# Phys 726 - Lecture 16

## Holstein-Primakov Method

→ bosonic operator approach to spin waves and their interactions (excitations are not independent)

→ accommodates arbitrary $S$

→ Some subtleties associated with an enlarged Hilbert space

* Begin by introducing a diagonal counting operator $\hat{n} = S - \hat{S}^z$ (which measures deviation from full polarization in the $z$ direction) and raising/lowering operators $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$

  → the eigenvalues of $\hat{n}$ are integer and range from 0 to $2S$

→ Suppose that $|m\rangle$ is an $\hat{S}^z$ eigenstate with eigenvalue $m = -S, -S+1, \ldots, S$.

Then the raising / lowering operators obey

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

and

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

→ Switch notation to states $|n\rangle$ satisfying

$$\hat{n}|n\rangle = n|n\rangle \quad \text{with } n = S - m = 0, 1, 2, \ldots, 2S$$

Then

$$\begin{aligned}(S-m)(S+m+1) &= (S-m)(2S - S + m + 1) \\ &= n(2S - n + 1) \\ &= 2Sn\left(1 - \frac{(n-1)}{2S}\right)\end{aligned}$$

and

$$\begin{aligned}(S+m)(S-m+1) &= (2S - S + m)(S - m + 1) \\ &= (2S - n)(n+1) \\ &= 2S\left(1 - \frac{n}{2S}\right)(1+n)\end{aligned}$$

→ New raising / lowering expressions

$$\hat{S}^+ |n\rangle = \sqrt{2S}\sqrt{n}\sqrt{1-\frac{(n-1)}{2S}}\,|n-1\rangle$$

$$\hat{S}^- |n\rangle = \sqrt{2S}\sqrt{1-\frac{n}{2S}}\sqrt{1+n}\,|n+1\rangle$$

→ Make the connection to bosonic ~~[illegible]~~ creation / annihilation operators

$$a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle$$

→ Holstein-Primakoff transformation

$$S^+ = \sqrt{2S}\left(1-\frac{a^\dagger a}{2S}\right)^{1/2} a$$

$$S^- = \sqrt{2S}\,a^\dagger\left(1-\frac{a^\dagger a}{2S}\right)^{1/2}$$

$$S^z = S - a^\dagger a$$

→ the transformation is exact, except that the spectrum of $\hat{n} = S - \hat{S}^z$ is bounded $(0,1,2,\ldots,2S)$ whereas that of $\hat{n} = a^\dagger a$ is not $(0,1,2,\ldots)$

Fortunately, the unwanted part of the enlarged Hilbert space is unreachable

$$S^- |m = \overset{-S}{\cancel{0}}\rangle = S^- |n = 2S\rangle$$

$$= \sqrt{2S}\, a^\dagger \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} |n=2S\rangle$$

$$= \sqrt{2S}\, a^\dagger \underbrace{\left(1 - \frac{2S}{2S}\right)^{1/2}}_{\equiv 0} |n=2S\rangle$$

* Consider the FM quantum Heisenberg model on the cubic lattice $\{\vec{r}\} = \mathbb{Z}\vec{e}_x + \mathbb{Z}\vec{e}_y + \mathbb{Z}\vec{e}_z$

$$\hat{H} = -\frac{1}{2} J \sum_{\vec{r}} \sum_{\vec{\eta} = \pm\vec{e}_x, \pm\vec{e}_y, \pm\vec{e}_z} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\eta}}$$

$$= -\frac{1}{2}J \sum_{\vec{R}} \sum_{\vec{\eta}} \left\{ \frac{1}{2}\left( S^+_{\vec{R}} S^-_{\vec{R}+\vec{\eta}} + S^-_{\vec{R}} S^+_{\vec{R}+\vec{\eta}} \right) + S^z_R S^z_{R+\eta} \right) \right\}$$

$$= -\frac{1}{2}J \sum_{\vec{R}} \sum_{\vec{\eta}} \left\{ \frac{1}{2}\left[ 2S \left(1 - \frac{a^+_{\vec{R}} a_{\vec{R}}}{2S}\right)^{1/2} a_{\vec{R}}\, a^+_{\vec{R}+\vec{\eta}} \left(1 - \frac{a^+_{\vec{R}+\vec{\eta}} a_{\vec{R}+\eta}}{2S}\right) \right.\right.$$

$$\left. + 2S\, a^+_{\vec{R}} \left(1 - \frac{a^+_{\vec{R}} a_{\vec{R}}}{2S}\right)^{1/2} \left(1 - \frac{a^+_{\vec{R}+\vec{\eta}} a_{\vec{R}+\vec{\eta}}}{2S}\right)^{1/2} a_{\vec{R}+\eta} \right]$$

$$\left. + \left(S - a^+_{\vec{R}} a_{\vec{R}}\right)\left(S - a^+_{\vec{R}+\vec{\eta}} a_{\vec{R}+\vec{\eta}}\right) \right\}$$

→ two simplifications:

(1) take advantage of translational invariance to build "magnon" creation annihilation ops

$$a_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\cdot\vec{R}_j} a_j = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} a_{\vec{R}}$$

$$a^+_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_j e^{-i\vec{q}\cdot\vec{R}_j} a^+_j = \frac{1}{\sqrt{N}} e^{-i\vec{q}\cdot\vec{R}} a^+_{\vec{R}}$$

obeying $[a_{\vec{q}}, a^+_{\vec{q}'}] = \delta_{\vec{q},\vec{q}'}$ $\quad [a_{\vec{q}}, a_{\vec{q}'}] = [a^+_{\vec{q}}, a^+_{\vec{q}'}] = 0$

(2) Expand the square root in powers of $a^\dagger a/2S$:

$$S^+ = \sqrt{2S}\left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} a$$

$$= \sqrt{2S}\left(1 + \frac{1}{2}\left(-\frac{a^\dagger a}{2S}\right) - \frac{1}{8}\left(-\frac{a^\dagger a}{2S}\right)^2 + \cdots\right) a$$

$$= \sqrt{2S}\left(1 - \frac{a^\dagger a}{4S} - \frac{a^\dagger a a^\dagger a}{32S^2} + \cdots\right) a$$

$$S^- = \sqrt{2S}\, a^\dagger\left(1 - \frac{a^\dagger a}{4S} - \frac{a^\dagger a a^\dagger a}{32S^2} + \cdots\right)$$

→ With (1) and (2) both applied, we get

$$S^+_{\vec{R}} = \left(\frac{2S}{N}\right)^{1/2}\left[\sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{R}} a_{\vec{q}} - \frac{1}{4SN}\sum_{\vec{q}_1\vec{q}_2\vec{q}_3} e^{i(\vec{q}_1 - \vec{q}_2 - \vec{q}_3)\cdot\vec{R}} a^\dagger_{\vec{q}_1} a_{\vec{q}_2} a_{\vec{q}_3} + \cdots\right]$$

$$S^-_{\vec{R}} = \left(\frac{2S}{N}\right)^{1/2}\left[\sum_{\vec{q}} e^{+i\vec{q}\cdot\vec{R}} a^\dagger_{\vec{q}} - \frac{1}{4SN}\sum_{\vec{q}_1\vec{q}_2\vec{q}_3} e^{i(\vec{q}_1 + \vec{q}_2 - \vec{q}_3)} a^\dagger_{\vec{q}_1} a^\dagger_{\vec{q}_2} a_{\vec{q}_3} + \cdots\right]$$

$$\hat{S}^z_{\vec{R}} = S - \frac{1}{N}\sum_{\vec{q}_1\vec{q}_2} e^{i(\vec{q}_1-\vec{q}_2)\cdot\vec{R}}\, a^\dagger_{\vec{q}_1} a_{\vec{q}_2}$$

* Substitution into the Hamiltonian gives

$$\hat{H} = -\frac{1}{2} J N z S^2 + \hat{H}_0 + \text{beyond bilinear terms}$$

$N$: number of sites; $z$: coordination ($z=6$)

where

$$\hat{H}_0 = -\frac{1}{2} J z S \sum_{\vec{q}} \left(\gamma_{\vec{q}}\, a_{\vec{q}} a^\dagger_{\vec{q}} + \gamma_{-\vec{q}}\, a^\dagger_{\vec{q}} a_{\vec{q}} - 2 a^\dagger_{\vec{q}} a_{\vec{q}}\right)$$

$$\gamma_{\vec{q}} = \frac{1}{z}\sum_{\eta} e^{i\vec{q}\cdot\vec{\eta}}$$

$$= \frac{1}{3}\left(\cos q_x + \cos q_y + \cos q_z\right)$$

Hence

$$\hat{H}_0 = \sum_{\vec{q}} J z S (1-\gamma_{\vec{q}})\, a^\dagger_{\vec{q}} a_{\vec{q}}$$

→ describes a magnon gas with dispersion

$$JzS\left(1-\frac{1}{3}\left(1-\frac{1}{2}q_x^2+\dots+1-\frac{1}{2}q_y^2+\dots+1-\frac{1}{2}q_z^2+\dots\right)\right)$$

$$= J\frac{zS}{6}\left(q_x^2+q_y^2+q_z^2+\dots\right)$$

$$\sim JSq^2$$

→ thermodynamics of bosons

$$U = \sum_{\vec{q}} \hbar\omega_q \langle \hat{n}_q \rangle = \sum_{\vec{q}} \hbar\omega_q \frac{1}{e^{\beta\hbar\omega_{\vec{q}}}-1}$$

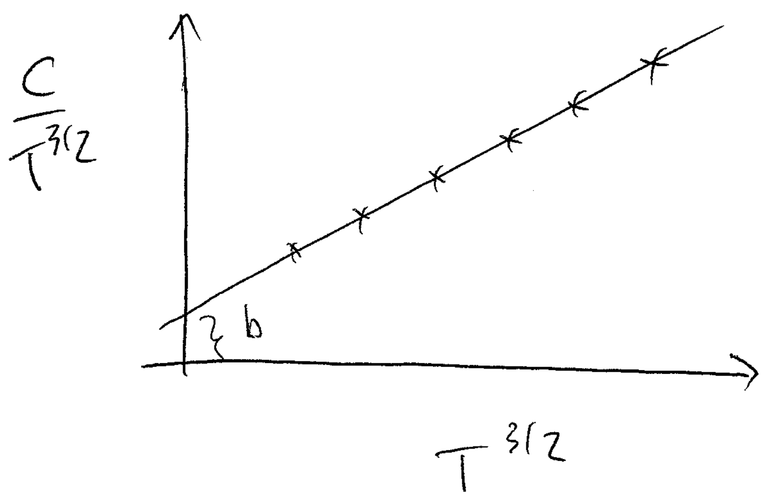
$$= V\int \frac{d^3q}{(2\pi)^3} \frac{JSq^2}{e^{\beta JSq^2}-1} = \frac{VJS}{8\pi^3}\int^{\text{cutoff}} 4\pi q^2 dq \cdot \frac{q^2}{e^{\beta JSq^2}-1}$$

$$= \frac{VJS}{2\pi^2}\int \frac{q^4 dq}{e^{\beta JSq^2}-1} \sim T^{5/2}$$

and $C_V \sim T^{3/2}$

→ in real materials, we expect to see both a phonon and magnon contribution

$$C = aT^3 + bT^{3/2}$$




→ total magnetization is

$$\left\langle \sum_{\vec{R}} \hat{S}^z_{\vec{R}} \right\rangle = \left\langle NS - \sum_{\vec{q}} a^\dagger_{\vec{q}} a_{\vec{q}} \right\rangle$$

and the change in magnetization from its saturation value is

$$\Delta M = \sum_{\vec{q}} \langle \hat{n}_{\vec{q}} \rangle = V \int^{\text{cutoff}} \frac{d^3 q}{(2\pi)^3} \frac{1}{e^{\beta J S q^2} - 1}$$

$$= \frac{V}{2\pi^2}\int \frac{q^2\,dq}{e^{\beta J S q^2}-1} \sim T^{3/2}$$

when $\Delta M \sim NS$ then the magnetism is destroyed

$$M(T) = M(0)\left(1-\left(\frac{T}{T_c}\right)^{3/2}\right)$$

$\Rightarrow$ proliferation of spin wave excitations melts the long-range order

<u>EXERCISE</u> : Redo this for the AFM case. What does the dispersion relation look like now?