Spin-Wave Approximation (Ferromagnetic Case)

- In the ordered state of magnetic systems, small deviation from the strictly ordered configuration may propagate as a wave. Such "spin waves" are quantized, and called magnons.

- We consider localized spins; electrons responsible to magnetization are bound to respective atoms, specified by its spatial position x:

We have geralized $S=1/2 \to S \geq 1/2$

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

$$\mathcal{H} = -J\sum_{(x,x')} \mathbf{S}_x \cdot \mathbf{S}_{x'} - H\sum_x S^z_x$$

$$= -J\sum_{(x,x')}\left(\frac{1}{2}(S^+_x S^-_{x'} + S^-_x S^+_{x'}) + S^z_x S^z_{x'}\right) - H\sum_x S^z_x \quad ①$$

(The g-factor and the Bohr magneton μ_B has been absorbed in the definition of H ($g\mu_B H \to H$).)

- Remember the effect of S^+_x, S^-_x and S^z_x on the state $|S_z = m\rangle$:

$$S^+_x |S^z = m\rangle = ((S-m)(S+m+1))^{1/2} |S^z = m+1\rangle$$
$$S^-_x |S^z = m+1\rangle = ((S-m)(S+m+1))^{1/2} |S^z = m\rangle$$
$$S^z_x |S^z = m\rangle = m |S^z = m\rangle$$

By defining $|n\rangle \equiv |S^z = S-n\rangle$, these equations will be

$$\left.\begin{aligned} S^+_x |n+1\rangle &= ((n+1)(2S-n))^{1/2} |n\rangle \\ S^-_x |n\rangle &= ((n+1)(2S-n))^{1/2} |n+1\rangle \\ S^z |n\rangle &= (S-n)|n\rangle \end{aligned}\right\} \quad ②$$

- We assume that the deviation from complete alignment (= the ground state) is small. In other words, we assume that almost all spins are in the state $|0\rangle$ or $|1\rangle$.
  Then we can assume $n=0$ in the first two equations of (2):

$$S_x^+ |1\rangle = \sqrt{2S}\, |0\rangle$$
$$S_x^- |0\rangle = \sqrt{2S}\, |1\rangle$$

Therefore, if we define the boson system with creation/annihilation operator b_x, b_x^+ and consider the new Hamiltonian that can be obtained by replacing the spin operator in (1) by b_x and b_x^+ according to the correspondence

$$S_x^+ \to \sqrt{2S}\, b_x \quad S_x^- \to \sqrt{2S}\, b_x^+ \quad S_x^z \to S - b_x^+ b_x$$

then, the resulting bosonic system should have essentially the same properties as the original spin system as far as the low-excitation condition ($n \leq 1$) is satisfied.

- The bosonic Hamiltonian

$$\mathcal{H} = -\sum_{(xx')} \left(JS(b_x^+ b_{x'} + b_x b_{x'}^+) + J(S-\hat{n}_x)(S-\hat{n}_{x'}) \right)$$
$$- H \sum_x (S - \hat{n}_x) \qquad (\hat{n}_x \equiv b_x^+ b_x)$$

- Spin wave Hamiltonian (justified for low temperature since $\langle \hat{n} \rangle \ll 1$)

We may further neglect the $n_x n_{x'}$ term, yielding

$$\mathcal{H}_{SW} = +JS \sum_{(x x')} (b_x^\dagger - b_{x'}^\dagger)(b_x - b_{x'})$$

$$- JS^2 d N - H \sum_x (S - b_x^\dagger b_{x'})$$

$$= E_0 + t \sum_{(x, x')} (b_x^\dagger - b_{x'}^\dagger)(b_x - b_{x'}) - \mu \sum_x b_x^\dagger b_x \quad \text{— ③}$$

$$(E_0 \equiv -dJS^2 N - HS, \quad t \equiv JS, \quad \mu \equiv -H)$$

$$(N \equiv L^d / a^d = (\#\text{ of unit cells}) = (\#\text{ of spins}))$$

- The solution

Since the spin-wave Hamiltonian is quadratic in b, it can be diagonalized. By introducing b_k s.t.

$$b_x = \frac{1}{\sqrt{N}} \sum_k e^{ikx} b_k$$

The μ-term becomes $-\mu \sum_k b_k^\dagger b_k$

The t-term becomes

$$+t \sum_{x, \delta} (b_x^\dagger - b_{x+\delta}^\dagger)(b_x - b_{x+\delta}) \quad (\delta = e_x, e_y, e_z)$$

$$= +t \frac{1}{N} \sum_{x, \delta} \sum_{k k'} (e^{-ikx} - e^{-ik(x+\delta)}) b_k^\dagger (e^{ik'x} - e^{ik'(x+\delta)}) b_{k'}$$

$$= +\frac{t}{N} \sum_{x \delta k k'} e^{i(k'-k)x} (1 - e^{-ik\delta})(1 - e^{ik'\delta}) b_k^\dagger b_{k'}$$

$$= +t \sum_{\delta k} \left(+4 \sin^2 \frac{k\delta}{2}\right) b_k^\dagger b_k = \sum_k \epsilon_k b_k^\dagger b_k$$

$$\epsilon_k \equiv 2t \sum_\delta (1 - \cos k\delta)$$

Putting together

$$\mathcal{H}_{SW} = E_0 + \sum_k (\epsilon_k - \mu)\, b_k^\dagger b_k$$

$$\epsilon_k \equiv 2t \sum_\delta (1 - \cos(k\delta)) \simeq \underbrace{t a^2}_{\equiv \alpha} k^2 \quad (ka \ll 1)$$

∘ Consistency of the approximation. $(\alpha = t a^2 = JS a^2)$

In the case $H=0$ $(\mu=0)$, the present approximation is expected to be exact in the low-density limit. Except for the $k=0$ mode, which corresponds to the global rotation and therefore can be neglected in discussion of the quasi-particle excitation, the excitation energy is strictly positive. Therefore the excitation density goes to zero in the low-T limit. This argument suggests that the spin-wave approximation is asymptotically exact for the present (ferromagnetic) case.

∘ Heat capacity

$$E = \langle \mathcal{H}_{SW} \rangle = (\mathrm{const}) + \sum_k \epsilon_k \langle \hat{n}_k \rangle$$

$$= \sum_k \epsilon_k \frac{1}{e^{\beta\epsilon_k} - 1}$$

$$= L^3 \int \frac{d^3k}{(2\pi)^3} \frac{\epsilon_k}{e^{\beta\epsilon_k} - 1} = L^3 \int \frac{d^3k}{(2\pi)^3} \frac{\alpha k^2}{e^{\beta\alpha k^2} - 1}$$

$$= L^3 \left(\frac{1}{\beta\alpha}\right)^{5/2} \cdot \alpha \int \frac{d^3x}{(2\pi)^3} \frac{x^2}{e^{x^2} - 1}$$

$$= A L^3 \frac{(k_B T)^{5/2}}{\alpha^{3/2}}$$

$$E/L^3 = A \frac{(k_B T)^{5/2}}{\alpha^{3/2}}$$

$$\left(\begin{array}{l} A \equiv \int \frac{d^3x}{(2\pi)^3} \frac{x^2}{e^{x^2}-1} \fallingdotseq 0.0452 \\ \alpha = JSa^2 \end{array} \right)$$

The specific heat per unit cell is

$$C_{magnon} \fallingdotseq 0.113\, k_B \left(\frac{k_B T}{JS}\right)^{3/2} \propto T^{3/2}$$

There are some real magnetic systems for which the magnon contribution and the phonon contribution ($\propto T^3$) are two dominant contributions in the low-T regime. (Ex. Yttrium iron garnet (YIG))

- The nemerical constant A

$$A \equiv \int \frac{d^3x}{(2\pi)^3} \frac{x^2}{e^{x^2}-1}$$

$$= \int_0^\infty \frac{dx}{(2\pi)^3} 4\pi x^2 \frac{x^2}{e^{x^2}-1}$$

$x^2 \equiv \xi$

$d\xi = 2x\,dx$

$$= \frac{1}{2\pi^2} \int_0^\infty \frac{d\xi}{2\sqrt{\xi}} \frac{\xi^2}{e^{\xi}-1}$$

$$= \frac{1}{4\pi^2} \int_0^\infty d\xi \frac{\xi^{3/2}}{e^{\xi}-1}$$

$$= \frac{1}{4\pi^2} \int_0^\infty d\xi \sum_{p=0}^\infty e^{-\xi} \left(e^{-\xi}\right)^p \xi^{3/2}$$

$$= \frac{1}{4\pi^2} \sum_{p=0}^\infty \int_0^\infty d\xi \; e^{-(1+p)\xi} \xi^{3/2}$$

$$= \frac{1}{4\pi^2} \sum_{p=0}^\infty \int_0^\infty d\xi \; e^{-\xi} \xi^{3/2} (1+p)^{-\frac{5}{2}}$$

$$= \frac{1}{4\pi^2} \Gamma\left(\frac{5}{2}\right) \zeta\left(\frac{5}{2}\right)$$

$$= \frac{1}{4\pi^2} \times \frac{3\sqrt{\pi}}{4} \times 1.34148 \cdots$$

$$= 0.0253303 \times 1.32934 \times 1.34148$$

$$\doteqdot 0.0452$$

∘ Deviation from the saturated magnetization

$$S - \langle S^z_x \rangle = \frac{1}{N} \sum_x \langle n_x \rangle \quad (N \cdots \# \text{ of the unit cells})$$

$$= \frac{1}{N} \sum_k \langle n_k \rangle = \frac{1}{N} \sum_k \frac{1}{e^{\beta\epsilon} - 1}$$

$$= \frac{\Omega}{N} \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\epsilon} - 1} \quad (\Omega \equiv L^3)$$

$$= a^3 \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\alpha k^2} - 1} = a^3 (\beta\alpha)^{-\frac{3}{2}} \int \frac{d^3\xi}{(2\pi)^3} \frac{1}{e^{\xi^2} - 1}$$

$$= B\, a^3 \left(\frac{k_B T}{\alpha}\right)^{3/2} \quad \left(B \equiv \int_{-\infty}^{\infty} \frac{d^3\xi}{(2\pi)^3} \frac{1}{e^{\xi^2} - 1} \right)$$

$$= B \left(\frac{k_B T}{J S}\right)^{3/2}$$

$$\propto T^{3/2}$$

$$\left(\begin{aligned} B &= \int_0^{\infty} d\xi \frac{\xi^2}{2\pi^2} \frac{1}{e^{\xi^2} - 1} \\ &= \int_0^{\infty} dx \frac{1}{4\pi^2} \frac{\sqrt{x}}{e^x - 1} \\ &= \frac{1}{4\pi^2} \zeta\left(\frac{3}{2}\right) \Gamma\left(\frac{3}{2}\right) \\ &\fallingdotseq \frac{1}{4\pi^2} \times 2.612 \times \frac{\sqrt{\pi}}{2} \fallingdotseq 0.0586 \end{aligned} \right)$$

Spin-Wave Theory of Antiferromagnets

The Ground State

- The ground state of the antiferromagnetic Heisenberg model

The antiferromagnetic case is more complicated. Our intuition and also mean-field approximations suggest that the ground state is a state in which the spins alternate, e.g., something like checkerboard in the case of the square lattice:

$$\begin{matrix} \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \end{matrix} \quad \cdots \text{ Neél State}$$

However, it's also easy to show that the perfect Neél state defined by

$$S_i^z |\Psi\rangle = \begin{cases} +\frac{1}{2} |\Psi\rangle & (i \in A\text{-sublattice}) \\ -\frac{1}{2} |\Psi\rangle & (i \in B\text{-sublattice}) \end{cases}$$

can't be the ground state. (Show it!)
Instead, the true ground state is "imperfect" Neél state:

$$\langle\Psi| S_i^z |\Psi\rangle = \begin{cases} +m & (i \in A) \\ -m & (i \in B) \end{cases}$$

with $|m| < \frac{1}{2}$, even if the Neél state is the ground state in some way. In other words, we have some quantum fluctuation even at $T=0$ in the antiferromagnetic model. In what follows, we estimate the amplitude of the quantum fluctuation and discuss the Neél state is really the ground state or not.

※ The simplest mean-field approximation to the Heisenberg model yields exactly the same result as the mean-field approximation to the Ising model. Therefore, it predicts finite temperature phase transitions for all spatial dimensions, and spontaneous (staggered) magnetization for the ground state. This result is correct for $d \geq 3$. However, it is widely accepted that in $d=2$ there is no finite-T phase transition in the Heisenberg model though the ground state still has the spontaneous magnetization. In $d=1$, the true ground state is not the Neél state at all.

$$\mathcal{H} = -J \sum_{(xx')} \left(S_x^x S_{x'}^x + S_x^y S_{x'}^y + S_x^z S_{x'}^z \right)$$

$$\xrightarrow[\text{approx}]{\text{mean-field}} -J \sum_{(xx')} \left(S_x^x \langle S_{x'}^x \rangle + S_x^y \langle S_{x'}^y \rangle + S_x^z \langle S_{x'}^z \rangle + \langle S_x^x \rangle S_{x'}^x + \cdots \right)$$

$$= -zJ \sum_x \left(m^x S_x^x + m^y S_x^y + m^z S_x^z \right)$$

$$= -zJ \sum_x \mathbf{m} \cdot \mathbf{S}_x \qquad \left(\mathbf{m} \equiv \langle \mathbf{S}_x \rangle \right)$$

$$\xrightarrow[\text{rotation}]{\text{basis}} -zJm \sum S_x^z$$

(the same as the mean-field Hamiltonian for the Ising model)

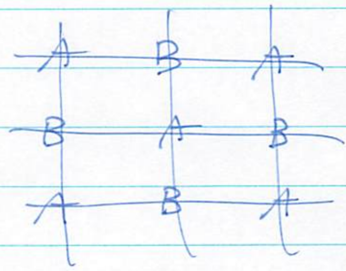
Spin wave theory

- The antiferromagnetic case can also be treated in a similar way to the ferromagnetic case.

- However, there are a few differences.
  (i) The ground state is not the fully-polarized state. This means that even in the low-T limit, the number of "flipped" spins doesn't go to zero. This causes the quantum shrink of the magnetization. Because of this, we should not expect that the approximation is asymptotically exact in the $T \to 0$ limit, unlike ferromagnets.
  (ii) The dispersion relation is essentially different: the excitation energy is proportional to k, in contrast to k^2 for the ferromagnetic case. This changes all the T-dependences of various quantities in low-T limit.

- Hamiltonian

$$\mathcal{H} = J \sum_{(x,x')} \boldsymbol{S}_x \cdot \boldsymbol{S}_{x'}$$



- The ground state

In contrast to the ferromagnetic case, we don't know any compact expression for the ground state. We just know (or at least assume) that we have finite "staggard" magnetization:

$$m \equiv \frac{1}{N} \sum_{x} (-1)^x S_x^z \neq 0 \qquad (-1)^x = \begin{cases} 1 & (x \in A) \\ -1 & (x \in B) \end{cases}$$

because of the spontaneous symmetry breaking. Note that the "fully-polarized" state ($|m| = S$) cannot be the exact ground state. This is in a strong contrast to the ferromagnetic case where $|m| = 1$ state is the exact ground state.

- The magnon creation/annihilation

For the spins on the A sublattice ($x \in A$) we do the same as in the ferromagnetic case, and we swap the creation op. and the annihilation op. for the B sublattice:

$$\begin{aligned} S_x^z &\Rightarrow S - a_x^\dagger a_x & &\Rightarrow -S + b_x^\dagger b_x \\ S_x^+ &\Rightarrow \sqrt{2S}\, a_x & &\Rightarrow \sqrt{2S}\, b_x^\dagger \\ S_x^- &\Rightarrow \sqrt{2S}\, a_x^\dagger & &\Rightarrow \sqrt{2S}\, b_x \\ & \quad (\text{on } A) & & \quad (\text{on } B) \end{aligned}$$