TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Solid State Theory (SS2020)

Lecture 22: Ground state and excitations in Heisenberg models

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§ 6.2 Ground state and excitations

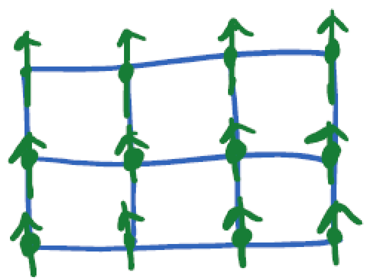
- Classical Heisenberg model:

$$H = \frac{J}{2} \sum_{\vec{r}, \vec{\delta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}}$$

$$\begin{cases} S_j^x = \sin\theta_j \cos\varphi_j \\ S_j^y = \sin\theta_j \sin\varphi_j \\ S_j^z = \cos\theta_j \end{cases}$$

FM:

$J < 0$



$\theta_j = 0$

(or rotate every spin by the same angle)

§ 6.2 Ground state and excitations

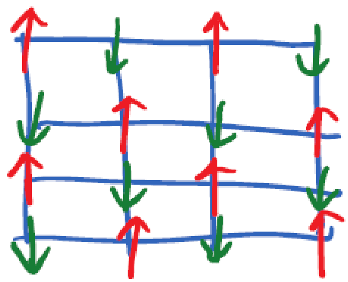
- Classical Heisenberg model:

$$H = \frac{J}{2} \sum_{\vec{r},\vec{\delta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}}$$

$$\begin{cases} S_j^x = \sin\theta_j \cos\varphi_j \\ S_j^y = \sin\theta_j \sin\varphi_j \\ S_j^z = \cos\theta_j \end{cases}$$

AFM:

$J > 0$



$\uparrow$ $\theta_j = 0$

$\downarrow$ $\theta_j = \pi$

➢ Rotating all spins by the same angle gives other ground states.

§ 6.2 Ground state and excitations

The degeneracy is due to the spin-rotational symmetry:

$$S_j^a \longrightarrow S_j^{a\,\prime} = \sum_b O_{ab} S_j^b \qquad (a,b = x,y,z)$$

orthogonal transformation

$$O^T O = O^T O = I_{3\times 3}$$

§ 6.2 Ground state and excitations

$$\vec{S}_i \cdot \vec{S}_j = \sum_a S_i^a S_j^a$$

$$\rightarrow \sum_{a,b,c} \underbrace{O_{ab} S_i^b}\; \underbrace{O_{ac} S_j^c}$$

$$= \sum_{b,c} \Big(\underbrace{\sum_a O^T_{ba} O_{ac}}_{\substack{\parallel \\ (O^T O)_{bc} = I_{bc} = \delta_{bc}}} \Big) S_i^b S_j^c$$

$$= \sum_b S_i^b S_j^b$$

$$= \vec{S}_i \cdot \vec{S}_j$$

§ 6.2 Ground state and excitations

The degeneracy is due to the spin-rotational symmetry:

$$S_j^a \longrightarrow S_j^{a\prime} = \sum_b O_{ab} S_j^b \qquad (a, b = x, y, z)$$

The Hamiltonian has spin-rotational symmetry,
(no prefered direction)

but the ground/thermal state may have FM/AFM order.

This is the so-called "symmetry breaking".

§ 6.2 Ground state and excitations

- Spontaneous symmetry breaking and order parameters:

Symmetry breaking is characterized by order parameters.

FM $\Longleftrightarrow$ magnetization

AFM $\Longleftrightarrow$ staggered magnetization
(bipartite lattice)

➢ However, the definition of order parameters is a bit tricky…

§ 6.2 Ground state and excitations

Finite temperature:

$$\beta = 1/k_B T$$

$$Z = \int d\vec{S}_1 \cdots d\vec{S}_N \; e^{-\beta H(\vec{S}_1 \cdots \vec{S}_N)}$$

$$d\vec{S}_j = \sin\theta_j \, d\theta_j \, d\varphi_j$$

$$\langle S_j^z \rangle_T = \frac{1}{Z} \int d\vec{S}_1 \cdots d\vec{S}_N \; \vec{S}_j \, e^{-\beta\left(H - h\sum_j S_j^z\right)}$$

magnetization $M = \lim_{h \to 0^+} \lim_{N \to \infty} \langle S_j^z \rangle_T$

§ 6.2 Ground state and excitations

Finite temperature :

$\beta = 1/k_B T$

$$Z = \int d\vec{S}_1 \cdots d\vec{S}_N \; e^{-\beta H(\vec{S}_1 \cdots \vec{S}_N)}$$

$$d\vec{S}_j = \sin\theta_j \, d\theta_j \, d\varphi_j$$

$$\langle (-1)^j S_j^z \rangle_T = \frac{1}{Z} \int d\vec{S}_1 \cdots d\vec{S}_N \; (-1)^j S_j^z \, e^{-\beta[H - h\sum_j (-1)^j S_j^z]}$$

staggered magnetization $M = \lim_{h \to 0^+} \lim_{N \to \infty} \langle (-1)^j S_j^z \rangle_T$

§ 6.2 Ground state and excitations

Correlation function:

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle = \frac{1}{Z} \int d\vec{S}_1 \cdots d\vec{S}_N \; \vec{S}_i \cdot \vec{S}_j \, e^{-\beta H}$$

$$\lim_{|j-i| \to \infty} \lim_{N \to \infty} \langle \vec{S}_i \cdot \vec{S}_j \rangle = \begin{cases} \text{const.} & \text{FM} \\ \underbrace{(-1)^{j-i}}_{\text{bipartite lattice}} \cdot \text{const.} & \text{AFM} \end{cases}$$

§ 6.2 Ground state and excitations

- Mermin-Wagner theorem (classical version):

Spontaneously breaking of continuous symetry cannot happen in classical models with local interactions at $T>0$ in $d<3$.

$\Rightarrow$ FM/AFM do NOT survive at any $T>0$ in $d=1$ & $d=2$ classical Heisenberg models.

§ 6.2 Ground state and excitations

- Quantum Heisenberg models: ferromagnetic case

$$H = \frac{J}{2} \sum_{\vec{r}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}} \qquad J < 0$$

Ground state : fully polarized

(and many others by spin rotations…)

$$|g\rangle = \prod_{\vec{r}} |S\rangle_{\vec{r}}$$

$$H|g\rangle = E_0 |g\rangle$$

§ 6.2 Ground state and excitations

Proof :

$$\vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}} = S^x_{\vec{r}} S^x_{\vec{r}+\vec{\delta}} + S^y_{\vec{r}} S^y_{\vec{r}+\vec{\delta}} + S^z_{\vec{r}} S^z_{\vec{r}+\vec{\delta}}$$

$$= \frac{1}{2}\left(S^+_{\vec{r}} S^-_{\vec{r}+\vec{\delta}} + S^-_{\vec{r}} S^+_{\vec{r}+\vec{\delta}} \right) + S^z_{\vec{r}} S^z_{\vec{r}+\vec{\delta}}$$

$$S^+_{\vec{r}} S^-_{\vec{r}+\vec{\delta}} \, |s\rangle_{\vec{r}} \, |s\rangle_{\vec{r}+\vec{\delta}} = 0$$

$$S^-_{\vec{r}} S^+_{\vec{r}+\vec{\delta}} \, |s\rangle_{\vec{r}} \, |s\rangle_{\vec{r}+\vec{\delta}} = 0$$

$$S^z_{\vec{r}} S^z_{\vec{r}+\vec{\delta}} \, |s\rangle_{\vec{r}} \, |s\rangle_{\vec{r}+\vec{\delta}} = s^2 \, |s\rangle_{\vec{r}} \, |s\rangle_{\vec{r}+\vec{\delta}}$$

§ 6.2 Ground state and excitations

$$H|g\rangle = \frac{J}{2}\sum_{\vec{r},\vec{\delta}}\left(\frac{1}{2}S^+_{\vec{r}}S^-_{\vec{r}+\vec{\delta}} + \frac{1}{2}S^-_{\vec{r}}S^+_{\vec{r}+\vec{\delta}} + S^z_{\vec{r}}S^z_{\vec{r}+\vec{\delta}}\right)\prod_{\vec{r}}|S\rangle_{\vec{r}}$$

$$= \frac{J}{2}\sum_{\vec{r},\vec{\delta}}\left(0+0+S^2\right)\prod_{\vec{r}}|S\rangle_{\vec{r}}$$

$$= \frac{J}{2}NzS^2|g\rangle$$

number of sites

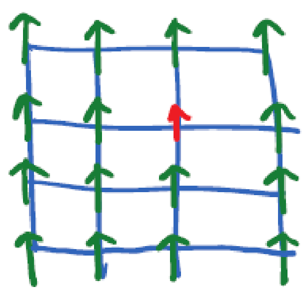
$z = \sum_{\vec{\delta}}$ coodination number

(e.g. $z=4$ for square lattice)

Ground-state energy: $E_0 = \frac{J}{2}NzS^2$

§ 6.2 Ground state and excitations

First excited state:



$\uparrow \longrightarrow \uparrow \quad (|S\rangle \to |S-1\rangle)$

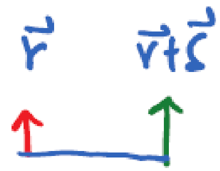
$(\uparrow \longrightarrow \downarrow$ for $S = 1/2)$

$$|S\rangle_{\vec{r}} \Rightarrow |S-1\rangle_{\vec{r}} = \frac{1}{\sqrt{2S}} S^-_{\vec{r}} |S\rangle_{\vec{r}}$$

single-spin flip

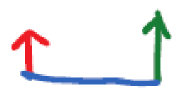
Define $|e_{\vec{r}}\rangle = \frac{1}{\sqrt{2S}} S^-_{\vec{r}} |g\rangle \qquad H|e_{\vec{r}}\rangle = ?$

§ 6.2 Ground state and excitations

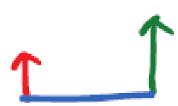
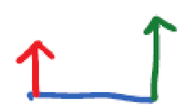
$S^+_{\vec r}\, S^-_{\vec r+\vec\delta}$ 

$= 2S$ 

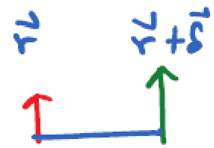
$\left(S^+_{\vec r}\,|s-1\rangle_{\vec r} = \sqrt{2s}\,|s\rangle_{\vec r}\,,\quad S^-_{\vec r+\vec\delta}\,|s\rangle_{\vec r+\vec\delta} = \sqrt{2s}\,|s-1\rangle_{\vec r+\vec\delta} \right)$

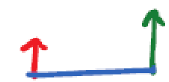
$S^-_{\vec r}\, S^+_{\vec r+\vec\delta}$  $= 0$

$\left(S^+_{\vec r+\vec\delta}\,|s\rangle_{\vec r+\vec\delta} = 0 \right)$

$S^z_{\vec r}\, S^z_{\vec r+\vec\delta}$  $= s(s-1)$ 

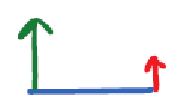
§ 6.2 Ground state and excitations

$\Rightarrow \quad \vec S_{\vec r}\cdot\vec S_{\vec r+\vec\delta}$ 

$= \frac{1}{2}\left(S^{+}_{\vec r}S^{-}_{\vec r+\vec\delta} + S^{-}_{\vec r}S^{+}_{\vec r+\vec\delta}\right)$ 

$+ S^{z}_{\vec r}S^{z}_{\vec r+\vec\delta}$ 

$= S$  $+ \; S(S-1)$ 

$= S\Big($  $-$  $\Big) + S^2$ 

$$H\,|e_{\vec r}\rangle = JS\sum_{\vec\delta}\Big(|e_{\vec r+\vec\delta}\rangle - |e_{\vec r}\rangle\Big) + E_0\,|e_{\vec r}\rangle$$

not an eigenstate !

§ 6.2 Ground state and excitations

Spin-wave / magnon ansatz :

$$|e_{\vec{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} |e_{\vec{r}}\rangle \qquad \vec{k} \in FBZ$$

§ 6.2 Ground state and excitations

$$\Rightarrow \quad H|e_{\vec{k}}\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} JS \sum_{\vec{\delta}} |e_{\vec{r}+\vec{\delta}}\rangle$$

$$- \frac{1}{\sqrt{N}}\sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} JS \sum_{\vec{\delta}} |e_{\vec{r}}\rangle + E_0|e_{\vec{k}}\rangle$$

$$= \Big[E_0 + \underbrace{JS\Big(\sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}} - z\Big)}\Big] |e_{\vec{k}}\rangle$$

eigenstate !

spin-wave/magnon excitation energy $\omega_{\vec{k}}$

$\omega_{\vec{k}} \to |\vec{k}|^2$ for $\vec{k} \to 0$ (gapless excitation)

§ 6.2 Ground state and excitations

Spin-wave / magnon ansatz :

$$|e_{\vec{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} |e_{\vec{r}}\rangle \qquad \vec{k} \in \text{FBZ}$$

higher excited states ? difficult !

create more spin waves ? collisions ...

§ 6.2 Ground state and excitations

- Quantum Heisenberg models: antiferromagnetic case

$$H = \frac{J}{2} \sum_{\vec{r},\vec{\delta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}} \qquad J > 0$$

Ground state $\overset{?}{=}$ Néel state

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

§ 6.2 Ground state and excitations

$$\qquad\quad \vec{r} \quad \vec{r}+\vec{\delta}$$

$$S^+_{\vec r}\, S^-_{\vec r+\vec\delta} \;\uparrow\!\_\!\_\!\downarrow \;=\; 0 \qquad \left(S^+_{\vec r}\,|s\rangle = 0 \right)$$

$$S^-_{\vec r}\, S^+_{\vec r+\vec\delta} \;\uparrow\!\_\!\_\!\downarrow \;=\; 2S \;\uparrow\!\_\!\_\!\downarrow \qquad \left(\begin{array}{l} S^-_{\vec r}\,|s\rangle = \sqrt{2S}\,|s-1\rangle \\ S^+_{\vec r}\,|-s\rangle = \sqrt{2S}\,|-s+1\rangle \end{array} \right)$$

$$S^z_{\vec r}\, S^z_{\vec r+\vec\delta} \;\uparrow\!\_\!\_\!\downarrow \;=\; -S^2 \;\uparrow\!\_\!\_\!\downarrow$$

$$H\,|\text{Néel}\rangle = \underset{\substack{\uparrow \\ O(N) \text{ terms}}}{\cdots}$$

$O(N)$ terms (spin flips everywhere!)

$\Rightarrow$ $|\text{Néel}\rangle$ is not an eigenstate!

§ 6.2 Ground state and excitations

Ground state of AFM Heisenberg model: open problem
(except for $d=1$ spin-1/2 AFM Heisenberg model, which can be solved by Bethe ansatz)

Very relevant question:

Does magnetic order survive at $T=0$?

§ 6.2 Ground state and excitations

Ground state of AFM Heisenberg model: open problem
(except for $d=1$ spin-1/2 AFM Heisenberg model,
which can be solved by Bethe ansatz)

A lot of surprises, e.g.

Haldane gap in $d=1$ spin-1 AFM Heisenberg model
(Nobel prize in 2016)

§ 6.2 Ground state and excitations

- Mermin-Wagner theorem (quantum version):

Requirement: short-range interaction

+ continuous spin-rotational symmetry

(NOT limited to Heisenberg models)

FM: order at $T=0$, abitrary d

$$\begin{cases} \text{no order at } T>0, & d=1 \ \& \ 2 \\ \text{order for } T<T_c, & d\geq 3 \end{cases}$$

§ 6.2 Ground state and excitations

- Mermin-Wagner theorem (quantum version):

AFM: $\begin{cases} \text{no order at } T=0 \text{ for } d=1 \\ \text{possible order at } T=0 \text{ for } d \geq 2 \end{cases}$

→ spin liquid with no order?

$\begin{cases} \text{no order at } T>0 \text{ for } d=1 \ \& \ 2 \\ \text{possible order for } T<T_c,\ d \geq 3 \end{cases}$

➢ $T = 0,\ d = 1$ and 2: strong quantum fluctuations, leading to a zoo of exotic phases!

§ 6.2 Ground state and excitations

- Mermin-Wagner theorem (quantum version):

Goldstone theorem:

magnetic order in the present context.

If continuous symmetry is broken, there are gapless excitations (Goldstone bosons).

- See lecture notes (part 1 and part 2) on the spin-wave theory based on large S expansion.