = 1$)[5].

A simple physical explanation to the tendency toward collinear ordering by quantum fluctuations is given by Henley.[6, 7] *What happens when external fields \mathbf{h}_i are applied to an antiferromagnet?* If \mathbf{h}_i is uniform, it is a familiar fact that the fixed-length spins

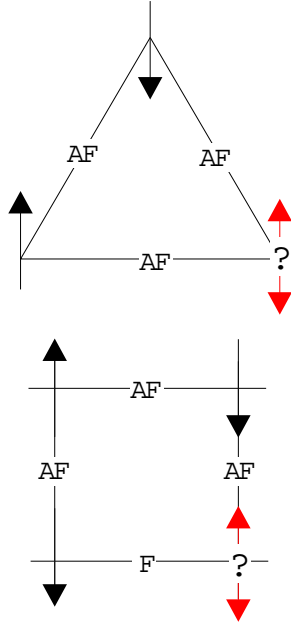


Figure 1. Top: A triangle of three Ising spins with antiferromagnet interaction, exhibiting “geometrical frustration” which results two-fold degenerate ground state manifold. **Bottom:** A square of four spins interacting antiferromagnetically except for one ferromagnetic bond (which could be induced by site disorder), illustrating frustration common to most spin glasses.[2]

in each sublattice prefer to be transverse to the field because they can gain energy by relaxing towards it. This happens because there is no net coupling of the field to the ground state in first order;

$$\sum_i^N \mathbf{h}_i \cdot \mathbf{S}_i = 0 \quad (2)$$

If each \mathbf{S}_i turns transverse, each \mathbf{S}_i can deviate towards \mathbf{h} and gains energy to $O(h^2)$. This is illustrated in Fig. 3.

Now, because of disorder (fluctuations), the exchange field acting on (say) the even sublattice has a random fluctuating component from the odd sublattice as illustrated schematically in Figure 3. As argued above, the even sublattice should prefer to be transverse to the ground state orientations of the odd spins. One can check that this fluctuating field satisfies condition in Eq. (2), too. Consequently, *the even and odd sublattices must align collinear*. They can do this either sense (parallel or antiparallel), so the continuous degeneracy of the classical system is reduced to that of Ising-one. For the case of *BCC antiferromagnet* shown in Fig. 2, remaining Ising type degeneracy is the true

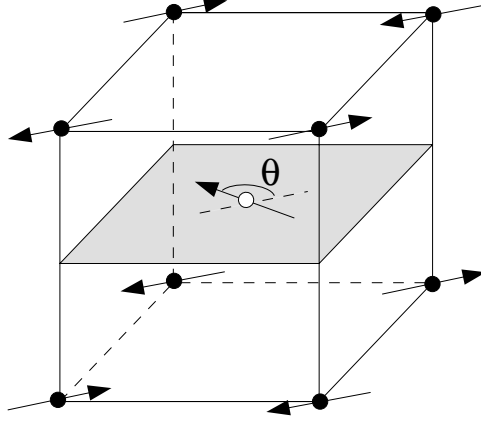


Figure 2. Two antiferromagnetic sublattices on a BCC lattice. Note that the mean field due to spins in one sublattice (i.e. spins at the corners shown by filled circles) on the spins in other sublattice (i.e. spin at the center shown by open circle) is zero. Therefore in the classical limit, the energy of the system is independent of θ , resulting an infinite degenerate ground state manifold.

symmetry of the system and can not be removed[5]. Hence, the ground state selection by quantum fluctuation in this simple example is as complete as symmetry allows.

Based on this argument, Henley[6, 7] proposed that this effect could be described phenomenologically by an effective biquadratic exchange interaction of the form $K[\mathbf{S}_i \cdot \mathbf{S}_j]^2$, where the results of Ref. [4] indicated that K is of order $J'^2/(JS)$, where J and J' are coupling constants introduced below. Subsequently many examples of ground state selection via quantum fluctuations have been analyzed.[8, 9, 10, 11, 12, 14] This phenomenon is the analog of *ordering by disorder* due to thermal fluctuations, a concept first discussed by Villain[13] for Ising systems and then extended to vector spin systems by Henley.[6, 7] The same effect can be realized by configurational fluctuations associated with random substitution in alloys.[7]

A related question in frustrated systems concerns the nature of the elementary excitations. The Goldstone theorem indicates that at zero wavevector there should be one zero-energy mode. In view of the classical degeneracy associated with the relative rotation of decoupled sublattices, one finds additional zero-energy modes. However, in the presence of quantum fluctuations which remove the classical degeneracy, one can understand the results of Ref. [4], namely that quantum fluctuations cause the extra zero-energy modes to now have a nonzero energy at relative order $J'^2/(JS)^2$. Such “quantum gaps” have been observed by inelastic scattering of neutrons.[18, 19] As we shall see, and similar to the results of Ref. [4], in contrast to ground state selection, the gaps still occur at relative order $J'^2/JS^2/S$, even though one must go to higher order in J'/J to completely

resolve the structural degeneracy. Here we will calculate the quantum gap at relative order $1/S$ using the Dyson–Maleev[15] transformation. This provides an alternative, and possibly simpler, calculation than in Ref. [4].

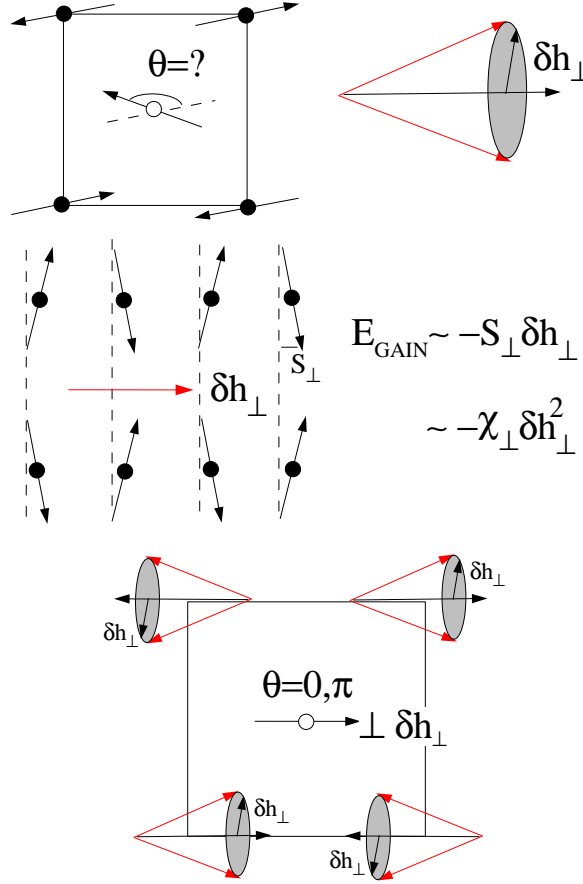


Figure 3. A schematic illustration of *ordering by disorder*. Top right figure shows the quantum zero point fluctuations which give rise to a random field δh_{\perp} perpendicular to the direction of the ordered moment. On the middle we show how an antiferromagnet orients itself to an external field. On the bottom, we consider the fluctuating component of the spins in one sublattice as an external field acting on the spins in other sublattice. This leads to collinear ordering by zero-point fluctuations of the spins. See text for detail discussion.

Since the work of Shender[4] and Henley[6, 7], a large number of systems have been studied, such as AF spins on a square and cubic lattice with nearest and next-nearest neighbor interactions, AF spins on a pyrochlore lattice, etc. In the case of interest to us here, it is found that quantum fluctuations favor states in which spins are collinear.

Hence, for a system where all possible collinear states are symmetry equivalent, the removal of the infinite degeneracy of the ground state manifold by quantum fluctuations is as complete as permitted by symmetry and one has a ground state with no accidental degeneracy. To the best of our knowledge all collinear systems studied so far are of this type and hence it is of interest to study *how quantum fluctuations select a unique ground state if the collinear states are not all symmetry equivalent*. Recently we have addressed this issue in Refs.[12, 14] by studying two particular systems, namely quantum spins with nearest neighbor AF interactions on a body-centered tetragonal (BCT) and on a face-centered cubic (FCC) lattices[12, 14]. In the BCT system, the Shender mechanism can only resolve the continuous degeneracy of the ground state manifold into an infinite discrete Ising type degeneracy. We analyzed the selection of a unique ground state out of this infinite Ising type degenerate manifold by higher order effects of quantum fluctuations in detail using interacting spin wave theory. Another case where collinear configurations are not equivalent by symmetry is provided by the "second kind of AF ordering" on an FCC lattice[5] where one has two inequivalent collinear states; type A and type B. We studied this system[5] and found that quantum fluctuations favor the state of type A.

In systems discussed above, number of parameters describing the ground state manifold is finite (i.e. one for BCC and four for FCC antiferromagnet and even infinite for BCT case but not macroscopic (i.e. (number of zero energy modes/N) $\rightarrow 0$ as $N \rightarrow \infty$ where N is the total number of spins)). In such systems it seems that the complete removal of degeneracy of the ground state manifold occurs at the first order in $1/S$. However there are systems where this is not the case. Kagomé lattice with only nearest antiferromagnetic interaction is probably the best example for this. As we shall discuss below, in kagomé antiferromagnet the number of zero-energy modes is macroscopic (i.e. it is proportional to the number of spin sites in the system) and therefore removal of degeneracy of the ground state manifold by quantum disorder is much more complicated than BCT case. A unique ground state selection involves higher order quantum corrections in $1/S$, which prefers coplanar ordering.

Briefly this paper is organized as follows. In the next section, we study *ordering by disorder* in a simple model. We demonstrate how to get the effective quantum interaction between two subsystems which are classically decoupled. In this section we also study the spin waves and gaps due to quantum fluctuations by treating spin-wave interactions using the standard Hartree decoupling of the higher order interaction terms introduced by the Dyson-Maleev transformation[15] to bosons. Here we show that the effects of quantum fluctuations can be well approximated (only at zero wavevector) by the effective biquadratic interaction mentioned above. We also show how to calculate the quantum gap induced by zero-point fluctuations and its temperature dependence in a simple way using Hartree decoupling approach. In Sec. III we considered FCC and BCT antiferromagnets where a unique ground state selection by disorder occurs at higher order in (J'/J) but still at first order in $1/S$. Sec. IV is devoted to kagomé antiferromagnet where ground state selection due to disorder occurs at second order in $1/S$. Our conclusion will be given in the Sec. V.

2. Order by Disorder: A Simple Case

Let us consider a Heisenberg antiferromagnet on a body centred cubic (BCC) lattice, with short range exchange. We consider only nearest neighbor (nn) couplings, J' , and next nearest neighbor (nnn) couplings, J , and take J to be antiferromagnetic. When J' is sufficiently small, the system forms two simple cubic antiferromagnetic sublattices. We therefore write the Hamiltonian of the system as

$$\mathcal{H} = J \sum_{\langle \alpha, i, j; 2 \rangle} \mathbf{S}_\alpha(i) \mathbf{S}_\alpha(j) + J' \sum_{\langle \alpha i, \beta j; 1 \rangle} \mathbf{S}_1(i) \mathbf{S}_2(j), \quad (3)$$

where $S_\alpha(i)$ denotes the i th spin on sublattice α ($\alpha = 1$ and 2). The first term on the right-hand side of Eq. (3) is the interaction within the sublattices and second term is that between sublattices.

Within the classical approximation the two sublattices may assume arbitrary relative orientations in the ground state because of the vanishing local field of one subsystem on the other (see Fig.2). This therefore gives a degeneracy additional to the global Heisenberg rotational invariance of \mathcal{H} . The additional degeneracy has consequences for the exciton spectrum of the system. It leads to an excitation spectrum consisting of two acoustic branches, each with a zero mode at $\mathbf{q} = 0$. The Goldstone, or zero-energy mode of one of these branches is due to the global Heisenberg invariance, while the second branch is due to the out of phase rotation of spins in different subsystems. The absence of a gap is a consequence of the additional degeneracy of the ground state structure considered above. Therefore in the classical treatment we have a one-dimensional infinite degenerate manifold of ground state with two zero energy modes at $\mathbf{q} = 0$.

It is now well known that in such a situation quantum fluctuations select collinear structures out of infinite degenerate ground state manifold[4, 16, 17] and opens a gap at $\mathbf{q} = 0$. We will reproduce this result here by evaluating the zero-point energy when the two sublattices are arbitrarily oriented. However, in the interest of simplicity, we will assume that the spin structure is coplanar, so that all spins lie in the yz -plane and each sublattice, α , is characterized by a wave vector \mathbf{Q} and a phase θ_α . For the spin-wave expansion we introduce the following local axes at site i in sublattice α , so that the S'_z -axis lies along the direction in which the spin points in the ground state:

$$\mathbf{S}_\alpha(i) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\mathbf{Q} \cdot \mathbf{r}_i + \theta_\alpha) & 0 \\ 0 & 0 & \cos(\mathbf{Q} \cdot \mathbf{r}_i + \theta_\alpha) \end{pmatrix} \mathbf{S}'_\alpha(i), \quad (4)$$

where, using Dyson-Maleev transformation, we have

$$S'^x_\alpha(i) = \sqrt{\frac{S}{2}} \left[a^+_\alpha(i) + a_\alpha(i) - \frac{1}{2S} a^+_\alpha(i) a^+_\alpha(i) a_\alpha(i) \right] \quad (5)$$

$$S'^y_\alpha(i) = i\sqrt{\frac{S}{2}} \left[a^+_\alpha(i) - a_\alpha(i) - \frac{1}{2S} a^+_\alpha(i) a^+_\alpha(i) a_\alpha(i) \right] \quad (6)$$

$$S'^z_\alpha(i) = S - a^+_\alpha(i) a_\alpha(i) \quad (7)$$

and

$$\mathbf{Q} = (\pi/a, \pi/a, \pi/a) , \quad (8)$$

where a is the cubic lattice constant. The spin-wave expansion for the other configurations can be easily obtained by taking other \mathbf{Q} values (i.e. $\mathbf{Q} = (\pi/a, \pi/a, 0)$ for ferromagnetic ordering along c -axis). From Eq. (4) we see that the angle $\phi_\alpha(i)$ that a spin i in sublattice α makes with the crystal z -axis is

$$\phi_\alpha(i) = \mathbf{Q} \cdot \mathbf{r}_i + \theta_\alpha . \quad (9)$$

From Eq. (4) one can write

$$\mathbf{S}_\alpha(i) \cdot \mathbf{S}_\beta(j) = S^2 \cos(\theta_{j\beta, i\alpha}) + \hat{O}_{j\beta, i\alpha}^{(2)} + \hat{O}_{j\beta, i\alpha}^{(4)} + \text{O}(1/S) , \quad (10)$$

where the quadratic term is

$$\begin{aligned} \hat{O}_{j\beta, i\alpha}^{(2)} = & -S \cos(\theta_{j\beta, i\alpha}) \left[a_\alpha^+(i) a_\alpha(i) + a_\beta^+(j) a_\beta(j) \right] \\ & + \frac{1}{2} S \left[1 + \cos(\theta_{j\beta, i\alpha}) \right] \left[a_\alpha^+(i) a_\beta(j) + a_\alpha(i) a_\beta^+(j) \right] \\ & + \frac{1}{2} S \left[1 - \cos(\theta_{j\beta, i\alpha}) \right] \left[a_\alpha^+(i) a_\beta^+(j) + a_\alpha(i) a_\beta(j) \right] , \end{aligned} \quad (11)$$

where

$$\theta_{j\beta, i\alpha} = \mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_i) + \theta_\beta - \theta_\alpha \quad (12)$$

is the angle between spin i in sublattice α and spin j in sublattice β . In Eq. (10) $\hat{O}_{j\beta, i\alpha}^{(4)}$ is the four-operator term which is discussed in Sec. II.A.2.

Using Eq. (11) we may write the Hamiltonian up to terms quadratic in the boson operators as

$$\mathcal{H} = E_0 + \mathcal{H}_0 + \mathcal{H}_I , \quad (13)$$

where

$$E_0 = -6NJS^2 \left[1 + (1/S) \right] , \quad (14)$$

$$\mathcal{H}_0 = 3JS \sum_{\alpha=1,2, \mathbf{q}} \left(a_\alpha^+(\mathbf{q}) a_\alpha(\mathbf{q}) + a_\alpha(\mathbf{q}) a_\alpha^+(\mathbf{q}) + \gamma(\mathbf{q}) \left[a_\alpha^+(\mathbf{q}) a_\alpha^+(-\mathbf{q}) + a_\alpha(\mathbf{q}) a_\alpha(-\mathbf{q}) \right] \right) , \quad (15)$$

where

$$\gamma(\mathbf{q}) = \frac{1}{6} \sum_{\vec{\Delta}} e^{i\mathbf{q} \cdot \vec{\Delta}} = (1/3) \left[\cos(q_x a) + \cos(q_y a) + \cos(q_z a) \right] . \quad (16)$$

Also N is the number of the sites in each of the two simple cubic antiferromagnetic sublattice, \mathbf{q} is summed over N values in the interval $-\pi < aq_\alpha < \pi$ ($\alpha = x, y, z$), and we introduced Fourier transformed variables by

$$a_\alpha^+(i) = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} a_\alpha^+(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}_i} . \quad (17)$$

The interaction between sublattices is

$$H_I = 2J'S \sum_{\alpha,\beta,\mathbf{q}} \left(A_{\alpha\beta}(\mathbf{q}) \left[a_\alpha^+(\mathbf{q})a_\beta(\mathbf{q}) + a_\alpha(\mathbf{q})a_\beta^+(\mathbf{q}) \right] \right. \\ \left. + B_{\alpha\beta}(\mathbf{q}) \left[a_\alpha^+(\mathbf{q})a_\beta^+(-\mathbf{q}) + a_\alpha(\mathbf{q})a_\beta(-\mathbf{q}) \right] \right) , \quad (18)$$

where $A_{\alpha\alpha} = B_{\alpha\alpha} = 0$, and, for $\alpha \neq \beta$, we have

$$A_{\alpha\beta}(\mathbf{q}) = \frac{1}{8} \sum_{\vec{\delta}_{\alpha,\beta}} \left[1 + \cos(\mathbf{Q} \cdot \vec{\delta}_{\alpha,\beta} + \theta_\beta - \theta_\alpha) \right] e^{-i\mathbf{q}\cdot\vec{\delta}_{\alpha,\beta}} , \quad (19a)$$

$$B_{\alpha\beta}(\mathbf{q}) = \frac{1}{8} \sum_{\vec{\delta}_{\alpha,\beta}} \left[1 - \cos(\mathbf{Q} \cdot \vec{\delta}_{\alpha,\beta} + \theta_\beta - \theta_\alpha) \right] e^{-i\mathbf{q}\cdot\vec{\delta}_{\alpha,\beta}} , \quad (19b)$$

where $\vec{\Delta}$ is summed over second-neighbor vectors, and $\vec{\delta}_{\alpha,\beta}$ is summed over the four first-neighbor vectors which connect sublattices α and β .

We may characterize the orientation of sublattices with respect to each other by a single parameter θ , so that the angle between spin at the corner (0,0,0) and at the center (1/2,1/2,1/2) is

$$\theta = \frac{3}{2}\pi + \theta_2 - \theta_1 \quad (20)$$

One see that with this definition Eq. (19) can be rewritten as

$$A_{\alpha\beta}(\mathbf{q}) = C_{\alpha\beta}(\mathbf{q}) + S_{\alpha\beta}(\mathbf{q}) \quad (21a)$$

$$B_{\alpha\beta}(\mathbf{q}) = C_{\alpha\beta}(\mathbf{q}) - S_{\alpha\beta}(\mathbf{q}) , \quad (21b)$$

where $C_{\alpha\beta}(\mathbf{q})$ and $S_{\alpha\beta}(\mathbf{q})$ are the matrix elements of the matrices

$$\mathbf{C}(\mathbf{q}) = \begin{bmatrix} 0 & c(\mathbf{q}) \\ c(\mathbf{q}) & 0 \end{bmatrix} \quad (22)$$

and

$$S(\mathbf{q}) = \begin{bmatrix} 0 & \cos(\theta)s(\mathbf{q}) \\ \cos(\theta)s(\mathbf{q}) & 0 \end{bmatrix} , \quad (23)$$

where $s(\mathbf{q})$ and $c(\mathbf{q})$ are

$$\begin{aligned} s(\mathbf{q}) &= \sin(q_x a/2) \sin(q_y a/2) \sin(q_z a/2) , \\ c(\mathbf{q}) &= \cos(q_x a/2) \cos(q_y a/2) \cos(q_z a/2) . \end{aligned} \quad (24)$$

The bilinear Hamiltonian in Eq. (13) can be written in matrix form as

$$\mathcal{H} = E_0 + \frac{1}{2} \sum_{\mathbf{q}} \mathbf{X}^+(\mathbf{q}) \mathbf{M}(\mathbf{q}) \mathbf{X}(\mathbf{q}) . \quad (25)$$

Here

$$\mathbf{X}(\mathbf{q}) = \begin{pmatrix} \mathbf{V}(\mathbf{q}) \\ \mathbf{V}^+(-\mathbf{q}) \end{pmatrix} , \quad (26)$$

with

$$\mathbf{V}(\mathbf{q}) = \begin{pmatrix} a_1(\mathbf{q}) \\ a_2(\mathbf{q}) \end{pmatrix} \quad (27)$$

and the matrix $\mathbf{M}(\mathbf{q})$ is

$$\mathbf{M}(\mathbf{q}) = \begin{pmatrix} \mathbf{H}_1(\mathbf{q}) & \mathbf{H}_2(\mathbf{q}) \\ \mathbf{H}_2(\mathbf{q}) & \mathbf{H}_1(\mathbf{q}) \end{pmatrix} , \quad (28)$$

where \mathbf{H}_1 and \mathbf{H}_2 are the two dimensional matrices

$$\mathbf{H}_1(\mathbf{q}) = 6JS \left[\mathbf{I} + [2J'/(3J)] \mathbf{A}(\mathbf{q}) \right] \quad (29a)$$

$$\mathbf{H}_2(\mathbf{q}) = 6JS \left[\gamma(\mathbf{q}) \mathbf{I} + [2J'/(3J)] \mathbf{B}(\mathbf{q}) \right] . \quad (29b)$$

Here \mathbf{I} is the two dimensional unit matrix and the matrix elements of $\mathbf{A}(\mathbf{q})$ and $\mathbf{B}(\mathbf{q})$ were given in Eqs. (21). After diagonalizing the matrix $\mathbf{M}(\mathbf{q})$, one finds that the Hamiltonian in Eq. (25) can be written in terms of normal mode operators $c_\alpha^+(\mathbf{q})$ and $c_\alpha(\mathbf{q})$ as

$$\mathcal{H} = E_0 + \Delta E_Q + \sum_{\alpha, \mathbf{q}} \epsilon_\alpha(\mathbf{q}) c_\alpha^+(\mathbf{q}) c_\alpha(\mathbf{q}) , \quad (30)$$

where $\alpha = 1, 2$ labels the eigenvalues of $\mathbf{M}(\mathbf{q})$ and where the first quantum correction, ΔE_Q , is

$$\Delta E_Q = \frac{1}{2} \sum_{\alpha, \mathbf{q}} \epsilon_\alpha(\mathbf{q}) . \quad (31)$$

Here the $\epsilon_\alpha(\mathbf{q})$ are the positive square roots of the roots of the characteristic equation of the dynamical matrix $\mathbf{D}(\mathbf{q})$

$$\mathbf{D}(\mathbf{q}) = \left[\mathbf{H}_1(\mathbf{q}) + \mathbf{H}_2(\mathbf{q}) \right] \left[\mathbf{H}_1(\mathbf{q}) - \mathbf{H}_2(\mathbf{q}) \right] \quad (32)$$

$$= E_0^2(\mathbf{q}) \left[\mathbf{I} + 4j\mathbf{P}(\mathbf{q}) \right] \left[\mathbf{I} + 4j\mathbf{R}(\mathbf{q}) \right] , \quad (33)$$

where

$$j = J'/(3J) \quad (34)$$

$$E_0(\mathbf{q}) = 6JS\sqrt{1 - \gamma^2(\mathbf{q})} \quad (35)$$

and the matrices \mathbf{P} and \mathbf{R} are

$$\mathbf{P}(\mathbf{q}) = \frac{1}{2[1 + \gamma(\mathbf{q})]} \left[\mathbf{A}(\mathbf{q}) + \mathbf{B}(\mathbf{q}) \right] = \frac{1}{1 + \gamma(\mathbf{q})} \mathbf{C}(\mathbf{q}) \quad (36)$$

$$\mathbf{R}(\mathbf{q}) = \frac{1}{2[1 - \gamma(\mathbf{q})]} \left[\mathbf{A}(\mathbf{q}) - \mathbf{B}(\mathbf{q}) \right] = \frac{1}{1 - \gamma(\mathbf{q})} \mathbf{S}(\mathbf{q}) . \quad (37)$$

We may use Eq. (31) to express the zero-point energy per site in dimensionless units, $\Delta E'_Q$, as

$$\begin{aligned} \Delta E'_Q &\equiv \Delta E_Q / (6NJS^2) = \frac{1}{12NJS^2} \sum_{\mathbf{q}} \text{tr}(\sqrt{\mathbf{D}}) \\ &= \frac{1}{12NJS^2} \sum_{\mathbf{q}} E_0(\mathbf{q}) \text{tr}(\sqrt{\mathbf{I} + \mathbf{Y}_{\mathbf{q}}}) \\ &\equiv \frac{1}{2S} \langle \text{tr}(\sqrt{\mathbf{I} + \mathbf{Y}_{\mathbf{q}}}) \rangle_{\mathbf{q}} \equiv \frac{1}{S} \Delta e_Q , \end{aligned} \quad (38)$$

so that $S^{-1} \Delta e_Q$ is the correction to the ground state energy in dimensionless units at relative order $1/S$, and

$$\mathbf{Y}_{\mathbf{q}} = 4j \left(P(\mathbf{q}) + R(\mathbf{q}) \right) + 16j^2 P(\mathbf{q}) R(\mathbf{q}) \quad (39)$$

and $\langle \dots \rangle_{\mathbf{q}}$ represents the following \mathbf{q} -summation over the first Brillouin zone

$$\langle f(\mathbf{q}) \rangle_{\mathbf{q}} = \frac{1}{6NJS} \sum_{\mathbf{q}} E_0(\mathbf{q}) f(\mathbf{q}) = \left(\frac{a}{2\pi} \right)^3 \int_{-\pi/a}^{\pi/a} dq_x \int_{-\pi/a}^{\pi/a} dq_y \int_{-\pi/a}^{\pi/a} dq_z \sqrt{1 - \gamma(\mathbf{q})^2} f(\mathbf{q}) . \quad (40)$$

To get an analytical expression for the effective interaction between antiferromagnetic sublattices, we now follow Ref. [12] and expand Δe_Q in powers of j . For the regime of interest $|J'| < |J|$, $j = [J'/(3J)] < 1/3$. Therefore we write Δe_Q in Eq. (38) as

$$\Delta e_Q = \sum_{n=0}^{\infty} C_n \langle \text{tr}(\mathbf{Y}_{\mathbf{q}}^n) \rangle_{\mathbf{q}} \quad C_n = (-1)^{n-1} \frac{(2n)!}{2^{2n+1} (n!)^2 (2n-1)} \quad (41)$$

and then collect the terms which are of the same order in j to get Δe_Q in the form

$$\Delta e_Q = \Delta e_Q^{(0)} + \Delta e_Q^{(2)} j^2 + \mathcal{O}(j^4) . \quad (42)$$

In above expansion we note that odd terms in j (and thus in $\cos(\theta)$) do not survive after \mathbf{q} -summation over the first Brillouin zone. From Eqs. (39) and (41) we see that

$$\Delta e_Q = \text{Const.} + 16C_2 \langle \text{tr}(\mathbf{P}^2 + \mathbf{R}^2) \rangle_{\mathbf{q}} j^2 + O(j^4) . \quad (43)$$

where Const. denotes terms which are independent of the $\cos(\theta)$. After a little algebra one finds that

$$\begin{aligned} \Delta e_Q &= \text{Const.} - 2 \langle \hat{c}^2(\mathbf{q}) + \hat{s}^2(\mathbf{q}) \cos(\theta)^2 \rangle_{\mathbf{q}} j^2 \\ &= \text{Const.} - 2 \langle \hat{c}^2(\mathbf{q}) \rangle_{\mathbf{q}} \left[1 + \cos(\theta)^2 \right] j^2 , \end{aligned} \quad (44)$$

where

$$\hat{s}(\mathbf{q}) = \frac{1}{1 - \gamma(\mathbf{q})} \sin\left(\frac{q_x a}{2}\right) \sin\left(\frac{q_y a}{2}\right) \sin\left(\frac{q_z a}{2}\right) \quad (45)$$

$$\hat{c}(\mathbf{q}) = \frac{1}{1 + \gamma(\mathbf{q})} \cos\left(\frac{q_x a}{2}\right) \cos\left(\frac{q_y a}{2}\right) \cos\left(\frac{q_z a}{2}\right) \quad (46)$$

In writing above expressions, we used the fact that from symmetry $\langle \hat{s}^2(\mathbf{q}) \rangle_{\mathbf{q}} = \langle \hat{c}^2(\mathbf{q}) \rangle_{\mathbf{q}}$. From this equation, we see that zero-point fluctuations select the collinear spin arrangement where $\cos(\theta)^2 = 1$ as the ground state.[5]

Spin Waves and Gap Due to Quantum Fluctuations

In the previous section we showed that in the classical picture there are infinite degenerate spin structures and that the quantum fluctuations remove this degeneracy and select the spin structure with $\cos(\theta)^2 = 1$ (i.e. collinear ordering) as the ground state. Here we will consider the effect of the quantum fluctuations on the other quantities, such as spin waves and spin gap for the ground state structure, i.e. for $\cos(\theta)^2 = 1$. We first note that the Hamiltonian matrices H_1 and H_2 (or matrices \mathbf{C} and \mathbf{S}) in Eqs. (29) commute ($[H_1, H_2] = 0$) and thus we can diagonalize them simultaneously. This enables us to perform the diagonalization analytically at any \mathbf{q} -point, and obtain the spin-wave spectrum as

$$\omega_m^2(\mathbf{q}) = (6JS)^2 \left(1 + \gamma(\mathbf{q}) + (-1)^m 4jc(\mathbf{q}) \right) \left(1 - \gamma(\mathbf{q}) + (-1)^m 4 \cos(\theta) js(\mathbf{q}) \right) \quad m = 1, 2. \quad (47)$$

Here $c(\mathbf{q})$ and $s(\mathbf{q})$ are given in Eqs. (24).

It is particularly important to note that the two spin-wave modes all have zero energy at $\mathbf{q} = 0$ ($\gamma(\mathbf{q}) \rightarrow 0$ and $s(\mathbf{q}) \rightarrow 0$ as $\mathbf{q} \rightarrow 0$). This is exactly what one expects in the classical limit, i.e. $S \rightarrow \infty$ where the two antiferromagnetic sublattices are decoupled in the mean field sense. However the absence of a spin-wave gap is a little surprising at first glance, as we included quantum fluctuations via linear spin-wave theory in our calculation, and it is these fluctuations which give rise to an effective interaction between the AF-sublattices and force them to be collinear. Hence one would expect that including

the effect of quantum fluctuations should open a gap at the zone center, as first pointed out in Ref. [4] and verified by experiment.[18, 19] Thus, even though the linear spin-wave theory is able to predict an effective interaction due to zero-point motions of the spins, it is not capable of predicting the expected gap at $\mathbf{q}=0$. Here we use an approach alternate to that of Ref. [4], based on the use of the Dyson-Maleev[15] transformation to treat spin-wave interactions correctly to leading order in $(1/S)$. In agreement with Ref. [4] we find that the magnitude of this gap is of relative order (J'/J^2S) . We will estimate this gap here in two different approaches. First we will do this by introducing an effective biquadratic interactions between sublattices to account the effect of quantum fluctuations:

$$\Delta E_Q \sim -\frac{Q}{S^3}(\mathbf{S}_1 \cdot \mathbf{S}_2)^2 . \quad (48)$$

This approach will be practically very useful to obtain the degeneracy and a qualitative estimate of the spin-wave gaps at $\mathbf{q}=0$. In the next subsection we will corroborate this approach by analyzing the effect of the four-operator terms in the boson Hamiltonian. At the end of this section, we will discuss the experimental consequences of the spin gap, its temperature dependence, etc.

2.1. Effective Biquadratic Exchange Interactions

Here we show that the effect of the quantum fluctuations on the ground state and *the spin-wave spectrum at zero wave vector* at the lowest order in (J'/J) can be represented by an effective biquadratic interaction[6] of the form

$$\Delta E_Q^{\text{eff}} = -\frac{1}{2}Q \sum_{i\alpha, j\beta} (\mathbf{S}_\alpha(i) \cdot \mathbf{S}_\beta(j))^2 / S^3 , \quad (49)$$

where the sum is over the nearest neighbor spins. Here Q is of order $(J'/J)^2$. In the next subsection we will show that the spin-wave spectrum at zero wavevector can indeed be obtained from the effective interaction of Eq. (49), and we will thereby obtain an evaluation of Q in terms of the parameters J and J' of our model. We point out that the biquadratic interaction given above does not break the degeneracy between the collinear states but is the dominant term which opens the spin-wave gap at $\mathbf{q}=0$.

From Eq. (10), one obtains, after keeping only the quadratic interactions,

$$(\mathbf{S}_\alpha(i) \cdot \mathbf{S}_\beta(j))^2 / S^3 = S \cos^2(\theta_{j\beta, i\alpha}) + \frac{2}{S} \cos(\theta_{j\beta, i\alpha}) \hat{O}_{j\beta, i\alpha}^{(2)} . \quad (50)$$

Remembering that $\cos(\theta_{j\beta, i\alpha})^2 = 1$ for collinear spin structures, and using Eq. (11), one can write

$$\begin{aligned} \Delta E_Q^{\text{eff}} = \text{Const.} + \sum_{i\alpha, j\beta} & \left\{ Q \left[a_\alpha^+(i) a_\alpha(i) + a_\beta^+(j) a_\beta(j) \right] \right. \\ & \left. - \frac{Q}{2} \left[1 + \cos(\theta_{j\beta, i\alpha}) \right] \left[a_\alpha^+(i) a_\beta(j) + a_\alpha(i) a_\beta^+(j) \right] \right\} \end{aligned}$$

$$+\frac{Q}{2}\left[1-\cos(\theta_{j\beta,i\alpha})\right]\left[a_{\alpha}^{+}(i)a_{\beta}^{+}(j)+a_{\alpha}(i)a_{\beta}(j)\right]\left.\right\}. \quad (51)$$

A comparison of this equation with Eq. (11) indicates that adding ΔE_Q^{eff} to the Hamiltonian in Eq. (13) leads replacing the matrices \mathbf{I} , $\mathbf{A}(\mathbf{q})$, and $\mathbf{B}(\mathbf{q})$ in Eqs. (29) as

$$\begin{aligned} \mathbf{I} &\rightarrow \left(1 + \frac{4Q}{3JS}\right)\mathbf{I} \\ \mathbf{A}(\mathbf{q}) &\rightarrow \left(1 - \frac{Q}{2J'S}\right)\mathbf{A}(\mathbf{q}) \\ \mathbf{B}(\mathbf{q}) &\rightarrow \left(1 + \frac{Q}{2J'S}\right)\mathbf{B}(\mathbf{q}) \end{aligned} \quad (52)$$

such that the matrices \mathbf{H}_1 and \mathbf{H}_2 given in Eqs. (29) now are

$$\mathbf{H}_1(\mathbf{q}) = 6JS\left[\left(1 + \frac{4Q}{3JS}\right)\mathbf{I} + [2J'/(3J)]\left(1 - \frac{Q}{2J'S}\right)\mathbf{A}(\mathbf{q})\right] \quad (53a)$$

$$\mathbf{H}_2(\mathbf{q}) = 6JS\left[\gamma(\mathbf{q})\mathbf{I} + [2J'/(3J)]\left(1 + \frac{Q}{2J'S}\right)\mathbf{B}(\mathbf{q})\right]. \quad (53b)$$

After inserting the above replacements into the expressions of the spin-wave modes in Eq. (32), the modes when quantum fluctuations are included are

$$\begin{aligned} \omega_m^2(\mathbf{q}) &= \text{Tr}[(H_1(\mathbf{q}) + H_2(\mathbf{q}))(H_1(\mathbf{q}) - H_2(\mathbf{q}))] \\ &= (6JS)^2\left(1 + \gamma(\mathbf{q}) + \frac{4Q}{3JS}(1 - (-1)^m s(\mathbf{q})) + \frac{4J'}{3J}(-1)^m c(\mathbf{q})\right) \\ &\quad \times \left(1 - \gamma(\mathbf{q}) + \frac{4Q}{3JS}(1 - (-1)^m c(\mathbf{q})) + \frac{4J'}{3J}(-1)^m s(\mathbf{q})\right) \end{aligned} \quad (54)$$

Here $c(\mathbf{q})$ and $s(\mathbf{q})$ are given in Eqs. (24). As $\mathbf{q} \rightarrow 0$ one has $\gamma(\mathbf{q}) \rightarrow 1$, $s(\mathbf{q}) \rightarrow 0$, $c(\mathbf{q}) \rightarrow 1$ and therefore

$$\begin{aligned} \omega_m^2(\mathbf{q} \rightarrow 0) &\approx (6JS)^2 2(1 - (-1)^m)\left(\frac{4Q}{3JS}\right) \\ &= 192JSQ \quad \text{for } m = 1 \\ &= 0 \quad \text{for } m = 2. \end{aligned} \quad (55)$$

This result indicates that in the two-fold manifold of zero wavevector modes which are degenerate within linearized spin-wave theory, quantum fluctuations give a nonzero energy so that only one Goldstone mode remains at zero energy.

2.2. Interacting Spin-Wave Theory– Hartree Decoupling of Fourth Order Interaction Terms

The objective of this subsection is to obtain the spin-wave gap by including the effect of quantum zero-point motion. In the previous subsection we showed that a biquadratic

exchange interaction given in Eq. (49) predicts a spin gap with one zero-energy mode at $\mathbf{q} = 0$ (Goldstone mode). Here we perform an interacting spin-wave calculation using the standard Hartree decoupling of the fourth order interaction terms which is known to give correctly all contributions to the spin-wave energies at relative order $(1/S)$. Since the procedure gives the same structure of the spin-wave spectrum at zero wavevector, we may use its result to determine the strength of the biquadratic interaction, Q in Eq. (49):

$$Q = -\frac{J'}{2} \left([\langle a_\alpha^+(i) a_\beta^+(j) \rangle]_{ap} + [\langle a_\alpha^+(i) a_\beta(j) \rangle]_p \right), \quad (56)$$

where $\langle \dots \rangle$ indicates a ground state expectation value and the subscripts "p" and "ap" indicate that $\alpha(i)$ and $\beta(j)$ must be associated with parallel or antiparallel spins, respectively.

For this purpose we use the Dyson-Maleev transformation given in Eqs. (5-7) and the local quantization axis defined by the rotation matrix in Eq. (4). Thus, one can obtain

$$\mathbf{S}_\alpha(i) \cdot \mathbf{S}_\beta(j) = S^2 \cos(\theta_{j\beta,i\alpha}) + \hat{O}_{j\beta,i\alpha}^{(2)} + \hat{O}_{j\beta,i\alpha}^{(4)} + O(1/S), \quad (57)$$

where $\hat{O}_{j\beta,i\alpha}^{(2)}$ is given in Eq. (11) and the four operator term $\hat{O}_{j\beta,i\alpha}^{(4)}$ is

$$\begin{aligned} \hat{O}_{j\beta,i\alpha}^{(4)} = & \frac{1}{4} [1 + \cos(\theta_{j\beta,i\alpha})] [2n_\alpha(i)n_\beta(j) - a_\alpha^+(i)a_\alpha^+(i)a_\alpha(i)a_\beta(j) - a_\beta^+(j)a_\beta^+(j)a_\beta(j)a_\alpha(i)] \\ & - \frac{1}{4} [1 - \cos(\theta_{j\beta,i\alpha})] [2n_\alpha(i)n_\beta(j) + a_\alpha^+(i)a_\alpha^+(i)a_\alpha(i)a_\beta^+(j) + a_\beta^+(j)a_\beta^+(j)a_\beta(j)a_\alpha(i)] \end{aligned} \quad (58)$$

In first order in $1/S$ we simply take out all contractions of operator averages, to get an effective biquadratic interaction from $\hat{O}_{j\beta,i\alpha}^{(4)}$,

$$\begin{aligned} \hat{O}_{j\beta,i\alpha}^{(2),\text{eff}} = & \text{Const.} + \frac{L-M}{2} [n(i) + n(j)] + \frac{L+M}{2} \cos(\theta_{j\beta,i\alpha}) [n(i) + n(j)] \\ & - \frac{1}{2} L [1 + \cos(\theta_{j\beta,i\alpha})] [a_\alpha^+(i)a_\beta(j) + a_\beta^+(j)a_\alpha(i)] \\ & - \frac{1}{2} M [1 - \cos(\theta_{j\beta,i\alpha})] [a_\alpha^+(i)a_\beta^+(j) + a_\beta(j)a_\alpha(i)], \end{aligned} \quad (59)$$

where i and j are neighboring sites on different sublattices α and β and

$$\begin{aligned} L = & \langle a_\alpha^+(i)a_\alpha(i) \rangle - [\langle a_\alpha^+(i)a_\beta(j) \rangle]_p, \\ M = & \langle a_\alpha^+(i)a_\alpha(i) \rangle + [\langle a_\alpha^+(i)a_\beta^+(j) \rangle]_{ap}. \end{aligned} \quad (60)$$

In order to get above expressions, we used the fact that operator averages of the terms which have the factor $[1 + \cos(\theta_{j\beta,i\alpha})]$ only need to be taken over parallel spins. Similarly those terms which have the factor $[1 - \cos(\theta_{j\beta,i\alpha})]$ need to be averaged over antiparallel spins. We also note that

$$[\langle a_\alpha^+(i)a_\beta^+(j) \rangle]_p = [\langle a_\alpha^+(i)a_\beta(j) \rangle]_{ap} = 0 \quad (61)$$

Using the same argument given in the previous section, one can easily see that adding $\hat{O}_{j\beta,i\alpha}^{(2).eff}$ into the Hamiltonian leads to the following replacements

$$\begin{aligned}\mathbf{I} &\rightarrow \left(1 + \frac{2J'(L-M)}{3JS}\right) \mathbf{I} \\ \mathbf{A}(\mathbf{q}) &\rightarrow [1 - (L/S)]\mathbf{A}(\mathbf{q}) \\ \mathbf{B}(\mathbf{q}) &\rightarrow [1 - (M/S)]\mathbf{B}(\mathbf{q}),\end{aligned}\quad (62)$$

so that the matrices \mathbf{H}_1 and \mathbf{H}_2 given in Eqs. (29) now are

$$\mathbf{H}_1(\mathbf{q}) = 6JS \left[\left(1 + \frac{2J'(L-M)}{3JS}\right) \mathbf{I} + \frac{2J'}{3J} \left(1 - \frac{L}{S}\right) \mathbf{A}(\mathbf{q}) \right] \quad (63)$$

$$\mathbf{H}_2(\mathbf{q}) = 6JS \left[\gamma(\mathbf{q})\mathbf{I} + \frac{2J'}{3J} \left(1 - \frac{M}{S}\right) \mathbf{B}(\mathbf{q}) \right]. \quad (64)$$

Therefore the new spin-wave modes are

$$\begin{aligned}\omega_m^2(\mathbf{q}) &= (6JS)^2 \\ &\times \left(1 + \frac{2J'(L-M)}{3JS} + \gamma(\mathbf{q}) + (-1)^m \frac{2J'}{3J} \left[\left(1 - \frac{L}{S}\right)(c(\mathbf{q}) + s(\mathbf{q})) + \left(1 - \frac{M}{S}\right)(c(\mathbf{q}) - s(\mathbf{q})) \right] \right) \\ &\times \left(1 + \frac{2J'(L-M)}{3JS} - \gamma(\mathbf{q}) + (-1)^m \frac{2J'}{3J} \left[\left(1 - \frac{L}{S}\right)(c(\mathbf{q}) + s(\mathbf{q})) \left(1 - \frac{M}{S}\right)(c(\mathbf{q}) - s(\mathbf{q})) \right] \right) \quad (65)\end{aligned}$$

As \mathbf{q} goes to zero, one obtains

$$\begin{aligned}\omega_m^2(\mathbf{q}) &\approx (6JS)^2 2 \frac{2J'(L-M)}{3JS} \left(1 - (-1)^m\right) \\ &\approx -48JJ'S \left([\langle a_\alpha^+(i)a_\beta^+(j) \rangle]_{ap} + [\langle a_\alpha^+(i)a_\beta(j) \rangle]_p \right) \left(1 - (-1)^m\right),\end{aligned}\quad (66)$$

where m takes the values 1 and 2. Comparing this with Eq. (55) one identifies Q as in Eq. (56). Note that because Eqs. (54) and (65) are not of the same form, this identification of Q only applies to the zero wavevector spectrum. However, for the actual values of J', J, L , and M , the modified spin-wave spectrum obtained from Eq. (65) or from the effective biquadratic interaction given in Eq. (54) (with Q from above equation) is almost identical in the whole zone.[14] From our calculation, it is apparent that the quantum corrections to the spin waves mainly occur at wavevectors close to the zone center, where they open a gap at $\mathbf{q} = 0$, leaving one Goldstone mode at zero energy.

One might think that the above procedure could be used to determine the temperature dependence of the gap, if the averages were interpreted as thermal averages, rather than ground state averages. This approach would lead us to believe that the quantum gaps would *increase* as the temperature is increased. This behavior strongly disagrees with experiments,[19] which showed that the quantum gap has a temperature dependence close

to that of the order parameter. In the boson calculation as outlined above, the result is that the quantum gap energy, ω_q for a fixed value of J'/J is given by

$$\omega_q = (1/S)f_1[kT/(JS)] , \quad (67)$$

where df/dx is positive. More generally one would expect a result of the form

$$\omega_q = (1/S)f_1[kT/(JS)] + (1/S^2)f_2[kT/(JS)] + O(1/S^3) . \quad (68)$$

Presumably, the second term dominates at all but the very lowest temperatures. A possible mechanism for this is that the spectral weight functions in a bosonic formulation are usually replaced, in a more accurate calculation, by spectral weight functions associated with spin operators, which have an amplitude proportional to $\langle S_z \rangle$ rather than to unity. Replacement of $\langle a_\alpha^+(i)a_\beta^+(j) \rangle_T$ by $\langle S_z \rangle_T \langle a_\alpha^+(i)a_\beta^+(j) \rangle_T$ would lead to the experimental result. We are presently considering how to make this argument in detail.

3. Systems with More Than One Zero Modes

All of the studies on a very large number of frustrated magnetic systems show that "order by disorder" is very general in that it should exist in many quantum systems with a classically degenerate ground state. In the cases of interest to us here, it is found that quantum fluctuations favor states in which spins are collinear. Hence, for a system where all possible collinear states are symmetry equivalent, the removal of the infinite degeneracy of the ground state manifold by quantum fluctuations is as complete as permitted by symmetry and one has a ground state with no accidental degeneracy. To the best of our knowledge all collinear systems studied so far are of this type and hence it is of interest to study how quantum fluctuations select a unique ground state if the collinear states are not all symmetry equivalent. This issue is addressed in this section by studying two particular systems, namely quantum spins with nearest neighbor AF interactions on a body-centered tetragonal (BCT) lattice and on a face-centered cubic (FCC) lattice. In these systems, the Shender mechanism can only resolve the continuous degeneracy of the ground state manifold into an infinite discrete Ising type degeneracy, as we discussed above. The selection of a unique ground state out of this infinite Ising type degenerate manifold requires higher order effects of quantum fluctuations. We will briefly discuss this below.

3.1. Ground State Selection in FCC Antiferromagnets

In this section we are concerned with the determination of the ground state of quantum Heisenberg antiferromagnets on a face-centered cubic (FCC) lattice in the case when the second neighbor isotropic antiferromagnetic interaction of the form $J\mathbf{S}_i \cdot \mathbf{S}_j$ dominates the isotropic nearest neighbor interaction (with coupling constant J'), as illustrated in Figure 4.

A seminal study of the classical ground state of this system was given by Yamamoto and Nagamiya.[20] In particular, a relevant structure to study is that which they called

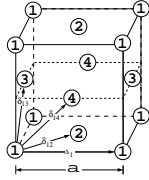


Figure 4. Four antiferromagnetic sublattices on a FCC lattice. Nearest neighbors within a given simple cubic sublattice are specified by vectors Δ , of which one is shown. Interactions between nearest neighbors on the same sublattice are proportional to J and those between sublattices by J' . A few nearest-neighbor vectors $\delta_{\alpha,\beta}$ connecting different sublattices α and β are shown.

type AF-II (we will refer to it as the "second kind"), which has a two-fold degeneracy between inequivalent structures called type A and type B, as shown in Fig. 5, and whose domain of stability for the classical ($S \rightarrow \infty$) case is $|J'| < 2|J|$. [21] This degeneracy of the ordering of the second kind was found to be extremely robust: it was not removed by either a tetragonal distortion, or by tetragonal anisotropy. [20] This system may be viewed as four interpenetrating simple cubic antiferromagnetic sublattices in which the mean field on one sublattice due to any of the other vanishes. Thus this system provides yet another example of one which classically has a continuous degeneracy which we expect to be lifted by quantum fluctuations. [1] The phenomenological biquadratic interaction mentioned above causes the sublattices to be collinear, but it does not resolve the degeneracy between structures of type A and type B. As we shall see, the degeneracy between type A and type B structures is removed when the effects of quantum fluctuations are included to higher order in J'/J . For this type of calculation the formalism introduced in the previous section is convenient. We also point out that in real systems there may be mechanisms other than quantum fluctuations which could remove the degeneracy between the collinear states. For example, dipolar interactions, single-ion anisotropy, biquadratic exchange interactions, or elastic strain effects due to the dependence of the exchange tensor on atomic displacements, *etc.* may play an important role. However, for the purpose of this paper, we are interested in understanding the effects that quantum fluctuations alone can have on the ground state selection and therefore we will give little consideration to other possible interactions not included in the Hamiltonian given below.

We start with the following Hamiltonian

$$\mathcal{H} = \sum_{\langle ij;1 \rangle} J' \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle ij;2 \rangle} J \mathbf{S}_i \cdot \mathbf{S}_j, \quad (69)$$

where $\langle ij; n \rangle$ indicates that the sum is over pairs of n th nearest neighbors. We are mainly concerned with the case when J is dominant, and the system can be considered to be four interpenetrating simple cubic antiferromagnetic sublattices. As we mentioned previously, the effect of quantum fluctuations at second order in J'/J is to cause the spins to be

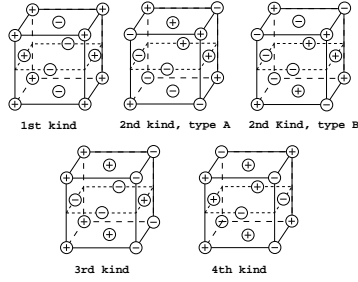


Figure 5. Various non-equivalent collinear spin arrangements in the face-centered cube. (–) and (+) represent spins up and down with respect to any given direction.

arranged collinearly.[4] Therefore, for the α th simple cubic antiferromagnetic sublattice we introduce an Ising variable σ_α to specify its phase, so that σ_α gives the value of S_z for the spin at position τ_α , where τ_α is $(0,0,0)$ for $\alpha = 1$ and $(0.5,0.5,0.5)$ for $\alpha = 2$. In terms of these variables, the ground state energy, i. e. the effective interaction, denoted \mathcal{H}_{eff} , then must be of the form:

$$\mathcal{H}_{\text{eff}}/J = C_0 + C_2(\sigma_1\sigma_2 + \dots + \sigma_3\sigma_4) + C_4\sigma_1\sigma_2\sigma_3\sigma_4 , \quad (70)$$

where the coefficients C_n depend on J'/J and $1/S$. In writing this result we omitted odd-order terms in the σ_i , since the original Hamiltonian of Eq. (69) is invariant under $\mathbf{S}_i \rightarrow -\mathbf{S}_i$ for all i . Now it is possible to eliminate some terms in Eq. (70) using the symmetry operations of the system. First of all, the reflection operation with respect to the $[100]$, $[010]$ or $[001]$ planes should not change the energy. Since these symmetry operations change the sign of any two σ_i , the coefficients C_2 in Eq. (70) must be zero. Thus we have

$$\mathcal{H}_{\text{eff}}/J = C_0 + C_4\sigma_1\sigma_2\sigma_3\sigma_4 . \quad (71)$$

Since there is no symmetry operation which changes the sign of the only one σ_i (or equivalently, three of them), the term $\sigma_1\sigma_2\sigma_3\sigma_4$ is allowed by symmetry. It therefore follows that we have two inequivalent collinear spin arrangement in which $\sigma_1\sigma_2\sigma_3\sigma_4$ is minus or plus one. (See Fig. 5.) The first one where $\sigma_1\sigma_2\sigma_3\sigma_4 = -1$ is called “the second kind of type A.” For this configuration it is possible to find a unique $[111]$ direction, perpendicular to which, each net plane contains a ferromagnetic array of spins and the sequence of such net planes is stacked antiferromagnetically. In other words, this structure has trigonal crystal symmetry and therefore subject to a rhombohedral distortion. In contrast, ordering of “the second kind of the type B” (also shown in Fig. 5) for which ($\sigma_1\sigma_2\sigma_3\sigma_4 = 1$), still has cubic symmetry.

In order to determine which of these structures is really the ground-state configuration, we therefore need to know the sign of C_4 in Eq. (71). In Ref.[14] we studied the complete removal of the remaining degeneracy between these two inequivalent of

collinear structures by analyzing the contribution to the spin-wave zero-point energy which is shown to be of the form;

$$\mathcal{H}_{\text{eff}}/J = C_0 + C_4\sigma_1\sigma_2\sigma_3\sigma_4(J'/J)^4 + O(J'/J)^5,$$

where C_4 is a positive constant. (The term of order $(J'/J)^5$ is also given in Ref. [14] explicitly.) Therefore the spin structure with $\sigma_1\sigma_2\sigma_3\sigma_4 = -1$, known as *second kind of type A*, is chosen to be the ground state by quantum fluctuations. We note that in this particular spin configuration, the magnetic symmetry is trigonal and therefore the magnetic ordering should give rise to a structural distortion away from cubic symmetry. In fact, most of the monoxides of the iron group elements, [20, 22, 23] such as MnO, have the magnetic structure found here and exhibit a small trigonal distortion from cubic symmetry. However we mention a caution that in these real systems there may be other energies, such as single ion anisotropy, dipolar, further neighbor, or magnetoelastic interactions, which should be considered together with those discussed here.

3.2. 3D Ordering in BCT Antiferromagnets

Three dimensional magnetic ordering in BCT antiferromagnet is of special interest because the magnetic properties of such structures are believed to be relevant to high temperature superconductivity. The most important example of such layered structures is perhaps La_2CuO_4 [24] in which long-range magnetic order is observed below $T_N \sim 300$ K. However it is now believed that most of the magnetic properties can be understood in terms of the Dzyaloshinskii–Moriya interaction which arises due to the orthorhombic distortion. [25] Recently, new systems which preserve the tetragonal symmetry at all temperatures have been studied. Rare-earth (R) cuprates, R_2CuO_4 [26] (which superconduct after electron doping [27]) and $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ [28] are the most studied ones. In particular, the latter compound is the best experimental realization of the system that we are going to study in this subsection. However, as we have discussed in Ref. [29], there are other type of interactions, such as the magnetic dipole interaction, magnetic anisotropy, and biquadratic exchange interactions, which may compete with the effective interactions due to quantum disorder we are going to calculate here. Accordingly, it is important to calculate the effective interaction due to quantum fluctuations in order to compare its strength with that of other interactions.

We now describe in detail the model that we are going to study. We consider a BCT antiferromagnet with dominant antiferromagnetic interactions between nearest neighbor in the same basal plane and weaker interactions between nearest neighbors in adjacent planes, as illustrated in Fig. 6. (The interplane interactions may be either ferromagnetic or antiferromagnetic.) We write the Hamiltonian as

$$\mathcal{H} = \sum_{p=1}^M H_p + \sum_{p=1}^{M-1} H_{p,p+1} \quad (72)$$

where H_p refers to the p -th plane alone and is given by

$$H_p = J \sum_{i, \delta_1} \mathbf{S}_p(\mathbf{r}_i) \cdot \mathbf{S}_p(\mathbf{r}_i + \delta_1) \quad (73)$$

and the interaction $H_{p,p+1}$ between the p th and $(p+1)$ -th planes is

$$H_{p,p+1} = 2J_\perp \sum_{i, \delta_2} \mathbf{S}_p(\mathbf{r}_i) \cdot \mathbf{S}_{p+1}(\mathbf{r}_i + \delta_2) \quad (74)$$

where $\mathbf{S}_p(\mathbf{r}_i)$ is the spin at position \mathbf{r}_i in plane p . Also δ_1 and δ_2 are the vectors joining a site to its NN's in-plane and NN's out-of-plane, respectively, as shown in Fig. 6.

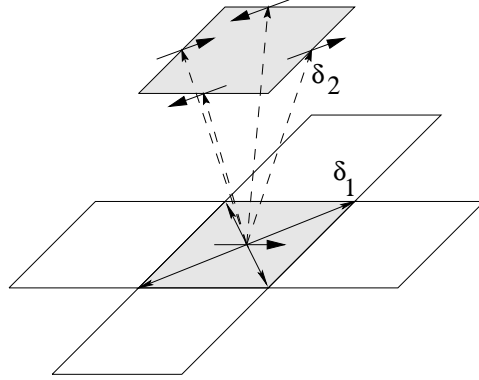


Figure 6. A spin with its interactions. The full lines show the nearest-neighbor vectors, $\vec{\delta}_1$ in the plane for the interaction J . The dashed lines show the nearest-neighbor vectors $\vec{\delta}_2$ from the p th plane to the $p+1$ st plane (above it) for the interaction J_\perp . Note that the mean field interaction between adjacent planes is zero and thus the direction of the staggered magnetization in each plane is arbitrary.

From the results of the previous section, we one may conclude that zero-point fluctuations give rise to a collinearity zero-point energy of order

$$\Delta E \sim -J_\perp^2 S [1 + (\hat{n}_i \cdot \hat{n}_{i+1})^2] / J, \quad (75)$$

where J (J_\perp) is the antiferromagnetic coupling between nearest-neighbor spins in the same (adjacent) basal plane of the BCT lattice and \hat{n}_i defines the orientation of the staggered magnetization in the i th plane. Thus the continuous degeneracy with respect to the orientations of the \hat{n} 's, is resolved into a two-fold degeneracy for each collinear \hat{n}_i . Actually, the exact symmetry of this Heisenberg system is such that if one fixes the \hat{n}_i for alternate (even-numbered, say) planes, then the configuration obtained by the replacement for all odd-numbered layers $\hat{n}_i \rightarrow -\hat{n}_i$ is degenerate in energy with

the original one. This exact symmetry (due to the four-fold axes of the tetragonal crystal) indicates that there is no possibility of finding an effective interaction of the form $C\hat{n}_i \cdot \hat{n}_{i+1}$. However, symmetry DOES allow an interaction of the form $C\hat{n}_i \cdot \hat{n}_{i+2}$, which would uniquely fix the orientation of all even numbered layers with respect to one another. One should note the physical origin of these zero-point effects: although the classical ground-state energy is independent of the \hat{n} 's, the spin-wave spectrum does depend on these variables. Thus the quantum zero-point motion, which involves a sum over spin-wave energies, can introduce a dependence on the \hat{n} 's and thus lead to ground-state selection.

In order to treat arbitrary configurations we take advantage of the well established fact that zero-point fluctuations favor collinear structures.[4] We study the complete removal of the remaining degeneracy of the collinear spin structures by assigning an arbitrary sign σ_i ($i = 1, 2, \dots, M$) to the staggered moment of the planes as shown in Fig. 7. We then develop an expansion scheme in which we can calculate the zero-point energy for an arbitrary set of these Ising variables. We carry the calculations of the ground-state energy up to the order in J_{\perp}/J at which the classical degeneracy is first removed.

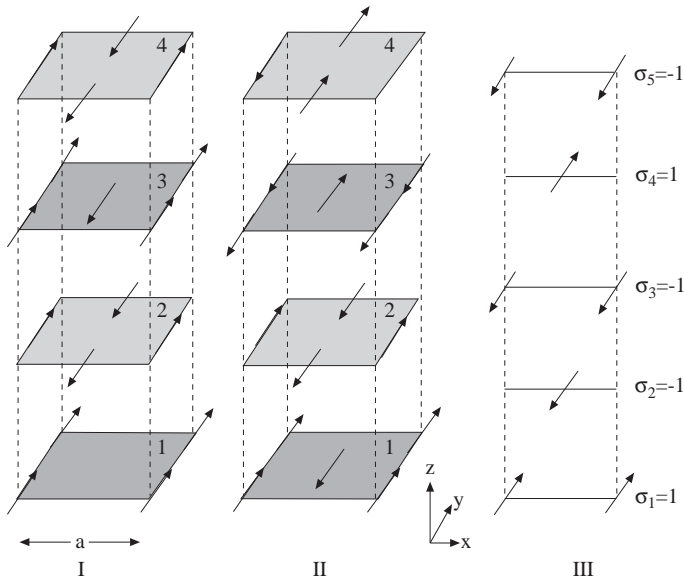


Figure 7. Various spin structures. Structures I and II have unit cells which span 2 and 4 planes (perpendicular to \hat{z}), respectively. In the right-most panel, spins of an arbitrary structure (III) in the plane $y = 0$ are shown. The values of σ_i for the i th plane perpendicular to \hat{z} are given.

If we write the quantum zero-point energy, E_Q as $E_Q = E_C[1 + \Delta e_Q]$, where E_C is the classical ground-state energy of a single plane, then Δe_Q can be calculated as a

perturbation series in j and $1/S$. At first order in $1/S$ and up to the sixth order in $j = J_{\perp}/J$, the leading contribution to Δe_Q which involves the configuration of the planes (assumed to be collinear) is

$$E(\{\sigma_i\}) = E_1 + CE_G(j^6/S) \left[-2\sigma_1\sigma_3 - 2\sigma_{M-2}\sigma_M + 2 \sum_{i=1}^{M-2} \sigma_i\sigma_{i+2} - 3 \sum_{i=1}^{M-3} \sigma_i\sigma_{i+1}\sigma_{i+2}\sigma_{i+3} \right],$$

where $C > 0$ and E_1 are constants independent of the σ 's, and E_G is the classical ground-state energy. (Here sums from i to j when $j < i$ are interpreted to be zero.) This result shows that for $M > 4$ second-neighboring planes are antiferromagnetically coupled in the ground state and thus the three dimensional spin structure can not be described by a single wave vector, as is often assumed. Thus the entire structure has only the degeneracy associated with the relative phase of the odd numbered layers relative to the even numbered layers. This degeneracy reflects a true symmetry of the system and can not be removed.

In this way we establish that structure II of Fig. 7 is stabilized by zero-point fluctuations, at least if one considers only effects at order $1/S$. This stabilization energy is of order $J_{\perp}^6 S/J^5$. Surprisingly, there is no σ -dependent contribution at order j^4/S . Since J_{\perp}/J can be very much smaller than $1/S$, we carried out perturbation theory in $1/S$, to locate contributions to the stabilization energy which were of order J_{\perp}^4/J^3 but were higher order in $1/S$. We found a stabilization energy of order $J_{\perp}^4/(J^3 S)$. As with the zero-point energy of linear spin-waves, this energy stabilizes structure II of Fig. 7.

An interesting result from the effective interaction given above is found for a system consisting of a small number of BCT layers. In particular, for a three-layer system, we find that the first and third layers are parallel to one another in the ground state. It would also be interesting to study experimentally a system with four BCT layers. In that case our results indicate that all configurations in which both next-nearest neighboring planes are parallel are degenerate with those in which both next-nearest neighboring planes are antiparallel. Although this degeneracy will no doubt be removed by higher order effects, it does suggest the possibility of obtaining unusual spin structures in extremely thin film systems.

4. Kagomé Antiferromagnet: a System With Macroscopic Zero Energy Modes

The nearest neighbor Heisenberg antiferromagnet on kagomé lattice, shown in Fig. 8, is one of the most studied example of a system with a macroscopic number of zero modes. The interest in kagomé antiferromagnet was initiated by its proposal as a model for two experimental systems; the insulating layered compound $\text{SrCr}_{8-x}\text{Ga}_{4+x}\text{O}_{19}$ [10] and a second layer of ^3He adsorbed on graphite[11]. From the theoretical point of view, the model is particularly interesting since it has all the ingredients such as low dimensionality,

strong frustration, and low coordination number, required for a disordered "spin liquid" ground state.

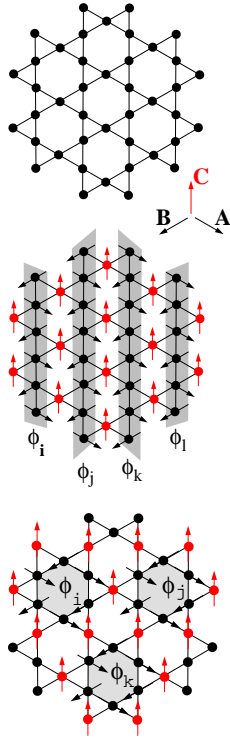


Figure 8. Top: Kagomé lattice for which the nearest neighbor antiferromagnet exhibits strong frustration. **Middle:** Kagomé lattice with $\mathbf{q}=0$ spin structure. Note that the classical ground state energy does not depend on the angles (shown as ϕ_i, ϕ_j , etc) of the infinitely long chains of A–B spins. **Bottom:** $\sqrt{3} \times \sqrt{3}$ structure in which each hexagon of A–B spins have an arbitrary angle (denoted as ϕ_i, ϕ_j , etc) with respect to C–spin axis.

The model considered here is described by the following Hamiltonian,

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (76)$$

where the sum runs over all the nearest-neighbor pairs on the kagomé lattice. In the classical limit, all ground states satisfy the "120° structure", in which the angle between each pair of nearest-neighbor spins is 120°. Two such spin structures (so called $\mathbf{q}=0$ and $\sqrt{3} \times \sqrt{3}$) are shown in Fig. 8. From these two particular spin structures, one can easily see that the degree of degeneracy in kagomé lattice is very large. For example, in the

$\mathbf{q}=0$ coplanar structure, one can generate new spin configurations by rotating an infinitely long chain of spins A–B about the spin direction C without changing the total energy as shown in Fig. 8. Similarly, in the $\sqrt{3} \times \sqrt{3}$ structure, rotation of A–B–A–B–A–B spins on a single hexagon about the spin direction C also does not change the energy of the system. Hence, unlike the cases of BCC, FCC, and even BCT antiferromagnets where number of zero–energy modes are not macroscopic, in the kagomé antiferromagnet the degree of freedom to describe the ground state manifold is macroscopic.

Kagomé antiferromagnet has been extensively studied by spin wave theory[30, 31, 32], by various numerical techniques such as quantum monte carlo[30] and exact diagonalization for finite systems[33, 34], by perturbation[35], high–temperature[30], and N expansion[36] techniques, etc. Hence, here we will not repeat any of these studies but will give only simple ideas to see how "order by disorder" work in this interesting system.

4.1. Coplanar Ordering by Disorder

In the case of BCC antiferromagnet discussed in Sec. II, the actual calculations of an effective interaction due to quantum fluctuations are not overly complicated, and in fact, a simplified calculation [3,4] is both quite short and quite easy to understand. However, the case of BCC antiferromagnet involves only the removal of a one–parameter degeneracy. In Sec. III we have seen that more complicated removal of degeneracy involving higher order corrections in J'/J , but still at first order in $1/S$ occur for the BCT and FCC antiferromagnets with strong second neighbor interactions. However the kagomé antiferromagnet [6] presents an even more pathological situation.

Consider the so-called " $\sqrt{3} \times \sqrt{3}$ " structure shown in Fig. 8. Here the C sublattice spin point along the positive z -direction, which we refer to as the 12 o'clock direction. In each hexagon of A and B spins one can place the A spins along the 4 o'clock direction and the B spins along the 8 o'clock direction. To fully specify the orientations of the A and B spins in a given hexagon we have to specify the angle ϕ which the normal to the face of the clock makes with a fixed axis. It is easy to see [7,8] that the ground–state manifold of the classical system includes the direct product space in which each A-B hexagon is assigned an arbitrary value of ϕ over the interval $[0, 2\pi]$. Furthermore, the classical spin–wave spectrum, or equivalently, the spectrum of noninteracting spin waves in the quantum model, has zero–energy local modes corresponding to varying the ϕ for any given hexagon of A-B spins [8,9]. Furthermore, as we will see below, the noninteracting spin wave spectrum is exactly the same for all coplanar configurations. This surprising hidden gauge symmetry has been previously noted by Calker et al.[8] In view of the discussion of Eqs. (44) we expect that the degeneracy present in the classical system is only completely removed by quantum fluctuations at relative order $1/S^2$. Thus this situation is decidedly more complicated than that analyzed by Shender [1]. Here a) the classical ground state degeneracy corresponds to the macroscopic entropy of a finite number of free angles per lattice site, and b) the removal of degeneracy is not complete at first order in $1/S$. Thus, the ground state energy, E_G , is of the form

$$E_G = -C_2^2 JS^2 \left(1 + \frac{\alpha}{S} + \frac{\beta}{S^2} \dots\right). \quad (77)$$

where C_2 (and later C_n) is a constant. A simple calculation analogous to that leading to the result of Eq. (44) here yields

$$\alpha = -C_4^2 \sum_{\langle i,j \rangle} |\sin(\phi_i - \phi_j)| \quad (78)$$

where i and j labels hexagons and $\langle i, j \rangle$ indicates a sum over pair of nearest neighboring hexagons both of which involve the same two sublattices (e. g. both are A,B hexagons, both are A,C hexagons, or both are B,C hexagons). Note that α is minimized for coplanar spin arrangement: $\phi_i - \phi_j = 0, \text{ mod } \pi$. Thus at this order all A-B hexagons must have their spins in the same plane. Thus we set $\exp(i\phi_i) = \sigma_i$, and coplanarity requires that each σ_i is $+$ or $-$ 1. But since, at this order in $1/S$, each of these variables can be chosen independently in the ground state manifold, there remains an Ising degeneracy. This remaining Ising degeneracy is only resolved by including the term in Eq. (77) proportional to β . As we discuss below, this term favors the so-called " $\sqrt{3} \times \sqrt{3}$ " structure discussed by Elser[30] and by Harris *et al*[31].

The corresponding calculation of the spin-wave spectrum is much more delicate. If one includes spin-wave interactions within lowest order perturbation theory one would expect to obtain a finite energy for the modes in view of the effective potential of Eq. (78) induced by quantum interactions. Indeed, a simple decoupling of the fourth-order spin-wave interactions as done in Sec.II leads to the local mode frequency, ω_l as

$$\omega_l^2 = C_4^2 S \langle n \rangle, \quad (79)$$

where n is the number of Bose excitations and $\langle \rangle$ indicates a ground state average. However, this calculation is not self-consistent because a frequency of order $S^{1/2}$ leads to $\langle n \rangle$ being of order $S^{1/2}$. The self-consistent version of Eq. (79) is

$$\omega_l^2 = C_5^2 S(S/\omega_l) \quad (80)$$

which leads to

$$\omega_l \sim S^{2/3}. \quad (81)$$

It seems likely, then, that the effective potential favors coplanarity, as in Eq. (78), but would have a different dependence on S than given in that equation.

The final question one has to consider is the removal of the Ising degeneracy characterized by the σ_i 's. A calculation[37] of the lowest order perturbation contribution to the energy which depends on these variables gives a contribution to β in Eq. (77) of the form

$$\beta \sim -C_6^2 \sum_{i,j} \sigma_i \sigma_j, \quad (82)$$

which favors a "ferromagnetic" arrangement of the σ 's. This arrangement is precisely the " $\sqrt{3} \times \sqrt{3}$ " structure studied previously [6,9]. The elementary excitations thus consist of Ising-like excitations from the ferromagnetic ground state of the σ variables. In addition, relative to any such Ising state there are spin-wave excitations. In true thermodynamic equilibrium these latter excitations would dominate the low-temperature thermodynamics. However, it is not entirely clear that it would be easy to establish equilibrium. We note that the energy barrier between different σ configurations involves the energy of order S in Eq. (77), whereas the difference between the different metastable minima (for different σ configurations) is, by Eqs. (77) and (82), of order 1. In the large S limit, one could easily envision very slow equilibration.

5. Conclusion

In this paper we briefly review the phenomenon *order by disorder* in frustrated quantum magnetic systems. We may summarize our conclusions as follows.

- It is shown that a ground state degeneracy arises as the system is unable to simultaneously satisfy the minimum energy condition for all bonds in the system; *phenomenon known as "frustration"*. Depending on the symmetry of the system, this extra degeneracy can develop finite, infinite (but not macroscopic) and even macroscopic (as in kagomé AF) number of zero energy modes in spin wave spectrum.
- Quantum disorder (fluctuations) have a special role in frustrated magnetic systems because they can lift the degeneracy of the ground state manifold and make the system more ordered. Particularly we showed that the infinite degeneracy of the ground state manifold of various systems such as FCC and BCT antiferromagnets is partially removed by collinear ordering at relative order $J'^2/(J^2S)$. The effective interaction between the decoupled (in the mean field sense) sublattices is of the form

$$E_{ZPE} \approx -\left(\frac{J'^2S}{J}\right) \left[1 + \cos(\theta)^2\right]$$

It is shown that high order quantum fluctuations removes the remaining Ising-type degeneracy of the ground state manifold.

- In order to include the effect of quantum fluctuations on the spin-wave modes, we performed an interacting spin-wave calculations using the standard Hartree decoupling of the fourth order interaction terms described by Dyson-Malev transformation to boson. Quantum fluctuations are found to modify the spin-wave spectrum significantly at small \mathbf{q} -vectors. Particularly at $\mathbf{q} = 0$ zero energy modes split into a nonzero modes and one zero energy mode (Goldstone mode). Next we showed that this gap and the modified spin-wave spectrum due to quantum fluctuations can be very well modeled (only at small wavevector) by an effective biquadratic interactions of the form:

$$\Delta E_Q^{\text{eff}} = -\frac{1}{2}Q \sum_{i\alpha, j\beta} (\mathbf{S}_\alpha(i) \cdot \mathbf{S}_\beta(j))^2 / S^3$$

where Q is estimated to be

$$Q = -\frac{J'}{2} \left([\langle a_{\alpha}^{\dagger}(i)a_{\beta}^{\dagger}(j) \rangle]_{ap} + [\langle a_{\alpha}^{\dagger}(i)a_{\beta}(j) \rangle]_p \right),$$

where $\langle \dots \rangle$ indicates a ground-state expectation value.

- We point out that above equation does not form a basis for a consistent calculation of the temperature dependence of the gap because of the reasons discussed in the text. The temperature dependence can be used to demonstrate whether or not the gap is due to quantum fluctuations.[18, 19] It is an open question to show definitively that this temperature dependence is nearly the same as that of the order parameter.
- Finally we consider the AF spins on a kagomé lattice, which forms a system with macroscopic phason modes. It is shown that the degeneracy in the ground state manifold of a classical Heisenberg antiferromagnet on a kagomé lattice is also removed by quantum fluctuations. In the classical ground state one can assign an azimuthal angle ϕ to each independent hexagon of coplanar spins. Quantum fluctuations to lowest order in $1/S$ (i. e. involving zero-point energy of non-interacting spin waves) partially resolve this degeneracy, so that at this order the ground state has all hexagons coplanar, i. e. $\phi_i - \phi_j = 0, \text{mod}\pi$, where ϕ_i is the azimuthal angle of hexagon i . This Ising gauge symmetry is only removed at second order in $1/S$. We discuss that including spin-wave interactions to first order in $1/S$ causes the local modes which classically have zero energy to have a nonzero energy, which is self-consistently calculated to be of order $S^{2/3}$.

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