

Local Ferromagnetism In The Holstein–Primakoff Transformation Approach

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Abstract

When the temperature T go from $T_c \rightarrow 0$, the magnetic moment $\langle m_z \rangle$ will increasing until it reach either $\langle m_z \rangle = m_0$ or $\langle m_z \rangle = -m_0$ at $T = 0$. At the $T \neq 0$ and without the external field, the spin will oscillate around the Oz axis, their collective equation frequency can be considered as the quasi-particle, called Magnon. This work use the Holstein-Primakoff transformation for the spin operator to showing the quantization of the quasi-particle Magnon.

1 Independence Magnon Hamiltonian

1.1 Derivation

Considering the hopping Hamiltonian of the spin configuration in the form:

$$\mathcal{H} = - \sum_{m,n \neq m} J_{nm} \vec{S}_n \cdot \vec{S}_m. \quad (1)$$

In this Hamiltonian, we will not considering the external field, which will be considered later. In the Hamiltonian (1), the spin operator \vec{S} satisfies the cyclic commutation:

$$[S_n^i, S_m^j] = \delta_{nm} \epsilon^{ijk} S_n^k. \quad (2)$$

The idea will be, since the Boson is have the integer spin and each bosonic excited state corresponding to the degree of the projection of the magnetic moment on the Oz axis, we will choose the "vacuum states" $|0\rangle$ to be the maximum projection. The corresponding creation operator will decrease the spin projection by 1:

$$|s, m = s - n\rangle \rightarrow \frac{1}{\sqrt{n}} (a^\dagger)^n |0\rangle$$

We usually using the ladder operator S_+, S_- , its will link with the annihilation and creation operator through Holstein-Primakoff transformation, respectively:

$$S^+ = \sqrt{2s} \sqrt{1 - \frac{a^\dagger a}{2s}}, \quad S^- = \sqrt{2s} a^\dagger \sqrt{1 - \frac{a^\dagger a}{2s}}, \quad S^z = s - a^\dagger a \quad (3)$$

Usually, this expression useful when we have a large s , to express the square root in term of s . But in this case, we're dealing the the single electron and $s = 1/2$. But luckily, the density of magnon is very low, give us the approximation:

$$S_n^+ = \sqrt{2s} a, \quad S^- = \sqrt{2s} a^\dagger, \quad S^z = s - a^\dagger a \quad (4)$$

Projecting the Hamiltonian onto the parallel and perpendicular plane:

$$H = H_{\parallel} + H_{\perp} = - \sum_{m,n \neq m} J_{mn} S_n^z S_m^z - \sum_{m,n \neq m} J_{mn} \left(S_n^x S_m^x + S_n^y S_m^y \right), \quad (5)$$

a little bit massage on H_{\perp} will give us

$$S_n^x S_m^x + S_n^y S_m^y = \frac{1}{2} \left(S_n^+ S_m^- + S_n^- S_m^+ \right), \quad (6)$$

assuming the hopping energy is symmetry: $J_{mn} = J_{nm}$ and neglect the density of magnon in each ladder operator, then a little of changing the variable of the summation give:

$$H_{\perp} = - \sum_{m,n \neq m} J_{mn} \left(S_n^x S_m^x + S_n^y S_m^y \right) = - \sum_{m,n \neq m} J_{mn} S_n^- S_m^+, \quad (7)$$

$$H_{\perp} = -2s \sum_{m,n \neq m} J_{mn} a_n^{\dagger} a_m.$$

Along with that, we talked about the symmetry of the hopping coefficient, let change the index according to $l = m - n$, and use the definition of the Fourier transform ¹:

$$H_{\perp} = -2s \sum_{l \neq 0} J_l \sum_n a_n^{\dagger} a_{l+n} = -2s \sum_{l \neq 0} J_l \sum_n \sum_{q_1 q_2} a_{q_1}^{\dagger} a_{q_2} e^{iq_1 n} e^{-iq_2(l+n)},$$

the sum over index n will yield $\delta_{q_1 q_2}$, giving the form of:

$$H_{\perp} = -2s \sum_q \sum_{l \neq 0} J_l e^{-iq l} a_q^{\dagger} a_q.$$

Defining the hopping coefficient $J\gamma_q = \frac{1}{Z} \sum_{l \neq 0} J_l e^{-iq l}$ with Z is the number of the nearest neighbor to get:

$$H_{\perp} = -2s Z J \sum_q \gamma_q a_q^{\dagger} a_q. \quad (8)$$

Now, consider the parallel part:

$$\begin{aligned} H_{\parallel} &= - \sum_{m,n \neq m} J_{mn} S_m^z S_n^z = - \sum_{m,n \neq m} J_{mn} (s - a_m^{\dagger} a_m)(s - a_n^{\dagger} a_n) \\ &= -Js^2 N^2 + 2s \sum_{m,n \neq m} J_{mn} a_m^{\dagger} a_m = -Js^2 N^2 + 2s \sum_{m,n \neq m} J_{mn} \sum_{q_1 q_2} a_{q_1}^{\dagger} a_{q_2} e^{im(q_1 - q_2)} \\ &= -Js^2 N^2 + 2s \sum_{l \neq 0} J_l \sum_q a_q^{\dagger} a_q = -Js^2 N^2 + 2JZs \sum_q a_q^{\dagger} a_q. \end{aligned} \quad (9)$$

Combining (9) and (8):

$$H = -Js^2 N^2 + 2sJZ \sum_q (1 - \gamma_q) a_q^{\dagger} a_q$$

$$H - E_0 = \sum_q 2sJZ(1 - \gamma_q) \left(a_q^{\dagger} a_q + \frac{1}{2} \right) \equiv \sum_q \varepsilon_q \left(a_q^{\dagger} a_q + \frac{1}{2} \right), \quad (10)$$

$$\varepsilon_q = 2JZs(1 - \gamma_q). \quad (11)$$

So, from the spin Hamiltonian and the density independent Holstein–Primakoff Transformation, we derived the second quantization of magnon Hamiltonian.

1.2 Simple Cubic Lattice

Let see an example for this derivation, the simple cubic lattice will have the hopping energy $J_{mn} = \delta_{|n-m|1}$:

$$\gamma_q = \frac{1}{Z} \sum_{l \neq 0} J_l e^{ilq} = \frac{2}{6} \cos(q_i a_i), \quad i \in \{x, y, z\}. \quad (12)$$

Using the longwave approximation to have:

$$\cos(q_i a_i) = 1 - \frac{q_i^2 a_i^2}{2} \rightarrow \gamma_q \approx \frac{2}{6} \left(3 - \frac{q_i^2 a_i^2}{2} \right) = 1 - \frac{q_i^2 a_i^2}{6}.$$

The energy dispersion will have the parabola form:

$$\varepsilon_q = 12Js \left(1 - 1 + \frac{q_i^2 a_i^2}{6} \right) = 2Js q_i^2 a_i^2 \propto \mathbf{q}^2. \quad (13)$$

The energy dispersion have the form of the ideal bosonic gas form, therefore we can use the same approach for the grand canonical, define the effective Hamiltonian in the form:

$$\mathcal{H}_{eff.}(q) = \left(\frac{\hbar^2 q^2}{2m} - \mu \right) a_q^{\dagger} a_q \quad (14)$$

This express give us the Bose-Einstein distribution:

$$n(q) = \frac{1}{e^{\frac{\varepsilon(q) - \mu}{T}} - 1} \quad (15)$$

Or the Free energy corresponding with it:

$$\mathcal{Z} = \frac{1}{1 - e^{\frac{\mu - \varepsilon(q)}{T}}} \rightarrow F = -T \ln(\mathcal{Z}) = T \ln \left(1 - e^{\frac{1}{T}(\mu - \varepsilon)} \right) \quad (16)$$

¹The Fourier transform give a coefficient $1/N$, but it will eventually gone after the first sum, so let ignore it :v.

2 Further Approximation - The Interaction Term

We can take the interaction into account by considering again (5) under the higher order approximation of the HP transformation:

$$S_n^+ = \sqrt{2s} \left(1 - \frac{a^\dagger a}{4s}\right) a, \quad S^- = \sqrt{2s} a^\dagger \left(1 - \frac{a^\dagger a}{4s}\right), \quad S^z = s - a^\dagger a \quad (17)$$

Substituting it into the spin operators part of (5):

$$\begin{aligned} S_n^z S_m^z + \frac{1}{2} \left(S_n^+ S_m^- + S_n^- S_m^+ \right) &= (s - n_n)(s - n_m) + \frac{1}{2} \left[2s \left(1 - \frac{n_n}{4s}\right) a_n a_m^\dagger \left(1 - \frac{n_m}{4s}\right) + a_n^\dagger \left(1 - \frac{n_n}{4s}\right) \left(1 - \frac{n_m}{4s}\right) a_m \right] \\ &= s^2 - s(n_n + n_m) + n_n + n_m + s \left[a_n a_m^\dagger + a_n^\dagger a_m - \frac{1}{4s} \left(n_n a_n a_m^\dagger + a_n a_m^\dagger n_m + a_n^\dagger n_n a_m + a_n^\dagger n_m a_m \right) \right] + n_n n_m \\ &= s^2 + s(a_n a_m^\dagger + a_n^\dagger a_m - n_n - n_m) + \frac{1}{4} \left[4n_n n_m - n_n a_n a_m^\dagger - a_n a_m^\dagger n_m - a_n^\dagger n_n a_m - a_n^\dagger n_m a_m \right] \\ &= s^2 + s(a_n^\dagger - a_m^\dagger)(a_m - a_n) + \frac{1}{4} \left[4n_n n_m - a_m^\dagger a_n^\dagger (a_n^2 + a_m^2) - (a_m^{\dagger 2} + a_n^{\dagger 2}) a_n a_m \right] \\ &= s^2 - s(a_n^\dagger - a_m^\dagger)(a_n - a_m) - \frac{1}{4} \left[a_n^\dagger a_m^\dagger (a_n - a_m)^2 - (a_n^\dagger - a_m^\dagger)^2 a_n a_m \right]. \end{aligned}$$

Therefore,

$$H = -J \frac{N(N-1)}{2} s^2 + s \sum_{m,n \neq m} J_{mn} (a_n^\dagger - a_m^\dagger)(a_n - a_m) + \sum_{m,n \neq m} \frac{J_{mn}}{4} \left[a_n^\dagger a_m^\dagger (a_n - a_m)^2 - (a_n^\dagger - a_m^\dagger)^2 a_n a_m \right] \quad (18)$$

$$\equiv E_0 + H_0 + H_{\text{int}}$$

The first term is the background energy, which can be chose to be vanished. The second term H_0 is the energy dispersion of the Magnon and the final term corresponding with the magnon-magnon interaction. We can show the dispersion of the hopping energy have the form correspond to the tight-binding hopping energy:

$$\begin{aligned} H_0 &= s \sum_{n,m \neq n} J_{mn} (a_n^\dagger - a_m^\dagger)(a_n - a_m) = s \sum_{m,n \neq m} J_{nm} (a_n^\dagger a_n + a_m^\dagger a_m) - s \sum_{n,l \neq 0} J_l (a_n^\dagger a_{n+l} + a_{n+l}^\dagger a_n) \\ &= 2s \sum_{l \neq 0} J_l \sum_q a_q^\dagger a_q - s \sum_q \sum_{l \neq 0} J_l (e^{iql} + e^{-iql}) a_q^\dagger a_q = 2s \sum_q \sum_{l \neq 0} J_l (1 - \cos(\mathbf{q} \cdot \mathbf{l})) a_q^\dagger a_q = \sum_q \varepsilon(\mathbf{q}) a_q^\dagger a_q, \end{aligned}$$

in which,

$$\varepsilon(q) \equiv 2s \sum_{l \neq 0} J_l (1 - \cos(\mathbf{q} \cdot \mathbf{l})) \xrightarrow{\text{long wave approx.}} 2sq^2 \sum_{l \neq 0} J_l l^2, \quad (19)$$

We re-obtained the parabola energy dispersion around the minima, giving the ferromagnetic phenomenon.

3 Anti-ferromagnetic:

So, we have seen that, the micro-interaction between then spin momentum create the macro ferromagnetic phenomenon. But sometime, the nearest neighbor interaction more favor to be anti-align with the other, result in two nearest neighbors have the difference direction of spinor. This phenomenon is called anti-ferromagnetic. This phenomenon can be easily described in a bi-lattice, where two Bravais lattice go with the other. But the fascinating phenomenon will happen in the system where many ground states have the same energy, called "geometrical frustration", when the system is in the superposition of the many-fold of that ground states.

3.1 Holstein-Primakoff Transformation In Bi-lattice:

Working with two difference aligned sub-lattice, called A and B, respectively, we will choose the axis for the whole system aligned with the magnetic moment of sub-lattice A.

3.1.1 Sub-lattice A:

The system total magnetic aligned with the sub-lattice A, the representation of the spin-operator will be keep as²:

$$\begin{aligned} S_A^+ &= \sqrt{2s - a^\dagger a} \approx \sqrt{2s} a \\ S_A^- &= a^\dagger \sqrt{2s - a^\dagger a} \approx \sqrt{2s} a^\dagger \\ S_A^z &= s - a^\dagger a \end{aligned}$$

²We will assume the low density right now to work in the simplest approximation

These spin-representation satisfy the SU(2) commutations: $[S_A^x, S_A^y] = iS_A^z \rightarrow [S_A^+, S_A^-] = 2S_A^z = 2s$ (at ground states).

3.1.2 Sub-lattice B:

For the atom belong to the sub-lattice B (called atom B for short), the spin-operator will be opposite with the atom in sub-lattice A (called atom A):

$$\begin{aligned} S_B^- &= \sqrt{2s - b^\dagger b} \approx \sqrt{2s} b \\ S_B^+ &= b^\dagger \sqrt{2s - b^\dagger b} \approx \sqrt{2s} b^\dagger \\ S_B^z &= b^\dagger b - s \end{aligned}$$

3.2 Heisenberg Anti-ferromagnet:

Same as ferromagnetic, but now we considering only nearest neighbors hopping energy for two sub-lattice:

$$\begin{aligned} H &= -J \sum_{\langle m, n \rangle} \vec{S}_n \cdot \vec{S}_m = -J \sum_{\langle m, n \rangle} (S_n^x S_m^x + S_n^y S_m^y + S_n^z S_m^z) \\ &= -J \sum_{\langle m, n \rangle} \left(\frac{1}{2} (S_n^- S_m^+ + S_n^+ S_m^-) + S_n^z S_m^z \right) \end{aligned}$$

Without the lose of generality, let assume $n \in A, m \in B$, then using the Fourier transformation ³

$$\begin{aligned} S_n^- &= \sqrt{2s} \sum_q a_q^\dagger e^{-iqn}, \quad S_n^+ = \sqrt{2s} \sum_q a_q e^{iqn}, \quad S_n^z = s - \sum_{q_1, q_2} a_{q_1}^\dagger a_{q_2} e^{i(q_2 - q_1)n} \\ S_m^- &= \sqrt{2s} \sum_q b_q e^{-iqm}, \quad S_m^+ = \sqrt{2s} \sum_q b_q^\dagger e^{iqm}, \quad S_m^z = \sum_{q_1, q_2} b_{q_1}^\dagger b_{q_2} e^{i(q_1 - q_2)m} - s. \end{aligned}$$

To have

$$\begin{aligned} \sum_{\langle m, n \rangle} (S_n^- S_m^+ + S_n^+ S_m^-) &= 2s \sum_{\langle m, n \rangle} \sum_{q_1, q_2} (a_{q_1}^\dagger b_{q_2}^\dagger e^{i(q_2 m - q_1 n)} + a_{q_1} b_{q_2} e^{i(q_1 n - q_2 m)}) \\ &= 2s \sum_q \sum_{\{l, |l|=|m-n|=1\}} (a_q^\dagger b_q^\dagger e^{iq_l} + a_q b_q e^{-iq_l}) = 2s \sum_q \gamma_q (a_q^\dagger b_q^\dagger + a_q b_q), \end{aligned}$$

in which,

$$\gamma_q = \frac{1}{Z} \sum_l e^{iq_l}, \quad (20)$$

with Z is the number of nearest neighbors, we also considering the symmetry of the sum over l as the nearest neighbour (run from $\{-|l| \rightarrow |l|\}$, ⁴). The parallel part will be:

$$\begin{aligned} \sum_{\langle m, n \rangle} S_n^z S_m^z &= \sum_{\langle m, n \rangle} \left(-s^2 + s \sum_{q_1, q_2} (a_{q_1}^\dagger a_{q_2} e^{i(q_2 - q_1)n} + b_{q_1}^\dagger b_{q_2} e^{i(q_1 - q_2)m}) \right) + O(n^2) \\ &= -s^2 N Z + s \sum_{\langle l \rangle, q} (a_q^\dagger a_q + b_q^\dagger b_q) = -s^2 N Z + s Z \sum_q (a_q^\dagger a_q + b_q^\dagger b_q) \end{aligned}$$

Due to the anti-ferromagnetic assumption, the hopping become:

$$J = -\delta_{|n-m|=1} |J| \quad (21)$$

Loosenly allow us to merge into our transformation as:

$$\begin{aligned} H &= -|J| s^2 N Z + s Z |J| \sum_q (a_q^\dagger a_q + b_q^\dagger b_q) + \frac{2s|J|Z}{2} \sum_q \gamma_q (a_q^\dagger b_q^\dagger + a_q b_q) \\ H - E_0 &= s Z |J| \sum_q (a_q^\dagger a_q + b_q^\dagger b_q + \gamma_q (a_q^\dagger b_q^\dagger + a_q b_q)) \end{aligned} \quad (22)$$

Again, we use Bogoliubov transformation to diagonalize this Hamiltonian, to address this, let make it into the form of matrix multiplication:

$$I = \begin{pmatrix} a^\dagger & b \end{pmatrix} \begin{pmatrix} 1 & \gamma_q \\ \gamma_q & 1 \end{pmatrix} \begin{pmatrix} a \\ b^\dagger \end{pmatrix} \quad (23)$$

³Same argument, the coefficient will be canceled out.

⁴if $J \rightarrow J_{mn}$, the assumption of γ_q holds

Assuming the Bogoliubov transformation matrix U so that⁵:

$$\begin{pmatrix} a^\dagger \\ b \end{pmatrix} = U \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (24)$$

so that

$$\begin{aligned} I &= (\alpha^\dagger \quad \beta) U^{-1} \begin{pmatrix} 1 & \gamma_q \\ \gamma_q & 1 \end{pmatrix} U^{-1} \begin{pmatrix} \alpha \\ \beta^\dagger \end{pmatrix} \\ &= (\alpha^\dagger \quad \beta) \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} 1 & \gamma_q \\ \gamma_q & 1 \end{pmatrix} \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} \alpha \\ \beta^\dagger \end{pmatrix} \\ &= (\alpha^\dagger \quad \beta) \begin{pmatrix} \varepsilon_q & 0 \\ 0 & \varepsilon_q \end{pmatrix} \begin{pmatrix} \alpha \\ \beta^\dagger \end{pmatrix} \end{aligned}$$

with $\varepsilon_k = \sqrt{1 - \gamma_q^2}$ is the eigenenergy of the quasi-particle. The matrix elements of U will be:

$$u = 12 \quad (25)$$

$$v = sd \quad (26)$$

A QuBit Dynamic

Since we are working with the 2-state system, therefore, the density matrix have the form 2×2 and Hermitian, therefore can be described by the group $SU(2)$ or the Pauli matrix in the form of:

$$\rho = \frac{1}{2} \left(1 + \frac{\vec{n} \cdot \vec{\sigma}}{2} \right). \quad (27)$$

Vector $\vec{n} \in \mathbf{R}^3$ is the pointing of the magnetic moment, so called Bloch vector. This particle been placed in the external field \vec{B} , give it the energy:

$$H = -\frac{1}{2} \vec{B} \cdot \vec{\sigma} \quad (28)$$

The evolution of the spin momentum can be described through the equation of motions:

$$\begin{aligned} id_t \rho &= [H, \rho] \\ id_t \frac{1}{2} n_i \sigma_i &= -\frac{B_j}{4} [\sigma_j, \sigma_k] n_k = -\frac{B_j}{4} 2i \sigma_i \epsilon^{jki} n_k \\ d_t n_i &= -\epsilon^{jki} B_j n_k \\ \Rightarrow d_t \vec{n} &= -\vec{B} \times \vec{n} \end{aligned}$$

B Effectively Diagonalize Bogoliubov Transformation

Start from:

$$\begin{pmatrix} \alpha \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} u & -v \\ -v & u \end{pmatrix} \begin{pmatrix} a \\ b^\dagger \end{pmatrix} \quad (29)$$

For both set of basis $(\alpha, \beta); (a, b)$ is canonical, it have to satisfy: $[a, a^\dagger] = [b, b^\dagger] = [\alpha, \alpha^\dagger] = [\beta, \beta^\dagger] = 1$:

$$\begin{aligned} [\alpha, \alpha^\dagger] &= [au - vb^\dagger, a^\dagger u - vb] = [au, ua^\dagger - vb] - [vb^\dagger, a^\dagger u - vb] \\ &= u^2 [a, a^\dagger] - uv [a, b] - vu [b^\dagger, a^\dagger] + v^2 [b^\dagger, b] = 1 \\ \Rightarrow u^2 - v^2 &= 1 \Rightarrow \det U = \begin{vmatrix} u & -v \\ -v & u \end{vmatrix} = 1 \Rightarrow \det U^{-1} = 1 \end{aligned}$$

And from that, we have:

$$\begin{aligned} I &= (\alpha^\dagger \quad \beta) \begin{pmatrix} v(\gamma_q u + v) + u(\gamma_q v + u) & u(\gamma_q u + v) + v(\gamma_q v + u) \\ u(\gamma_q u + v) + v(\gamma_q v + u) & v(\gamma_q u + v) + u(\gamma_q v + u) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta^\dagger \end{pmatrix} \\ &= (\alpha^\dagger \quad \beta) \begin{pmatrix} \varepsilon_k & 0 \\ 0 & \varepsilon_k \end{pmatrix} \begin{pmatrix} \alpha \\ \beta^\dagger \end{pmatrix}, \end{aligned}$$

so that,

$$\gamma_q(u^2 + v^2) + 2uv = 0$$

Or,

$$\begin{aligned} \gamma_q &= -\frac{2uv}{u^2 + v^2} \\ \varepsilon_k &= 2uv\gamma_q + u^2 + v^2 \end{aligned}$$

⁵By any meaning in this case, we don't have any Unitary transformation since this is not a complete basic set, which should be $\psi = \begin{pmatrix} a & b & a^\dagger & b^\dagger \end{pmatrix}^\dagger$