2. Local moments and microscopic models

≙ Ingredients for frustrated magnetism in insulators

2.1. Spin and SU(2)

SU(2): special unitary group, unitary 2×2 matrices with det = +1

Spin ≙ internal angular momentum of quantum particles

Angular momentum algebra (= SU(2) algebra)

$$\left[\hat{S}_i, \hat{S}_k\right] = i\hbar\,\varepsilon_{ikl}\,\hat{S}_l$$

realizable with integer and half-integer S.

(Eigenvalues of $\hat{S}_z$: $-S, \dots, S$ ⇝ $2S$ must be integer; $S = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \dots$; $\hat{\vec{S}}^2 = \hbar^2 S(S+1)$)

Specifically $S = 1/2$ (≙ fundamental representation of SU(2))

$m = \pm\frac{1}{2}$ ⇝ states $|\uparrow\rangle, |\downarrow\rangle$ with $\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1$, $\langle\uparrow|\downarrow\rangle = 0$

$$\hat{S}_x = \frac{\hbar}{2}\left(|\downarrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow|\right)$$
$$\hat{S}_y = i\frac{\hbar}{2}\left(|\downarrow\rangle\langle\uparrow| - |\uparrow\rangle\langle\downarrow|\right)$$
$$\hat{S}_z = \frac{\hbar}{2}\left(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|\right)$$

$$\hat{\vec{S}} = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \hbar/4 \cdot \mathbb{1} \cdot 3 = \tfrac{3}{4}\hbar^2$$

$$\hat{S}_z \left|\uparrow_\downarrow\right\rangle = \pm\frac{\hbar}{2}\left|\uparrow_\downarrow\right\rangle$$

$$\left\langle\uparrow_\downarrow\right|\hat{S}_x\left|\uparrow_\downarrow\right\rangle = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar}{2}\underline{\underline{\sigma}}_x$$
$$\left\langle\uparrow_\downarrow\right|\hat{S}_y\left|\uparrow_\downarrow\right\rangle = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \frac{\hbar}{2}\underline{\underline{\sigma}}_y$$
$$\left\langle\uparrow_\downarrow\right|\hat{S}_z\left|\uparrow_\downarrow\right\rangle = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{\hbar}{2}\underline{\underline{\sigma}}_z$$

$\underline{\underline{\sigma}}_i$ ≙ Pauli spin matrices

$$\left[\underline{\underline{\sigma}}_i, \underline{\underline{\sigma}}_k\right] = 2i\,\varepsilon_{ikl}\,\underline{\underline{\sigma}}_l$$

$$\underline{\underline{\sigma}}_i\,\underline{\underline{\sigma}}_k = i\,\varepsilon_{ikl}\,\underline{\underline{\sigma}}_l + \delta_{ik}\,\underline{\underline{\mathbb{1}}}$$

Rotation operator in spin space

$\hat{D}_{\vec{\varphi}} = e^{i/\hbar\, \vec{\varphi}\cdot\hat{\vec{S}}}$ (analogous to $\hat{D}_{\varphi} = e^{i/\hbar\, \vec{\varphi}\cdot\hat{\vec{L}}}$)

$\rightsquigarrow \hat{D}_{2\pi,z} = e^{i/\hbar\, 2\pi(\pm\frac{\hbar}{2})} = \ominus 1$ different from $SO(3)$

$$\left\langle \begin{matrix}\uparrow\\ \downarrow\end{matrix} \right| e^{i/\hbar\, \vec{\varphi}\cdot\hat{\vec{S}}} \left| \begin{matrix}\uparrow\\ \downarrow\end{matrix} \right\rangle = \left\langle \begin{matrix}\uparrow\\ \downarrow\end{matrix} \right| 1 + \frac{i}{2}\vec{\varphi}\cdot\vec{\sigma} - \frac{1}{2!}\frac{1}{2^2}\vec{\varphi}^2 - \frac{1}{3!}\frac{1}{2^3}\vec{\varphi}^2\,\vec{\varphi}\cdot\vec{\sigma} + \dots \left| \begin{matrix}\uparrow\\ \downarrow\end{matrix} \right\rangle$$

$$= \begin{pmatrix} \cos\frac{\varphi}{2} + i\frac{\varphi_z}{\varphi}\sin\frac{\varphi}{2} & \frac{i\varphi_x+\varphi_y}{\varphi}\sin\frac{\varphi}{2} \\ \frac{i\varphi_x-\varphi_y}{\varphi}\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} - i\frac{\varphi_z}{\varphi}\sin\frac{\varphi}{2} \end{pmatrix}$$

$$\det\left| e^{i/2\,\vec{\varphi}\cdot\vec{\sigma}} \right| = +1$$

Higher spin

Spin $S \;\hat{=}\; (2S+1)$ - dimensional representation of $SU(2)$

Eg. $S=1 \rightsquigarrow$ 3-dim rep.

$$\hat{S}_x = \hbar\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\hat{S}_y = \hbar\frac{1}{\sqrt{2}i}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\hat{S}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Generalization $SU(2) \rightarrow SU(N)$

N „flavors" (instead of $\uparrow, \downarrow$)

Generators $S^{mm'}$ with $m, m' = 1, \dots, N$ (instead of $\hat{S}^x, \hat{S}^y, \hat{S}^z$)

Algebra $\left[S^{mm'}, S^{\mu\mu'}\right] = \delta_{m'\mu} S^{m\mu'} - \delta_{m\mu'} S^{\mu m'}$

Useful for different degree of freedom (e.g. spin & orbital); for novel approximations ($SU(N)$ with $N\to\infty$); in cold atoms, –

2.2. Electrons in solids

Electrons in magnetic field (no lattice)

$$\hat{H} = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - g\mu_B \vec{S}\cdot\vec{H} \qquad \mu_B = \frac{e\hbar}{2mc}$$

Magnetic response of free electrons:

- Landau diamagnetism (recall: orbital $\vec{B}$-field ↝ Landau levels)

$$\chi_{Landau} = -\frac{(N/V)e^2}{4mc^2 p_F^2} = -\frac{e^2 p_F}{12\pi^2 mc^2}$$

(p_F: Fermi momentum)

- Pauli paramagnetism

$$\chi_{Pauli} = \mu_B^2\, g(E_F) = \frac{e^2 p_F}{4\pi^2 mc^2}$$

(E_F: Fermi energy)

$$\rightsquigarrow \quad \underline{\chi_{Landau} = -\frac{1}{3}\chi_{Pauli}}$$

With lattice: Periodic potential

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\vec{r}) \qquad (+\ \vec{B}\text{-field terms})$$

$$U(\vec{r}) = U(\vec{r} + \vec{R}_n)$$

($\vec{R}_n$: lattice vector)

$$\rightsquigarrow \quad \underline{\psi_{m\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{m\vec{k}}(\vec{r})} \qquad \text{with } u_{m\vec{k}}(\vec{r}) = u_{m\vec{k}}(\vec{r} + \vec{R}_n)$$

Bloch theorem

$\vec{k} \in 1.\,BZ$, m band index

$$\hat{H}\psi_{m\vec{k}} = \varepsilon_m(\vec{k})\psi_{m\vec{k}}, \quad \text{formally } \varepsilon_m(\vec{k}) = \varepsilon_m(\vec{k} + \vec{G}_n)$$

($\vec{G}_n$: reciprocal lattice vector)

$$\vec{R}_n \cdot \vec{G}_m = 2\pi\ell$$

Wannier state (localized at $\vec{R}_i$):

$$\phi_{m,\vec{R}_i}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{k\in 1.BZ} \psi_{m,\vec{k}}(\vec{r} - \vec{R}_i) = \frac{1}{\sqrt{N}}\sum_{k\in 1.BZ} e^{-i\vec{k}\cdot\vec{R}_i}\psi_{m,\vec{k}}(\vec{r})$$

Bloch electrons display Landau diamag & Pauli paramag, but in general $\sqrt{\chi_{Landau}} \neq \frac{1}{3}\chi_{Pauli}$.

Localized magnetic moments

arise in partially filled inner shells (see Sec 2.4)

and with strong Coulomb interaction (see Sec 2.5)

Examples are transition metals (3d: Mn, Fe, Co, Ni, especially in oxides like NiO, Fe_2O_3, ...)

rare earths (4f: Gd, Eu, Dy, ...)

actinides (5f: U, Np, Am, ...)

Their main magnetic response comes from Zeeman term, $-g\mu_B \vec{S}\cdot\vec{H}$.

If interaction between moments can be neglected, their susceptibility follows a Curie law:

$$\chi = \left\langle \frac{\partial M}{\partial H} \right\rangle = N g^2 \mu_B^2 \frac{S(S+1)}{3 k_B T}$$

2.3. Exchange interaction

Magnetism in solids $\hat{=}$ ordering of spin moments due to interactions

Dipolar interaction is weak ($\lesssim 1K$)

Dominant interaction comes from combination of
- electron kinetic energy (hopping)
- Pauli principle
- Coulomb repulsion

} ↝ exchange interaction

∃ different forms of exchange interaction:
non-trivial problem of quantum chemistry, material-dependent

Most important: direct exchange (typically ferromagnetic)
superexchange (typically antiferromagnetic)

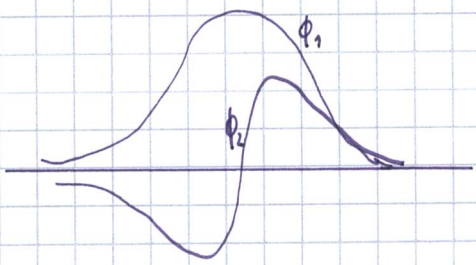
Simplest form of exchange interaction is $J\,\vec{S}_i \cdot \vec{S}_j$ (SU(2)-symmetric), anisotropies arise from effects of spin-orbit coupling.

(a) Direct exchange

relevant for electrons in orthogonal, but spatially overlapping orbitals

In order to reduce Coulomb repulsion energy, electrons want to avoid each other. This is best done with antisymmetric real-space two-particle wavefunction, which requires a symmetric spin state.

↳ ferro spin alignment



Formally: Coulomb interaction in 2nd quantization

$$V = \frac{1}{2} \int d^3x\, d^3y\; v(\vec{x},\vec{y}) \sum_{ss'} \psi_s^\dagger(\vec{x})\, \psi_{s'}^\dagger(\vec{y})\, \psi_{s'}(\vec{y})\, \psi_s(\vec{x})$$

Express this in orbital basis $\psi_s^+(\vec{x}) = \sum_{i=1}^{2} \phi_i^*(\vec{x})\, c_{is}^+$

and bring in form

$$V = \sum_{i \neq i'} U_{ii'}\, n_i n_{i'} + \sum_i U_{ii}\, n_{i\uparrow} n_{i\downarrow} + \sum_{ss',\, i \neq i'} J^F\, c_{is}^+ c_{i's'}^+ c_{is'} c_{i's}$$

$n_i = n_{i\uparrow} + n_{i\downarrow}$, $n_{is} = c_{is}^+ c_{is}$

$$-2J^F\left(\vec{S}_i \cdot \vec{S}_{i'} + \frac{n_i n_{i'}}{4}\right)$$

$\vec{S}_i = \frac{1}{2} \sum_{ss'} c_{is}^+\, \vec{\sigma}_{ss'}\, c_{is'}$

Explicitely:

$$U_{ii'} = \frac{1}{2} \int d^3x\, d^3y\; v(\vec{x},\vec{y})\; |\phi_i(\vec{x})|^2 |\phi_{i'}(\vec{y})|^2$$

$$J^F = \frac{1}{2} \int d^3x\, d^3y\; v(\vec{x},\vec{y})\; \phi_i(\vec{x})\, \phi_{i'}^*(\vec{x})\, \phi_{i'}(\vec{y})\, \phi_i^*(\vec{y})$$

One can prove that $J^F > 0$ (↷ ferromagnetic)

for short-range interactions ($v = \delta(\vec{x}-\vec{y})$ ↷ obvious) and

for Coulomb interactions (see Auerbach book)

Direct exchange is relevant for Hund's rule:

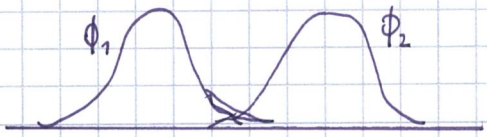
Electrons occupy orbitals in open shells as to maximize S_{tot}.

(b) Superexchange

relevant for electrons in non-orthogonal but spatially separated orbitals

In order to reduce (i.e. gain) kinetic energy, electrons want to hop between orbitals. Due to Pauli principle, this requires antiparallel spins.

↳ antiferro spin alignment



Formally, this can be efficiently calculated using second-order perturbation theory in the electron hopping between orbitals 1 and 2.

Consider:

$$H^t = -t \sum_s \left(c_{1s}^\dagger c_{2s} + c_{2s}^\dagger c_{1s} \right) \qquad \text{inter-orbital hopping}$$

$$H^U = U \sum_i n_{i\uparrow} n_{i\downarrow} \qquad \text{intra-orbital Coulomb}$$

Assume $t \ll U$ (small overlap of orbitals).

Unperturbed state is ground state of H^U: 4fold degenerate space

$\{0\} = |s_1 s_2\rangle$ $(s = \uparrow, \downarrow)$

Action of H^t: transitions in/out of $\{0\}$.

Second-order effective Hamiltonian H_{eff}:

$$\langle a | H_{eff} | b \rangle = - \sum_{n \notin \{0\}}{}' \frac{\langle a | H^t | n \rangle \langle n | H^t | b \rangle}{\langle n | H^U | n \rangle}, \quad a, b \in \{0\}$$

↖ intermediate state with two electrons in same orbital (virtual double occupancy)

E.g. $|\uparrow,\downarrow\rangle \xrightarrow{H^t} |\uparrow\downarrow, 0\rangle \xrightarrow{H^t} |\downarrow, \uparrow\rangle$

Collect all contributions:

$$\underline{H_{eff} = J \left(\vec{S}_1 \cdot \vec{S}_2 - \tfrac{1}{4} \right)}, \quad J = 4 \frac{t^2}{U} > 0$$

2.4. Magnetic ions in solids (brief, see Yosida book for details)

Small overlap (of WF) between neighboring ions ↝ nearly localized states

⊕ Partially filled shells ↝ Mott insulator w/ Coulomb

Consider isolated ion ↝ to understand relevant level structure.
in crystal !!

Recall hydrogen atom: $E_n = -\frac{1}{2n^2}$,

Degeneracies split by LS coupling & Coulomb interaction w/ other electrons.

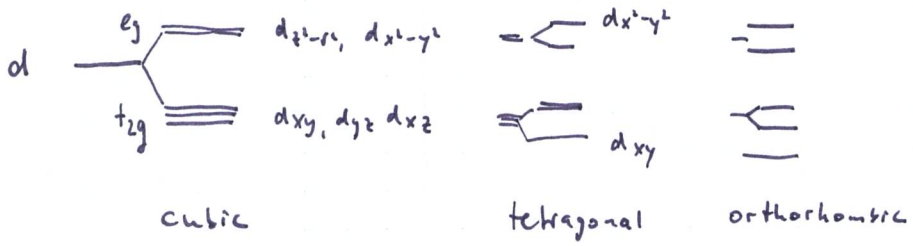
Remaining $(n\ell)$ shell has $(2\ell+1) \times 2$ states
↖ spin.

Substructure is determined by <u>Crystalline electric field</u>

(electrostatic potential of surrounding ions ↝ depends on <u>symmetry</u> of crystal)

e.g. $d_{x^2-y^2}$ ✿ and d_{xy} ✿ can split !

<u>Examples</u>



(Energetic sequence of multiplets depends on details, degeneracies do NOT)

Cuprates $3d^9$ ↝ 1 hole in $d_{x^2-y^2}$

Non-degenerate CEF (ground) state $\langle 0|\vec{L}|0\rangle = 0$ ↝ quenched orbital ang. momentum

(because CEF Hamiltonian is real, L is imaginary)

2.5. Local-moment formation and spin interactions

Local moments form as a result of Coulomb interaction.

Consider Hubbard model:

$$H = -t \sum_{\langle ij \rangle} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

at half filling (on average one electron per site, $\langle n_i \rangle = 1$).

For $U \gg t$ doubly occupied sites are costly

↝ at $\langle n \rangle = 1$ the low-energy sector is given by $n = 1$. (all sites singly occupied)

↝ charge fluctuation suppressed, no electron transport

↝ Mott insulator (with local spin-$\frac{1}{2}$ moment on sites)

$n = 1$ defines manifold of 2^N spin states ($N \hat{=}$ number of sites).

These are degenerate for $t/U \to 0$, but degeneracy is lifted by virtual hopping. Effective Hamiltonian by second-order perturbation theory & projection into low-energy subspace (see 2.3).

Result:

$$H = J \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right) \quad , \quad J = 4 \frac{t^2}{U} > 0$$

Heisenberg model

$$\vec{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} c_{i\sigma}^{\dagger} \vec{\sigma}_{\sigma\sigma'} c_{i\sigma'}$$

($\vec{\sigma}$: Pauli)

Signatures of local-moment formation:

- magnetic susceptibility Curie-like, $\chi = C/T$ for $J \ll T \lesssim U$
- Single-particle spectra show Hubbard bands (→ literature)

Spin anisotropies (breaking of SU(2) spin symmetry, deviations from Heisenberg)

arise from spin-orbit coupling $\vec{L} \cdot \vec{S}$ (SOC)

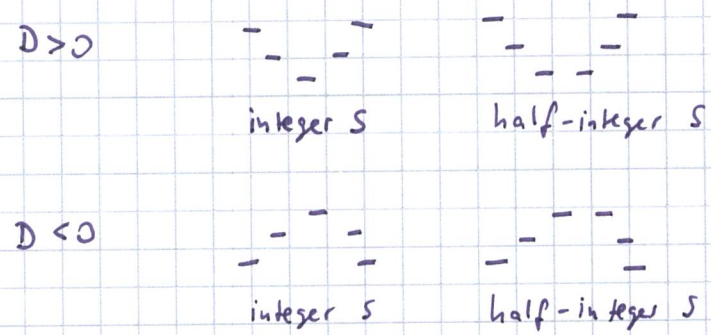
Often, anisotropies can be treated as perturbations.

When derived from Hubbard-like model, they arise from higher ionic states.

(a) Single-ion anisotropy

$$H_{SI} = D S_z^2 + E (S_x^2 - S_y^2)$$

Levels from D (assume E = 0):



states with different S_z split in energy
($E \neq 0$: couples states with $\Delta S_z = \pm 2$)

↷ ground state can be unique or doubly degenerate

Notes:
- H_{SI} obeys crystal symmetries!
  Cubic system has $D = 0$, $E = 0$, but $(S_x^4 + S_y^4 + S_z^4)$ term.
- Lattice with basis can have <u>local</u> (instead of global) anisotropy axes
- H_{SI} does not act for $S = 1/2$: $S_x^2 = S_y^2 = S_z^2 = \text{const} = 1/4$

(b) Exchange anisotropies

D-M vector

Dzyaloshinsky – Moriya: $\vec{D} \cdot (\vec{S}_1 \times \vec{S}_2)$ — first order in SOC

Pseudodipolar: $\vec{S}_1 \cdot \overleftrightarrow{\Gamma} \cdot \vec{S}_2$ — second order in SOC

($\overleftrightarrow{\Gamma}$: symmetric tensor)

Ising: $S_1^z S_2^z$

D-M interaction requires broken inversion symmetry to exist.

2.6. Symmetry breaking and mean-field theory

Recall Noether's theorem: Every continuous symmetry is associated with a conservation law.

Symmetry operation $\hat{S}$

Continuous symmetry has generator $\hat{g}\,(=\hat{g}^\dagger)$: $\hat{S} = e^{i\alpha\hat{g}}$ ($\hat{S}$: e.g. translation; $\hat{g}$: e.g. momentum)

$[\hat{H}, \hat{S}] = 0 \iff [\hat{H}, \hat{g}] = 0$

Spontaneous symmetry breaking: $[\hat{H}, \hat{S}] = 0$, but $[\hat{\rho}, \hat{S}] \neq 0$ ($\hat{H}$: Hamiltonian; $\hat{\rho}$: density matrix)

Symmetry breaking in Gibbs ensemble:

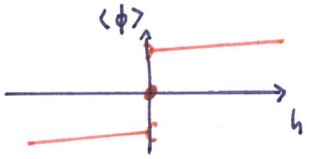
$[\hat{H}, \hat{S}] = 0$ implies $[e^{-\beta\hat{H}}, \hat{S}] = 0$ — can symmetry be broken?

Apply symmetry-breaking field $\hat{H} \to \hat{H} - h\hat{\phi}$

with $\hat{\phi} \equiv$ order parameter, i.e., $[\hat{\phi}, \hat{S}] \neq 0$

Spontaneous symmetry breaking $\hat{=}$ Limit $h \to 0$ singular

$\lim_{h\to 0} \hat{\rho}(h) \neq \hat{\rho}(h=0)$



e.g. ferromagnet

Symmetry breaking (at $T > 0$) requires thermodynamic limit, as finite systems cannot display a phase transition at $T > 0$

($e^{-\beta\hat{H}}$ = product of finite number of exponentials → regular function of $\beta = 1/k_B T$)

↝ Symmetry breaking implies $\lim_{h\to 0}\lim_{N\to\infty} \ldots \neq \lim_{N\to\infty}\lim_{h\to 0} \ldots$

Symmetry breaking also implies existence of gapless excitation modes, with $\omega(q) \to 0$ for $q \to 0$ (long-wavelength limit) ↝ Goldstone modes

(because $q = 0$ corresponds to symmetry-restoring uniform transformation)

Mean-field theory for ferromagnetic Heisenberg model

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

$\vec{h} \hat{=} g\mu_B \vec{B}$

$$\vec{S}_i \cdot \vec{S}_j = \underbrace{(\vec{S}_i - \langle \vec{S}_i \rangle) \cdot (\vec{S}_j - \langle \vec{S}_j \rangle)}_{\text{fluctuations} \to 0} + \vec{S}_i \cdot \langle \vec{S}_j \rangle + \langle \vec{S}_i \rangle \cdot \vec{S}_j - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle$$

MF approx $\hat{=}$ discard fluctuations $\to 0$

Assume homogeneous state $\langle \vec{S}_i \rangle = \langle \vec{S} \rangle$: coordination number

$$H_{MF} = -(\vec{h} + \vec{h}_{MF}) \cdot \sum_i \vec{S}_i + J N \frac{z}{2} \langle \vec{S} \rangle^2$$

with self-consistency condition

$$\vec{h}_{MF} = J z \langle \vec{S} \rangle$$

H_{MF} describes single spin in field $\vec{h}$

$\vec{h}_{MF}$ represents mean field (of environment acting on a particular spin).

H_{MF} can be solved. For $S = \frac{1}{2}$ and $\vec{h} \parallel \vec{h}_{MF} \parallel \langle \vec{S} \rangle$:

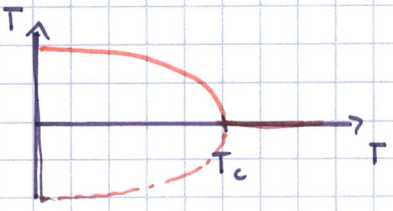
$$\langle S \rangle = \frac{1}{2} \tanh \frac{h + h_{MF}}{2 k_B T}$$

Self-consistency condition then yields full solution. $\left(\text{Solve } \frac{4 k_B T}{J z} x = \tanh x \right)$

For $h = 0$: $\exists\, T_c$: $T > T_c$: one solution $\langle S \rangle = 0$

$T < T_c$: three solutions $\langle S \rangle = \pm \#$ (↑ stable), $\langle S \rangle = 0$ (↑ unstable)

Ordering temperature : $\boxed{k_B T_c = \frac{J z}{4}}$ (recall $T_c \simeq J$ from chapter 1)



$\langle \vec{S} \rangle \neq 0$ implies spontaneous symmetry breaking.

State for $T < T_c$ displays long-range order :

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \overset{MF}{=} \langle \vec{S} \rangle^2 \neq 0 \quad \text{for } |i - j| \to \infty.$$

2.7. Paradigmatic models for frustrated magnets

Heisenberg $H = \sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$ $\quad J > 0$

Ising $H = \sum_{\langle ij \rangle} J_{ij}\, S_i^z S_j^z$

Compass / Kitaev $H = \sum_{\langle ij \rangle_\gamma} J_{ij}\, S_i^\gamma S_j^\gamma$ $\quad (\gamma \hat{=}$ different bonds on lattice)

- Triangular Ising: every triangle $\uparrow\uparrow\downarrow$ or $\uparrow\downarrow\downarrow$ ⇝ largely degenerate
  (Kagome Ising similar) ⇝ finite residual entropy $S/N \hat{=}$ classical spin liquid

- Triangular Heisenberg: classical $\sum_{i \in \Delta} \vec{S}_i = 0$ ⇝ unique 120° ground state (up to SU(2) rotations)

  $S = 1/2$ still 120° order

  ATTN: with external field $\sum_{i \in \Delta} \vec{S}_i = \frac{\vec{h}}{3J}$

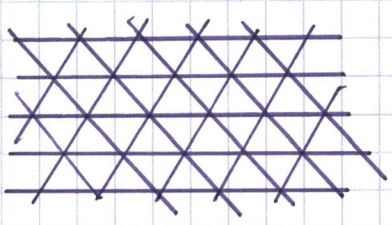
  ⇝ still SU(2) degenerate ⇝ order by disorder

- Kagome Heisenberg: classical $\sum_{i \in \Delta} \vec{S}_i = 0$ ⇝ largely degenerate (incl. non-coplanar states)

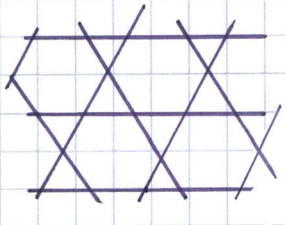
  $S = 1/2$ most likely quantum spin liquid

- Pyrochlore Heisenberg classical $\sum_{i \in \text{tetrahedron}} \vec{S}_i = 0$ ⇝ largely degenerate

  $S = 1/2$ perhaps quantum spin liquid



triangular



Kagome (corner-sharing triangles)

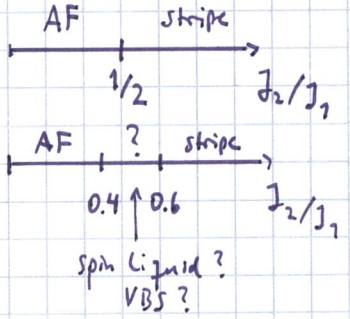
pyrochlore (corner-sharing tetrahedra)

Frustration can also be introduced by couplings beyond nearest neighbors.

first neighbor
second neighbor

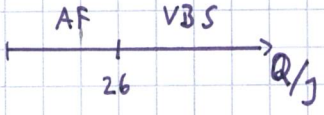
- Square lattice $J_1 - J_2$
  classical

  $S = 1/2$

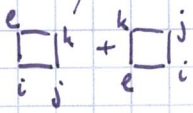


- Square lattice $J - Q$

  $S = 1/2$



$$H_Q = -Q \sum_{\langle ijke \rangle} (\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4})(\vec{S}_k \cdot \vec{S}_e - \tfrac{1}{4})$$



- Triangular lattice $J_1 - J_2$
  Classical

  $S = 1/2$