Quantum and thermal fluctuations in low D systems.

Example of quantum magnetizm

Holstein-Primakoff transformation

Bogoliubov transformation

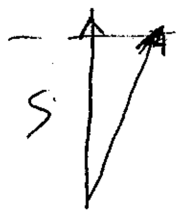
Mermin-Wagner theorem

O(3) quantum phase transition

Bose condensation of triplons

Holstein - Primakoff transformation.

We want to consider small deviations of a spin from the equilibrium direction



Algebra of spin is defined by commutation relations

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

In terms of $S_\pm = S_x \pm i S_y$ this is equivalent to

$$\begin{cases} [S_+, S_-] = 2 S_z \\ [S_+, S_z] = -S_+ \\ [S_-, S_z] = S_- \end{cases}$$

We want to introduce creation operater of magnon. Magnon is the spin deviation from the equilibrium,

a^+ - creation operater

$$\boxed{a a^+ - a^+ a = 1}$$: the usual bosonic commutation relation.

Halstein-Primakoff transformation:
transformation from spin to a.

$$\begin{cases} S_+ = \sqrt{2S}\sqrt{1-\dfrac{a^+a}{2S}}\,a \\ S_- = \sqrt{2S}\,a^+\sqrt{1-\dfrac{a^+a}{2S}} \\ S_z = S - a^+a \end{cases}$$

check commutation relations.

$$[S_+, S_z] = \sqrt{2s}\,[f a,\ s - a^+ a]$$

$$f = \sqrt{1 - \frac{a^+ a}{2s}} = \sqrt{1 - \frac{\hat{n}}{2s}}, \quad \hat{n} = a^+ a$$

obviously, $[f, \hat{n}] = 0$.

$$\sqrt{2s}\,[f a,\ s - a^+ a] = -\sqrt{2s}\,[f a, a^+ a] =$$

$$= -\sqrt{2s}\, f\, [a, a^+ a] = -\sqrt{2s}\, f\, \overbrace{[a a^+]}^{=1} a =$$

$$= -\sqrt{2s}\, f a = -S_+ \quad \underline{\text{OK}}$$

Similarly $[S_-, S_z] = S_-$

$$[S_+, S_-] = 2s\,[f a, a^+ f] = 2s\{f[a, a^+ f] +$$

$$+ [f, a^+ f] a\} = 2s\{f \underbrace{[a, a^+]}_{\shortparallel} f + f a^+ [a, f] +$$

$$+ [f, a^+] f a\} = 2s\left\{1 - \frac{a^+ a}{2s} + \underline{f a^+ [a, f] + [f, a^+] f a}\right\}$$

Let us calculate the underlined terms only up to the leading order in $\frac{1}{S}$, assuming that $S \gg 1$.

$$f = \sqrt{1 - \frac{a^+ a}{2S}} \approx 1 - \frac{a^+ a}{4S}$$

$$[a, f] = -\frac{1}{4S}[a, a^+ a] = -\frac{a}{4S}$$

Hence

$$f a^+ [a f] \approx [f a^+] f a \approx -\frac{a^+ a}{4S}$$

$$\boxed{[S_+, S_-] = 2S\left\{1 - \frac{a^+ a}{2S} - \frac{a^+ a}{4S} - \frac{a^+ a}{4S}\right\} = 2(S - a^+ a)}$$

OK.

The commutation relation can be checked in all orders in $1/S$.

Description of ferromagnet using second quantization.

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

We will keep only the leading order is $1/S$. This is equivalent to quadratic approximation in the operators a, a^+.

In this approximation

$$\begin{cases} S^+ \approx \sqrt{2S}\, a \\ S^- \approx \sqrt{2S}\, a^+ \\ S_z = S - a^+ a \end{cases}$$

Hence

$$H \approx -J\sum_{\langle ij\rangle}\left\{ (S - a_i^+ a_i)(S - a_j^+ a_j) + \frac{1}{2} 2S\left(a_i^+ a_j + a_j^+ a_i\right)\right\} \approx$$

$$\approx -JS^2 \sum_{\langle ij\rangle} + JS\sum_{\langle ij\rangle}\left[a_i^+ a_i + a_j^+ a_j - (a_i^+ a_j + a_j^+ a_i)\right]$$

$$\sum_{\langle ij\rangle} = \frac{ZN}{2};$$

$$\sum_{\langle ij\rangle}(\ldots) = \frac{1}{2}\sum_{i,\delta}(\ldots) \qquad \vec{j} = \vec{i} + \vec{\delta}$$

to avoid double counting.

$$JS\sum_{\langle ij\rangle}\left[a_i^+a_i + a_j^+a_j - (a_i^+a_j + a_j^+a_i)\right] =$$

$$= \frac{JS}{2}\sum_{n\delta}\left[a_n^+a_n + a_{n+\delta}^+a_{n+\delta} - (a_n^+a_{n+\delta} + a_{n+\delta}^+a_n)\right]$$

Fourier transform

$$a_n^+ = \frac{1}{\sqrt{N}}\sum_k a_k^+ e^{ikr_n}$$

$$a_n = \frac{1}{\sqrt{N}}\sum_k a_k e^{-ikr_n}, \quad \sum_k \equiv \int\frac{d^Dk}{(2\pi)^3}$$

Let us ~~work~~ work out the firs term

$$\frac{JS}{2}\sum_{n\delta} a_n^+a_n = \frac{JS}{2}\cdot Z\sum_{n,k,q}\frac{1}{N}e^{ikr_n}e^{-iqr_n}a_k^+a_q$$

$$\frac{1}{N}\sum_n e^{i(k-q)r_n} = \delta_{kq} = \begin{cases} 1 & \text{if } k=q \\ 0 & \text{if } k\neq q. \end{cases}$$

Hence

$$\frac{JS}{2}\sum_{n\delta} a_n^+ a_n = \frac{JSZ}{2}\sum_k a_k^+ a_k$$

Similarly $\frac{JS}{2}\sum_{n\delta} a_{n+\delta}^+ a_{n\delta}^+ = \frac{JSZ}{2}\sum_k a_k^+ a_k$

$$-\frac{JS}{2}\sum_{n\delta}\left(a_n^+ a_{n+\delta} + a_{n+\delta}^+ a_n\right) =$$

$$= -JS\sum_{k\delta} a_k^+ a_k e^{ik\bar{\delta}}$$

ground state energy.

$$H = -\frac{JS^2ZN}{2} + JS\sum_{k\delta} a_k^+ a_k\left(1 - e^{ik\bar{\delta}}\right) =$$

$$= -\frac{JS^2ZN}{2} + \sum_k \omega_k a_k^+ a_k$$

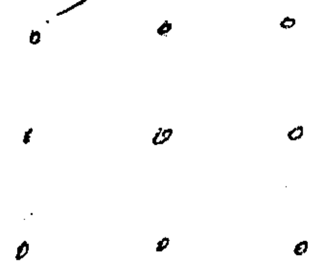
$$\boxed{\omega_k = JS\sum_\delta\left(1 - e^{ik\delta}\right)}$$

magnon spectrum.

For simple cubic lattice, $z = 6$

$$\omega_k = 6JS\left[1 - \frac{1}{3}(\cos k_x + \cos k_y + \cos k_z)\right]$$

For square lattice, $z = 4$,



$$\omega_k = 4JS\left[1 - \frac{1}{2}(\cos k_x + \cos k_y)\right]$$

This was a $1/S$ expansion, however, this approximation works well even for $S = 1/2$.

Antiferromagnet

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j$$

There are two sublattices, up and down

$$\begin{array}{cccc} A & B & & \\ \uparrow & \downarrow & \uparrow & \downarrow \end{array}$$

A-sublattice:

$$S^+ \approx \sqrt{2S}\, a$$
$$S^- \approx \sqrt{2S}\, a^+$$
$$S_z \approx S - a^+ a$$

B-sublattice

$$S^+ \approx \sqrt{2S}\, b^+$$
$$S^- \approx \sqrt{2S}\, b$$
$$S_z = -S + b^+ b$$

$$H = J \sum_{\substack{n \in A \\ \delta}} \left[S_n^z S_{n+\delta}^z + \frac{1}{2}\left(S_n^+ S_{n+\delta}^- + S_{n+\delta}^+ S_n^- \right) \right] \approx$$

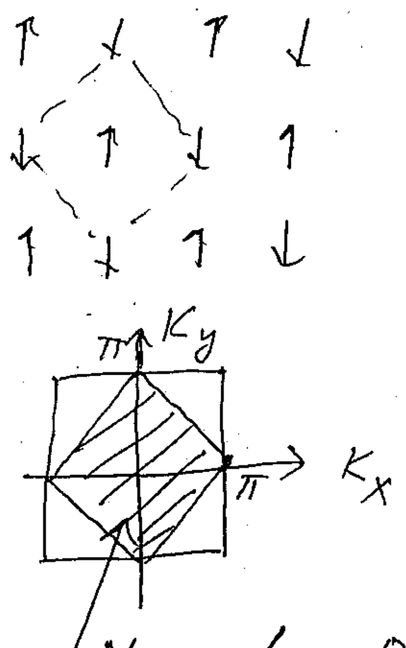
$$\approx J \sum_{n,\delta} \left[(S - a_n^+ a_n)(-S + b_{n+\delta}^+ b_{n+\delta}) + \frac{2S}{2}\left(a_n b_{n+\delta} + a_n^+ b_{n+\delta}^+ \right) \right]$$

$$\approx J \sum_{\substack{n \in A \\ \delta}} \left\{ -S^2 + S\left[a_n^+ a_n + b_{n+\delta}^+ b_{n+\delta} + (a_n b_{n+\delta} + a_n^+ b_{n+\delta}^+) \right] \right\}$$

Fourier transform

$$a_n^+ = \sqrt{\frac{2}{N}} \sum_{K \in MBZ} a_K^+ e^{i\vec{K}\vec{r}_n}$$

$$b_n^+ = \sqrt{\frac{2}{N}} \sum_{K \in MBZ} b_K^+ e^{i\vec{K}\vec{r}_n}$$



Magnetic BZ
MBZ

All K-summations below are performed over MBZ.

the first term in the Hamiltonian

$$J \sum_{\substack{n \in A \\ \delta}} (-S^2) = -JS^2 Z \frac{N}{2} \quad \text{– ground state energy.}$$

the second term in the Hamiltonian

$$JS \sum_{\substack{n \in A \\ \delta}} a_n^+ a_n = JSZ \sum_n \sum_{Kq} a_K^+ a_q \frac{2}{N} e^{i(\vec{K}-\vec{q})\vec{r}_n} = JSZ \sum_K a_K^+ a_K$$

Here I take into account the relation

$$\boxed{\frac{2}{N} \sum_{n \in A} e^{i(\vec{K}-\vec{q})\vec{r}_n} = \delta_{Kq}}$$

Altogether the Hamiltonian is

$$H = -\frac{JS^2 zN}{2} + JSz\sum_{K}\left[a_K^+ a_K + b_K^+ b_K + \gamma_K\left(a_K b_{-K} + a_K^+ b_{-K}^+\right)\right]$$

$$\boxed{\gamma_K = \frac{1}{z}\sum_{\delta} e^{i\vec{K}\vec{\delta}}}$$

For square lattice $\gamma_K = \frac{1}{4}\left(e^{iK_x} + e^{-iK_x} + e^{iK_y} + e^{-iK_y}\right) =$
$= \frac{1}{2}\left(\cos K_x + \cos K_y\right)$

<u>Bogoliubov transform</u>

$$\boxed{\begin{aligned} a_K &= u_K \alpha_K + v_K \beta_{-K}^+ \\ b_K &= u_K \beta_K + v_K \alpha_{-K}^+ \end{aligned}}$$

a, b, α, β are operators. u_K, v_K are usual numbers.

The transform must preserve the bosonic commutation relations

$$\begin{matrix} [a_K, a_K^+] = 1 \\ [b_K, b_K^+] = 1 \end{matrix} \iff \begin{matrix} [\alpha_K, \alpha_K^+] = 1 \\ [\beta_K, \beta_K^+] = 1 \end{matrix}$$

$$[u_K\alpha_K + v_K\beta_{-K}^+, u_K\alpha_K^+ + v\beta_{-K}] = u_K^2[\alpha_K, \alpha_K^+] + v^2[\beta_{-K}^+, \beta_K] =$$

$= u_K^2 - v_K^2$. Hence $\boxed{u_K^2 - v_K^2 = 1}$

Rewrite the quantum part of the Hamiltonian on page 209.

$$a_k^+ a_k + b_k^+ b_k + \gamma_k (a_k b_{-k} + a_k^+ b_{-k}^+) =$$

I omit the subscript k in u_k, v_k

$$= (u\alpha_k^+ + v\beta_{-k})(u\alpha_k + v\beta_{-k}^+) +$$
$$+ (u\beta_k^+ + v\alpha_{-k})(u\beta_k + v\alpha_{-k}^+) +$$
$$+ \gamma_k\left[(u\alpha_k + v\beta_{-k}^+)(u\beta_{-k} + v\alpha_k^+) + (u\alpha_k^+ + v\beta_{-k})(u\beta_{-k}^+ + v\alpha_k)\right] =$$

$$\left.\begin{aligned} &= u^2\alpha_k^+\alpha_k + v^2\beta_{-k}\beta_{-k}^+ + u^2\beta_k^+\beta_k + v^2\alpha_{-k}\alpha_{-k}^+ + \\ &+ \gamma_k uv\left[\alpha_k\alpha_k^+ + \beta_{-k}^+\beta_{-k} + \alpha_k^+\alpha_k + \beta_{-k}\beta_{-k}^+\right] + \\ &+ (\alpha_k^+\beta_{-k}^+ + \alpha_k\beta_{-k})\underbrace{\left[uv + uv + \gamma_k(u^2+v^2)\right]}_{=0} \end{aligned}\right\} \text{A}$$

$= 0 \leftarrow$ The condition of diagonalization

$$\boxed{\begin{aligned} &2u_k v_k + \gamma_k(u_k^2 + v_k^2) = 0 \\ &u_k^2 - v_k^2 = 1 \end{aligned}}$$

The solution is

$$u_k = \sqrt{\frac{1}{2}\left(\frac{1}{\sqrt{1-\gamma_k^2}} + 1\right)}, \quad v_k = -\mathrm{sign}(\gamma_k)\sqrt{\frac{1}{2}\left(\frac{1}{\sqrt{1-\gamma_k^2}} - 1\right)}$$

$$2u_k V_k = -\frac{\gamma_k}{\sqrt{1-\gamma_k^2}}$$

Continue to transform Eq (A) on page 210.

$$\alpha_k \alpha_k^+ = 1 + \alpha_k^+ \alpha_k \quad , \quad \beta_k \beta_k^+ = 1 + \beta_k^+ \beta_k$$

$$\longrightarrow 2(V_k^2 + \gamma_k u_k V_k) + \alpha_k^+ \alpha_k \left[u_k^2 + V_k^2 + 2\gamma_k u_k V_k \right] +$$

$$+ \beta_k^+ \beta_k \left[u_k^2 + V_k^2 + 2\gamma_k u_k \gamma_k \right]$$

$$u_k^2 + V_k^2 + 2\gamma_k u_k V_k = \sqrt{1-\gamma_k^2}$$

$$2(V_k^2 + \gamma_k u_k V_k) = \sqrt{1-\gamma_k^2} - 1$$

Hence the Hamiltonian reads

$$\boxed{\begin{aligned} \mathcal{H} &= -\frac{JS^2 zN}{2} + \sum_{k \in MBZ} JSz\left(\sqrt{1-\gamma_k^2} - 1\right) + \\ &+ \sum_{k \in MBZ} \omega_k \left(\alpha_k^+ \alpha_k + \beta_k^+ \beta_k\right) \\ &\omega_k = JSz\sqrt{1-\gamma_k^2} \end{aligned}}$$

The first term in the Hamiltonian is classical ground state energy.

The second term is quantum correction to the ground state energy

The third term gives the magnon excitation spectrum.