Magnetism at finite temperature
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Temperature is an important parameter since exchange energies and ordering temperatures are comparable to room temperature

Curie (Néel) temperature: 1044°K in Fe, 70°K in Eu0, 2292K in Gd, 525°K in NiO (AF)

Exchange: 0.01eV ≈ 100°K
Magnetocrystalline anisotropy: 1mK to 10K
Shape anisotropy: from 1mK to 1K
External field: 1T ≈ 1°K
Outline

- The Heisenberg model in molecular field approximation
- Landau theory of phase transitions
- Beyond mean field:
  - Magnons (spin waves)
  - Ginzburg-Landau theory
  - Critical behavior
  - Role of dimensionality: 1D and 2D systems
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- Role of dimensionality: 1D and 2D systems
Various microscopic mechanisms for exchange interactions in solids:

- Localized / itinerant spin systems
- Short / long range
- Ferro or antiferro

\[ H = - \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

Various types of ordered magnetic structures:

Type of magnetic order depends on the interactions

Also spin glasses, spin liquids... : no long range magnetic order
The various exchange mechanisms can usually be described by an effective exchange Hamiltonian: Heisenberg model

\[ H = - \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

\( J_{ij} \) can be long or short range, positive or negative

\( \vec{S}_i \): classical (vector) or quantum spin

It is an interaction between spins: if the magnetic moment is given by \( J \) instead of \( S \) (\( J=L+S \)), interaction can be rewritten as:

\[ \tilde{H} = - \sum_{ij} I_{ij} \vec{J}_i \cdot \vec{J}_j \]

If \( J = L+S \), and \( L+2S = g_J J \), then, \( S = (g-1)J \) and \( I_{ij} = (g-1)^2 J_{ij} \)

In this lecture: no anisotropy effect

\( K \) coefficients vary with \( T \) as \( M^n \)
What is mean field approximation?

One moment in a magnetic field $H_{\text{ext}}$: $M = M_0 \ g \left( \frac{\mu H}{k_B T} \right)$

Where the function $g$ is
- the Brillouin function (quantum case)
- or the Langevin function (classical spins)

Heisenberg model: $H = - \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$

Main assumption: $\vec{S}_i$ is replaced by its average $\langle \vec{S}_i \rangle$

$H = - \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \Rightarrow H_{\text{MF}} = - \sum_{ij} J_{ij} \left[ \langle \vec{S}_i \rangle \cdot \vec{S}_j + \langle \vec{S}_j \rangle \cdot \vec{S}_i - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle \right]$

(similar to molecular field, or Hartree-Fock approximation)
field acting on $\vec{S}_i$ due to the other spins $\vec{S}_j$:

$$h_i = - \sum_j J_{ij} \langle \vec{S}_j \rangle$$

If there is also an external field:

$$h_i = - \sum_j J_{ij} \langle \vec{S}_j \rangle + \vec{h}_{ext}$$

**Initial problem:** many-body system of interacting spins

**New problem:** collection of spins in static local magnetic field
Mean field approximation

The field created by the neighbors is static; i.e. all thermal and quantum fluctuations are neglected. When fluctuations are small, it is a good approximation.

Fluctuations are large
- at high temperature: near $T_c$ (critical behavior) and above $T_c$ (paramagnetic fluctuations)
- in low dimensional systems (1D, 2D)
- Small spin value (quantum fluctuations): effect of spin waves is more important for small $S$-value

If fluctuations are large, corrections to mean field are important
The molecular field approximation

\[ H = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{S}_i \cdot \mathbf{h}_{ext} \]

Each magnetic moment is in an effective field

\[ \mathbf{h}_{ext} + \sum_j 2J_{ij} \langle \mathbf{S}_j \rangle \]

external field + field created by the neighboring moments

Local magnetization: \[ M_i = g \mu_B \langle \mathbf{S}_i \rangle = M_0 g \left( \frac{\mu H_i}{k_B T} \right) \quad (g \text{ is Brillouin or Langevin function}) \]

Set of coupled equations to determine \( \langle \mathbf{S}_i \rangle \) on each site

In a ferromagnet, it becomes simple since \( \langle \mathbf{S}_i \rangle \) is uniform:

\[ \langle \mathbf{S}_i \rangle = m_F \Rightarrow m_F = m_F g \left( \frac{h_{ext} + \alpha m_F}{k_B T} \right), \alpha = 2 \sum_j J_{ij} \]
New problem: each spin is in a local field that depends on surroundings

\[ h_i = - \sum_j J_{ij} \langle S_j \rangle \]

Hypothesis on the nature of ground state:

Ferromagnetic state: \( \langle S_i \rangle = S, \langle h_i \rangle = h \) (uniform solution)

2 sublattices AF \( \langle S_i \rangle = \pm S, \langle h_i \rangle = \pm h \)

Helimagnets: \( \langle S_i \rangle = \vec{S}_e^{i q R_i}, \langle h_i \rangle = \vec{h}_e^{i (q R_i + \varphi)} \)

Recipe: for each solution, solve the self-consistent equations, calculate \( S \), calculate the corresponding free energy, compare the energy of the various solutions.
The molecular field approximation: ferromagnetic solution

Approximation: $S_j$ is replaced by its average $\langle S_j \rangle = S(T)$

If exchange only between nearest neighbors, $h_{\text{eff}} = h_{\text{ext}} + 2zJS(T)$, \((z=\text{number of nearest neighbors})\)

Simple problem: magnetic moment in a uniform field $h_{\text{eff}}$: \[ S(T) = SB_S \left( \frac{g\mu_B(h_{\text{ext}} + 2zJS(T))}{k_BT} \right) \] selfconsistent equation for $S(T)$ \((B_S: \text{Brillouin function for spin } S)\)

For Antiferromagnet: 2 coupled equations for $S_A$ and $S_B$ (2 sublattices)

(if spins are considered as classical spins: $B_S$ is replaced by Langevin function $L$)
Solution of the mean field equation:  

\[ S(T) = SB_S \left( \frac{g\mu_B(h_{\text{ext}} + 2zJS(T))}{k_BT} \right) \]

**If** \( h_{\text{ext}} = 0 \)

\[ \frac{S(T)}{S} = y \frac{k_BT}{g\mu_B zJS} \]

At \( T > T_c \): \( y = 0 \)

At \( T < T_c \): 1 solution \( y_0 \neq 0 \)

\( T_c \) is obtained when \( y_0 = 0 \)

Calculation of \( T_c \):

near \( y=0 \), \( B_S(y) = y \frac{S(S+1)}{3S} + ... \)

At \( T_c \) \( \frac{S(S+1)}{3S} = \frac{k_BT}{g\mu_B zJS} \)
Ferromagnet: Order parameter and Curie temperature

\[ k_B T_c = \frac{2S(S + 1)}{3} \sum_j J_{ij} = \frac{2S(S + 1)}{3} zJ \quad \text{(If only nearest neighbor interactions \( J \))} \]

Magnetization is calculated selfconsistently

At low \( T \): \( M(T) - M_0 \propto \exp \left( -\frac{2T_c}{T} \right) \)

Near \( T_c \): \( M(T) \propto (T_c - T)^{1/2} \)

Similar calculations for antiferromagnets or ferrimagnets (2 sublattices, 2 selfconsistent parameters \( S_A \) and \( S_B \)); also with longer range interactions
Predictions of mean field theories:

- $T < T_c$: $M(T)$ calculated selfconsistently
  
  $T_c = 2zJ S(S+1)/3k_B$

At low $T$: exponential decrease of $S(T)$
Near $T_c$: $S(T)$ vanishes as $(T_c - T)^{1/2}$ (critical exponent $\beta = 1/2$)

- $T > T_c$ susceptibility: Curie Weiss law

Calculated using

$$M(T) = SB_S \left( \frac{g\mu_B (h_{ext} + 2zJ M(T))}{k_B T} \right)$$

In the paramagnetic state: $M(T) = \chi h_{ext}$. Expansion of the Brillouin function:

Curie-Weiss law: $\chi = C/(T - T_c)$, $C = S(S+1)/3k_B$ (critical exponent $\gamma = 1$)

In general, at $T >> T_c$ $\chi = C/(T - \theta_p)$
with $\theta_p \neq T_c$. 
- Specific heat: partition function for one spin in the effective field $h_{\text{eff}}$

$$Z = e^{-\beta h_{\text{eff}}/2} + e^{+\beta h_{\text{eff}}/2}$$

$$F = -k_B T \ln Z, C_v = -T \frac{\partial^2 F}{\partial T^2}$$

Discontinuity of $C_v$ at $T_c$: critical exponent $\alpha = 0$

- Magnetocaloric effect:

At $T > T_c$: $\delta Q \propto \frac{T T_c}{(T - T_c)^2} \delta H^2$, $\delta T \propto \frac{1}{C_M T_c} \frac{T}{C_M} \delta M^2$

At $T < T_c$: $\delta T \propto \frac{1}{C_M} \delta M^2$
Generalization to describe more complex models: antiferromagnets, ferrimagnets, ….

Crystal field effects

Comparison with experiments: qualitatively correct but:

- **Mean field** $T_c$ generally too large

- Deviations at low $T$: $\frac{M(T)}{M_0} = 1 - AT^{3/2}$ (in a ferromagnet)
  
  $= 1 - AT^2$ (in antiferromagnet)

- Deviations near $T_c$:
  
  $\frac{M(T)}{M_0} = (T_c - T)^\beta$ with $\beta < 0.5$

- Deviations above $T_c$:
  
  $\chi(T) \propto (T - T_c)^\gamma$ with $\gamma > 1$
Mean field magnetization for antiferro, ferrimagnets;...

Several sublattices: A, B, C ..... 

Molecular field on each sublattice created by the neighbors $H_A$, $H_B$....

$H_A: \alpha M_A + \beta M_B + ...$

$M_A = B_A \left( g\mu (H_A + H_{ext}) / kT \right)$, $M_B = B_B \left( g\mu (H_B + H_{ext}) / kT \right)$
Advantages and limitations of mean field approximations

-Simplicity
-Simple calculations of thermodynamic properties
-Various magnetic order: ferro, ferri, AF, helimagnets
-Anisotropy can be taken into account
-1st step to investigate a model.
-Powerful method, can be applied to many problems in physics

But it is necessary to compare various mean field solutions

-At low T: \( M(T) - M_0 \approx \exp(-\Delta/kT) \) instead of \( T^\alpha \) (\( \alpha = 2 \) or \( 3/2 \)): possible corrections if spin waves are included
-Near \( T_c \) : critical exponents are not correct
-Overestimation of \( T_c \)
-Absence of magnetism above \( T_c \) (short range correlations are not included)
-Dimensionality effects are not described: absence of magnetism for \( d=1 \), \( T_c = 0 \) for \( d=2 \) (Heisenberg case)- In MF \( T_c \) is determined by \( z \) only
Estimation of $T_c$

**Mean field:** $k_B T_c = \frac{2zJ S(S+1)}{3k_B}$ for Heisenberg model
$zJ$ for Ising model

Real $T_c$ is always smaller (even 0 for some models)

$T_c$ for the Ising model:

Table 5.2 Exact and approximate Curie temperatures for the Ising model (in units of $zJ/k_B$).

<table>
<thead>
<tr>
<th>lattice</th>
<th>$d$</th>
<th>$z$</th>
<th>mean-field</th>
<th>Oguchi</th>
<th>exact</th>
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<tbody>
<tr>
<td>linear chain</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>0.782</td>
<td>0.000</td>
</tr>
<tr>
<td>square</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>0.944</td>
<td>0.567</td>
</tr>
<tr>
<td>simple cubic</td>
<td>3</td>
<td>6</td>
<td>1</td>
<td>0.974</td>
<td>0.752</td>
</tr>
<tr>
<td>bcc</td>
<td>3</td>
<td>8</td>
<td>1</td>
<td>0.985</td>
<td>0.794</td>
</tr>
<tr>
<td>fcc</td>
<td>3</td>
<td>12</td>
<td>1</td>
<td>0.993</td>
<td>0.816</td>
</tr>
</tbody>
</table>

Mean field is better if $z$ is large!
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Landau expansion for 2\textsuperscript{nd} order phase transition

Free energy near $T_c$ can be expanded in powers of $M$:

$$F(M, h_{ext}, T) = F_0 + \frac{1}{2} a M^2 + \frac{1}{4} b M^4 + \frac{1}{6} c M^6 + \ldots - M h_{ext}$$

- $a$, $b$ and $c$ can be calculated for each model (Heisenberg, Hubbard, etc.)

- They depend on the microscopic parameters: $J_{ij}$, $U$, band structure...

- They depend on temperature

$\Rightarrow$ magnetization, specific heat, susceptibility above $T_c$ can be obtained from $F(M, H, T)$
Different situations depending on the coefficients \((c > 0)\)

\[
F(M, h_{\text{ext}}, T) = F_0 + \frac{1}{2} a M^2 + \frac{1}{4} b M^4 + \frac{1}{6} c M^6 + \ldots - M h_{\text{ext}}
\]

**Magnetization for** \(h_{\text{ext}}=0\) **is determined by:**

\[M(a + b M^2 + c M^4) = 0\]

1) \(a > 0\), and \(b^2 - 4ac < 0\): \(M = 0\)
(no magnetic order)

2) \(a < 0\) (and \(b^2 - 4ac > 0\)): \(M \neq 0\)

\(T_c\) is determined by \(a(T_c) = 0\) \(\Rightarrow a = a_0 (T - T_c)\)

And \(M(T) = (a_0/b)^{1/2} (T_c - T)^{1/2}\)

Above \(T_c\): if \(h_{\text{ext}} \neq 0\), \(h_{\text{ext}} = aM\)

\[\Rightarrow \text{Curie Weiss law: } M/h_{\text{ext}} = 1/a_0 (T - T_c)\]
\[ M(a + bM^2 + cM^4) = 0 \]

\( a > 0 \) and \( b^2 - 4ac > 0 \): \textbf{1st order transition is possible}

\[ T > T_c \]
\[ T < T_2 \]
\[ T = T_1 \]
\[ T < T_c \]

\( T < T_2 \): 2 minima \( M=0 \) and \( M=m \); \( F(m) > F(0) \) \( \rightarrow \) stable minimum for \( M=0 \)

\( T = T_1 \): \( F(m)=F(0) \)

\( T < T_1 \): 2 minima but \( F(m)<F(0) \) \( \rightarrow \) stable solution \( M= m \)

\( T < T_c \): 1 minimum \( m \) (\( a \) changes sign at \( T_c \))

Transition occurs at \( T_1 (> T_c) \) - 2 minima for \( T_c < T < T_1 \)

Hysteresis for \( T_c < T < T_1 \)
1st order transition under magnetic field: metamagnetism

Occurs if $a > 0$ and $b^2 - 4ac > 0$

$$F(M, h_{ext}, T) = F_0 + \frac{1}{2} aM^2 + \frac{1}{4} bM^4 + \frac{1}{6} cM^6 + \cdots - Mh_{ext}$$

This may occur if the Fermi level is located in a minimum of DOS
Thermodynamic properties within Landau theory

\[ F(M, h_{\text{ext}}, T) = F_0 + \frac{1}{2} a M^2 + \frac{1}{4} b M^4 + \frac{1}{6} c M^6 + \cdots - M h_{\text{ext}} \]

If \( a = a_0 (T - T_c) \)

Near \( T_c \): \( M \propto (T - T_c)^{1/2} \) (\( T < T_c \)), \( \chi \propto 1/((T_c - T) (T > T_c)) \)

Specific heat jump at \( T_c \): \( a_0 T_c/b \)

At \( T_c \) \( M \propto h_{\text{ext}}^{1/3} \)

**Critical exponents**

\( \beta = \frac{1}{2}, \gamma = 1, \alpha = 0, \delta = 3 \)

\[ \Rightarrow \text{Mean field exponents} \]

1st order transition: discontinuity of \( M \), susceptibility, specific heat
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Improving the mean field approximation: Ginzburg-Landau theory

In Landau theory $M(T) = 0$ at $T > T_c$

But near $T_c$, large fluctuations of $M$ ($\langle M \rangle = 0$, but $\langle M^2 \rangle \neq 0$)

Ginzburg-Landau theory: takes into account spatial fluctuations of $M$

$M \rightarrow M(r)$

Ginzburg-Landau free energy:

$$F(M, h_{ext}, T) - F_0 = \iiint d^3r \left( \frac{1}{2} a M(r)^2 + \frac{1}{4} b M(r)^4 + \frac{1}{2} g |\nabla M(r)|^2 - M(r) h_{ext} \right)$$

If $M(r) = M_0 + m(r)$ with $m(r) \ll M_0$,

$$\Delta F = \sum_{q \neq 0} \left( gq^2 + a + 3bM_0^2 \right) |m_q|^2$$
Why a \((\nabla M)^2\) contribution?

If variation of \(M(r)\) is « smooth »:

\[ S_i S_j = S^2 \cos(\theta_i - \theta_j) \approx S^2(1 - (\theta_i - \theta_j)^2/2) \]

Contribution to exchange energy:

\[ J(R_i - R_j)S^2 (\theta_i - \theta_j)^2/2 \approx A \left(\frac{\partial \theta}{\partial x}\right)^2 \text{ in the continuum limit} \]

If \(M(r) = M_0 (\cos \theta(x), \sin \theta(x), 0)\) (1D model)

\[ \nabla M = M_0 \frac{\partial \theta}{\partial x} (-\sin \theta(x), \cos \theta(x), 0) \text{ and } \nabla M = M_0^2 \left(\frac{\partial \theta}{\partial x}\right)^2 \]

The \((\nabla M)^2\) is justified if spatial fluctuations are small

Fourier transform:

\[ M(r) = \sum_q M(q)e^{iqr} \Rightarrow \nabla M(r) = \sum_q qM(q)e^{iqr} \]
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Ginzburg-Landau free energy:

$$F(M, h_{ext}, T) - F_0 = \iiint d^3r \left( \frac{1}{2} a M(r)^2 + \frac{1}{4} b M(r)^4 + + \frac{1}{2} g |\nabla M(r)|^2 - M(r) h_{ext} \right)$$

If $M(r) = M_0 + m(r)$ with $m(r) \ll M_0$,

$$\Delta F = \sum_{q \neq 0} \left( g q^2 + a + 3 b M_0^2 \right) |m_q|^2$$
Additional contribution to the free energy

\[ \Delta F = \sum_{q \neq 0} \left( gq^2 + a + 3bM_0^2 \right) |m_q|^2 \]

→ contribution to susceptibility, specific heat ...

\[ \Delta C_v \propto (T-T_c)^{-1/2} \]

Correlation length \( \xi \)

\[ \langle |m_q|^2 \rangle \propto \frac{kT}{q^2 + 1/\xi^2} \]

with \( \xi \propto \sqrt{\frac{gT_c}{T-T_c}} \) (Orstein-Zernike Critical exponent \( v=1/2 \))

in real space: \( \langle m(r).m(r') \rangle \propto \exp\left( -\frac{(r-r')}{\xi} \right) \)

Small \( q \) fluctuations are large

\( q=0 \) fluctuations and correlation length diverge at \( T_c \)

\( \xi \) can be measured with neutrons
Landau Ginzburg: spatial fluctuations (Landau Lifshitz Gilbert: dynamic)

Valid only if: \(1 >> |T - T_c| / T_c >> AT_c^2\) (Ginzburg criterion)

Near \(T_c\): better description of critical behavior.

Description of phase transitions: sophisticated techniques (renormalization group) - Universality of the critical behavior at 2nd order phase transitions

Define the order parameter \(M\)

if \(t = (T - T_c) / T_c\), and \(h = \mu H / kT_c\)

values in M. F. approximation

\[
\begin{align*}
M(T) & \sim t^\beta \quad (h=0) \\
M(h) & \sim h^{1/\delta} \quad (t=0) \\
x(T) & \sim t^{-\gamma} \\
\zeta(T) & \sim t^{-\gamma} \\
C(T) & \sim t^{-\alpha} \\
S(k) & \sim k^{-2+\eta} \quad (t=0)
\end{align*}
\]

\(\beta = 1/2\)  
\(\delta = 3\)  
\(\gamma = 1\)  
\(\alpha = 0\)
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Magnetic transition is an example of phase transitions

-Liquid-solid transition: spontaneous symmetry breaking at $T_c$
-Order parameter (spatial)
-A liquid has more symmetries than a solid: complete translational and rotational invariance
-Para-ferromagnetic transition is similar
Different types of phase transitions:

<table>
<thead>
<tr>
<th>Phenomenon</th>
<th>High $T$ Phase</th>
<th>Low $T$ Phase</th>
<th>Order parameter</th>
<th>Excitations</th>
<th>Rigidity phenomenon</th>
<th>Defects</th>
</tr>
</thead>
<tbody>
<tr>
<td>crystal</td>
<td>liquid</td>
<td>solid</td>
<td>$\rho G$</td>
<td>phenons</td>
<td>rigidity</td>
<td>dislocations, grain boundaries</td>
</tr>
<tr>
<td>ferromagnet</td>
<td>paramagnet</td>
<td>ferromagnet</td>
<td>$M$</td>
<td>magnons</td>
<td>permanent magnetism</td>
<td>domain walls</td>
</tr>
<tr>
<td>antiferromagnet</td>
<td>paramagnet</td>
<td>antiferromagnet</td>
<td>$M$ (on sublattice)</td>
<td>magnons</td>
<td>(rather subtle)</td>
<td>domain walls</td>
</tr>
<tr>
<td>nematic (liquid crystal)</td>
<td>liquid</td>
<td>oriented liquid</td>
<td>$S = \frac{1}{2} (3 \cos^2 \theta - 1)$</td>
<td>director fluctuations</td>
<td>various</td>
<td>disclinations, point defects</td>
</tr>
<tr>
<td>ferroelectric</td>
<td>non-polar crystal</td>
<td>polar crystal</td>
<td>$P$</td>
<td>soft modes</td>
<td>ferroelectric hysteresis</td>
<td>domain walls</td>
</tr>
<tr>
<td>superconductor</td>
<td>normal metal</td>
<td>superconductor</td>
<td>$</td>
<td>\psi</td>
<td>e^{i\phi}$</td>
<td></td>
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</table>
Critical exponents
they depend on
- the model (Heisenberg, X-Y, Ising...)
- the dimensionality of the system

$$M(T) \propto (T_c - T)^\beta, \propto \chi(T) \propto (T - T_c)^{-\gamma}$$

<table>
<thead>
<tr>
<th></th>
<th>D=1</th>
<th>D=2</th>
<th>D=3</th>
<th>Mean field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heisenberg</td>
<td>No ordering</td>
<td>0.36, 1.39</td>
<td>0.36, 1.39</td>
<td>(\beta = 1/2) (\gamma = 1)</td>
</tr>
<tr>
<td>X-Y</td>
<td>No ordering</td>
<td>0.35, 1.32</td>
<td>0.35, 1.32</td>
<td></td>
</tr>
<tr>
<td>Ising</td>
<td>T_c = 0; (\chi \propto \exp(-a/T))</td>
<td>1/8, 7/4</td>
<td>0.32, 1.24</td>
<td></td>
</tr>
</tbody>
</table>

\[\alpha + 2\beta + \gamma = 2; \ D_v = 2 - \alpha\]
**Critical exponents**

They depend on:
- the model (Heisenberg, X-Y, Ising...)
- the dimensionality of the system

\[ M(T) \propto (T_c - T)^\beta, \propto \chi(T) \propto (T - T_c)^{-\nu} \]

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<tr>
<td></td>
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<td>0.36, 1.39</td>
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<tr>
<td>X-Y</td>
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<td></td>
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<td></td>
<td>Kosterlitz-Thouless</td>
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<td></td>
<td>( \chi \propto \exp(a/t^{1/2}) )</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>0.35, 1.32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ising</td>
<td>( T_c = 0 )</td>
<td>1/8, 7/4</td>
<td>0.32, 1.24</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \chi \propto \exp(-a/T) )</td>
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</tr>
</tbody>
</table>

Deviations from mean field indicate short range correlations near \( T_c \)
Comparison with experiments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mean field</th>
<th>Experiment</th>
<th>2D Ising</th>
<th>3D Ising</th>
<th>3D Heisenberg</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi(T) \propto (T - T_C)^{-\gamma}$</td>
<td>1</td>
<td>1.3–1.4</td>
<td>7/4</td>
<td>1.24</td>
<td>1.39</td>
</tr>
<tr>
<td>$M(T) \propto (T_C - T)^\beta$</td>
<td>1/2</td>
<td>$\approx 1/3$</td>
<td>1/8</td>
<td>0.324</td>
<td>0.362</td>
</tr>
<tr>
<td>$C(T) \propto</td>
<td>T - T_c</td>
<td>^{-\alpha}$</td>
<td>0</td>
<td>-0.1–0.1</td>
<td>log</td>
</tr>
<tr>
<td>$M(B, T = T_C) \propto</td>
<td>B</td>
<td>^{1/\delta}$</td>
<td>3</td>
<td>$\approx 5$</td>
<td>15</td>
</tr>
</tbody>
</table>

Critical exponents depend on the dimensionality

Critical exponent $\beta$ in thin Ni films on W:
- at 6 monolayers transition from 2- to 3-dimensional behavior
- crossover from Ising to Heisenberg due to anisotropy

(K. Baberschke)
Outline

- The Heisenberg model in molecular field approximation
- Landau theory of phase transitions
- Beyond mean field:
  - Magnons (spin waves)
  - Ginzburg–Landau theory
  - Critical behavior
  - Role of dimensionality: 1D and 2D systems
Improving mean field at low $T$: spin waves

1 dimensional model with ferromagnetic nearest neighbor exchange

$$H = -2 \sum_i J \vec{S}_i \cdot \vec{S}_{i+1} = -2J \sum_i S_i^z S_{i+1}^z - J \left( \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right)$$

Ground state: $\uparrow\uparrow\uparrow\uparrow\uparrow$ Energy: $-NJ/2$

Excited state with 1 reversed spin $\uparrow\uparrow\downarrow\uparrow\uparrow$ Not an eigenstate of $H$

$\Psi_i$: wave function with spin reversed on site $i$

$$-J \left( \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) \Rightarrow \text{The spin flip will propagate on sites } i-1 \text{ and } i+1$$

$$H\Psi_i = -J(\Psi_{i-1} + \Psi_{i+1}) + (-NJ/2 + J) \Psi_i$$
\[ H \psi_i = -J(\psi_{i-1} + \psi_{i+1}) + (-NJ/2 + J) \psi_i \]

Fourier transform: \( \Psi(q) = \sum \exp(iqR_i) \psi_i \)

\[ H \Psi(q) = -NJ/2 \Psi(q) + J(1-\cos qa) \Psi(q) \]

This is an eigenstate (no longer true for states with more spin flips)

**Excitation energy:** \( E(q) = J(1-\cos qa) \approx Ja^2/2 \; q^2 \)

**Low energy excitations**

\[ \langle \vec{S}_i, \vec{S}_{i+1} \rangle \propto \cos qa \]
« Classical » spin waves

Local field $h_i$ on each site: $h_i = J(m_{i-1} + m_{i+1})$

Moment on site $i$: precession in field $h_i$

$\frac{dm_i}{dt} = -\gamma m_i \times h_i$ (\(\gamma\) gyromagnetic factor)

$\frac{dm_i}{dt} = -\gamma J \, m_i \times (m_{i-1} + m_{i+1})$

1. Fourier transform (time and space) $\Rightarrow \, m_i(t) = m_0 \, e^{i\omega t} \, e^{iqR}$
2. Linearization of $\frac{dm}{dt}$
3. Similar to previous approach $\omega(q) = \gamma J(1-\cos qa)$
Spin waves in antiferromagnets

\[ H = -2 \sum_i J \vec{S}_i \cdot \vec{S}_{i+1} = -2J \sum_i S_i^z S_{i+1}^z - J \left( \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) \]

Not an eigenstate

\[ S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \]

More complicated calculations

\[ E(q) = J | \sin q \alpha | \]
Examples of spin wave spectra (inelastic neutrons)
Magnons: low T properties

In ferromagnets: at low k: \( E(k) \approx zJ M S(ka)^2 = k^2 \)

In antiferromagnets: \( E(k) \approx zJ M ka \)

Magnetization at low T: \( M(T) = M_0 - \text{number of excited magnons} \)

Magnons obey Bose-Einstein statistics

\[
N_{sw} = \sum_k <n_k> = \sum_k \frac{1}{e^{E(k)/T} - 1}
\]

\[
\langle S \rangle \approx S - \sum_k n_B(\omega_k)
\]

\[
\sum_k \rightarrow \int dk^d = \int dk \frac{k^{d-1}}{(2\pi)^d}
\]

At low T, in 3D systems: for a ferromagnet: \( M(T) = M_0 - A(k_BT/D)^{3/2} \)

for AF (sublattice magnetization): \( M(T) = M_0 - B(kT/C)^2 \)

(mean field exp(-A/k_BT))
Estimation of $T_c$ from spin waves:

$$\langle S \rangle \approx S - \sum_k n_B(\omega_k)$$

$T_c$ is determined by, $\langle S \rangle = 0 \rightarrow$ value for $T_c$ smaller by a factor 10 compared to mean field $(2zS(S+1)/3k_B)$

Specific heat: magnons contribute to energy

$$\Delta E = \sum \omega_k n_B(\omega_k) \rightarrow C_v \propto T^2 \text{ (Ferro)} \text{ or } T \text{ (AF)}$$

(mean field: $\exp(-A/k_B T)$)
Spin waves also exist in itinerant ferromagnets:

2 types of excitations:
- Stoner excitations: transition from a filled $\uparrow$ state to an empty $\downarrow$ state: gap $\Delta$ at $q=0$;
- Collective excitations: spin waves

Magnetic excitations in Ni ($\Delta_0 \approx 100\text{meV}$)
Outline

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  - Ginzburg-Landau theory
- Critical behavior
  - Role of dimensionality: 1D and 2D systems
Dimensionality effect

\[ \langle S \rangle \approx S - \sum_k n_B(\omega_k) \sum_k \rightarrow \int dk^d = \int dk \frac{k^{d-1}}{(2\pi)^d} \]

In ferromagnets: \( \omega_k = Dk^2 \)

\[ \int \frac{q^{d-1}}{\exp(Dq^2/k_B T) - 1} \]

becomes (\( x = Dq^2/kT \)):

\[ T^{d/2} \int \frac{x^{d/2-1}}{\exp(x) - 1} dx \]

At \( T \neq 0 \) integral is divergent for \( d=1 \) or \( 2 \)

\( \Rightarrow \text{No ferromagnetism in 1 and 2 dimensions at } T > 0 \)

In AF: \( \omega_k = Ck \) : integral is divergent in 1 dimension
Mermin-Wagner theorem: For Heisenberg model, no long range order in 1 and 2 dimensional systems at T>0

- Magnetism is possible at T=0

- Valid only in the absence of anisotropy

Anisotropy may stabilize ferromagnetism in 2-D systems (surfaces and thin films)

Mermin-Wagner theorem does not apply to Ising or XY models
Heisenberg spins with anisotropy

Uniaxial anisotropy: \(- KS_i^2\)

easy axis: \(K > 0\): spin wave gap at 0°K

\[ \varepsilon(k) = 2S[J(0) - J(q) + K] \]

Variation of magnetic moment at \(T \neq 0\): \(M(T) - M(0) = N_{SW}\)

In 2D; no divergence of NSW: at low \(T\):

\[ N_{SW} \propto T \exp \left( -\frac{A}{T} \right) \]

Easy plane anisotropy: \(K < 0\)

\[ \varepsilon(k) = \sqrt{Dk^2(Dk^2 + 2|K|)} \propto k \]

No spin gap; \(N_{SW}\) is divergent at finite \(T\). Order at \(T=0\)?

Anisotropy may stabilize ferromagnetism in 2-D systems
Ising model in 1D systems (Mermin-Wagner does not apply)

\[ H = -\sum_{i,j} J_{ij} S_i S_j \quad \text{with } S_i = \pm 1 \]

Describes many physical situations: A-B alloy, magnetic system with infinite uniaxial anisotropy, lattice-gas transition ….

Ising chain: \[ H = -\sum_{i=1}^{N-1} J_i S_i S_{i+1} \]

Exactly solvable

\[ Z_N(T) = 2^N \prod_{i=1}^{N-1} \cosh \left( \frac{J_i}{k_B T} \right) \]

No phase transition: \( F = U - TS \)

\( U \) is minimized if all spins are aligned: \[ \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \quad U = NJ, \quad S = 0 \]

1 defect: \[ \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \downarrow \]

Energy cost: \( \Delta U = 2J, \quad \Delta S = k \ln \Omega = k \ln N \quad \Delta F = 2J - kT \ln N \)

if \( T \neq 0 \), defects are always favored by entropy \( \Rightarrow \) no order (in 2D \( T_c \neq 0 \))
Examples of 2D systems:

- Compounds with in-plane interactions >> interplane interactions

examples: La$_2$CuO$_4$……

- Ultrathin films: 2d character if $d < \frac{2\pi}{k_F}$ 0.2 – 2 nm
  - $d<$exchange length: depends on the nature of exchange: 0.2 – 10 nm

- Surfaces of bulk materials

- Superlattices F/NM: interlayer interactions
Some low dimensional systems

A

B

cuprates

Li$_2$VO(Si,Ge)O$_4$

KCuF$_3$

(1D)

K$_2$CuF$_4$

(2D)
Reduction of Curie temperature

\[ T_c \text{ for Co thin films} \]

In 2D:
- no order if no anisotropy
- with anisotropy: reduced \( T_c \) (reduction of nb of nearest neighbors)

Magnetization of Ni films

\[ M(T) \text{ for different thickness (theory)} \]
From 3D to 2D behavior:

- In 3D systems correlation length diverges at $T_c$: 
  \[ \xi = \xi_0 \left| \frac{T - T_c}{T_c} \right|^{-\nu} \]

- Crossover from 2D to 3D when the thickness $d \approx \xi$

- Asymptotic form for $T_c$:
  \[ \frac{T_c(\infty) - T_c(d)}{T_c(d)} = \left( \frac{d}{\xi_0} \right)^{-\frac{1}{\nu}} \]

(Heisenberg: $\nu = 0.7$ Ising: 0.6)

Experimentally: $\nu \approx 0.7$
Close to Heisenberg

(Gradmann, 1993)
Summary

-Mean field approximation is easy to handle. Allows to compare easily different types of orderings

-In many cases (3D systems) is gives the correct qualitative ground state

-Temperature variation:
  - at low $T$: spin waves
  - $T_c$ too large, critical exponents not correct (short range fluctuations)

-Mean field wrong in low dimension systems
Some general reference books
S. Blundell: Magnetism in Condensed Matter (Oxford University Press, 2001)
J.M.D. Coey: Magnetism and Magnetic materials (Cambridge University Press 2009)
R. Skomski: Simple models of Magnetism (Oxford University Press, 2008)

More advanced books
N. Majilis: The quantum theory of magnetism (World scientific 2007) (in particular Molecular field approximation, magnons
P. Mohn: Magnetism in the solid state (Springer, 2006) (most devoted to itinerant magnetism; see also J. Kübler in 'Handbook of Magnetism and Magnetic materials', vol1 )