Magnetic ordering

- Types of magnetic structure
- Ground state of the Heisenberg ferromagnet and antiferromagnet
- Spin wave
- High temperature susceptibility
- Mean field theory
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.
Critical behaviors

Magnetization

\[ M(T) \sim (T_c - T)^\beta \]

Magnetic susceptibility

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 FM

Ferromagnetic Heisenberg Hamiltonian

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

\[ J(\mathbf{R} - \mathbf{R}') = J(\mathbf{R}' - \mathbf{R}) \geq 0 \]

Construct the ground state of Hamiltonian

\[ |0\rangle = \prod_{\mathbf{R}} |S\rangle_{\mathbf{R}}, \quad S_z(\mathbf{R}) |S\rangle_{\mathbf{R}} = S |S\rangle_{\mathbf{R}} \]

\[ H = -\frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} J(\mathbf{R} - \mathbf{R}') S_z(\mathbf{R}) S_z(\mathbf{R}') - g\mu_B H \sum_{\mathbf{R}} S_z(\mathbf{R}) \]

\[ -\frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} J(\mathbf{R} - \mathbf{R}') S_-(\mathbf{R}') S_+(\mathbf{R}) \]
The energy of ground state

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

where we have used the following relations

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

**Q:** Prove that you cannot find a state with lower energy than the energy of \(|0\rangle\).
Ground state of the Heisenberg AFM

Hamiltonian:

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

Estimation of ground state energy:

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

Only one-dimensional array of spin-half ions with coupling between nearest neighbors can be solved by Bethe ansatz exactly.
Order by symmetry breaking

Spin rotationally invariant Hamiltonian \( H_0 \)

Degenerate ground states

In presence of an external magnetic field

\[
H = H_0 - \hbar S^z_{\vec{q}}, \quad S^z_{\vec{q}} = \sum_i e^{i\vec{q} \cdot \vec{r}_i} S^z_i
\]

Spontaneously symmetry breaking

\[
\lim_{\hbar \to 0^+} \langle S^z_{\vec{q}} \rangle \neq 0
\]

Nambu-Goldstone theorem:

Spontaneously broken continuous symmetry implies the existence of low energy excitations called Goldstone modes which intend to recover the broken symmetry.
Mermin-Wagner theorem

For the quantum Heisenberg model

\[ H = \frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j, \]

with short-range interactions that obey

\[ \frac{1}{2N} \sum_{ij} \left| J_{ij} \right| \left| \vec{r}_i - \vec{r}_j \right|^2 < \infty, \]

there can not be spontaneously broken spin symmetry at finite temperature in one and two dimensions.

Goldstone modes: Spin waves

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

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

The above state differs from the ground state only in that the spin at site \( \mathbf{R} \) has had its z-component reduced from \( S \) to \( S-1 \)

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

To get the above equation, we need the following relations

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

$$S_z (\mathbf{R}') |\mathbf{R}\rangle = S |\mathbf{R}\rangle, \quad \mathbf{R}' \neq \mathbf{R}$$

$$= (S - 1) |\mathbf{R}\rangle, \quad \mathbf{R}' = \mathbf{R}$$
It implies that linear combination of $|\mathbf{R}\rangle$ are eigenstates.

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

We obtain

$$H|k\rangle = E_k |k\rangle$$

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

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

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

When $k \to 0$ we have

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

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

**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.

**AFM**: Spin wave excitation energy of Heisenberg AFM is linear in $k$ at long wavelengths.

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

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

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

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

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

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

Then, the correlation function is given by

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

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

The high temperature susceptibility is

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

with

\[ \theta = \frac{S(S + 1)}{3} \frac{J_0}{k_B}, \quad J_0 = \sum_{\mathbf{R}} J(\mathbf{R}) \]

where \( \theta \) can be positive or negative according to the coupling is ferromagnetic or antiferromagnetic.
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  \hspace{1cm} \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.

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

The zero-field susceptibility without interaction

\[
\chi_0 = \left( \frac{\partial M_0}{\partial H} \right)_{H=0} = \frac{M'_0(0)}{T} = \frac{N (g\mu_B)^2 S(S+1)}{V 3 \frac{k_B T}{k_B}} = \frac{C}{T}
\]

Curie law

The critical temperature \( T_c \)

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

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

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

\[ \theta > 0 \text{ for FM}, \quad \theta < 0 \text{ for AFM} \]

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

Remarks: reliable only at high temperature.
Summary

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

- Ground state of FM \(|↑↑↑↑\cdots↑\rangle\).

- 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 (high temperature correction).

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