

§6. Quantum magnetism

* Spin-wave theory

- FM Heisenberg model

$$H = \frac{J}{2} \sum_{\vec{r}, \vec{s}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{s}} \quad (J < 0)$$

$$= \frac{J}{2} \sum_{\vec{r}, \vec{s}} \left[\frac{1}{2} (S_{\vec{r}}^+ S_{\vec{r}+\vec{s}}^- + S_{\vec{r}}^- S_{\vec{r}+\vec{s}}^+) + S_{\vec{r}}^z S_{\vec{r}+\vec{s}}^z \right]$$

$$S_{\vec{r}}^+ S_{\vec{r}+\vec{s}}^- = \sqrt{2S - a_{\vec{r}}^+ a_{\vec{r}}^-} a_{\vec{r}}^- a_{\vec{r}+\vec{s}}^+ \sqrt{2S - a_{\vec{r}+\vec{s}}^+ a_{\vec{r}+\vec{s}}^-}$$

(still complicated...)

Ground state: $|g\rangle = \prod_{\vec{r}} |s\rangle_{\vec{r}} = \prod_{\vec{r}} |0\rangle_{\vec{r}}$

(vacuum of bosons)

\uparrow Spin language \downarrow boson language

First excited state: $|e_{\vec{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}} S_{\vec{r}}^- |g\rangle$

(one-boson state)

$$= \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}} a_{\vec{r}}^+ |g\rangle = \underbrace{a_{\vec{k}}^+}_{\sqrt{2S - a_{\vec{r}}^+ a_{\vec{r}}^-}} |0\rangle$$

Low-energy states: small number of bosons $\langle a_{\vec{r}}^+ a_{\vec{r}}^- \rangle$

Semiclassical treatment: S large

$$\Rightarrow \langle a_{\vec{r}}^+ a_{\vec{r}}^- \rangle \ll 2S$$

$$S_{\vec{r}}^+ = \sqrt{2S - a_{\vec{r}}^\dagger a_{\vec{r}}} a_{\vec{r}} \approx \sqrt{2S} \left(1 - \frac{1}{4S} a_{\vec{r}}^\dagger a_{\vec{r}} + \dots \right) a_{\vec{r}}$$

$$S_{\vec{r}}^- = a_{\vec{r}}^\dagger \sqrt{2S - a_{\vec{r}}^\dagger a_{\vec{r}}} \approx \sqrt{2S} a_{\vec{r}}^\dagger \left(1 - \frac{1}{4S} a_{\vec{r}}^\dagger a_{\vec{r}} + \dots \right)$$

(omitted in linear spin-wave theories)

$$\Rightarrow S_{\vec{r}}^+ S_{\vec{r}+\vec{s}}^- \approx 2S a_{\vec{r}} a_{\vec{r}+\vec{s}}^\dagger + O(1) \text{ terms}$$

$$\begin{aligned} S_{\vec{r}}^z S_{\vec{r}+\vec{s}}^z &= (S - a_{\vec{r}}^\dagger a_{\vec{r}})(S - a_{\vec{r}+\vec{s}}^\dagger a_{\vec{r}+\vec{s}}) \\ &= S^2 - S(a_{\vec{r}}^\dagger a_{\vec{r}} + a_{\vec{r}+\vec{s}}^\dagger a_{\vec{r}+\vec{s}}) + O(1) \text{ terms} \end{aligned}$$

$$\begin{aligned} \Rightarrow H &= \frac{J}{2} \sum_{\vec{r}, \vec{s}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{s}} \\ &\approx \frac{J}{2} \sum_{\vec{r}, \vec{s}} \left[\frac{1}{2} (2S a_{\vec{r}} a_{\vec{r}+\vec{s}}^\dagger + 2S a_{\vec{r}+\vec{s}} a_{\vec{r}}^\dagger) \right. \\ &\quad \left. + S^2 - S(a_{\vec{r}}^\dagger a_{\vec{r}} + a_{\vec{r}+\vec{s}}^\dagger a_{\vec{r}+\vec{s}}) \right] \\ &= \frac{1}{2} JS^2 N z + \frac{J}{2} S \sum_{\vec{r}, \vec{s}} (a_{\vec{r}}^\dagger a_{\vec{r}+\vec{s}}^\dagger + a_{\vec{r}+\vec{s}} a_{\vec{r}}^\dagger) \\ &\quad - JSz \sum_{\vec{r}} a_{\vec{r}}^\dagger a_{\vec{r}} \quad \xrightarrow{\quad a_{\vec{r}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} a_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \quad} \\ &= \frac{1}{2} JS^2 N z + \sum_{\vec{k}} \underbrace{w_{\vec{k}}}_{\vec{k} \in FBZ} a_{\vec{k}}^\dagger a_{\vec{k}} \quad \vec{k} \in FBZ \\ &\quad \xrightarrow{\quad w_{\vec{k}} = -JSz \left(1 - \frac{1}{z} \sum_{\vec{s}} e^{i\vec{k} \cdot \vec{s}} \right) \quad} \end{aligned}$$

$$H = \sum_{\vec{k}} \omega_{\vec{k}} a_{\vec{k}}^+ a_{\vec{k}} + E_0$$

ground state $|0\rangle$ ✓

first excited state $a_{\vec{k}}^+ |0\rangle$ ✓

higher excited states: $a_{\vec{k}_1}^+ a_{\vec{k}_2}^+ |0\rangle$ not exact eigenstates ...
 \vdots
 (Unphysical degrees of freedom with $a_{\vec{F}}^+ a_{\vec{F}} > 2S$ also appear!)

Spin-wave/magnon dispersion:

$$\omega_{\vec{k}} = -JSz \left(1 - \frac{1}{2} \sum_{\vec{s}} e^{i\vec{k} \cdot \vec{s}} \right)$$

$$= -JSz \left[1 - \frac{1}{2z} \sum_{\vec{s}} \log(\vec{k} \cdot \vec{s}) \right]$$

$$\sim -JS \underbrace{|\vec{k}|^2}_{\text{for } |\vec{k}| \rightarrow 0}$$

Magnetization for $T > 0$:

$$\begin{aligned} \langle S_{\vec{r}}^z \rangle_T &= \langle S - a_{\vec{r}}^+ a_{\vec{r}} \rangle_T = S - \frac{1}{N} \sum_{\vec{k}} \underbrace{\langle a_{\vec{k}}^+ a_{\vec{k}} \rangle_T}_{\downarrow \text{Bose-Einstein distribution}} \\ &= S - \frac{1}{N} \sum_{\vec{k}} \frac{1}{e^{\omega_{\vec{k}}/T} - 1} \end{aligned}$$

$d=3$, low T :

$$\begin{aligned}\langle S_j^2 \rangle &\approx S - \int \frac{d\vec{k}}{(2\pi)^3} \frac{1}{e^{-JS|\vec{k}|^2/T} - 1} \\ &= S - \frac{1}{2\pi^2} \int_0^\infty dk \frac{k^2}{e^{-JSk^2/T} - 1} \\ &\approx S - \text{const} \times T^{3/2}\end{aligned}$$

Internal energy:

$$\begin{aligned}U(T) &= \langle H \rangle_T = E_0 + \sum_{\vec{k}} \omega_{\vec{k}} \langle a_{\vec{k}}^\dagger a_{\vec{k}} \rangle_T \\ &= E_0 + \sum_{\vec{k}} \frac{\omega_{\vec{k}}}{e^{\omega_{\vec{k}}/T} - 1} \\ &= E_0 + \text{const} \times T^{5/2}\end{aligned}$$

Heat capacity:

$$C_V = \frac{\partial U}{\partial T} \sim T^{3/2}$$

$d=1 \& 2$: Mermin-Wagner theorem rules out Fm order.

$T > 0$

(Linearized spin-wave theory breaks down!)

— AFM Heisenberg model

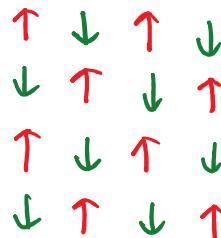
$$H = \frac{J}{2} \sum_{\vec{r}, \vec{s}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{s}} \quad (J>0)$$

$$= \frac{J}{2} \sum_{\vec{r}, \vec{s}} \left[\frac{1}{2} (S_{\vec{r}}^+ S_{\vec{r}+\vec{s}}^- + S_{\vec{r}}^- S_{\vec{r}+\vec{s}}^+) + S_{\vec{r}}^z S_{\vec{r}+\vec{s}}^z \right]$$

2d at $T=0$

3d at $T < T_c$: existence of AFM order

Consider bipartite lattice:



A sublattice

$$S_{\vec{r}}^+ = \sqrt{2S - a_{\vec{r}}^+ a_{\vec{r}}^-} a_{\vec{r}}$$

$$S_{\vec{r}}^- = a_{\vec{r}}^+ \sqrt{2S - a_{\vec{r}}^+ a_{\vec{r}}^-}$$

$$\underbrace{S_{\vec{r}}^z = S - a_{\vec{r}}^+ a_{\vec{r}}^-}_{\uparrow}$$

$$\langle S_{\vec{r}}^z \rangle \approx S$$

$$\Rightarrow \langle a_{\vec{r}}^+ a_{\vec{r}}^- \rangle \ll 2S$$



$$S_{\vec{r}}^+ \approx \sqrt{2S} a_{\vec{r}}^- + \dots$$

$$S_{\vec{r}}^- \approx \sqrt{2S} a_{\vec{r}}^+ + \dots$$

B sublattice

$$S_{\vec{r}}^+ = b_{\vec{r}}^+ \sqrt{2S - b_{\vec{r}}^+ b_{\vec{r}}^-} b_{\vec{r}}$$

$$S_{\vec{r}}^- = \sqrt{2S - b_{\vec{r}}^+ b_{\vec{r}}^-} b_{\vec{r}}$$

$$\underbrace{S_{\vec{r}}^z = b_{\vec{r}}^+ b_{\vec{r}}^- - S}_{\uparrow}$$

$$\langle S_{\vec{r}}^z \rangle \approx -S$$

$$\Rightarrow \langle b_{\vec{r}}^+ b_{\vec{r}}^- \rangle \ll 2S$$



$$S_{\vec{r}}^+ \approx \sqrt{2S} b_{\vec{r}}^- + \dots$$

$$S_{\vec{r}}^- \approx \sqrt{2S} b_{\vec{r}}^+ + \dots$$

$$H = \frac{J}{2} \sum_{\vec{r}, \vec{s}} \left[\frac{1}{2} (S_{\vec{r}}^+ S_{\vec{r}+\vec{s}}^- + S_{\vec{r}}^- S_{\vec{r}+\vec{s}}^+) + S_{\vec{r}}^z S_{\vec{r}+\vec{s}}^z \right]$$

A B (or vice versa)

$$\begin{aligned} S_{\vec{r} \in A}^+ S_{\vec{r} \in B}^- &\approx 2S a_{\vec{r} \in A}^\dagger b_{\vec{r} \in B} \\ S_{\vec{r} \in A}^- S_{\vec{r} \in B}^+ &\approx 2S a_{\vec{r} \in A}^\dagger b_{\vec{r} \in B}^\dagger \end{aligned} \quad \left. \right\} \text{pairing of bosons}$$

$$\begin{aligned} S_{\vec{r} \in A}^z S_{\vec{r} \in B}^z &= (S - a_{\vec{r} \in A}^\dagger a_{\vec{r} \in A}) (b_{\vec{r} \in B}^\dagger b_{\vec{r} \in B} - S) \\ &\approx -S^2 + S(a_{\vec{r} \in A}^\dagger a_{\vec{r} \in A} + b_{\vec{r} \in B}^\dagger b_{\vec{r} \in B}) \end{aligned}$$

$$\Rightarrow H \approx -\underbrace{\frac{1}{2} JS^2 N z}_{E_0} + JSz \left(\sum_{\vec{r} \in A} a_{\vec{r}}^\dagger a_{\vec{r}} + \sum_{\vec{r} \in B} b_{\vec{r}}^\dagger b_{\vec{r}} \right) + JS \sum_{\vec{r} \in A} \sum_{\vec{s}} (a_{\vec{r}} b_{\vec{r}+\vec{s}} + a_{\vec{r}}^\dagger b_{\vec{r}+\vec{s}}^\dagger)$$

Enlarged unit cells :

A and B sublattices separately define their
magnetic Brillouin zones!

$$\left\{ \begin{array}{l} a_{\vec{r}} = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}} a_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \\ b_{\vec{r}} = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}} b_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \end{array} \right.$$

defined in magnetic Brillouin zones
(N/2 \vec{k} -points!)

$$\begin{aligned}
 H = E_0 + JSz \sum_{\vec{k}} (a_{\vec{k}}^+ a_{\vec{k}} + b_{\vec{k}}^+ b_{\vec{k}}) \\
 + JSz \sum_{\vec{k}} \left[\gamma_{\vec{k}} (a_{\vec{k}}^+ b_{-\vec{k}}^+ + b_{-\vec{k}} a_{\vec{k}}) \right] \\
 \downarrow \\
 \nu_{\vec{k}} = \frac{1}{2} \sum_{\vec{s}} e^{i\vec{k} \cdot \vec{s}}
 \end{aligned}$$

not yet diagonalized ...

Bogoliubov transformation:

$$\begin{cases} a_{\vec{k}} = u_{\vec{k}} \alpha_{\vec{k}} + v_{\vec{k}} \beta_{\vec{k}}^+ & [\alpha_{\vec{k}}, \alpha_{\vec{k}'}^+] = [\beta_{\vec{k}}, \beta_{\vec{k}'}^+] = \delta_{\vec{k}\vec{k}'} \\ b_{-\vec{k}} = u_{\vec{k}} \beta_{\vec{k}} + v_{\vec{k}} \alpha_{\vec{k}}^+ & [\alpha_{\vec{k}}, \beta_{\vec{k}'}] = 0 \end{cases}$$

...

$$\Rightarrow [\alpha_{\vec{k}}, \alpha_{\vec{k}'}^+] = (\underbrace{u_{\vec{k}}^2 - v_{\vec{k}}^2}_{\rightarrow u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1}) \delta_{\vec{k}, \vec{k}'}, \quad (\alpha_{\vec{k}} \text{ and } \beta_{\vec{k}} \text{ are independent bosonic operators.})$$

$$\begin{aligned}
 & \sum_{\vec{k}} (a_{\vec{k}}^+ a_{\vec{k}} + b_{\vec{k}}^+ b_{\vec{k}}) + \sum_{\vec{k}} \gamma_{\vec{k}} (a_{\vec{k}}^+ b_{-\vec{k}}^+ + a_{\vec{k}} b_{-\vec{k}}) \\
 = & \sum_{\vec{k}} \left[u_{\vec{k}}^2 \alpha_{\vec{k}}^+ \alpha_{\vec{k}} + v_{\vec{k}}^2 \beta_{\vec{k}}^+ \beta_{\vec{k}} + \underbrace{u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^+ \beta_{\vec{k}}^+ + \alpha_{\vec{k}} \beta_{\vec{k}})}_{+ v_{\vec{k}}^2 \alpha_{\vec{k}} \alpha_{\vec{k}}^+ + u_{\vec{k}}^2 \beta_{\vec{k}} \beta_{\vec{k}}^+} \right. \\
 & \quad \left. + u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^+ \beta_{\vec{k}}^+ + \alpha_{\vec{k}} \beta_{\vec{k}}) \right] \\
 + & \sum_{\vec{k}} \gamma_{\vec{k}} \left[\underbrace{u_{\vec{k}}^2 \alpha_{\vec{k}}^+ \beta_{\vec{k}}^+ + v_{\vec{k}}^2 \alpha_{\vec{k}} \beta_{\vec{k}}^+}_{+ u_{\vec{k}}^2 \alpha_{\vec{k}} \beta_{\vec{k}} + v_{\vec{k}}^2 \alpha_{\vec{k}} \beta_{\vec{k}}^+} + u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^+ \alpha_{\vec{k}} + \beta_{\vec{k}}^+ \beta_{\vec{k}}) \right. \\
 & \quad \left. + u_{\vec{k}} v_{\vec{k}} (\alpha_{\vec{k}}^+ \alpha_{\vec{k}} + \beta_{\vec{k}}^+ \beta_{\vec{k}}) \right]
 \end{aligned}$$

"unwanted terms"

Require that the "unwanted" terms vanish:

$$2U_{\vec{K}}V_{\vec{K}} + P_{\vec{K}}(U_{\vec{K}}^2 + V_{\vec{K}}^2) = 0$$

Together with $U_{\vec{K}}^2 - V_{\vec{K}}^2 = 1$:

$$\Rightarrow \begin{cases} U_{\vec{K}}^2 = \frac{1}{2} \left(1 + \frac{1}{\sqrt{1-P_{\vec{K}}^2}} \right) \\ V_{\vec{K}}^2 = -\frac{1}{2} \left(1 - \frac{1}{\sqrt{1-P_{\vec{K}}^2}} \right) \end{cases}$$

Then, the Hamiltonian is given by

$$\begin{aligned} H &= JSz \sum_{\vec{K}} (U_{\vec{K}}^2 + V_{\vec{K}}^2 + 2P_{\vec{K}}U_{\vec{K}}V_{\vec{K}})(\alpha_{\vec{K}}^{\dagger}\alpha_{\vec{K}} + \beta_{\vec{K}}^{\dagger}\beta_{\vec{K}}) \\ &\quad + E_0 + JSz \sum_{\vec{K}} (2V_{\vec{K}}^2 + 2P_{\vec{K}}U_{\vec{K}}V_{\vec{K}}) \\ &= JSz \sum_{\vec{K}} \sqrt{1-P_{\vec{K}}^2} (\alpha_{\vec{K}}^{\dagger}\alpha_{\vec{K}} + \beta_{\vec{K}}^{\dagger}\beta_{\vec{K}}) \\ &\quad + E_0 + JSz \sum_{\vec{K}} (-1 + \sqrt{1-P_{\vec{K}}^2}) \\ &= \sum_{\vec{K}} w_{\vec{K}} (\alpha_{\vec{K}}^{\dagger}\alpha_{\vec{K}} + \beta_{\vec{K}}^{\dagger}\beta_{\vec{K}}) + E'_0 \\ &\quad \text{with } w_{\vec{K}} = JSz \sqrt{1-P_{\vec{K}}^2} \quad \text{and } E'_0 = E_0 + JSz \sum_{\vec{K}} (\sqrt{1-P_{\vec{K}}^2} - 1) \end{aligned}$$

long-wavelength limit: $|\vec{K}| \approx 0$,

$$P_{\vec{K}} \approx 1 - \frac{1}{2}(\vec{k})^2 \quad \vec{k} \approx (0, 0, \dots) \quad \text{classical energy}$$

$$w_{\vec{K}} \propto JS\sqrt{2z} |\vec{K}| \quad (\text{gapless, linear dispersion})$$

quantum fluctuations

Staggered magnetization:

$$\begin{aligned}\langle S_{\vec{r} \in A}^z \rangle &= \langle S - a_{\vec{r}}^+ a_{\vec{r}} \rangle \quad \xrightarrow{\text{a}_{\vec{R}} = u_{\vec{R}}^+ a_{\vec{R}} + v_{\vec{R}}^+ \beta_{\vec{R}}^+} \\ &= S - \frac{1}{N/2} \sum_{\vec{R}} \langle a_{\vec{R}}^+ a_{\vec{R}} \rangle \\ &= S - \frac{2}{N} \sum_{\vec{R}} \left(u_{\vec{R}}^2 \langle a_{\vec{R}}^+ a_{\vec{R}} \rangle + v_{\vec{R}}^2 \langle \beta_{\vec{R}}^+ \beta_{\vec{R}} \rangle \right)\end{aligned}$$

$$d=2, T=0: \quad \langle S_{\vec{r} \in A}^z \rangle = S - \frac{2}{N} \sum_{\vec{R}} v_{\vec{R}}^2$$

reduced staggered magnetization
(due to quantum fluctuations)

$$d=3, T>0: \quad \langle a_{\vec{R}}^+ a_{\vec{R}} \rangle_T = \langle \beta_{\vec{R}}^+ \beta_{\vec{R}} \rangle_T = \frac{1}{e^{w_{\vec{R}}/T} - 1}$$

$$\begin{aligned}\langle S_{\vec{r} \in A}^z \rangle &= S - \underbrace{\frac{2}{N} \sum_{\vec{R}} v_{\vec{R}}^2}_{\text{quantum fluctuations}} - \underbrace{\frac{2}{N} \sum_{\vec{R}} \frac{1}{e^{w_{\vec{R}}/T} - 1} (u_{\vec{R}}^2 + v_{\vec{R}}^2)}_{\text{thermal fluctuations}}\end{aligned}$$

$$= S - \frac{1}{N} \sum_{\vec{R}} \left(\frac{1}{\sqrt{1-y_{\vec{R}}^2}} - 1 \right) - \frac{2}{N} \sum_{\vec{R}} \frac{1}{e^{w_{\vec{R}}/T} - 1} \frac{1}{\sqrt{1-y_{\vec{R}}^2}}$$

$$\sim S - \text{const.} - \text{const.} \times T^2$$

heat capacity: $C_V \sim \text{const.} \times T^3$

$(d=3)$ (Debye's T^3 law for acoustic phonons)