Chapter 6

Spin waves and quantum fluctuations in Heisenberg magnets

For quantum spins, it is well known that, except in the very special case of ferromagnetic order, there are fluctuations even at zero temperature. When the classical ground state is unique, these fluctuations reduce the order parameter but rarely destroy it altogether in non-frustrated systems except in one dimension. In the presence of frustration, these fluctuations play a much more important role. First of all, they often select among the classical ground states through the zero-point energy, an effect analogous to that of thermal fluctuations and known as quantum order by disorder. Secondly, the reduction of the order parameter is in general significantly enhanced by the competition between exchange channels, often leading to the destruction of the order parameter even in two and three dimensional models, opening the way to quantum spin liquids.

6.1 Holstein-Primakoff expansion

For quantum spins, the components of $\vec{S}_i$ are operators that satisfy the $SU(2)$ algebra:

$$\left[S_i^x, S_i^y\right] = iS_i^z \quad (\hbar = 1) \tag{6.1}$$

and the other two commutation relations obtained by circular permutations of x, y and z. The magnitude S of the spin fixes the value of $\vec{S}^2$ according

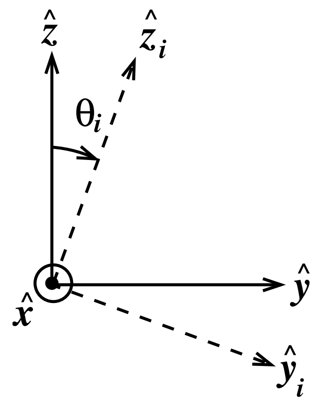

Figure 6.1: Definition of the local reference frame.

to:

$$\vec{S}^2 = S(S+1).$$

S can take all half-integer and integer values $S = 1/2$, 1, 3/2, etc.

The Hamiltonian can be written as:

$$H = \sum_{(i,j)} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{(i,j)} J_{ij} \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \tag{6.2}$$

or

$$H = \sum_{(i,j)} J_{ij} \left[\frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \right]$$

with $S_i^+ = S_i^x + iS_i^y$ and $S_i^- = S_i^x - iS_i^y$. These ladder operators increase or decrease the quantum number along z by 1 according to

$$S^+|S,m\rangle = \sqrt{S(S+1) - m(m+1)}\ |S,m+1\rangle$$
$$S^-|S,m\rangle = \sqrt{S(S+1) - m(m-1)}\ |S,m-1\rangle,$$

where $|S,m\rangle$ is the eigenstate of S^z of eigenvalue m.

If a classical ground state is obtained with the spins $\vec{S}_i$ parallel to $\hat{z}_i$, a natural guess for the quantum ground state is the state:

$$|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes \ldots \tag{6.3}$$

where $|\phi_i\rangle$ is an eigenstate of $\vec{S}_i \cdot \hat{z}_i$ with maximal eigenvalue:

$$\vec{S}_i \cdot \hat{z}_i \, |\phi_i\rangle = S \, |\phi_i\rangle \, . \tag{6.4}$$

However, this state is in general not an eigenstate of H. Indeed, let us consider 2 spins $\vec{S}_i$ and $\vec{S}_j$, and let us take the y and z component in the plane of the two spins (see Fig. 6.1). The scalar product takes the form

$$\vec{S}_i.\vec{S}_j = S_i^x S_j^x + S_i^{y_i} S_j^{y_j} \hat{y}_i.\hat{y}_j + S_i^{z_i} S_j^{z_j} \hat{z}_i.\hat{z}_j + S_i^{y_i} S_j^{z_j} \hat{y}_i.\hat{z}_j + S_i^{z_i} S_j^{y_j} \hat{z}_i.\hat{y}_j$$

or, defining the angle θ_i by

$$\hat{z}_i = \hat{z}\cos\theta_i + \hat{y}\sin\theta_i, \quad \hat{y}_i = -\hat{z}\sin\theta_i + \hat{y}\cos\theta_i,$$

the following form:

$$\vec{S}_i.\vec{S}_j = S_i^x S_j^x + (S_i^{y_i} S_j^{y_j} + S_i^{z_i} S_j^{z_j})\cos(\theta_i - \theta_j) + (S_i^{y_i} S_j^{z_j} - S_i^{z_i} S_j^{y_j})\sin(\theta_i - \theta_j).$$

The state $|\phi_i\rangle \otimes |\phi_j\rangle$ is not an eigenstate of $\vec{S}_i.\vec{S}_j$ because of the ladder operators. The only exception is the ferromagnetic case $\theta_i = \theta_j$. In that case, the last term drops, and the scalar product takes the usual form $\vec{S}_i.\vec{S}_j = \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + S_i^z S_j^z$. Since the projection of the spin along the quantization axis is maximum in $|\phi_i\rangle$ and $|\phi_j\rangle$, $S_i^+ |\phi_i\rangle = S_j^+ |\phi_j\rangle = 0$, and the ladder operators do not affect the states. In all other cases, ladder operators couple $|\phi_i\rangle \otimes |\phi_j\rangle$ to other states.

For simplicity, let us concentrate on coplanar ground states and let us assume that the spins lie in the plane perpendicular to x. As discussed in the previous chapter, the angles θ_i must satisfy the minimization condition

$$\sum_{i,j} J_{ij} \sin(\theta_i - \theta_j)$$

for the configuration defined by the θ_i's to be a ground state. Since we want to discuss fluctuations around a state where the projection of the spin $\vec{S}_i$ along z_i is maximal and equal to S, we can write $S_i^{z_i} = S - \delta S_i^{z_i}$ and assume that $\delta S_i^{z_i}$ is small. The last term of $\vec{S}_i.\vec{S}_j$ given by the S contribution to $S_i^{z_i}$ drops because of the minimization condition when summing over the lattice, leading to

$$H \simeq \sum_{(i,j)} J_{ij} [S_i^x S_j^x + (S_i^{y_i} S_j^{y_j} + S_i^{z_i} S_j^{z_j})\cos(\theta_i - \theta_j)]. \tag{6.5}$$

This form of the Hamiltonian is a convenient starting point to treat quantum fluctuations around coplanar, non-collinear ground states. We will just have to check that the terms that we have dropped are indeed negligible.

To treat quantum fluctuations, we perform a $1/S$ expansion starting from the Holstein-Primakoff representation of spins:

$$\begin{cases} S_i^{z_i} = S - a_i^\dagger a_i \\ S_i^+ = \sqrt{2S}\sqrt{1 - \frac{a_i^\dagger a_i}{2S}}\ a_i \\ S_i^- = \sqrt{2S} a_i^\dagger \sqrt{1 - \frac{a_i^\dagger a_i}{2S}} \end{cases} \tag{6.6}$$

where a_i, $a_i^\dagger$ are bosonic operators. Note that the operators S_i^+ and S_i^- are defined with respect to the local axis: $S_i^+ = S_i^x + iS_i^{y_i}$ and $S_i^- = S_i^x - iS_i^{y_i}$.

The first non trivial terms in an expansion in $1/S$ are proportional to S. Indeed, the terms we have dropped when deriving Eq. 6.5 are only $O(S^{1/2})$, and the other terms are $O(1)$. The terms proportional to S can be simply obtained by dropping the square roots and only keeping the terms proportional to S in $S_i^{z_i} S_j^{z_j}$. This leads to a quadratic Hamiltonian in terms of bosonic operators. Indeed, to this order,

$$S_i^x S_j^x = \frac{1}{4}(S_i^+ + S_i^-)(S_j^+ + S_j^-) = \frac{S}{2}(a_i^\dagger a_j + a_j^\dagger a_i + a_i a_j + a_i^\dagger a_j^\dagger),$$

$$S_i^{y_i} S_j^{y_j} = \frac{1}{4}(S_i^+ - S_j^-)(S_i^+ - S_j^-) = \frac{S}{2}(a_i^\dagger a_j + a_j^\dagger a_i - a_i a_j - a_i^\dagger a_j^\dagger)$$

and

$$S_i^{z_i} S_j^{z_j} = S^2 - S(a_i^\dagger a_i + a_j^\dagger a_j)$$

leading to the Hamiltonian:

$$\begin{aligned} H &= \sum_{(i,j)} J_{ij}[S^2 \cos(\theta_i - \theta_j) - S(a_i^\dagger a_i + a_j^\dagger a_j)\cos(\theta_i - \theta_j) \\ &+ \frac{S}{2}(a_i^\dagger a_j + a_j^\dagger a_i)(1 + \cos(\theta_i - \theta_j)) + \frac{S}{2}(a_i a_j + a_i^\dagger a_j^\dagger)(1 - \cos(\theta_i - \theta_j))]. \end{aligned}$$

The diagonalization of this Hamiltonian can be done explicitly if it can be decoupled into a sum of independent terms after a Fourier transform. Before we proceed with the diagonalization, let us look at two interesting examples where this is the case.

Helical states

In that case, the Hamiltonian takes the form

$$\begin{aligned} H &= \frac{1}{2}\sum_i \sum_{\vec{R}_n} J_{\vec{R}_n}[S^2 \cos(\vec{Q}.\vec{R}_n) - S(a_i^\dagger a_i + a_{i+\vec{R}_n}^\dagger a_{i+\vec{R}_n}) \cos(\vec{Q}.\vec{R}_n) \\ &+ \frac{S}{2}(a_i^\dagger a_{i+\vec{R}_n} + a_{i+\vec{R}_n}^\dagger a_i)(1+\cos(\vec{Q}.\vec{R}_n)) \\ &+ \frac{S}{2}(a_i a_{i+\vec{R}_n} + a_i^\dagger a_{i+\vec{R}_n}^\dagger)(1-\cos(\vec{Q}.\vec{R}_n)]. \end{aligned}$$

Replacing $\cos(\vec{Q}.\vec{R}_n)$ by $[\exp(i\vec{Q}.\vec{R}_n) + \exp(-i\vec{Q}.\vec{R}_n)]/2$ and introducing Fourier transforms of the bosonic operators:

$$a_{\vec{k}}^\dagger = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_i} a_i^\dagger, \quad a_i^\dagger = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_i} a_{\vec{k}}^\dagger, \tag{6.7}$$

this Hamiltonian can be rewritten after some algebra as

$$H = \frac{NS^2}{2} J_{\vec{Q}} + \sum_{\vec{k}} \left[B_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{2} A_{\vec{k}} \left(a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}} \right) \right]$$

with

$$\begin{cases} A_{\vec{k}} = \frac{S}{2}\left[J_{\vec{k}} - \frac{1}{2}(J_{\vec{k}+\vec{Q}} + J_{\vec{k}-\vec{Q}}) \right] \\ B_{\vec{k}} = \frac{S}{2}\left[J_{\vec{k}} + \frac{1}{2}(J_{\vec{k}+\vec{Q}} + J_{\vec{k}-\vec{Q}}) - 2J_{\vec{Q}} \right] \end{cases}$$

$J_1 - J_2$ model on square lattice

For the $J_1 - J_2$ model on the square lattice, as we saw earlier, there is a continuous degeneracy defined by the angle θ between the two Néel ordered J_2 sublattices so that $\cos(\theta_i - \theta_j)$ is equal to $\cos\theta$ on horizontal J_1 bonds, $-\cos\theta$ on vertical J_1 bonds, and -1 on J_2 bonds. The Hamiltonian of Eq. 6.5 can thus be written into a form that keeps the periodicity of the square lattice:

$$\begin{aligned} H &= \sum_i [\frac{J_1}{2}\sum_{\vec{\tau}_x} S_i^x S_{i+\vec{\tau}_x}^x + \cos\theta(S_i^y S_{i+\vec{\tau}_x}^y + S_i^z S_{i+\vec{\tau}_x}^z) \\ &+ \frac{J_1}{2}\sum_{\vec{\tau}_y} S_i^x S_{i+\vec{\tau}_y}^x - \cos\theta(S_i^y S_{i+\vec{\tau}_y}^y + S_i^z S_{i+\vec{\tau}_y}^z) \\ &+ \frac{J_2}{2}\sum_{\vec{\tau}_2}(S_i^x S_{i+\vec{\tau}_2}^x - S_i^y S_{i+\vec{\tau}_2}^y - S_i^z S_{i+\vec{\tau}_2}^z)], \end{aligned}$$

where the sums over $\vec{\tau}_x$, $\vec{\tau}_y$ and $\vec{\tau}_2$ run over vectors joining horizontal first neighbours, vertical first neighbours, and second neighbours respectively, and where we have dropped the explicit reference to the local axis in S_i^y and S_i^z for clarity.

Expressing the operators in terms of Holstein-Primakoff bosons, keeping terms of order S only, and performing a Fourier transform, this Hamiltonian takes the form

$$H = -2NS^2J_2 + \sum_{\vec{k}} \left[B_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2} A_{\vec{k}} \left(a^\dagger_{\vec{k}} a^\dagger_{-\vec{k}} + a_{\vec{k}} a_{-\vec{k}} \right) \right]$$

with

$$\begin{cases} A_{\vec{k}} = S\left[-2J_1(\cos^2\frac{\theta}{2}\cos k_x + \sin^2\frac{\theta}{2}\cos k_y) - 4J_2\cos k_x \cos k_y\right] \\ B_{\vec{k}} = S\left[2J_1(\sin^2\frac{\theta}{2}\cos k_x + \cos^2\frac{\theta}{2}\cos k_y) + 4J_2\right] \end{cases}$$

Summary

Quite generally, if the fluctuations can be described with one site per unit cell, after a Fourier transform the Hamiltonian is of the form:

$$H = E_{\mathrm{class}} S^2 + \sum_{\vec{k}} \left[B_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2} A_{\vec{k}} \left(a^\dagger_{\vec{k}} a^\dagger_{-\vec{k}} + a_{\vec{k}} a_{-\vec{k}} \right) \right]$$

where the classical energy E_{class} is the ground state energy for spins of length 1, and where the coefficients $B_{\vec{k}}$ and $A_{\vec{k}}$ are of order S.

6.2 Bogoliubov transformation

If a bosonic Hamiltonian is diagonal, $H = \sum_{\vec{k}} \omega_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}}$, it satisfies

$$\left[H, b_{\vec{k}}\right] = \omega_{\vec{k}} \left[b^\dagger_{\vec{k}} b_{\vec{k}}, b_{\vec{k}}\right] = -\omega_{\vec{k}} b_{\vec{k}}. \tag{6.8}$$

So, to diagonalize a Hamiltonian of the form

$$H = E_{\mathrm{class}} S^2 + \sum_{\vec{k}} \left[B_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2} A_{\vec{k}} \left(a^\dagger_{\vec{k}} a^\dagger_{-\vec{k}} + a_{\vec{k}} a_{-\vec{k}} \right) \right]$$

we look for operators $\alpha_{\vec{k}} = u_{\vec{k}} a_{\vec{k}} + v_{\vec{k}} a^\dagger_{-\vec{k}}$ satisfying the equation

$$\left[H, \alpha_{\vec{k}}\right] = -\omega_{\vec{k}} \alpha_{\vec{k}}. \tag{6.9}$$

Now

$$\left[H, a_{\vec{k}}\right] = -\frac{1}{2}(A_{\vec{k}} + A_{-\vec{k}})a^{\dagger}_{-\vec{k}} - B_{\vec{k}}a_{\vec{k}}$$

and

$$[H, a^{\dagger}_{-\vec{k}}] = \frac{1}{2}\left(A_{\vec{k}} + A_{-\vec{k}}\right)a_{\vec{k}} + B_{\vec{k}}a^{\dagger}_{-\vec{k}}$$

so that

$$\left[H, \alpha_{\vec{k}}\right] = u_{\vec{k}}\left(-A_{\vec{k}}a^{\dagger}_{-\vec{k}} - B_{\vec{k}}a_{\vec{k}}\right) + v_{\vec{k}}\left(A_{\vec{k}}a_{\vec{k}} + B_{\vec{k}}a^{\dagger}_{-\vec{k}}\right)$$

leading to the equation

$$u_{\vec{k}}\left(-A_{\vec{k}}a^{\dagger}_{-\vec{k}} - B_{\vec{k}}a_{\vec{k}}\right) + v_{\vec{k}}\left(A_{\vec{k}}a_{\vec{k}} + B_{\vec{k}}a^{\dagger}_{-\vec{k}}\right) = -\omega_{\vec{k}}\left(u_{\vec{k}}a_{\vec{k}} + v_{\vec{k}}a^{\dagger}_{-\vec{k}}\right).$$

To satisfy this equation, the coefficients of $a_{\vec{k}}$ resp. $a^{\dagger}_{-\vec{k}}$ must be the same on both sides, leading to:

$$\left\{\begin{array}{l} -B_{\vec{k}}u_{\vec{k}} + A_{\vec{k}}v_{\vec{k}} = -\omega_{\vec{k}}u_{\vec{k}} \\ -A_{\vec{k}}u_{\vec{k}} + B_{\vec{k}}v_{\vec{k}} = -\omega_{\vec{k}}v_{\vec{k}} \end{array}\right. \quad \Rightarrow \quad \left\{\begin{array}{l} \left(-B_{\vec{k}} + \omega_{\vec{k}}\right)u_{\vec{k}} + A_{\vec{k}}v_{\vec{k}} = 0 \\ -A_{\vec{k}}u_{\vec{k}} + \left(B_{\vec{k}} + \omega_{\vec{k}}\right)v_{\vec{k}} = 0 \end{array}\right. \tag{6.10}$$

$$\tag{6.11}$$

This homogeneous system has a non-zero solution if its determinant vanishes, leading to

$$\omega^2_{\vec{k}} - B^2_{\vec{k}} + A^2_{\vec{k}} = 0 \Rightarrow \omega_{\vec{k}} = \pm\sqrt{B^2_{\vec{k}} - A^2_{\vec{k}}}.$$

For the operators $\alpha_{\vec{k}}, \alpha^{\dagger}_{\vec{k}}$ to be bosonic, they must satisfy $[\alpha_{\vec{k}}, \alpha^{\dagger}_{\vec{k}}] = 1$, which implies $u^2_{\vec{k}} - v^2_{\vec{k}} = 1$. But

$$u^2_{\vec{k}} - v^2_{\vec{k}} = u^2_{\vec{k}}\frac{2\omega_{\vec{k}}}{B_{\vec{k}} + \omega_{\vec{k}}}$$

Now, $B_{\vec{k}}$ must be positive. Otherwise the spectrum would not be bounded from below. Then, since $|\omega_{\vec{k}}| < B_{\vec{k}}$, the frequency $\omega_{\vec{k}}$ must be positive, and the final solution is given by

$$\omega_{\vec{k}} = \sqrt{B^2_{\vec{k}} - A^2_{\vec{k}}}.$$

The coefficient $u_{\vec{k}}$ and $v_{\vec{k}}$, which are only defined up to a sign, can be chosen as

$$u_{\vec{k}} = \sqrt{\frac{B_{\vec{k}} + \omega_{\vec{k}}}{2\omega_{\vec{k}}}}, \quad v_{\vec{k}} = \mathrm{sign}(A_{\vec{k}})\sqrt{\frac{B_{\vec{k}} - \omega_{\vec{k}}}{2\omega_{\vec{k}}}}.$$

The final form of the Hamiltonian, including the constant, can be obtained by expressing the original operator $a_{\vec{k}}, a^\dagger_{\vec{k}}$ in terms of the new ones:

$$\begin{cases} a_{\vec{k}} = u_{\vec{k}}\alpha_{\vec{k}} - v_{\vec{k}}\alpha^\dagger_{-\vec{k}} \\ a^\dagger_{-\vec{k}} = u_{\vec{k}}\alpha^\dagger_{-\vec{k}} - v_{\vec{k}}\alpha_{\vec{k}} \end{cases}$$

and by injecting these expressions into the original Hamiltonian. After some algebra, the final result is:

$$H = E_{\text{class}}S^2 - \frac{1}{2}\sum_{\vec{k}} B_{\vec{k}} + \frac{1}{2}\sum_{\vec{k}}\omega_{\vec{k}} + \sum_{\vec{k}}\omega_{\vec{k}}\alpha^\dagger_{\vec{k}}\alpha_{\vec{k}}$$

Now, $-\frac{1}{2}\sum_{\vec{k}} B_{\vec{k}} = E_{\text{class}}S$. This can be shown for instance by calculating the expectation value of the Hamiltonian before and after the Fourier transform in a state with one boson of each wave-vector. In such a state, $\langle a^\dagger_{\vec{k}} a_{\vec{k}}\rangle = 1$ and $\langle a^\dagger_i a_j\rangle = \delta_{ij}$. In the expectation value in real space, the expression is the same as that of the classical energy with the coefficient S^2 replaced by $S^2 - 2S$ while in Fourier space the expectation value is $E_{\text{class}}S^2 + \sum_{\vec{k}} B_{\vec{k}}$.

Finally, the result can be put into the form:

$$H = E_{\text{class}}S(S+1) + \sum_{\vec{k}}\omega_{\vec{k}}\left(\alpha^\dagger_{\vec{k}}\alpha_{\vec{k}} + \frac{1}{2}\right).$$

The operators $\alpha^\dagger_{\vec{k}}, \alpha_{\vec{k}}$ are called Bogoliubov operators, and the excitations are called spin-waves or magnons.

Helical state

For a helical state of pitch vector $\vec{Q}$, the Hamiltonian takes the specific form

$$H = \frac{NJ_{\vec{Q}}}{2}S(S+1) + \sum_{\vec{k}}\omega_{\vec{k}}\left(\alpha^\dagger_{\vec{k}}\alpha_{\vec{k}} + \frac{1}{2}\right).$$

and the dispersion relation of the spin waves is given by

$$\omega_{\vec{k}} = S\sqrt{(J_{\vec{k}} - J_{\vec{Q}})\left[\frac{1}{2}(J_{\vec{k}+\vec{Q}} + J_{\vec{k}-\vec{Q}}) - J_{\vec{Q}}\right]}.$$

It vanishes at $\vec{k} = 0$ and $\vec{k} = \vec{Q}$.

6.3 Order by disorder

Since the frequencies $\omega_{\vec{k}}$ are positive, the ground state corresponds to the vacuum of $\alpha_{\vec{k}}$, and the ground state energy is given by:

$$E_0 = E_{\text{class}} S(S+1) + \frac{1}{2}\sum_{\vec{k}} \omega_{\vec{k}}$$

If the ground state is degenerate, the first term is the same for all ground states, but not the second one. Indeed the spin-wave spectrum depends on the ground state around which fluctuations take place. This second term, which is always positive, is often referred to as the zero-point energy. Note that the total correction to the classical energy, which is given by $-\frac{1}{2}\sum_{\vec{k}} B_{\vec{k}} + \frac{1}{2}\sum_{\vec{k}} \omega_{\vec{k}}$, is negative, as it should since quite generally quantum fluctuations reduce the energy.

Minimizing the zero point energy can thus be expected, in close analogy to thermal fluctuations, to select among the ground states, an effect also known as *quantum order by disorder*.

Connection to thermal fluctuations

Quantum fluctuations and thermal fluctuations are related but not strictly equivalent. In the case of coplanar states, the coefficients entering the classical and quantum expansions are related by:

$$A_{\vec{k}} = \frac{S}{2}(\beta_{\vec{k}} - \alpha_{\vec{k}}), \quad B_{\vec{k}} = \frac{S}{2}(\beta_{\vec{k}} + \alpha_{\vec{k}})$$

so that

$$B_{\vec{k}}^2 - A_{\vec{k}}^2 = \frac{S^2}{2}\alpha_{\vec{k}}\beta_{\vec{k}}$$

implying that

$$\sum_{\vec{k}} \ln \omega_{\vec{k}} = \frac{1}{2}N(2\ln S - \ln 2) + \frac{1}{2}\sum_{\vec{k}}(\ln \alpha_{\vec{k}} + \ln \beta_{\vec{k}}).$$

So, thermal order by disorder corresponds to minimizing $\sum_{\vec{k}} \ln \omega_{\vec{k}}$ while quantum order by disorder corresponds to minimizing $\sum_{\vec{k}} \omega_{\vec{k}}$. Since the logarithm is an increasing function, the same state is often selected, but this does not need to be the case. A counter example is provided by $SU(3)$ spins on the square lattice.

$J_1 - J_2$ model

For the $J_1 - J_2$ model on the square lattice for $J_2 > J_1/2$, $\sum_{\vec{k}} \omega_{\vec{k}}$ is minimal for $\theta = 0$ and π: the two helical states are selected, as for thermal order by disorder.

6.4 Order parameter

The other important effect of quantum fluctuations is to reduce the local magnetization in the $\hat{z}_i$ direction from the value S. Indeed, except for ferromagnets, the ground state has components with smaller values of $\vec{S}_i \cdot \hat{z}_i$. In a system where all sites are equivalent, this is easily quantified by defining an order parameter related to the local magnetization by:

$$m = \frac{1}{N} \sum_i \left\langle S_i^{z_i} \right\rangle = S - \frac{1}{N} \sum_i \langle a_i^\dagger a_i \rangle = S - \frac{1}{N} \sum_{\vec{k}} \langle a_{\vec{k}}^\dagger a_{\vec{k}} \rangle$$

Now,

$$\begin{aligned} a_{\vec{k}}^\dagger a_{\vec{k}} &= \left(u_{\vec{k}} \alpha_{\vec{k}}^\dagger - v_{\vec{k}} \alpha_{-\vec{k}} \right) \left(u_{\vec{k}} \alpha_{\vec{k}} - v_{\vec{k}} \alpha^\dagger_{-\vec{k}} \right) \\ &= u_{\vec{k}}^2 \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} + v_{\vec{k}}^2 \alpha^\dagger_{-\vec{k}} \alpha_{-\vec{k}} + v_{\vec{k}}^2 - u_{\vec{k}} v_{\vec{k}} \left(\alpha_{\vec{k}}^\dagger \alpha^\dagger_{-\vec{k}} + \alpha_{-\vec{k}} \alpha_{\vec{k}} \right). \end{aligned}$$

In the ground state, $\langle \alpha_{\vec{k}}^\dagger \alpha^\dagger_{-\vec{k}} \rangle = \langle \alpha_{-\vec{k}} \alpha_{\vec{k}} \rangle = \langle \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} \rangle = 0$, leading to the following expressions for the expectation value

$$\langle a_{\vec{k}}^\dagger a_{\vec{k}} \rangle = v_{\vec{k}}^2 = \frac{B_{\vec{k}} - \omega_{\vec{k}}}{2\omega_{\vec{k}}}$$

and for the order parameter:

$$m = S - \frac{1}{N} \sum_{\vec{k}} \frac{B_{\vec{k}} - \omega_{\vec{k}}}{2\omega_{\vec{k}}}.$$

The last term may be approximated by an integral:

$$\frac{1}{N} \sum_{\vec{k}} \frac{B_{\vec{k}} - \omega_{\vec{k}}}{2\omega_{\vec{k}}} \simeq \frac{1}{(2\pi)^2} \int \mathrm{d}k_x \int \mathrm{d}k_y \frac{B_{\vec{k}} - \omega_{\vec{k}}}{2\omega_{\vec{k}}}$$

The persistence of magnetic order depends on the magnitude of this integral. If it is larger than S, the basic assumption of the theory, the presence of magnetic order with fluctuations around that order, breaks down, and the ground state must be of a completely different nature.

Quite generally, the dispersion $\omega_{\vec{k}}$ vanishes linearly at one or several points in the Brillouin zone, as shown e.g. by the dispersion in a helical state. In one dimension, the integral giving the correction to the magnetization diverges logarithmically, and there can be no magnetic order at zero temperature (except of course ferromagnetic order since there are no fluctuations in that case). As we will see in the next chapters, the zero-temperature properties are radically different from those of ordered magnets and depend dramatically on the value of the spin S. For half-integer spins, the correlations decay algebraically, and the excitation spectrum is gapless, but elementary excitations are domain walls and not spin waves. For integer spins, the correlations decay exponentially and the spectrum is gapped.

In two and thee dimensions, the integral is convergent as long as the dispersion only vanishes at isolated points. However, because of frustration, it can happen that the spectrum becomes soft along lines or surfaces. This can for instance be expected if there is an infinite number of helical ground states with pitch vectors forming a line in the Brillouin zone: Fluctuations from one helical state with a wave-vector equal to the pitch vector of another ground state should occur at zero energy.

6.4.1 $J_1 - J_2$ model on the square lattice

As long as $J_2 < J_1/2$, the ground state is the Néel state with pitch vector (π, π). However, for $J_2 = J_1/2$, we saw that there is an infinite number of ground states with pitch vectors of the form (k_x, π), $0 \leq k_x \leq \pi$, or (π, k_y), $0 \leq k_y \leq \pi$. So we expect the spectrum in the Néel phase to become soft along these lines when $J_2 \to J_1/2$. Indeed, using the general formula for the dispersion in a helical magnet, the spectrum can be easily shown to be given by:

$$\omega_{\vec{k}} = S\ \sqrt{[4(J_1 - J_2) + 4J_2 \cos k_x \cos k_y]^2 - [2J_1(\cos k_x + \cos k_y)]^2}$$

For $J_2 = J_1/2$, this reduces to

$$\omega_{\vec{k}} = 2J_1 S\ \sqrt{(1 + \cos k_x)(1 + \cos k_y)(1 - \cos k_x)(1 - \cos k_y)},$$

or, more simply,

$$\omega_{\vec{k}} = 2J_1 S\ |\sin k_x|\ |\sin k_y|.$$

The spectrum indeed vanishes along the lines $k_x = \pi$ and $k_y = \pi$, as expected. It also vanishes along the lines $k_x = 0$ and $k_y = 0$, but this is somewhat accidental. It is a consequence of the symmetry $\omega_{\vec{Q}-\vec{k}} = \omega_{\vec{k}}$ when the pitch vector $\vec{Q}$ is equal to (π, π).

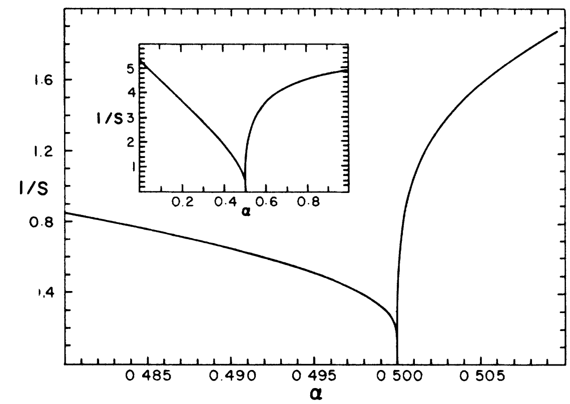

Figure 6.2: Phase diagram of the $J_1 - J_2$ model on the square lattice according to spin-wave theory (after Chandra and Douçot, 1988). The region above the lines is predicted to be disordered. α stands for the ratio J_2/J_1.

In any case, the presence of a line of zeroes implies that the integral giving the quantum correction to the order parameter diverges in two-dimensions, destroying the order whatever the value of S. Starting from the standard antiferromagnetic model with $J_2 = 0$, and increasing J_2, the spectrum becomes progressively softer upon approaching the point $J_2 = J_1/2$. Accordingly, the correction to the magnetization increases, and for any value of S there will be a critical value of J_2/J_1 at which the correction to the magnetization is equal to S. Beyond that ratio, this theory predicts that long-range order is destroyed by quantum fluctuations. The situation is the same when approaching the point $J_2 = J_1/2$ from above. The dispersion in the two degenerate helical states of wave vectors $(0,\pi)$ and $(\pi,0)$ only has zeroes at four points, $(0,0)$, $(0,\pi)$, $(\pi,0)$ and (π,π), and the correction to the order parameter remains finite as long as $J_2 > J_1/2$. But again it diverges in the limit $J_2 \to J_1/2$. As a consequence, in the plane $(1/S, J_2/J_1)$, there is a region encompassing all ratios J_2/J_1 when $1/S$ is large, and extending to the point $J_2 = J_1/2$ when $1/S \to 0$, where quantum fluctuations destroy long-range order. For any physical value of S, this theory thus predicts that there is a parameter range around $J_2 = J_1/2$ where long-range order is destroyed (see Fig. 6.2).

6.4.2 Kagome

For the planar configurations, one can show that there are three branches of spin waves given by:

$$\omega_1(\vec{k}) = 0 \tag{6.12}$$

$$\omega_{2,3}(\vec{k}) = JS\sqrt{2}\left(\sin^2\vec{k}\cdot\vec{u}_1 + \sin^2\vec{k}\cdot\vec{u}_2 + \sin^2\vec{k}\cdot\vec{u}_3\right)^{1/2} \tag{6.13}$$

where $\vec{u}_1$ is along x, while $\vec{u}_2$ and $\vec{u}_3$ are obtained from $\vec{u}_1$ by a rotation around z by $2\pi/3$ and $4\pi/3$ respectively.

The presence of a zero mode that extends over the entire Brillouin zone again leads to a divergence of the correction to the order parameter. This harmonic theory thus predicts that the kagome antiferromagnet on the kagome lattice is disordered for any spin S.

6.4.3 Beyond the quadratic theory

The theory developed in this chapter is based on the first relevant order in a $1/S$ expansion which leads to a simple quadratic bosonic Hamiltonian that can be diagonalized using a Bogoliubov transformation. As long as the order is only reduced but not destroyed by these harmonic fluctuations, one can expect this theory to be valid. When however this theory predicts that magnetic order is destroyed, one needs to go beyond this approach.

One obvious thing to try is to push the expansion to higher order in $1/S$. This is very cumbersome and will not be presented here. The main outcome in cases where this has been carried out is that the region where quantum fluctuations destroy long-range order is modified, sometimes reduced, but usually not suppressed altogether. For instance, for kagome, the spin-1/2 case is predicted to remain disordered, but long-range order is restored for large spins.

However, the example of one dimension suggests that more radical things could occur. This raises the main question of frustrated quantum magnetism: Which kind of ground state can replace magnetic long-range order? On pure logical grounds, one can distinguish three possibilities:

1. The $SU(2)$ rotational symmetry is broken, but there is no magnetic order. In that case, one generally talks of spin *nematic* order since the order parameter is a tensor of higher order, as in liquid crystals.

2. $SU(2)$ is not broken. By analogy with the classical correlations, and bearing in mind the one-dimensional case, one can think a priori of two possibilities:

- Correlations are algebraic, and the spectrum is gapless.
- Correlations decay exponentially, and the spectrum is gapped.

All possibilities have been actively studied. They are discussed in the next chapters.