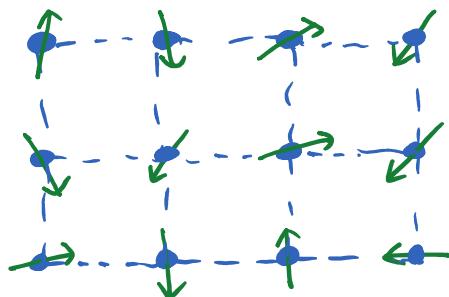


## § 6. Quantum magnetism

## \*) Heisenberg models



$$H = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Ground state? Low-energy excitations? ...

depend on dimensionality, lattice geometry, spin,  
sign/strength of interactions,  
temperature ...

Simplification: Heisenberg model (with nearest-neighbor  
interactions)

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$J < 0$  : ferromagnetic (FM)

$J > 0$  : antiferromagnetic (AFM)

- Definition of the problem :

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

all nearest neighbors of site  $\vec{r}$

spin-S :  $\vec{S}_{\vec{r}} = (S_{\vec{r}}^x, S_{\vec{r}}^y, S_{\vec{r}}^z), \quad \vec{S}_{\vec{r}}^2 = S(S+1)$

$$[S_{\vec{r}}^a, S_{\vec{r}'}^b] = \delta_{\vec{r}, \vec{r}'} \cdot i \sum_{abc} S_{\vec{r}}^c$$

spin operators at different sites  
commute with each other

Standard Commutation  
relation of angular  
momentum

$$S_{\vec{r}}^{\pm} = S_{\vec{r}}^x \pm i S_{\vec{r}}^y$$

$$\Rightarrow [S_{\vec{r}}^{\pm}, S_{\vec{r}'}^z] = \mp S_{\vec{r}}^{\pm} \delta_{\vec{r}, \vec{r}'}$$

$$[S_{\vec{r}}^{+}, S_{\vec{r}'}^{-}] = 2 S_{\vec{r}}^z \delta_{\vec{r}, \vec{r}'}$$

single-site basis :

$$|S, m\rangle$$

↑ magnetic quantum number  
spin quantum number

$$\begin{cases} \vec{S}_{\vec{r}}^2 |S, m\rangle = S(S+1) |S, m\rangle \\ S_{\vec{r}}^z |S, m\rangle = m |S, m\rangle \end{cases}$$

$m = -S, -S+1, \dots, S$

2S+1 states in a single site

$$\left\{ \begin{array}{l} S_{\vec{r}}^+ |s, m\rangle_{\vec{r}} = \sqrt{s(s+1) - m(m+1)} |s, m+1\rangle_{\vec{r}} \\ S_{\vec{r}}^- |s, m\rangle_{\vec{r}} = \sqrt{s(s+1) - m(m-1)} |s, m-1\rangle_{\vec{r}} \\ S_{\vec{r}}^z |s, m\rangle_{\vec{r}} = m |s, m\rangle_{\vec{r}} \end{array} \right. \rightarrow \begin{aligned} S_{\vec{r}}^+ |s, s\rangle_{\vec{r}} &= 0 \\ S_{\vec{r}}^- |s, -s\rangle_{\vec{r}} &= 0 \end{aligned}$$

$N$ -site basis: (tensor product of single-site basis)

$$\dots |s, m\rangle_{\vec{r}} |s, m'\rangle_{\vec{r}+\vec{\delta}} \dots$$

↙  $(2s+1)^N$ -dimensional Hilbert space!

We will simplify notation below:  $|s, m\rangle \rightarrow |m\rangle$   
( $s$  is the same for every site)

— Classical limit ( $s \rightarrow \infty$ )

$$\left[ \frac{\hat{S}^a}{s}, \frac{\hat{S}^b}{s} \right] = \underbrace{\frac{1}{s} \cdot i \epsilon_{abc}}_{0 \text{ for } s \rightarrow \infty} \frac{\hat{S}^c}{s}$$

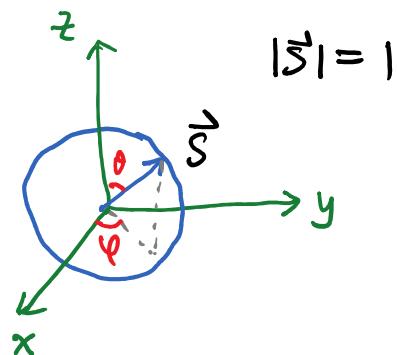
$$\langle s | \frac{\hat{S}^z}{s} | s \rangle = 1 \Rightarrow \langle \frac{\hat{S}^z}{s} \rangle \leq 1$$

Rescaled spin operators commute in the Large- $S$  limit!

Classical spin: unit vectors

$$\vec{s}_j = (s_j^x, s_j^y, s_j^z)$$

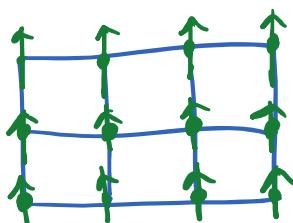
$$\left\{ \begin{array}{l} s_j^x = \sin \theta_j \cos \varphi_j \\ s_j^y = \sin \theta_j \sin \varphi_j \\ s_j^z = \cos \theta_j \end{array} \right.$$



$$|\vec{s}| = 1$$

Ground state: minimize the energy functional  $H$   
( $T=0$ ) with respect to  $(\theta_j, \varphi_j)$

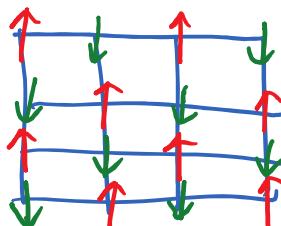
FM:



$$\theta_j = 0$$

(or rotate every spin by the same angle)

AFM:



$$\begin{array}{l} \uparrow \theta_j = 0 \\ \downarrow \theta_j = \pi \end{array}$$

bipartite lattice: A-sublattice ↑  
B-sublattice ↓ Néel order

nonbipartite lattice: ?



frustration!

The degeneracy is due to the spin-rotational symmetry:

$$\begin{aligned}
 S_j^a &\rightarrow S_j^{a'} = \sum_b O_{ab} S_j^b \quad (a,b=x,y,z) \\
 \Rightarrow \vec{S}_i \cdot \vec{S}_j &= \sum_a S_i^a S_j^a \quad \xrightarrow{\text{orthogonal transformation}} \quad O^T O = O^T O = I_{3 \times 3} \\
 &\rightarrow \sum_{a,b,c} O_{ab} S_i^b O_{ac} S_j^c \\
 &= \sum_{b,c} \underbrace{\left( \sum_a O_{ba}^T O_{ac} \right)}_{\parallel} S_i^b S_j^c \\
 &\quad (O^T O)_{bc} = I_{bc} = \delta_{bc} \\
 &= \sum_b S_i^b S_j^b \\
 &= \vec{S}_i \cdot \vec{S}_j
 \end{aligned}$$

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

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

This is the so-called "symmetry breaking".

Symmetry breaking is characterized by order parameters.

FM  $\Leftrightarrow$  magnetization

AFM  $\Leftrightarrow$  staggered magnetization  
(bipartite lattice)

Finite temperature:

$$Z = \int d\vec{s}_1 \dots d\vec{s}_N e^{-\beta H(\vec{s}_1, \dots, \vec{s}_N)}$$

$\beta = 1/k_B T$

$d\vec{s}_j = \sin\theta_j d\theta_j d\varphi_j$

$$\langle S_j^z \rangle_T = \frac{1}{Z} \int d\vec{s}_1 \dots d\vec{s}_N \vec{s}_j e^{-\beta(H - h_s s_j^z)}$$

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

$$\langle \underbrace{(-1)^j}_{\text{magnetic field}} \vec{s}_j^z \rangle_T = \frac{1}{Z} \int d\vec{s}_1 \dots d\vec{s}_N (-1)^j s_j^z e^{-\beta[H - h \sum_j (-1)^j s_j^z]}$$

staggered magnetization  $M = \lim_{h \rightarrow 0^+} \lim_{N \rightarrow \infty} \langle (-1)^j \vec{s}_j^z \rangle_T$

Correlation function:

$$\langle \vec{s}_i \cdot \vec{s}_j \rangle = \frac{1}{N} \int d\vec{s}_1 \cdots d\vec{s}_N \vec{s}_i \cdot \vec{s}_j e^{-\beta H}$$

$$\lim_{|i-j| \rightarrow \infty} \lim_{N \rightarrow \infty} \langle \vec{s}_i \cdot \vec{s}_j \rangle = \begin{cases} \text{const.} & \text{FM} \\ (-1)^{j-i} \cdot \text{const.} & \text{AFM} \end{cases}$$

↓  
bipartite lattice

Spontaneous symmetry breaking!

(Hamiltonian rotationally invariant, ground/thermal state picks up a particular direction.)

Mermin-Wagner theorem (classical version):

Spontaneously breaking of continuous symmetry

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.