Lecture 29

Consider ~~[illegible]~~ fluctuation corrections to the mean-field solution for Heisenberg ferromagnet. Fluctuations are conveniently taken into account using second-quantized representation of the spin operators:

$$S_i^z = S - b_i^+ b_i$$

$$S_i^+ = \sqrt{2S - b_i^+ b_i}\, b_i$$

$$S_i^- = b_i^+ \sqrt{2S - b_i^+ b_i}$$

– Holstein–Primakoff representation of spin operators.

Here $[b_i, b_j^+] = \delta_{ij}$

b^+, b are the exact analogs of ladder operators for harmonic oscillator:

$$H = \hbar\omega\left(b^+ b + \tfrac{1}{2}\right)$$

Hilbert space of harmonic oscillator:

$$|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$$

$$b^+ b\,|n\rangle = n\,|n\rangle$$

In the case of spin operators:

$$|0\rangle = |S^z = S\rangle,\ |1\rangle = |S^z = S-1\rangle, \ldots,$$

$$|2S\rangle = |-S\rangle$$

Thus the important difference from harmonic oscillator is that the Hilbert space of b's is restricted.

Check that commutation relations are satisfied:

$$[S^\alpha, S^\beta] = i\,\varepsilon_{\alpha\beta\gamma} S^\gamma$$

$[S^+, S^-] = 2S^z$ – check that this is satisfied.

$$[S^+, S^-] = \left[\sqrt{2S-b^+b}\; b,\; b^+\sqrt{2S-b^+b}\right] =$$

$$= \sqrt{2S-b^+b}\; b b^+ \sqrt{2S-b^+b} \;-$$

$$- b^+\sqrt{2S-b^+b}\sqrt{2S-b^+b}\; b =$$

Use $[b, b^+] = bb^+ - b^+b = 1$

$$= \sqrt{2S-b^+b}\,(1+b^+b)\sqrt{2S-b^+b} - b^+(2S-b^+b)b =$$

$$= 2S - b^+b + b^+b(2S-b^+b) - 2S\,b^+b + b^+b^+bb =$$

$$= 2S - b^+b - b^+b\,b^+b + b^+(bb^+-1)b =$$

$$= 2S - b^+b - \cancel{b^+b\,b^+b} + \cancel{b^+b\,b^+b} - b^+b =$$

$$= 2S - 2b^+b = 2(S - b^+b) = 2S^z$$

What we want is obtain the correct temperature dependence of the magnetization in a ferromagnet at low T.

MFT predicts : $\frac{M(0)-M(T)}{M(0)} = \frac{\Delta M(T)}{M(0)} = 2e^{-\frac{2T_c}{T}}$

Correct result : $\frac{\Delta M(T)}{M(0)} \sim T^{3/2}$

Approximation we will use: expand the square roots in the S^+ and S^- expressions to leading order and ignore constraint on the Hilbert space of b's.

$$\sqrt{2S - b^+b} = \sqrt{2S}\,\sqrt{1-\frac{b^+b}{2S}} \approx \sqrt{2S}\left(1-\frac{b^+b}{4S}+\cdots\right)$$

This is a good approximation for large S when we are considering small fluctuations about fully polarized state at $T=0$ in which all spins are polarized in the z-direction and $\langle b^+b\rangle = 0$ on every site.

Rewrite the Heisenberg model Hamiltonian in terms of the magnon creation-annihilation operators.

$$H = -\frac{J}{2}\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j = -\frac{J}{2}\sum_{\langle ij\rangle}\left[S_i^z S_j^z + \frac{1}{2}\left(S_i^+S_j^- + S_i^-S_j^+\right)\right]$$

$$S_i^z S_j^z = \left(S - b_i^+b_i\right)\left(S - b_j^+b_j\right) \approx S^2 - S\left(b_i^+b_i + b_j^+b_j\right)$$

$$S_i^+ \approx \sqrt{2S}\, b_i$$

$$S_i^- \approx \sqrt{2S}\, b_i^+$$

$$S_i^+ S_j^- = 2S\, b_j^+ b_i$$

Throwing out constant terms, the Hamiltonian becomes:

$$\mathcal{H} = \frac{JS}{2} \sum_{\langle ij \rangle} \left[b_i^+ b_i + b_j^+ b_j - b_i^+ b_j - b_j^+ b_i \right]$$

This looks very similar to tight-binding Hamiltonian for electrons on a lattice.

Diagonalize by Fourier transform:

$$b_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} b_k e^{i\vec{k}\cdot\vec{r}}$$

Here $\vec{k}$ belongs to the first Brillouin zone ~~of~~ the lattice.

$$\mathcal{H} = \frac{JS}{2} \sum_{\langle ij \rangle} \frac{1}{N} \sum_{k_1 k_2} \Big[b_{k_1}^+ b_{k_2} e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}_i} +$$

$$+ b_{k_1}^+ b_{k_2} e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}_j} - b_{k_1}^+ b_{k_2} e^{-i\vec{k}_1\cdot\vec{r}_i} e^{i\vec{k}_2\cdot\vec{r}_j} -$$

$$- b_{k_1}^+ b_{k_2} e^{-i\vec{k}_1\cdot\vec{r}_j} e^{i\vec{k}_2\cdot\vec{r}_i} \Big]$$

$\vec{r}_j = \vec{r}_i + \vec{\lambda}$, where $\vec{\lambda}$ is a nearest-neighbor vector.

- $$\mathcal{H} = \frac{JS}{2}\sum_k \Big[2z\, b_k^+ b_k -$$

$$- \frac{JS}{2}\sum_k b_k^+ b_k \left(e^{i\vec{k}\cdot\vec{\lambda}} + e^{-i\vec{k}\cdot\vec{\lambda}} \right)$$

let $\gamma_k = \frac{1}{z}\sum_{\vec{\lambda}} \cos(\vec{k}\cdot\vec{\lambda})$

Then the Hamiltonian becomes,

$$\mathcal{H} = JzS \sum_k (1-\gamma_k)\, b_k^+ b_k$$

- let $\omega_k = JzS(1-\gamma_k)$ – magnon dispersion.

$$\mathcal{H} = \sum_k \omega_k\, b_k^+ b_k$$

The particles, created by b_k^+ are called magnons or spin waves. ω_k is the energy of a magnon with momentum $\vec{k}$.

Note that $\omega_k \xrightarrow[k\to 0]{} 0$ – this is a consequence of symmetry – magnetization of a ferromagnet, in the absence of an external field, can point in any direction – long-wavelength magnetization waves cost very little energy.

Specialize to cubic lattice in 3D.

Consider ω_k at small k:

$$\gamma_k = \frac{1}{6}\cdot 2\left[\cos k_x a + \cos k_y a + \cos k_z a\right] \simeq$$

$$\simeq \frac{1}{3}\left[3 - \frac{1}{2}\left(k_x^2 + k_y^2 + k_z^2\right)a^2\right] = 1 - \frac{1}{6}k^2 a^2$$

$$\omega_k = 6JS\left(1 - \gamma_k\right) = JS\,k^2 a^2$$

Thus $\omega_k \sim k^2$ at small k – characteristic magnon dispersion in a ferromagnet.

We want to calculate:

$$\langle S^z \rangle = \frac{1}{N}\sum_i \langle S_i^z \rangle = S - \frac{1}{N}\sum_i \langle b_i^+ b_i \rangle =$$

$$= S - \frac{1}{N}\sum_k \langle b_k^+ b_k \rangle$$

$$\langle b_k^+ b_k \rangle = \frac{1}{Z}\,\mathrm{Tr}\left(b_k^+ b_k\, e^{-\frac{H}{k_B T}}\right) =$$

$$= \frac{1}{Z}\sum_{n_k=0}^{\infty} n_k\, e^{-\frac{\omega_k n_k}{k_B T}}$$

$$Z = \sum_{n_k=0}^{\infty} e^{-\frac{n_k \omega_k}{k_B T}} = \frac{1}{1 - e^{-\frac{\omega_k}{k_B T}}}$$

$$\sum_{n_k=0}^{\infty} n_k e^{-\frac{n_k \omega_k}{k_B T}} = -k_B T \frac{\partial}{\partial \omega_k} \sum_{n_k=0}^{\infty} e^{-\frac{n_k \omega_k}{k_B T}} =$$

$$= -k_B T \frac{\partial}{\partial \omega_k} \frac{1}{1 - e^{-\frac{\omega_k}{k_B T}}} = \frac{e^{-\frac{\omega_k}{k_B T}}}{\left(1 - e^{-\frac{\omega_k}{k_B T}}\right)^2}$$

Thus we obtain:

$$\langle b_k^+ b_k \rangle = \frac{e^{-\frac{\omega_k}{k_B T}}}{\left(1 - e^{-\frac{\omega_k}{k_B T}}\right)^2} \cdot \left(1 - e^{-\frac{\omega_k}{k_B T}}\right) =$$

$$= \frac{e^{-\frac{\omega_k}{k_B T}}}{1 - e^{-\frac{\omega_k}{k_B T}}} = \frac{1}{e^{\frac{\omega_k}{k_B T}} - 1} \equiv n_B(\omega_k)$$

$$n_B(\varepsilon) = \frac{1}{e^{\frac{\varepsilon}{k_B T}} - 1}$$ – Bose–Einstein distribution.

Thus we obtain:

$$\langle S^z \rangle = S - \frac{1}{N} \sum_k \langle b_k^+ b_k \rangle = S - \frac{1}{N} \sum_k n_B(\omega_k)$$

Convert the sum to an integral:

$$\frac{1}{V} \sum_{\vec{k}} n_B(\omega_k) = \frac{1}{N a^3} \sum_{\vec{k}} n_B(\omega_k) = \int \frac{d\vec{k}}{(2\pi)^3} n_B(\omega_k).$$

$$\langle S^z \rangle = S - a^3 \int \frac{d\vec{k}}{(2\pi)^3} n_B(\omega_k)$$

Can use the small-k approximation for ω_k:

$$\omega_k = JSk^2a^2$$

$$a^3 \int \frac{d\vec{k}}{(2\pi)^3} n_B(\omega_k) = \frac{a^3}{2\pi^2} \int_0^\infty dk \cdot k^2 \frac{1}{e^{\frac{JSk^2a^2}{k_B T}} - 1}$$

let $x = \dfrac{JSk^2a^2}{k_B T}$

$$k = \frac{1}{a} \sqrt{\frac{k_B T}{JS}} \sqrt{x} \; ; \; dk = \frac{1}{a} \sqrt{\frac{k_B T}{JS}} \frac{dx}{2\sqrt{x}}$$

$$k^2 dk = \frac{k_B T x}{JSa^2} \cdot \frac{1}{2a}\sqrt{\frac{k_B T}{JS}}\,\frac{dx}{\sqrt{x}} =$$

$$= \frac{1}{2a^3}\left(\frac{k_B T}{JS}\right)^{3/2}\sqrt{x}\,dx$$

Thus we obtain:

$$a^3 \int \frac{d\vec{k}}{(2\pi)^3}\, n_B(\omega_k) = \frac{1}{4\pi^2}\left(\frac{k_B T}{JS}\right)^{3/2}\int_0^\infty dx\,\frac{\sqrt{x}}{e^x - 1} =$$

$$= \frac{1}{4\pi^2}\left(\frac{k_B T}{JS}\right)^{3/2}\frac{\sqrt{\pi}}{2}\,\zeta\left(\frac{3}{2}\right)$$

Thus we obtain:

$$M(T) = g\mu_B \langle S^z \rangle = M(0) -$$

$$- g\mu_B \frac{1}{8}\,\zeta\left(\frac{3}{2}\right)\left(\frac{k_B T}{JS}\right)^{3/2}$$

$\frac{\Delta M(T)}{M(0)} \sim T^{3/2}$ – This leads to much faster decay of M at low T, compared to the mean-field theory prediction.