Magnetic ordering

- Types of magnetic structure
- Ground state of the Heisenberg ferro and antiferro-magnet
- Spin wave
- High temperature susceptibility
- Mean field theory
- Summary
In some solids, individual magnetic ions have non-vanishing average magnetic moments below a critical temperature $T_c$. Such solids are called *magnetically ordered*. 

**Ferromagnetic order**: net magnetization, $T_c$: Curie temperature.

**Antiferromagnetic order**: no net magnetization, $T_c$: Neel temperature, can be probed by elastic neutron scattering.

(a), (b), (c): ferromagnetic, antiferromagnetic and ferrimagnetic ordering.
Thermodynamic properties at the onset of magnetic ordering

The observed magnetization just below $T_c$ is well described by a power law

$$M(T) \sim (T_c - T)^\beta$$

The susceptibility in a ferromagnet and a antiferromagnet

- **FM** \( \chi(T) \sim (T - T_c)^{-\gamma} \)
- **AFM**

Specific heat

$$c(T) \sim (T - T_c)^{-\alpha}$$

alpha, beta, gamma are universal exponents.
Ground state of the Heisenberg ferromagnet

Ferromagnetic Heisenberg Hamiltonian

$$H = -\frac{1}{2} \sum_{RR'} S(R) \cdot S(R') J(R - R') - g\mu_B H \sum_R S_z(R)$$

$$J(R - R') = J(R' - R) \geq 0$$

Construct the ground state of Hamiltonian

$$|0\rangle = \prod_R |S\rangle_R, \quad S_z(R)|S\rangle_R = S|S\rangle_R$$

$$H = -\frac{1}{2} \sum_{RR'} J(R - R') S_z(R) S_z(R') - g\mu_B H \sum_R S_z(R)$$

$$- \frac{1}{2} \sum_{RR'} J(R - R') S_-(R') S_+(R)$$
The energy of ground state

\[ H |0\rangle = E_0 |0\rangle, \quad E_0 = -\frac{1}{2} S^2 \sum_{\mathbf{R}, \mathbf{R}'} J(\mathbf{R} - \mathbf{R}') - N g \mu_B HS \]

We have used the following relations

\[ S_\pm(\mathbf{R}) |S_z\rangle_\mathbf{R} = \sqrt{(S \mp S_z)(S + 1 \pm S_z)} |S_z \pm 1\rangle_\mathbf{R} \]

Prove that you cannot find a state with lower energy than the energy of \(|0\rangle\)
Ground state of the Heisenberg antiferromagnet

\[ H = \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}'} \mathbf{S}(\mathbf{R}) \cdot \mathbf{S}(\mathbf{R}') |J(\mathbf{R} - \mathbf{R}')| \]

\[-\frac{1}{2} S(S + 1) \sum_{\mathbf{R}, \mathbf{R}'} |J(\mathbf{R} - \mathbf{R}')| \leq E_0 \leq -\frac{1}{2} S^2 \sum_{\mathbf{R}, \mathbf{R}'} |J(\mathbf{R} - \mathbf{R}')| \]

Only one-dimensional array of spin-half ions with coupling between nearest neighbors can be solved by Bethe ansatz.
Spin wave

To construct low-lying states of ferromagnet, we consider a state

$$|R\rangle = \frac{1}{\sqrt{2S}} S_-(R)|0\rangle$$

The above state differs from the ground state only in that the spin at site R has had its z-component reduced from S to S-1.

$$H|R\rangle = E_0|R\rangle + g\mu_B H|R\rangle + S \sum_{R'} J(R - R')[|R\rangle - |R'\rangle]$$

To get the above equation, we need the following relations

$$S_-(R')S_+(R)|R\rangle = 2S|R'\rangle$$

$$S_z(R')|R\rangle = \begin{cases} S|R\rangle, & R' \neq R \\ (S - 1)|R\rangle, & R' = R \end{cases}$$
It implies that linear combination of $|\mathbf{R}\rangle$ are eigenstates.

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} |\mathbf{R}\rangle$$

We obtain

$$H|\mathbf{k}\rangle = E_k |\mathbf{k}\rangle$$

$$E_k = E_0 + g\mu_B H + S \sum_{\mathbf{R}} J(\mathbf{R})(1 - e^{i\mathbf{k} \cdot \mathbf{R}})$$

If $J(-\mathbf{R}) = J(\mathbf{R})$, we can write the excited energy

$$\varepsilon(\mathbf{k}) = E_k - E_0 = 2S \sum_{\mathbf{R}} J(\mathbf{R}) \sin^2 \left(\frac{1}{2} \mathbf{k} \cdot \mathbf{R}\right) + g\mu_B H$$

When $k \to 0$ we have

$$\varepsilon(\mathbf{k}) \approx \frac{S}{2} \sum_{\mathbf{R}} J(\mathbf{R})(\mathbf{k} \cdot \mathbf{R})^2 + g\mu_B H$$
- The total spin in the state $|k\rangle$ is NS-1.

- The lower spin is distributed with equal probability $1/N$.

- The orientations of the transverse components of two spins separated by $\mathbf{R} - \mathbf{R}'$ differ by an angle $k \cdot (\mathbf{R} - \mathbf{R}')$.

Figure 33.7
Schematic representations of the orientations in a row of spins in (a) the ferromagnetic ground state and (b) a spin wave state.
The mean number of spin waves (magnon) with wave vector \( k \) at temperature \( T \) is

\[
n(k) = \langle n_k \rangle = \frac{1}{e^{\varepsilon(k)/k_B T} - 1}
\]

Then the magnetization at temperature \( T \) satisfies

\[
M(T) = M(0) \left[ 1 - \frac{V}{NS} \int \frac{dk}{(2\pi)^3} \frac{1}{e^{\varepsilon(k)/k_B T} - 1} \right]
\]

At low temperature, only small excitation energies contribute to the integral, the spontaneous magnetization is given by

\[
M(T) = M(0) \left[ 1 - \frac{V}{NS} (k_B T)^{3/2} \int \frac{dq}{(2\pi)^3} \left\{ \exp \left[ S \sum_{\mathbf{R}} J(\mathbf{R}) \frac{(\mathbf{q} \cdot \mathbf{R})^2}{2} \right] - 1 \right\}^{-1} \right]
\]

Implication 1: Bloch \( T^{3/2} \) law
Implication 2: No spontaneous magnetization in one- and two-dimensional isotropic Heisenberg model, which is agree with Mermin-Wagner theorem.

Spin wave excitation energy of Heisenberg antiferro-magnet is linear in $k$ at long wavelengths.

Spin wave spectrum can be detected by inelastic neutron scattering.
High temperature susceptibility

\[ \chi(T) = \frac{g\mu_B}{V} \left( \sum_{\mathbf{R}} S_z(\mathbf{R}) \right) |_{H=0} = \frac{1}{V} \frac{1}{k_B T} (g\mu_B)^2 \left( \sum_{\mathbf{R} \neq \mathbf{R}'} S_z(\mathbf{R}) S_z(\mathbf{R}') \right) |_{H=0} \]

\[ = \frac{1}{V} \frac{1}{k_B T} (g\mu_B)^2 \sum_{\mathbf{R} \neq \mathbf{R}'} \Gamma(\mathbf{R}, \mathbf{R}') \]

In the limit of infinite temperature, spins at different sites are completely uncorrelated.

\[ \langle S_z(\mathbf{R}) S_z(\mathbf{R}') \rangle = \langle S_z(\mathbf{R}) \rangle \langle S_z(\mathbf{R}') \rangle = 0, \quad \mathbf{R} \neq \mathbf{R}' \]

\[ \langle S_z(\mathbf{R}) S_z(\mathbf{R}) \rangle = \frac{1}{3} \langle S(\mathbf{R})^2 \rangle = \frac{1}{3} S(S + 1) \]

Then, the correlation function is given by

\[ \Gamma(\mathbf{R}, \mathbf{R}') \approx \frac{1}{3} S(S + 1) \delta_{\mathbf{R} \mathbf{R}'} - \beta \langle S_z(\mathbf{R}) S_z(\mathbf{R}') H_0 \rangle \]

\[ \frac{1}{1 - \beta \langle H_0 \rangle} \]
Finally, we have

$$\Gamma(R, R') = \frac{S(S+1)}{3} \left[ \delta_{RR'} + \frac{S(S+1)}{3} \beta J(R - R') + O(\beta J)^2 \right]$$

The high temperature susceptibility is

$$\chi(T) = \frac{N}{V} \frac{(g\mu_B)^2}{3k_BT} S(S+1) \left[ 1 + \frac{\theta}{T} + O\left(\frac{\theta}{T}\right)^2 \right]$$

with

$$\theta = \frac{S(S+1)}{3} \frac{J_0}{k_B}, \quad J_0 = \sum_R J(R)$$

\(\theta\) can be positive or negative according to the coupling is ferromagnetic or antiferromagnetic etc.
Mean field theory

The Heisenberg Hamiltonian corresponding to site $R$

$$\Delta H(R) = -S(R) \cdot \left( \sum_{R \neq R'} J(R - R')S(R') + g\mu_B H \right)$$

It has the form of the energy of a spin in an effective external field:

$$H_{\text{eff}} = H + \frac{1}{g\mu_B} \sum_{R'} J(R - R')S(R')$$  \hspace{1cm} \text{the second term: molecular field (Weiss field)}

The mean field approximation: we replace effective field by its thermal equilibrium mean value.

Use

$$\langle S(R) \rangle = \frac{V}{N} \frac{M}{g\mu_B}$$

$$H_{\text{eff}} = H + \lambda M, \quad \lambda = \frac{V}{N (g\mu_B)^2}, \quad J_0 = \sum_R J(R)$$
The solution of magnetization is given by \[ M = M_0 \left( \frac{H_{\text{eff}}}{T} \right) \]

The spontaneous magnetization is \[ M(T) = M_0 \left( \frac{\lambda M}{T} \right) \]

We can write the above mean field equation as the pair of equations.

\[
\begin{align*}
M(T) &= M_0(x) \\
M(T) &= \frac{T}{\lambda} x
\end{align*}
\]
A nonzero solution implies
\[ \frac{T_c}{\chi} = M'_0(0) \]

The zero-field susceptibility without interaction
\[ \chi_0 = \left( \frac{\partial M_0}{\partial H} \right)_{H=0} = \frac{M'_0(0)}{T} \]
\[ = \frac{N (g \mu_B)^2}{V} \frac{S(S+1)}{3 k_B T} = \frac{C}{T} \]

Curie law

The critical temperature \( T_c \)
\[ T_c = \frac{S(S+1)}{3 k_B} J_0 \]

The susceptibility in the MF approximation
\[ \chi = \frac{\partial M}{\partial H} = \frac{\partial M_0}{\partial H_{\text{eff}}} \frac{\partial H_{\text{eff}}}{\partial H} = \chi_0 (1 + \lambda \chi) \]
\[ \chi = \frac{\chi_0}{1 - \lambda \chi_0} \]

Curie-Weiss law
\[ \chi = \frac{C}{T - \theta} \]

\( \theta > 0 \) FM, \( \theta < 0 \) AFM

\[ C = \frac{N (g \mu_B)^2}{V} \frac{S(S+1)}{3 k_B} \]

Remarks: just reliable at high temperature.
Summary

- The types of magnetic ordering: ferromagnetic, antiferromagnetic ordering.

- Ground state of FM: $|\uparrow\uparrow\uparrow\cdots\uparrow\rangle$.

- Spin wave: Bloch $T^{3/2}$ law for FM, the parabolic and the linear dispersion for FM and AFM spin wave at long wavelengths.

- Mean field theory, and Curie-Weiss law $\chi = \frac{C}{T - \theta}$ (high temperature correction).