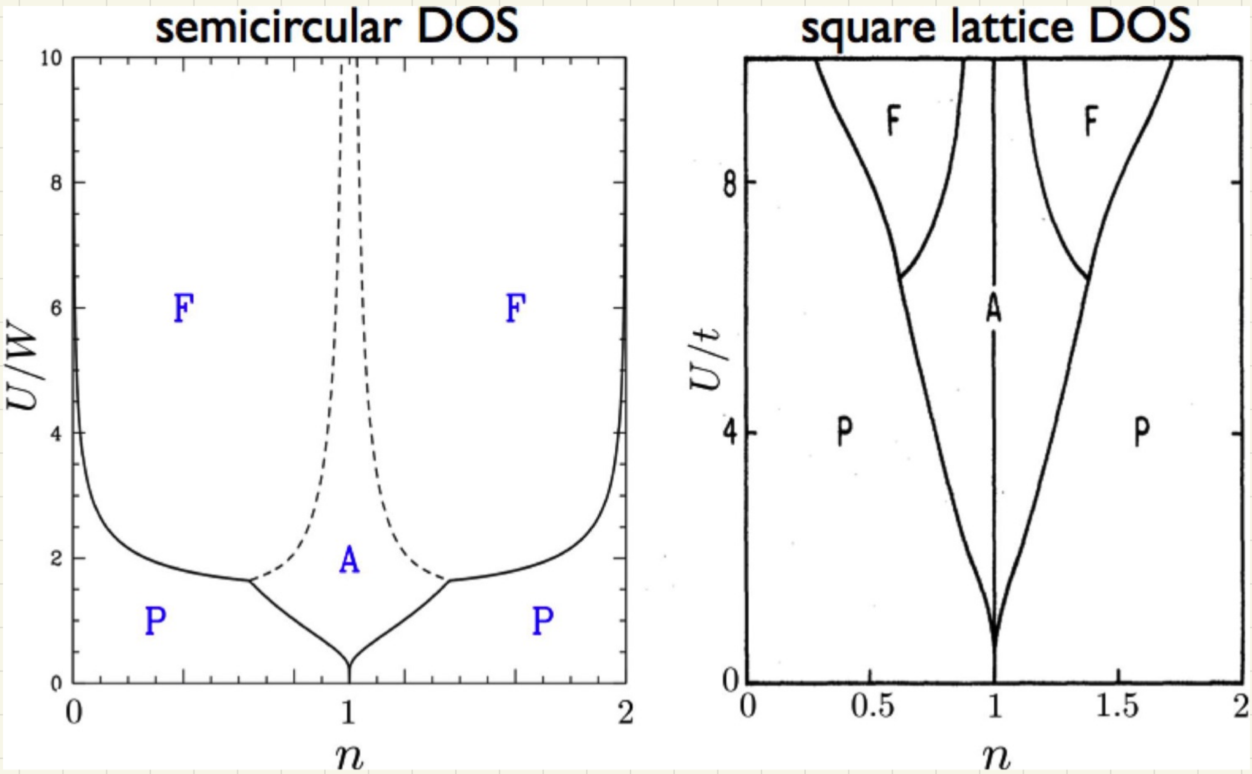
A paramagnetic solⁿ with $m=0$ always exists, in which case ② no longer applies.

Mean field phase diagrams at $T=0$:



In fact, FM is quite difficult to obtain in reality and seems to require $U/t \gtrsim 100$ on the square lattice.

Lecture 21 (March 11)

Heisenberg model: interacting local moments

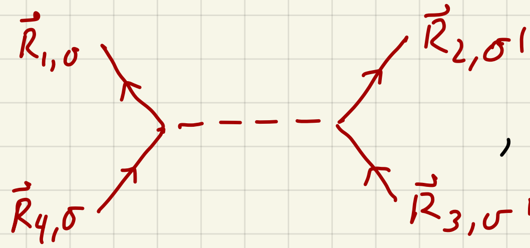
Electrons have a magnetic dipole moment $\vec{m} = -\mu_B \vec{\sigma}$.
How strong is the dipole-dipole interaction in solids?

$$E_{d-d} = \frac{\vec{m}_1 \cdot \vec{m}_2 - 3(\hat{n}\cdot\vec{m}_1)(\hat{n}\cdot\vec{m}_2)}{|\vec{r}_1 - \vec{r}_2|^2} \simeq \frac{\mu_B^2}{R^3} = \underbrace{\frac{e^2}{2a_B}}_{13.6\,eV} \cdot \underbrace{\left(\frac{e^2}{\hbar c}\right)^2}_{5.3\times10^{-5}} \cdot \underbrace{\left(\frac{a_B}{R}\right)^3}_{10^{-2}}$$

$= 7\,\mu eV$

if we assume $R \simeq 2.5\,\text{Å}$. This is tiny! Overwhelmingly, magnetism in solids is due to the Coulomb interaction. For example, with s-orbitals,

$$\hat{V} = \frac{1}{2} \sum_{\substack{\vec{R}_1,\vec{R}_2 \\ \vec{R}_3,\vec{R}_4}} \sum_{\sigma,\sigma'} \langle \vec{R}_1 \vec{R}_2 | \frac{e^2}{|\vec{r}-\vec{r}\,'|} | \vec{R}_4 \vec{R}_3 \rangle \, c^\dagger_{\vec{R}_1\sigma} c^\dagger_{\vec{R}_2\sigma'} c_{\vec{R}_3\sigma'} c_{\vec{R}_4\sigma}$$

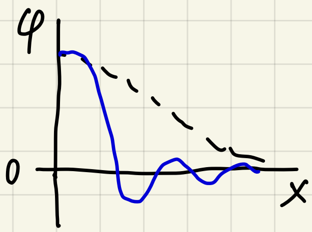
corresponding to the processes  , with

$$\langle \vec{R}_1 \vec{R}_2 | \frac{e^2}{|\vec{r}-\vec{r}\,'|} | \vec{R}_4 \vec{R}_3 \rangle = \int d^3r \int d^3r' \, \varphi^*(\vec{r}-\vec{R}_1)\, \varphi^*(\vec{r}\,'-\vec{R}_2) \times \frac{e^2}{|\vec{r}-\vec{r}\,'|}\, \varphi(\vec{r}\,'-\vec{R}_3)\, \varphi(\vec{r}-\vec{R}_4)$$

where $\langle \vec{r} | \vec{R} \rangle = \varphi(\vec{r}-\vec{R})$ is an s-band Wannier function, for which $\langle \vec{R} | \vec{R}' \rangle = \delta_{\vec{R}\vec{R}'}$. Due to the overlap factors, the Coulomb matrix element will be small unless $\vec{R}_4 = \vec{R}_1$ and $\vec{R}_3 = \vec{R}_2$, which yields the **direct Coulomb interaction**,

$$V(\vec{R}-\vec{R}') = \langle \vec{R} \vec{R}' | \frac{e^2}{|\vec{r}-\vec{r}\,'|} | \vec{R} \vec{R}' \rangle$$

$$= \int d^3r \int d^3r' \, \underbrace{|\varphi(\vec{r}-\vec{R})|^2}_{\rho_{\vec{R}}(\vec{r})} \frac{e^2}{|\vec{r}-\vec{r}\,'|} \underbrace{|\varphi(\vec{r}\,'-\vec{R}')|^2}_{\rho_{\vec{R}'}(\vec{r}\,')}$$



This decays as $|\vec{R}-\vec{R}'|^{-1}$ at long distances. If we were to neglect all but the direct matrix elements, we'd have

$$\hat{V}_{\text{direct}} = V(0) \sum_{\vec{R}} n_{\vec{R}\uparrow} n_{\vec{R}\downarrow} + \frac{1}{2} \sum_{\vec{R},\vec{R}'}{}' \, V(\vec{R}-\vec{R}')\, n_{\vec{R}}\, n_{\vec{R}'}$$

$\vec{R} \neq \vec{R}'$

where $n_{\vec{R}} \equiv \sum_\sigma n_{\vec{R}\sigma} = n_{\vec{R}\uparrow} + n_{\vec{R}\downarrow}$. The first term is the Hubbard interaction, with $U = V(0)$.

A second class of matrix elements is given by the case $\vec{R}_3 = \vec{R}_1 \equiv \vec{R}$ and $\vec{R}_4 = \vec{R}_2 \equiv \vec{R}'$, with $\vec{R} \neq \vec{R}'$. We define

$$\begin{aligned} J(\vec{R}-\vec{R}') &\equiv \langle \vec{R}\,\vec{R}' \,|\, \frac{e^2}{|\vec{R}-\vec{R}'|} \,|\, \vec{R}'\,\vec{R} \rangle \\ &= \int\! d^3r \int\! d^3r'\; \varphi^*(\vec{r})\,\varphi(\vec{r}+\vec{R}-\vec{R}')\, \frac{e^2}{|\vec{r}-\vec{r}'|}\, \varphi^*(\vec{r}'+\vec{R}-\vec{R}')\,\varphi(\vec{r}') \end{aligned}$$

Note $J(\vec{R}-\vec{R}') \in \mathbb{R}$. We define

$c^\dagger_{\vec{R}\uparrow} c_{\vec{R}'\uparrow} \, c^\dagger_{\vec{R}\downarrow} c_{\vec{R}'\downarrow}$

$$\begin{aligned} \hat{V}_{\text{exchange}} &= -\frac{1}{2} \sum_{\vec{R},\vec{R}'}{}' \sum_{\sigma,\sigma'} J(\vec{R}-\vec{R}')\, c^\dagger_{\vec{R}\sigma}\, c_{\vec{R}\sigma'}\, c^\dagger_{\vec{R}'\sigma'}\, c_{\vec{R}'\sigma} \\ &= -\frac{1}{4} \sum_{\vec{R},\vec{R}'} J(\vec{R}-\vec{R}') \left(\vec{\sigma}_{\vec{R}} \cdot \vec{\sigma}_{\vec{R}'} + n_{\vec{R}}\, n_{\vec{R}'} \right) \end{aligned}$$

We may lump the $n_{\vec{R}} n_{\vec{R}'}$ piece with the corresponding term in $\hat{V}_{\text{direct}}$, leaving

$$\hat{V}_{\text{Heis}} = -\sum_{\vec{R},\vec{R}'}{}' \, J(\vec{R}-\vec{R}')\, \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}'}$$

which is the Heisenberg interaction. Usually $J(\vec{R}-\vec{R}') > 0$, in which case this term promotes ferromagnetism.

Under conditions of spin rotation invariance (i.e. SU(2) symmetry) and lattice translation symmetry, the most general spin Hamiltonian is of the form

$$\hat{H} = \sum_{i<j} F_{ij}(\vec{S}_i \cdot \vec{S}_j) + \sum_{i<j<k} G_{ijk}(\vec{S}_i \cdot \vec{S}_j, \vec{S}_j \cdot \vec{S}_k) + \dots$$

where F_{ij}, G_{ijk}, H_{ijkl}, etc. are finite order polynomials in their arguments. The local spin operators satisfy the algebraic relations

$$[S_i^\alpha, S_j^\beta] = i\epsilon_{\alpha\beta\gamma} S^\gamma \qquad (\hbar = 1)$$

with $\vec{S}_i^2 = S_i(S_i+1)$. Thus, S_i is the total spin quantum number at site i. Typically, the dominant terms in the spin Hamiltonian are of the Heisenberg form, in which case

$$\hat{H} = -\sum_{i<j} J_{ij}\, \vec{S}_i \cdot \vec{S}_j - \gamma \sum_i \vec{H}_i \cdot \vec{S}_i$$

with $J_{ij} = J(|\vec{R}_i - \vec{R}_j|)$. We have included the Zeeman term in the presence of finite local fields $\{\vec{H}_i\}$. When $J_{ij} > 0$, the interaction between the spins $\vec{S}_i$ and $\vec{S}_j$ is ferromagnetic. When $J_{ij} < 0$, the interaction is antiferromagnetic.

Mean field theory of magnetic order:

Do the mean field thang:

$$\vec{S}_i = \vec{m}_i + \delta\vec{S}_i \qquad \text{with} \qquad \vec{m}_i \equiv \langle \vec{S}_i \rangle$$

Then

$$\vec{S}_i \cdot \vec{S}_j = \vec{m}_i \cdot \vec{m}_j + \vec{m}_i \cdot \delta\vec{S}_j + \vec{m}_j \cdot \delta\vec{S}_i + \overbrace{\delta\vec{S}_i \cdot \delta\vec{S}_j}^{(\text{flucts})^2 \to \text{drop it}}$$

$$= -\vec{m}_i \cdot \vec{m}_j + \vec{m}_i \cdot \vec{S}_j + \vec{m}_j \cdot \vec{S}_i + \cancel{\delta\vec{S}_i \, \delta\vec{S}_j}$$

and we obtain the mean field Hamiltonian

$$\hat{H}^{MF} = +\sum_{i<j} J_{ij} \, \vec{m}_i \cdot \vec{m}_j - \sum_i \Big(\gamma \vec{H}_i + \sum_j J_{ij} \, \vec{m}_j\Big) \cdot \vec{S}_i$$

$$\equiv E_0 - \gamma \sum_i \vec{H}_i^{\text{eff}} \cdot \vec{S}_i$$

where

$$\vec{H}_i^{\text{eff}} = \underbrace{\vec{H}_i}_{\text{applied field}} + \underbrace{\gamma^{-1} \sum_j J_{ij} \, \vec{m}_j}_{\text{internal field}}$$

and $E_0 = \sum_{i<j} J_{ij} \, \vec{m}_i \cdot \vec{m}_j$. Self-consistency now requires

$$\vec{m}_i = \langle \vec{S}_i \rangle = \frac{\mathrm{Tr}\, \vec{S}_i \exp(\gamma \vec{H}_i^{\text{eff}} \cdot \vec{S}_i / k_B T)}{\mathrm{Tr} \exp(\gamma \vec{H}_i^{\text{eff}} \cdot \vec{S}_i / k_B T)}$$

The mean field free energy is then

$$F(\{\vec{m}_i\}, \{\vec{H}_i\}, T) = \frac{1}{2} \sum_{i<j} J_{ij} \, \vec{m}_i \cdot \vec{m}_j - k_B T \sum_i \ln \mathrm{Tr} \exp\left(\frac{(\gamma \vec{H}_i + \overbrace{J_{ij} \, \vec{m}_j}^{\text{sum on } j}) \cdot \vec{S}_i}{k_B T}\right)$$

This formalism may now be applied to various models, both classical and quantum.

Magnetic order occurs below a critical temperature T_c, where the solution to the MF eqns which minimizes the free energy is of the form

$$\vec{m}_i = \sum_{\vec{Q}} \hat{\vec{m}}_{\vec{Q}}\, e^{i\vec{Q}\cdot\vec{R}_i}$$

where the sum is over a finite number of ordering wavevectors $\vec{Q}$, and where $\hat{\vec{m}}_{\vec{Q}}$ are the **order parameters.** As an example, consider spin-S quantum Heisenberg antiferromagnet on a BCC lattice. Recall the elementary DLVs and RLVs:

$$\vec{a}_1 = \tfrac{1}{2}a(\bar{1}\,1\,1) \quad , \quad \vec{a}_2 = \tfrac{1}{2}a(1\,\bar{1}\,1) \quad , \quad a_3 = \tfrac{1}{2}a(1\,1\,\bar{1})$$

$$\vec{b}_1 = \frac{2\pi}{a}(0\,1\,1) \quad , \quad \vec{b}_2 = \frac{2\pi}{a}(1\,0\,1) \quad , \quad \vec{b}_3 = \frac{2\pi}{a}(1\,1\,0)$$

which satisfy $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$. DLVs are all of the form

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

and sites with $n_1+n_2+n_3$ even are on the A sublattice, while those with $n_1+n_2+n_3$ odd are on the B sublattice. Note that with $\vec{Q} \equiv \frac{1}{2}(\vec{b}_1+\vec{b}_2+\vec{b}_3) = \frac{2\pi}{a}(1\,1\,1)$ we have $\exp(i\vec{Q}\cdot\vec{R}) = (-1)^{n_1+n_2+n_3}$. Thus $\vec{Q}$ is the ordering wavevector, and thus $\vec{m}_i = \vec{m}\, e^{i\vec{Q}\cdot\vec{R}_i}$, so $m_{A,B} = \pm\vec{m}$ and for $\vec{H}=0$ the internal field is $\vec{H}^{int}_{A,B} = -z\gamma^{-1}J m_{\vec{B},\vec{A}} = \pm z\gamma^{-1}J\vec{m}$. We then obtain the equations (see §14.7.2)

$$m_A = S B_S(zJSm_B/k_BT)$$
$$m_B = S B_S(zJSm_A/k_BT)$$

where $z=8$ for BCC, and $B_S(x)$ is the Brillouin function. Since $m_A = m_B = m$ ($\vec{m}_A = -\vec{m}_B = m\hat{n}$), we obtain the Néel temperature $T_N = S(S+1)zJ/3k_B$. (When $\vec{H} \neq 0$, there is a spin flop for weak fields.)

Magnetic susceptibility: When $T > T_c$, the system is paramagnetic and

$$\chi^{\mu\nu}_{ij} = \frac{\partial M^\mu_i}{\partial H^\nu_j}\bigg|_{\vec{H}=0} = \gamma \frac{\partial m^\mu_i}{\partial H^\nu_j}\bigg|_{\vec{H}=0} = -\frac{\partial^2 F}{\partial H^\mu_i \partial H^\nu_j}\bigg|_{\vec{H}=0}$$

$$= \frac{\gamma^2}{k_B T}\left\{\langle S^\mu_i S^\nu_j \rangle - \langle S^\mu_i \rangle \langle S^\nu_j \rangle\right\}_{\vec{H}=0}$$

The MF Hamiltonian is again $\hat{H}^{MF} = -\gamma \sum_i \vec{H}^{eff}_i \cdot \vec{S}_i$, with $\vec{H}^{eff}_i = \vec{H}_i + \gamma^{-1} J_{ij} \vec{m}_j$, which is a sum of local (single site) Hamiltonians. The response is then local, i.e.

$$\vec{M}_i = \chi_0 \vec{H}^{eff}_i = \chi_0 \vec{H}_i + \gamma^{-2} \chi_0 J_{ij} \vec{M}_j$$

where

$$\chi^{\mu\nu}_0 = \frac{\gamma^2}{k_B T} \cdot \frac{Tr(S^\mu S^\nu)}{Tr(1)} = \chi_0 \, \delta^{\mu\nu}$$

Thus $\chi^0 = N^{-1} Tr(\vec{S}^2)/Tr\,1$, where N is the number of components of S^μ. For the Ising model, $N=1$ and $\chi_0^{Ising} = \gamma^2/k_B T$. For the spin-$S$ quantum Heisenberg model, $\chi_0^{Heis} = S(S+1)\gamma^2/3k_B T$. We now have

$$(\delta_{ij} - \gamma^{-2}\chi_0 J_{ij})\vec{M}_j = \chi_0 \vec{H}_i$$

and thus

$$\chi_{ij}^{\mu\nu} = \left[\chi_0^{-1} - \gamma^{-2} J\right]_{ij}^{-1} \delta^{\mu\nu}$$

In Fourier space,

$$\hat{\chi}(\vec{q}) = \frac{\chi_0}{1 - \gamma^{-2}\chi_0 \hat{J}(\vec{q})} \quad ; \quad \hat{J}(\vec{q}) = \sum_{\vec{R}} J(R) e^{-i\vec{q}\cdot\vec{R}}$$

Note that $\hat{\chi}(\vec{q})$ will in general diverge at a (set of) special wavevector(s) as T is decreased from $T = \infty$, since $\chi_0 \propto T^{-1}$. The first such divergence corresponds to $T = T_c$.

In cases where there is single ion anisotropy, e.g.

$$\hat{H}_D = D \sum_i (S_i^z)^2$$

such that $D < 0 \Rightarrow$ easy axis and $D > 0 \Rightarrow$ easy plane, then $\chi_0 \to \chi_0^{\mu\nu}$ has a matrix structure in internal space, with

$$\chi_0^{\mu\nu} = \frac{\gamma^2}{k_B T} \langle S^\mu S^\nu \rangle$$

and the average is wrt the local (single site) Hamiltonian. Then

$$\hat{\chi}^{\mu\nu}(\vec{q}) = \chi_0^{\mu\lambda} \left[\mathbb{1} - \gamma^{-2} \hat{J}(\vec{q}) \chi_0\right]_{\lambda\nu}^{-1}$$

Just below $T = T_c$: Recall

$$\hat{\chi}(\vec{q}, T) = \frac{\chi_0(T)}{1 - \gamma^{-2}\chi_0(T)\hat{J}(\vec{q})}$$

This first diverges at the wavevector $\vec{Q}$ which maximizes the function $\hat{J}(\vec{q})$, and at temperature T_c, where

$$\gamma^{-2}\,\chi_0(T_c)\,\hat{J}(\vec{Q}) = 1$$

NB: It may be that $\hat{J}(\vec{q})$ is maximized on a set $\{\vec{Q}_1, \vec{Q}_2, \ldots\}$ of symmetry-related wavevectors. Let's expand $\hat{J}(\vec{q})$ about one such maximum and write

$$\hat{J}(\vec{q}) = \hat{J}(\vec{Q})\left\{1 - (\vec{q}-\vec{Q})^2 R_*^2 + \ldots\right\}$$

Then

$$\begin{aligned}
\hat{\chi}(\vec{q},T) &= \frac{1}{\left[\chi_0^{-1}(T) - \gamma^{-2}\hat{J}(\vec{Q})\right] + \gamma^{-2}\left[\hat{J}(\vec{Q}) - \hat{J}(\vec{q})\right]} \\
&\approx \frac{1}{\gamma^{-2}\hat{J}(\vec{Q})} \cdot \frac{1}{\left[\gamma^{2}\hat{J}(\vec{Q})\,\chi_0^{-1}(T) - 1\right] + (\vec{q}-\vec{Q})^2 R_*^2} \\
&\approx \frac{\chi_0(T)/R_*^2}{\xi^{-2}(T) + (\vec{q}-\vec{Q})^2}
\end{aligned}$$

where

$$\begin{aligned}
\xi^{-2}(T) &\equiv \left[1 - \gamma^{-2}\,\hat{J}(\vec{Q})\,\chi_0(T)\right]\cdot R_*^{-2} \\
&\approx -\frac{\hat{J}(\vec{Q})}{\gamma^2 R_*^2}\,\chi_0'(T_c)\,(T-T_c) > 0
\end{aligned}$$

is the **correlation length**. Note that $\xi(T) \propto (T-T_c)^{-1/2}$ just above T_c.

- **ferromagnet:** here we have $\vec{Q}=0$. For a hypercubic lattice,

$$\hat{J}(\vec{q}) = 2J\left\{\cos(q_1 a) + \ldots + \cos(q_d a)\right\} = \sum_{\vec{R}} J(\vec{R})\, e^{-i\vec{q}\cdot\vec{R}}$$

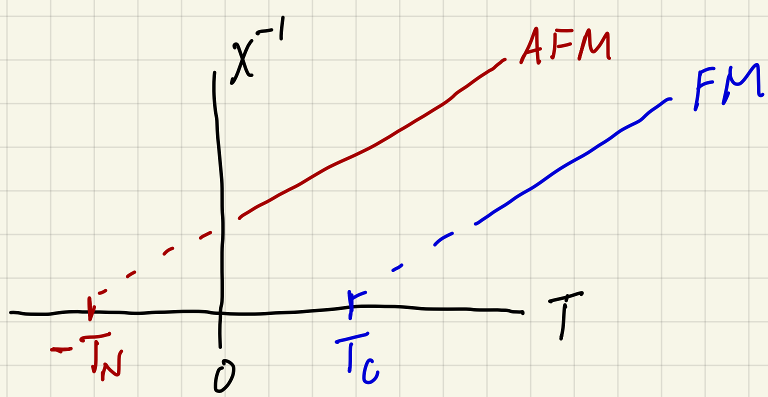
and $\hat{J}(\vec{Q}) = \hat{J}(0) = 2dJ$. For the spin-$S$ Heisenberg model, find $T_c = 2dS(S+1)J/3k_B$, the **Curie temperature**, and

$$\chi(\vec{q}=0,T) \approx \frac{\gamma^2 S(S+1)}{3k_B(T-T_c)}$$

- **antiferromagnet:** just like FM above, but with $J<0$ (assuming bipartite lattice). On d-dim^l hypercubic lattice, we have $\vec{Q}=\left(\frac{\pi}{a},\frac{\pi}{a},\ldots,\frac{\pi}{a}\right)$, and $\hat{J}(\vec{Q}) = -2dJ = +2d|J|$. The **staggered susceptibility** $\hat{\chi}(\vec{q}=\vec{Q},T)$ then diverges at the **Néel temperature** $T_N = 2dS(S+1)|J|/3k_B$. However the **uniform susceptibility** $\hat{\chi}(\vec{q}=0,T)$ remains finite through the transition:

$$\hat{\chi}(\vec{q}=0,T) \approx \frac{\gamma^2 S(S+1)}{3k_B(T+T_N)} \quad , \quad \hat{\chi}(\vec{q}=\vec{Q},T) \approx \frac{\gamma^2 S(S+1)}{3k_B(T-T_N)}$$

Thus, one expects

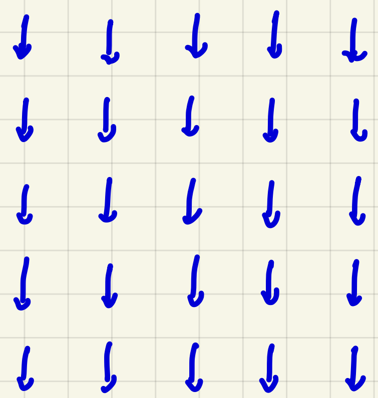


Spin wave theory : behavior near $T=0$

Heisenberg model (spin S) : $\hat{H} = -J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$ (NN only)

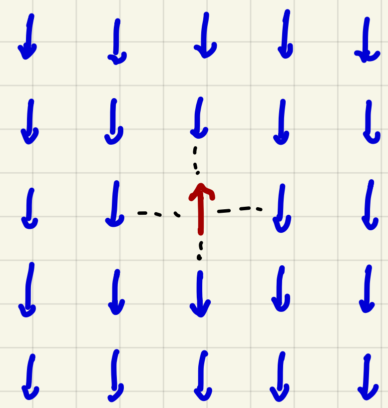
For **Ising** magnets,

FM ground state :



$$\mathcal{E}_{link} = -JS^2$$
$$E^0_{tot} = -\frac{1}{2}NzJS^2$$

FM excited state :

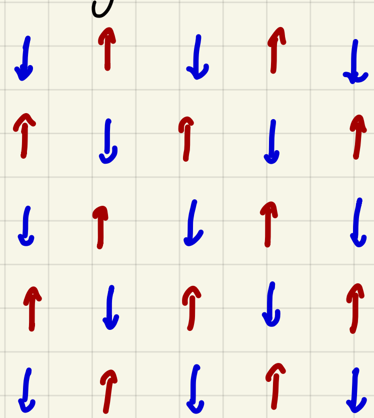


$$E_{tot} = E^0_{tot} + 2zJS^2$$
$$w_{exc} = 2zJS^2$$

single spin flip

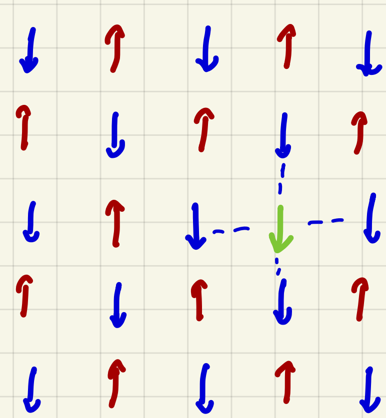
$$H^{Heis}_{ij} = -J\left(\frac{1}{2}S_i^+S_j^- + \frac{1}{2}S_i^-S_j^+ + S_i^zS_j^z\right)$$

AFM ground state :



$$\mathcal{E}_{link} = -|J|S^2$$
$$E^0_{tot} = -\frac{1}{2}Nz|J|S^2$$

AFM excited state :



$$E_{tot} = E^0_{tot} + 2z|J|S^2$$
$$w_{exc} = 2z|J|S^2$$

single spin flip

For the Heisenberg model, must obey QM:

$$[S_i^\mu, S_j^\nu] = i\epsilon_{\mu\nu\lambda} S_i^\lambda \delta_{ij} \Rightarrow [S^z, S^\pm] = \pm S^\pm, \quad [S^+, S^-] = 2S^z$$

On a single site, can describe by bosonic ladder operators a and $a^\dagger$ with $[a, a^\dagger] = 1$ (**Holstein-Primakoff transformation**):

$$\begin{aligned} S^+ &= a^\dagger \sqrt{2S - a^\dagger a} \\ S^- &= \sqrt{2S - a^\dagger a}\, a \\ S^z &= a^\dagger a - S \end{aligned} \quad \Longleftrightarrow \quad \begin{array}{lcccccc} S^z \equiv m: & -S & -S+1 & \cdots & +S & \Big| & \\ a^\dagger a \equiv n: & \underbrace{0 \quad 1 \quad \cdots \quad 2S}_{\text{phys}} & & & & \Big| & \overbrace{2S+1 \; \cdots}^{\text{unphys}} \end{array}$$

S^+ S^-

$n = S + m$

NONE SHALL PASS!

To take the square root of the operator $2S - a^\dagger a$, simply evaluate in the eigenbasis of $a^\dagger a$:

$$\begin{aligned} S^+ |S^z = m\rangle &= a^\dagger \sqrt{2S - a^\dagger a}\, |n = S + m\rangle \\ &= \sqrt{2S - (S+m)}\, a^\dagger |n = S+m\rangle \\ &= \sqrt{S - m}\sqrt{S+m+1}\, |n = S+m+1\rangle \\ &= \sqrt{S(S+1) - m(m+1)}\, |S^z = m+1\rangle \quad ✓ \end{aligned}$$

Thus, we obtain the correct matrix elements. To make further progress, assume $S \gg 1$ and that we are at low T. Expand

$$(2S - a^\dagger a)^{1/2} = \sqrt{2S}\left\{1 - \frac{1}{2}\left(\frac{a^\dagger a}{2S}\right) - \frac{1}{8}\left(\frac{a^\dagger a}{2S}\right)^2 + \cdots\right\}$$

as a power series in $a^\dagger a / 2S$. Then find

$$\vec{S}_i \cdot \vec{S}_j = \frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ + S_i^z S_j^z$$

$$= \underbrace{S^2}_{\mathcal{O}(S^2)} + \underbrace{S\left(a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j\right)}_{\mathcal{O}(S)}$$

$$+ \underbrace{\Big\{a_i^\dagger a_i a_j^\dagger a_j - \tfrac{1}{4} a_i^\dagger a_i^\dagger a_i a_j - \tfrac{1}{4} a_i^\dagger a_j^\dagger a_j a_j - \tfrac{1}{4} a_j^\dagger a_i^\dagger a_i a_i - \tfrac{1}{4} a_j^\dagger a_j^\dagger a_j a_i\Big\}}_{\mathcal{O}(S^0)} + \mathcal{O}(S^{-1})$$

Thus,

$$\hat{H} = \underbrace{-S^2 \sum_{i<j} J_{ij}}_{\substack{\text{classical ground}\\ \text{state energy}\\ \mathcal{O}(S^2)}} + \underbrace{S \sum_{i<j} J_{ij}\left(a_i^\dagger a_i + a_j^\dagger a_j - a_i^\dagger a_j - a_j^\dagger a_i\right)}_{\substack{\hat{H}_{sw} = \text{spin-wave Hamiltonian}\\ \mathcal{O}(S)}} + \underbrace{\mathcal{O}(S^0)}_{\substack{\text{spin-wave}\\ \text{interactions}}}$$

On a Bravais lattice, FT :

$$a_i = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{R}_i} a_{\vec{q}} \quad , \quad a_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{+i\vec{q}\cdot\vec{R}_i} a_i$$

Note $[a_i, a_{i'}^\dagger] = \delta_{ii'}$ and $[a_{\vec{q}}, a_{\vec{q}'}^\dagger] = \delta_{\vec{q}\vec{q}'}$. Using

$$\frac{1}{N} \sum_i e^{i(\vec{q}-\vec{q})\cdot\vec{R}_i} = \delta_{\vec{q}\vec{q}'}$$

we have

$$\hat{H}_{sw} = S \sum_{\vec{q}} \left[\hat{J}(0) - \hat{J}(\vec{q})\right] a_{\vec{q}}^\dagger a_{\vec{q}}$$

Thus,

$$\hbar\omega_{\vec{q}} = S\left[\hat{J}(0) - \hat{J}(\vec{q})\right] = \frac{1}{6} S \sum_{\vec{R}} \vec{R}^2 J(\vec{R})\, \vec{q}^{\,2} + \mathcal{O}(q^4)$$

Correlations:

$$\langle \delta_{a_i^\dagger a_i, k} \rangle$$

$$\langle S_i^z \rangle = -S + \langle a_i^\dagger a_i \rangle$$

$$= -S + \Omega \int_{\hat{\Omega}} \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\hbar \omega_k / k_B T} - 1} \qquad \text{(site-independent)}$$

This expression corresponds to a "poor man's" version of the HMW theorem. At finite T, we have as $k \to 0$

$$\frac{1}{e^{\hbar \omega_k / k_B T} - 1} = \frac{k_B T}{\hbar \omega_k} \propto \frac{T}{k^2}$$

and we see that $\langle S_i^z \rangle$ diverges if $d \leq 2$. This means that we've expanded about the wrong density matrix and there is no long-ranged spin order.

The transverse spin correlations are given by

$$\langle S_i^+ S_j^- \rangle = 2S\Omega \int_{\hat{\Omega}} \frac{d^d k}{(2\pi)^d} \frac{e^{i k \cdot (\vec{R}_i - \vec{R}_j)}}{e^{\hbar \omega_k / k_B T} - 1}$$

For $d > 2$, these correlations fall off as $|\vec{R}_i - \vec{R}_j|^{2-d}$. Note that our vacuum state here is $|0\rangle = |F\rangle$, the ferromagnet in which $a_i^\dagger a_i |0\rangle = 0 \Rightarrow S_i^z = -S$.