3. Spin-wave theory: Collinear vs. non-collinear states

3.1. Classical limit for Heisenberg models

Classical spins $\hat{=}$ commuting (unit) vectors

For SU(2) spins, classical limit is reached for $S \to \infty$,

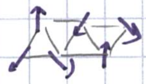
because $[S^x, S^y]_- = i\hbar S^z$

which is $[\frac{1}{S} S^x, \frac{1}{S} S^y]_- = \frac{1}{S} i\hbar \frac{S^z}{S}$ $\qquad \frac{1}{S} \to 0$

This limit is important, because quantum corrections can be calculated in $1/S$ expansion.

Classical states: Specified by direction of (unit) vector

Ferromagnet $\uparrow\uparrow\uparrow\uparrow$

Antiferromagnet $\uparrow\downarrow\uparrow\downarrow$  $\nwarrow \nearrow \nwarrow \nearrow$

(frustrated) (in magnetic field $\parallel \hat{z}$)

Theorem:

For classical Heisenberg spins and lattice with single site per unit cell (and no external field), the state with minimal energy is given by a single-Q spiral state, where the ordering wavevector $\vec{Q}$ minimizes the interaction function $J(\vec{q})$.

Single-Q spiral: $\langle \vec{S}_i \rangle = \mathrm{Re}\left(\vec{n}\, e^{i\vec{Q}\cdot\vec{R}_i}\right)$

$\vec{n} = \vec{n}_1 + i\vec{n}_2$; $\vec{n}_1, \vec{n}_2$ real, $\vec{n}_1 \cdot \vec{n}_2 = 0$

$\vec{Q} = 0$: $\uparrow\uparrow\uparrow\uparrow$

$\vec{Q} = (\pi,\pi)$: $\uparrow\downarrow\uparrow\downarrow$ (Néel state)
$\downarrow\uparrow\downarrow\uparrow$

$\vec{Q} = \pi/5$ $\uparrow\nearrow\nearrow\rightarrow\searrow\downarrow\swarrow\swarrow\nwarrow\nwarrow\uparrow$ (spiral) to avoid double counting of bonds; $J_{ij} = J_{ji}$

<u>Proof</u>: $$H = \frac{1}{2} \sum_{ij} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$

Introduce $$\vec{S}(\vec{q}) = \frac{1}{\sqrt{N}} \sum_i \vec{S}_i \, e^{-i \vec{q} \cdot \vec{R}_i}$$ (works on Bravais lattice) (with N sites)

Then
$$H = \frac{1}{2} \sum_q J(\vec{q}) \, \vec{S}(\vec{q}) \cdot \vec{S}(-\vec{q})$$

with $$J(\vec{q}) = \frac{1}{N} \sum_{ij} J_{ij} \, e^{i \vec{q} \cdot (\vec{R}_j - \vec{R}_i)} = \sum_{\vec{\Delta}} J_{\vec{\Delta}} \, e^{i \vec{q} \cdot \vec{\Delta}}$$

translation invariance $(\vec{\Delta} = \vec{R}_j - \vec{R}_i)$

$J_{ij} = J_{i, i+\Delta} = J_\Delta$

Length constraint $|\vec{S}_i| = 1$

$$\rightsquigarrow \sum_q \vec{S}(\vec{q}) \cdot \vec{S}(-\vec{q}) = N$$

$\rightsquigarrow$ H is minimized for $S(\vec{q}) = \begin{cases} N & \vec{q} = \vec{Q} \\ 0 & \text{otherwise} \end{cases}$ with $\vec{Q}: J(\vec{q}) \to \min$

<u>Examples</u> Cubic lattice $$J(\vec{q}) = 2J(\cos q_x + \cos q_y + \cos q_z)$$

$J > 0 \rightsquigarrow \vec{Q} = (\pi, \pi, \pi)$ antiferromagnet

$J < 0 \rightsquigarrow \vec{Q} = 0$ ferromagnet

Triangular lattice $$J(\vec{q}) = 2J\left(\cos q_x + 2 \cos \frac{q_x}{2} \cos \frac{\sqrt{3} q_y}{2}\right)$$

$J > 0 \rightsquigarrow \vec{Q} = (\frac{4}{3}\pi, 0)$ 120° state

$J < 0 \rightsquigarrow \vec{Q} = 0$ ferromagnet

3.2. Spin representations and $1/S$ expansion ($\hbar=1$)

Many-body calculation are often easier with bosons or fermions than for spins $\rightsquigarrow$ represent spins by bosons or fermions (many options)
(Hilbert space usually enlarged!)

General S: Represent $(2S+1)$ states, preserve $[S^\alpha, S^\beta] = i\varepsilon_{\alpha\beta\gamma} S^\gamma$

Holstein-Primakoff

$$\boxed{\begin{aligned} S^z &= S - a^+a \\ S^+ &= \sqrt{2S - a^+a}\; a \\ S^- &= a^+ \sqrt{2S - a^+a} \end{aligned}}$$

Hilbert-space constraint: $a^+a \le 2S$ (for physical Hilbert space)

Approximations rely on $\langle a^+a\rangle \ll 2S$ $\rightsquigarrow$ good for symmetry-broken states with $\langle S^z\rangle \neq 0$

$1/S$ expansion: expand all observables in Taylor series in $1/S$,

by expanding in $a^+a/_{2S}$ $(n = a^+a)$:

$$\sqrt{2S-n} = \sqrt{2S}\left(1 - \frac{n}{4S} - \frac{n^2}{32S^2} + - \dots\right)$$

Holstein-Primakoff representation <u>chooses</u> a reference state direction for each spin: $S \parallel \hat{z}$ $(a^+a = 0 \;\hat{=}\; S^z = S)$. For antiferromagnets different reference direction must be chosen for each spin. For non-collinear states (e.g. $\nwarrow \nearrow \nwarrow \nearrow$) these directions may themselves depend on $1/S$ (see later).

Dyson-Maleev

$$\begin{aligned} S^z &= S - a^+a \\ S^+ &= \sqrt{2S}\left(1 - \frac{a^+a}{2S}\right) a \\ S^- &= \sqrt{2S}\; a^+ \end{aligned}$$

Similar to Holstein-Primakoff, with two differences:

- $(S^-)^+ \neq S^+$ $\rightsquigarrow$ awkward calculations
- $1/S$ expansion does not involve $\sqrt{}$ expansion $\rightsquigarrow$ only finite number of terms

Holstein - Primakoff and Dyson - Maleev representations are <u>NOT</u> suitable for symmetric phases. Alternatives:

<u>Schwinger bosons</u>

$$S^z = \frac{1}{2}\left(a^+a - b^+b\right)$$
$$S^+ = a^+b$$
$$S^- = b^+a$$

Hilbert-space constraint: $a^+a + b^+b = 2S$

States $|S, m\rangle = (a^+)^{S+m}(b^+)^{S-m} \frac{1}{\sqrt{(S+m)!}} \frac{1}{\sqrt{(S-m)!}} |0\rangle$

For $S = 1/2$ more representations have been developed, e.g.

<u>Abrikosov fermions</u>

$$\left.\begin{aligned} S^z &= \frac{1}{2}\left(c_\uparrow^+c_\uparrow - c_\downarrow^+c_\downarrow\right) \\ S^+ &= c_\uparrow^+c_\downarrow \\ S^- &= c_\downarrow^+c_\uparrow \end{aligned}\right\} \quad S^\alpha = \frac{1}{2}\sum_{ss'} c_s^+ \underset{\substack{\uparrow \\ \text{Pauli}}}{\sigma_{ss'}^\alpha} c_{s'}$$

Hilbert-space constraint: $c_\uparrow^+c_\uparrow + c_\downarrow^+c_\downarrow = 1$

<u>Majorana fermions</u>
(Kitaev)

$$S^\alpha = b\,c^\alpha \qquad (\alpha = x, y, z)$$

$b = b^+$, $c^\alpha = c^{\alpha +}$

Hilbert-space constraint $\quad b\,c^x c^y c^z = 1 \quad$ (see later)

3.3. Spin-wave theory for ferromagnets

Spin-wave theory: describes properties of <u>ordered</u> magnetic phases, expands about classical reference state, formally is a $1/S$ expansion

Simplest case: Heisenberg ferromagnet (lattice arbitrary, specified later)

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - h \sum_i S_i^z$$

pairs of nearest neighbors

Assumption: $\vec{S}_i \parallel z$ $\curvearrowright$ $S_i^z = S - a_i^+ a_i$

(expand about fully polarized state) $S_i^+ = \sqrt{2S - a_i^+ a_i}\; a_i$

Insert:
$$H = -J \sum_{\langle ij \rangle} \Big(S^2 - S a_i^+ a_i - S a_j^+ a_j + a_i^+ a_i a_j^+ a_j + \frac{1}{2} \underbrace{a_i^+ \sqrt{2S - a_i^+ a_i}}_{S_i^-} \underbrace{\sqrt{2S - a_j^+ a_j}\; a_j}_{S_j^+} + \frac{1}{2} a_j^+ \sqrt{2S - a_j^+ a_j} \sqrt{2S - a_i^+ a_i}\; a_i \Big)$$
$$- h \sum_i (S - a_i^+ a_i)$$

Rewrite
$$H = -J \overbrace{\sum_{\langle ij \rangle}}^{= N\frac{z}{2}} S^2 - h \overbrace{\sum_i}^{= N} S \qquad H_0$$
$$- JS \sum_{\langle ij \rangle} (-a_i^+ a_i - a_j^+ a_j + a_i^+ a_j + a_j^+ a_i) + h \sum_i a_i^+ a_i \qquad H_2$$
$$- J \sum_{\langle ij \rangle} \Big(a_i^+ a_i a_j^+ a_j - \frac{1}{4} \big(a_i^+ a_i^+ a_i a_j + a_i^+ a_j^+ a_j a_j + a_j^+ a_j^+ a_j a_i + a_j^+ a_i^+ a_i a_i \big)\Big) \qquad H_4$$
$$- J \frac{1}{S} \sum_{\langle ij \rangle} [\, 6\ a^+, a \text{ operators} \,] \qquad H_6$$
$$+ \mathcal{O}(1/S^2)$$

H_n contains n a^+, a operators

Observations:
- organized in powers of $1/S$, higher powers $\hat{=}$ more operators
- equal number of a^+ & a $\hat{=}$ S^z conserved
- since leading term in energy is $\mathcal{O}(S^2)$, external field should be taken $\mathcal{O}(S)$ such that $h S^z$ is also $\mathcal{O}(S^2)$.

The re-writing of H is exact, but represents a strongly interacting problem of bosons. Strategy: Work at large S, such that higher-order terms are small.

H_0 is classical ground-state energy (i.e. energy of ideal ferromagnet in field)

H_2 is bilinear in bosons and can be solved — This is linear spin-wave theory.

To this end:

Define $\quad a_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} a_i \quad , \quad \vec{k} \in$ first Brillouin zone

$\quad a_i = \frac{1}{\sqrt{N}} \sum_k e^{-i\vec{k}\cdot\vec{R}_i} a_{\vec{k}} \quad , \quad N =$ no. of lattice sites

and $\quad J(\vec{k}) = \frac{2}{N} \sum_{\langle ij\rangle} J e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} = J \sum_{\vec{\Delta}} e^{i\vec{k}\cdot\vec{\Delta}}$

$\vec{\Delta}$: nearest-neighbor vectors

(For general interactions $\quad H = \frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad : \quad J(\vec{k}) = \frac{1}{N} \sum_{ij} J_{ij} e^{i\vec{k}(\vec{R}_j - \vec{R}_i)}$)

Insert:

$$H_2 = \sum_{\vec{k}\in BZ}{}' \omega_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}}$$

with
$$\omega_{\vec{k}} = S\left[J(0) - J(\vec{k})\right] + h = JSz(1-\gamma_{\vec{k}}) + h$$

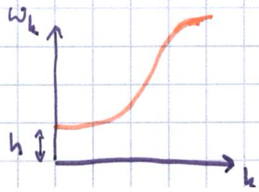
$$J(\vec{k}) =: Jz\gamma_{\vec{k}}$$

Interpretation of H_2: Excitations of classical ground state are bosons, created by $a^\dagger_{\vec{k}}$, these are spin waves with momentum $\vec{k}$.

$\omega_{\vec{k}}$ is energy (dispersion) of spin waves.

For $h=0$: $\omega_{\vec{k}=0} = 0$ and $\omega_{\vec{k}} = Dk^2$ for small $\vec{k}$ $\hat{=}$ Goldstone mode

E.g. cubic lattice $(z=6)$
$$J(\vec{k}) = 2J\,(\cos k_x + \cos k_y + \cos k_z) = J\sum_{\vec{\Delta}}^{6} e^{i\vec{k}\cdot\vec{\Delta}}$$
$$\gamma_{\vec{k}} = \frac{1}{3}\,(\cos k_x + \cos k_y + \cos k_z)$$



Note: Ground state of H_2 is vacuum of a_k,

this is state with $a_i^+ a_i = 0 \quad \forall i$

$\rightsquigarrow$ fully polarized ferromagnet $| \uparrow\uparrow\uparrow\uparrow \dots \rangle$

This is in fact the <u>exact</u> ground state of H.

Note: One-magnon state is $a_k^+ \, |\uparrow\uparrow\uparrow \dots \rangle$;

this is an <u>exact</u> eigenstate of H.

Observables can now be calculated from $H_0 + H_2$.

Example: Magnetization

$$M = \frac{1}{N} \sum_i S_i^z = \underset{\text{classical value}}{S} - \underbrace{\frac{1}{N} \sum_k a_k^+ a_k}_{\Delta M \text{ quantum correction}}$$

Within linear spin-wave theory, the a_k are independent bosons.

Thermal occupation from Bose gas: $\quad n_k = \langle a_k^+ a_k \rangle = \dfrac{1}{e^{\beta \omega_k} - 1}$

$$\rightsquigarrow \quad \Delta M = \frac{1}{N} \sum_k \frac{1}{e^{\beta \omega_k} - 1} \qquad \beta = \frac{1}{k_B T}$$

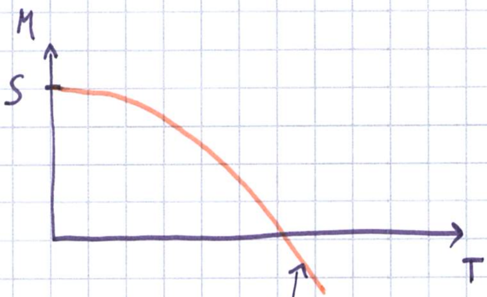
For small T $(T \ll J)$ n_k is only sizeable for $k \ll 1$.

$$\rightsquigarrow \quad \Delta M \underset{\substack{\uparrow \\ \text{no field}}}{\simeq} \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta D k^2} - 1} \propto T^{d/2} \underbrace{\int_0^{x_{max}} dx \, \frac{1}{e^x - 1} \, x^{\frac{d-2}{2}}}_{\text{divergent for } d \leq 2}$$

$\rightsquigarrow$ ordered state is destroyed by fluctuations at any finite T

(Mermin-Wagner theorem)

$d = 3$:



$M < 0$ unphysical $\rightsquigarrow$ approximation (ie. assumption of ordered state) breaks down

$T|_{M=0}$ is estimate for Curie temperature.

$H_4, H_6, \dots$

Effect of interactions: Perturbation theory!

 finite magnon lifetime for $T > 0$

 corrections to free energy (energy exact!)

$\vdots$

3.4. Spin-wave theory for collinear antiferromagnets

Bipartite lattice, nearest-neighbor AF interaction $\rightsquigarrow$ $\uparrow\downarrow\uparrow\downarrow$ (Neél state)

Expand around classical AF state $\parallel \hat{z}$

$$\underline{H = J \sum_{\langle ij \rangle}' \vec{S}_i \cdot \vec{S}_j - h \sum_i' S_i^z - \frac{D}{2} \sum_i {S_i^z}^2}$$

Single-ion anisotropy

Two options:

a) Two sublattices $\rightsquigarrow$ two sets of operators

b) Rotate every second spin $\rightsquigarrow$ classical AF state is $\uparrow\uparrow\uparrow$ $\rightsquigarrow$ one set of ops (not useful for $h \neq 0$)

(result identical, but care is needed w/ Brillouin zone)

$\boxed{\text{Here a)}}$ A sublattice
$$S_i^z = S - a_i^+ a_i \qquad \uparrow_A \downarrow_B \uparrow_A \downarrow_B$$
$$S_i^+ = \sqrt{}\, a_i$$

B sublattice
$$S_j^z = -S + b_j^+ b_j$$
$$S_j^- = \sqrt{}\, b_j$$

Insert:

$$H = -J N \frac{z}{2} S^2 - \frac{D}{2} N S^2 \qquad H_0 \text{ classical}$$

$$\underbrace{+ J S \sum_{\langle ij \rangle}' \left(a_i^+ a_i + b_j^+ b_j + a_i b_j + a_i^+ b_j^+ \right) + h \left(\sum_i a_i^+ a_i - \sum_j b_j^+ b_j \right) + DS \left(\sum_i a_i^+ a_i + \sum_j b_j^+ b_j \right)}_{H_2}$$

$$+ J \sum_{\langle ij \rangle}' \left(-a_i^+ a_i b_j^+ b_j + \frac{1}{4} \left(a_i^+ b_j^+ b_j^+ b_j + \dots \right) \right)$$

$$+ \mathcal{O}(1/S)$$

Observations:

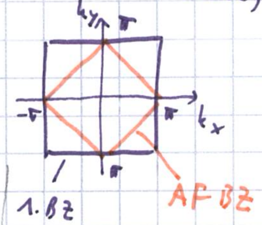
- total Particle number, $n_a + n_b$ not conserved! Vacuum is not eigenstate!
- S^z conservation is $n_a - n_b = \text{const}$
- field acts asymmetrically on both sublattices

H_2 is again bilinear and can be solved.

Introduce Fourier-transformed boson operators on both sublattices:

$$a_{\vec{k}} = \sqrt{2/N} \sum_i e^{i\vec{k}\cdot\vec{R}_i} a_i \quad , \quad i \in A$$
$$b_{\vec{k}} = \sqrt{2/N} \sum_j e^{i\vec{k}\cdot\vec{R}_j} a_j \quad , \quad j \in B$$

Here, $N/2$ is number of sites per sublattice, and $k \in$ „antiferromagnetic" Brillouin zone, i.e. the Brillouin zone of one sublattice. E.g. square lattice:



Insert:

$$H_2 = JzS \sum_{\vec{k}\in AF\,BZ} \Big[(1+\tilde{h}+\tilde{d})\, a^+_{\vec{k}} a_{\vec{k}} + (1-\tilde{h}+\tilde{d})\, b^+_{\vec{k}} b_{\vec{k}} + \gamma_{\vec{k}} \left(a_{\vec{k}} b_{-\vec{k}} + a^+_{\vec{k}} b^+_{-\vec{k}} \right) \Big]$$

where $\quad \tilde{d} = \frac{D}{Jz} \quad , \quad \tilde{h} = \frac{h}{JzS} \quad , \quad \gamma_{\vec{k}} = J(\vec{k})/Jz$

Particle number not conserved! Solve by Bogoliubov transformation (see BCS theory).

Introduce new bosonic operators α_k, β_k to eliminate anomalous terms.

$$\boxed{\begin{aligned} a_{\vec{k}} &= u_{\vec{k}}\, \alpha_{\vec{k}} - v_{\vec{k}}\, \beta^+_{-\vec{k}} \\ b_{-\vec{k}} &= -v_{\vec{k}}\, \alpha^+_{\vec{k}} + u_{\vec{k}}\, \beta_{-\vec{k}} \end{aligned}} \qquad u_{\vec{k}}, v_{\vec{k}} \text{ real}$$

$[\alpha_k, \alpha^+_{k'}] = \delta_{kk'}$ and $[\beta_k, \beta^+_{k'}] = \delta_{kk'}$ require $u_k^2 - v_k^2 = 1$

$\curvearrowright$ parametrize $u_k = \cosh \vartheta_k \;,\; v_k = \sinh \vartheta_k$.

Anomalous terms $\alpha_k \beta_{-k}$ are eliminated by choice $\tanh 2\vartheta_k = \frac{\gamma_k}{1+\tilde{d}}$.

Then

$$\underline{H_2 = JzS \sum_{\vec{k}\in AF\,BZ} \Big[\omega^+_k \alpha^+_k \alpha_k + \omega^-_k \beta^+_k \beta_k + \underbrace{\tfrac{1}{2}\left(\omega^+_k + \omega^-_k - 2(1+\tilde{h}+\tilde{d})\right)}_{\text{quantum correction to ground-state energy}} \Big]}$$

with mode energies

$$\underline{\omega_k^{\pm} = \sqrt{(JzS)^2(1-\gamma_k^2) + 2JzS^2D + S^2D^2} \pm h}$$

Discussion of spectrum $\omega_k^\pm$

- $h = 0,\ D = 0$:

$$\omega_k^+ = \omega_k^- = JzS\sqrt{1-\gamma_k^2}$$

$\omega_k^\pm = 0$ for $|\gamma_k| = 1$ (recall $\gamma_k = \frac{1}{z}\sum_\Delta e^{i\vec{k}\vec{\Delta}}$)

$\gamma_k = 1$ for $k = 0$ $\rightsquigarrow$ expand $\gamma_k = 1 - \frac{1}{z}k^2$

$\rightsquigarrow$ $\underline{\omega_k^\pm = c|k|}$ for small k, with velocity $c = JS\sqrt{2z}$

Goldstone mode

(Square lattice: ordering wavevector $Q = (\pi,\pi)$,

but recall $k \in$ AF BZ ($(0,0) \hat{=} (\pi,\pi)$).

$c = JS\,2\sqrt{2}$)

- $h = 0,\ D > 0$:

$\omega_k^+ = \omega_k^-$ gapped ($\hat{=}$ anisotropy gap)

$$\omega_{k=0} = S\sqrt{2JzD + D^2} \quad \propto \sqrt{JD} \text{ for small } D$$

- $h \neq 0,\ D = 0$:

$\omega_k^- < 0$ $\rightsquigarrow$ unstable

Collinear order ∥ field cannot exist;

canted state is realized instead. ↖↗↖↗

- $h \neq 0,\ D > 0$:

$\omega_k^\pm \geq 0$ for $h < h_c$, unstable for $h > h_c$

$$h_c = S\sqrt{JzD + D^2} \qquad \text{Spin-flop field}$$

$h < h_c$: ↑↓↑↓ , $h > h_c$ ↖↗↖↗

<u>Staggered magnetization:</u> (order parameter of collinear AFM)

$$\vec{m}_{stagg} = \sum_{i\in A}' \langle \vec{S}_i \rangle - \sum_{j\in B}' \langle \vec{S}_j \rangle$$

Here $\vec{m}_{stagg} \parallel \hat{z}$.

$$m_{stagg} = NS - \sum_i \langle a_i^+ a_i \rangle - \sum_j \langle b_j^+ b_j \rangle$$

$$= NS - 2 \sum_{k\in AFBZ}' \Big[\cosh^2\vartheta_k \langle \alpha_k^+ \alpha_k \rangle + \sinh^2\vartheta_k \langle \beta_k \beta_k^+ \rangle - \sinh\vartheta_k \cosh\vartheta_k \left(\langle \alpha_k^+ \beta_{-k}^+ \rangle + h.c. \right) \Big]$$

<u>T=0:</u> Ground state is vacuum of α, β (not of a, b).

$$\rightsquigarrow \quad m_{stagg} = NS - 2 \sum_k' \sinh^2\vartheta_k$$

$$= NS \Big(1 - \frac{1}{S} \underbrace{\Big(\frac{1}{N} \sum_k \frac{1}{\sqrt{1-\gamma_k^2}} - 1 \Big)}\Big)$$

hypercubic

$d=1$:	IR log divergent $\rightsquigarrow$ no order
$d=2$:	0.197
$d=3$:	0.078

$S = \frac{1}{2}$ square lattice $\quad m_{stagg} = 0.60 \, m_{class}$ (agrees w/ numerics !!)

<u>Ground-state wavefunction</u> Néel state is not eigenstate of H, because $S_i^- S_j^+$ change state

$\uparrow$ vacuum of a, b.

Ground state is vacuum of α, β: $\alpha|0\rangle = \beta|0\rangle = 0$

One can show that $|0\rangle = \exp\left(\frac{u_k}{v_k} a_k^+ b_{-k}^+ \right) |\text{Néel}\rangle$

(in linear spin-wave approximation)

3.5. Spin-wave theory for non-collinear antiferromagnets

Non-collinear classical states < non-bipartite lattice, e.g. triangular $\swarrow \uparrow \searrow$; AF + field $\nwarrow \nearrow \nwarrow \nearrow$

Expand around classical non-collinear state ($\sim 1/S$ expansion)

ATTN: Directions of $\langle \vec{S}_i \rangle$ can be functions of $1/S$

$\rightsquigarrow$ need $1/S$ expansion for directions / angles

Here: Simplest example of triangular lattice AF

$$H = J \sum_{\langle ij \rangle}' \vec{S}_i^0 \cdot \vec{S}_j^0$$

Follow option b): rotate spins to obtain ferromagnetic reference state.

Coplanar states: one angle

Non-coplanar states: two angles

Here: coplanar in xz plane $\swarrow \searrow \uparrow \swarrow \searrow \uparrow \dots$

$$S_i^{z_0} = S_i^z \cos\theta_i - S_i^x \sin\theta_i$$
$$S_i^{x_0} = S_i^z \sin\theta_i + S_i^x \cos\theta_i$$

„lab frame" rotating frame, $\Theta_i = \vec{Q}\cdot\vec{r}_i$

$\vec{Q} = (4/3\,\pi, 0)$

$$\rightsquigarrow \quad H = J \sum_{\langle ij \rangle} \Big(S_i^y S_j^y + \cos(\theta_i - \theta_j)\,(S_i^z S_j^z + S_i^x S_j^x) + \sin(\theta_i - \theta_j)\,(S_i^z S_j^x - S_i^x S_j^z) \Big)$$

follow Chernyshev / Zhitomirsky PRB 79, 144416 (2009)

$$S_i^z = S - a_i^\dagger a_i$$
$$S_i^+ = \sqrt{}\; a_i$$

$$\rightsquigarrow \quad H = H_0 + H_1 + H_2 + H_3 + H_4 + \dots$$

$H_n \propto S^{2-n/2}$, n boson operators

Presence of odd-N terms is main difference to collinear case!

$H_0 = -\frac{3}{2} J S^2 N$ classical ground-state energy

$H_1 = S^{3/2} \sum_i' \underbrace{\#}_{0} (a_i + a_i^+) = 0$ must vanish for reference state which minimizes classical energy

(non-zero a, a^+ terms $\hat{=}$ spin rotation)

(alternative interpretation: for classical minimum, the linear term of Taylor expansion vanishes)

H_2 : bilinear spin-wave piece

$$H_2 = \sum_k' \left[A_k a_k^+ a_k - \frac{1}{2} B_k \left(a_k a_{-k} + a_k^+ a_{-k}^+ \right) \right]$$

with $A_k = 3JS \left(1 + \gamma_{\vec{k}}/2 \right)$, $B_k = JS \frac{9}{2} \gamma_{\vec{k}}$

and $\gamma_k = \frac{1}{6} \sum_{\Delta}' e^{i\vec{k}\cdot\vec{\Delta}} = \frac{1}{3} \left(\cos k_x + 2\cos\frac{k_x}{2} \cos\frac{\sqrt{3}}{2} k_y \right)$

6 NN vectors

Bogoliubov trafo $a_k = u_k \alpha_k + v_k \alpha_{-k}^+$, $u_k^2 - v_k^2 = 1$

$$\rightsquigarrow \quad H_2 = \sum_k' \left[\omega_k \alpha_k^+ \alpha_k + \frac{1}{2} \left(\omega_k - A_k \right) \right]$$

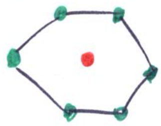
with mode energy

$$\omega_k = \sqrt{A_k^2 - B_k^2} = 3JS \sqrt{(1-\gamma_k)(2\gamma_k + 1)}$$

Discussion of spectrum: ($k \in$ full BZ!)

ω_k vanishes for $\underline{k = 0}$ $\quad (\gamma_k = 1)$

$\underline{k = \pm \vec{Q}}$ $\quad (\gamma_k = -\frac{1}{2})$



Near $k = 0$: $\quad \omega_k = c_1 |k|$ $\qquad c_1 > c_2$

$k = Q$: $\quad \omega_k = c_2 |q|$ for $\vec{k} = \vec{Q} + \vec{q}$

Two different Goldstone modes:
- $k = 0 \;\hat{=}\;$ in-plane rotation of spins
- $k = \pm Q \;\hat{=}\;$ out-of-plane rotation

Staggered magnetization: (in rotated frame simply $m_{stagg} = \sum_i{}' \langle S_i^z \rangle$)

$$m_{stagg} = SN - \underbrace{\sum_i \langle a_i^\dagger a_i \rangle}_{N \cdot 0.261 \text{ at } T=0}$$

For $S = \frac{1}{2}$: $\quad m_{stagg} = 0.48\, m_{class}$, numerics 0.41

(recall square lattice: 0.60 $\qquad 0.60$)

Higher-order corrections ($H_3, H_4 \ldots$) – angle corrections (not for triangular lattice)
- spectrum corrections
- lifetimes etc.

(all in $1/S$ expansion)

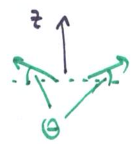
Zhitomirsky / Nikuni
PRB 57, 5013 (1998)

Spin-wave theory for canted AF

(as example for non-trivial angles)

Square-lattice AF with uniform field

$$\underline{H = J \sum_{\langle ij \rangle}' \vec{S}_i \cdot \vec{S}_j - h \sum_i S_i^z}$$



Assume spins in x-z plane, two sublattices.

Rotate:

$$S_i^{x_0} = S_i^z e^{i\vec{Q}\cdot\vec{R}_i} \cos\Theta - S_i^x \sin\Theta$$

$$S_i^{z_0} = S_i^z \sin\Theta + S_i^x e^{i\vec{Q}\cdot\vec{R}_i} \cos\Theta \quad , \quad \vec{Q} = (\pi, \pi)$$

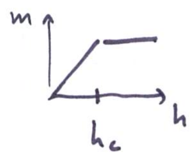
H-P representation

$$S_i^z = S - a_i^\dagger a_i$$

$$S_i^+ = \sqrt{\quad}\; a_i$$

Classical ground state $\sin\Theta = h/h_c$ with $h_c = h_{sat} = 8SJ$.

Classical magnetization curve



Insert in H:

$$\underline{H = H_0(\Theta) + H_1(\Theta) + H_2(\Theta) + H_3(\Theta) + \ldots}$$

Θ will have non-trivial $1/S$ expansion (!):

$$\Theta = \Theta^{(0)} + \frac{1}{S}\Theta^{(1)} + \frac{1}{S^2}\Theta^{(2)} + \ldots$$

$$\curvearrowright \quad H_0 = \underbrace{H_0(\Theta^{(0)})}_{\sigma(S^2)} + \underbrace{\frac{1}{S}\Theta^{(1)} \left.\frac{\partial H_0}{\partial \Theta}\right|_{\Theta^{(0)}}}_{\sigma(S)} + \ldots$$

Θ is determined from demanding that no linear terms in a, a^+ appear (linear term $\hat{=}$ a condensate $\hat{=}$ rotated spin)

Correct classical angles $\curvearrowright$ $H_1(\Theta^{(0)}) = 0$ $\quad (\mathcal{O}(S^{3/2}))$

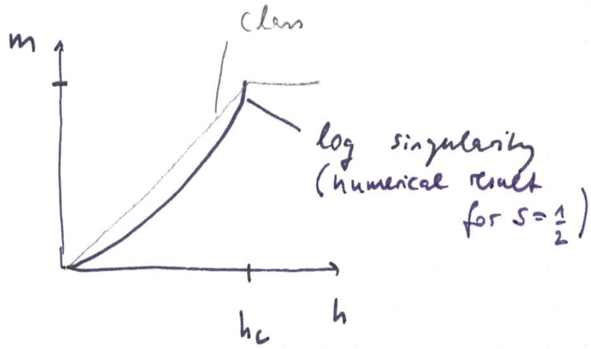
Higher-order corrections arise from $H_3, H_5, \ldots$ as follows:
H_3 contains $a_i^+ a_j^+ a_j$, $a_i a_j^+ a_j$ etc. These contribute linear terms which can be obtained by normal ordering in terms of α operators ($\alpha^+\alpha^+\alpha + \# \alpha^+ + \# \alpha$) or by mean-field decoupling ($a_i^+ a_j^+ a_j \to \langle a_i^+ a_j^+ \rangle a_j + \ldots$).
The resulting linear a, a^+ terms are $\mathcal{O}(S^{1/2})$ and need to be cancelled against $\frac{1}{S}\Theta^{(1)} \partial H_1/\partial\Theta|_{\Theta^{(0)}}$. $\curvearrowright$ $\Theta^{(1)}$.

H_2 yields spin-wave spectrum as before.

Uniform magnetization is now non-trivial.
Classical result $m = S \sin\Theta^{(0)} = S\, h/h_c$ for $h < h_c$.

$1/S$ Corrections from $<$ quantum fluct $\langle a^+ a \rangle$ $\hat{=}$ amplitude corrections; angle corrections $\hat{=}$ direction corrections (!)

$$\curvearrowright \quad m = S\left(1 - \tfrac{1}{S}\langle a_i^+ a_i \rangle\right)\left(\sin\Theta^{(0)} + \tfrac{1}{S}\Theta^{(1)}\cos\Theta^{(0)}\right) + \mathcal{O}(S^{-1})$$



Result for $S = \frac{1}{2}$:

ATTN: $h_c = 8SJ$ ($/\!/\, h_{sat}$) does not receive quantum corrections
(high-field state is exact, one-magnon state at high fields is exact)

Mourigal et al PRB (2010)
Chernyshev PRL (2006)

→ Zhitomirsky / Chernyshev, Rev Mod Phys 85, 219 (2013)

3.6. Magnon decay

AF magnons acquire finite lifetime even at $T=0$ (leading term $\mathcal{O}(S^0)$)

(recall: cubic vertices exist for non-collinear states only)

Near $k=0$, $k=Q$ decay rate Γ is small (Goldstone).
Details depend on problem (multiple modes, phase space)

E.g. hypercubic lattice $\Gamma \sim k^2$ ($d>2$)

triangular $\begin{cases} k^2 & k\to 0 \\ k^{7/2} & k\to Q \end{cases}$

ATTN: 2d $T_N=0$ $\curvearrowright$ finite ξ. (need $k \gg \xi^{-1}$ ... decay rate $\propto k\, T^2 \ln T$)

<u>Problem</u>: $1/S$ expansion can break down.
(Limit $S\to\infty$ for lifetime singular.)

In practice: Result to certain order in $1/S$ diverges.
(Example: Square-lattice AF in fields $h^* < H < h_{sat}$)
(related to curvature of spin-wave spectrum;
usual  ; singular  w/cubic vertex)

Need self-consistent calc for fixed S.

<u>Result</u> Conventional ordered magnets can have strongly broadened (ill-defined) magnons
(typically requires cubic vertices)