Magnetism at finite temperature: molecular field, phase transitions

- The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  - critical exponents
  - spin waves
  - Dimensionality effects: absence of phase transition in 1D and 2D models
Magnetism at finite temperature: molecular field, phase transitions

- The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  critical exponents
  spin waves
  Dimensionality effects: absence of phase transition in 1D and 2D models
What is mean field approximation?

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

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 $\langle \vec{S}_i \rangle$

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \Rightarrow \vec{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \langle \vec{S}_j \rangle$$

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

$$\vec{H}_i = \sum_j J_{ij} \langle \vec{S}_j \rangle$$

If there is also an external field:

$$\vec{H}_i = \sum_j J_{ij} \langle \vec{S}_j \rangle + \vec{H}_{ext}$$
\[ M = M_0 \, g\left(\frac{\mu H}{kT}\right) \quad \Rightarrow \quad M_i = M_0 \, g\left(\frac{\mu H_i}{kT}\right) \]

\[ \bar{H}_i = \sum_j J_{ij} \, \langle \vec{S}_j \rangle + \bar{H}_{ext} \]

\( H_i \) is a local field due to
- the interaction with neighboring spins (« molecular field »)
- the external field

In a ferromagnet: \( \langle \vec{S}_j \rangle \) is constant: \( \langle \vec{S}_j \rangle = \frac{M}{g\mu_B} \)

\( \Rightarrow \) molecular field is the same on all sites:
\[ \bar{H}_{ferro} = \bar{M} \sum_j J_{ij} + \bar{H}_{ext} \]
Solution of the mean field equation:

\[ M_i = M_0 \, g\left(\frac{\mu H_i}{kT}\right) \]

In a ferromagnet:

\[ M_i = M_0 = g\left(\frac{\mu (H + zJM_0)}{kT}\right) \]

\((g(x)\) is the Brillouin or Langevin function)
Ferromagnet: Order parameter and Curie temperature

If only nearest neighbor interactions $J$

$$k_B T_c = \frac{2S(S + 1)}{3} \sum_j J_{ij} = \frac{2S(S + 1)}{3} zJ$$

If only nearest neighbor interactions $J$

Magnetization is calculated selfconsistently

At low $T$: $M(T) - M_0 \propto \exp(-2T_c/T)$
Near $T_c$: $M(T) \propto (T_c - T)^{1/2}$

Similar calculations for antiferromagnets, or longer range interactions
Thermodynamics of a ferromagnet in mean field approximation

- Calculate the partition function $Z$ of the system: one spin in an effective field $H_{\text{eff}}$ ($H_{\text{eff}} = H_{\text{ext}} + zJM_0$)

For $S = \frac{1}{2}$:

\[ E_\downarrow = +g\mu_B H_{\text{eff}}/2 \]
\[ E_\uparrow = -g\mu_B H_{\text{eff}}/2 \]

\[ Z = e^{-E_\uparrow/kT} + e^{-E_\downarrow/kT} \]

-Free energy: $F = -kT \ln Z$

⇒ Susceptibility $\chi = -\frac{\partial^2 F}{\partial H^2}$

\[ \chi = \frac{C}{T-T_c}, C = \frac{(g\mu_B)^2}{3k} S(S+1) \]

⇒ Curie –Weiss law above $T_c$:

⇒ Specific heat: $C_v = -T \frac{\partial^2 F}{\partial T^2}$

⇒ Discontinuity at $T_c$: $\Delta C_v = 3k_B/2$
Same calculation can be done for an antiferromagnet with 2 sublattices: \( H_i \) is site-dependent (\( H_A \) and \( H_B \))

Also ferrimagnetism, helicoidal order, commensurate and incommensurate orderings…

Free energy and thermodynamics: \( F = \) free energy of a moment in an effective field

\[
\overline{H}_i = \sum_j J_{ij} \langle \hat{S}_j \rangle + \overline{H}_{ext}
\]
General case: - interactions $J_{ij}$ between 1st, 2nd, 3rd ....
- Any kind of Bravais lattice (1 magnetic site per unit cell)

Energy:  
$$E = - \sum_{i,j} J(R_i - R_j) \langle \vec{S}_i \cdot \vec{S}_j \rangle$$

In mean field approximation:  
$$E = - \sum_{i,j} J(R_i - R_j) \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle$$

Fourier transforms:  
$$J(q) = \frac{1}{N} \sum_{i,j} e^{iq(R_i - R_j)} J(R_i - R_j)$$

$$\vec{S}(q) = \frac{1}{N} \sum_i \langle \vec{S}_i \rangle e^{iqR_i}$$

$$E = - \sum_q J(q) S(q) \cdot S(-q)$$

Energy is minimum at $q_0$ for which $J(q)$ is maximum
The phase diagram for the 1D chain:

\[ J(q) = -J_1 \cos qa - J_2 \cos 2qa \]

Extrema of \( J(q) \):
- \( q = 0 \) (ferro)
- \( q = \pi/a \) (antiferro)
- \( \cos qa = -J_1/4J_2 \) (if \( |J_1/4J_2| \leq 1 \))

-The helimagnetic state is stabilized in the frustrated region \((J_2 < 0)\)

-It is in general incommensurate with the lattice periodicity
Example: multiferroics $\text{RMn}_2\text{O}_5$

4 commensurate structures

IC: incommensurate orderings
Magnetism at finite temperature: molecular field, phase transitions

-The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  critical exponents
  spin waves
  Dimensionality effects: absence of phase transition in 1D and 2D models
Itinerant magnetic systems

In 3d: overlap of 3d wave functions of nearest neighbors atoms: metallic systems

⇒ Competition between magnetic and kinetic energy: itinerant magnetism

Itinerant spin systems: magnetic moment is due to electrons in partially filled bands (3d band of transition metals)
Magnetism of 3d metals: due to itinerant 3d electrons

Band structure of Ni

\[ \sum_{k\sigma} \varepsilon_k n_{k\sigma} + Un_{i\downarrow}n_{i\downarrow} \] (\(+\) longer range interactions)
One band: degeneracy of the 3d band neglected

Coulomb repulsion: electrostatic interactions between electrons \( V(r) = -\frac{e^2}{r} \)

In solids this interaction is screened by the other charges:

\[
V(r) = -\frac{e^2 \exp(-qr)}{r}
\]

In metals \( 1/q \) is very small (\(<\) interatomic distance). \(\Rightarrow\) Only short range interactions are important

Local Coulomb repulsion: \( U n_{i\uparrow} n_{i\downarrow} \)

Hubbard model:

\[
H = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]

\(\Rightarrow\) from Pauli paramagnet to itinerant magnet and localized magnetic systems with increasing \( U \)
Mean field approximation on the term $U n_{i\downarrow} n_{i\downarrow}$:

$$U n_{i\uparrow} n_{i\downarrow} = U/4(n_{i\uparrow} + n_{i\downarrow})^2 - U/4(n_{i\uparrow} - n_{i\downarrow})^2$$

1st term: $\frac{U}{4} (n_{i\uparrow} + n_{i\downarrow})^2 = \frac{U}{4} n_i^2$  
Charge fluctuations are small  
⇒ constant potential

2nd term: $-\frac{U}{4} (n_{i\uparrow} - n_{i\downarrow})^2 = -US_{iz}^2$

Mean field approximation on the 2nd term:

$$-US_{iz}^2 \approx -2US_{iz} <S_{iz}> + U\langle S_{iz}\rangle^2 \text{ where } S_{iz} = (n_{i\uparrow} - n_{i\downarrow})/2$$

This 2nd term induces a spin-dependent potential on each site:

$$V_{i\sigma} = -\sigma U/2\langle n_{i\uparrow} - n_{i\downarrow}\rangle$$
Itinerant ferromagnetism: Stoner model at T=0

Description of 3d metals: narrow band + Coulomb interactions

Local Coulomb repulsion: \( U n_{i\uparrow}n_{i\downarrow} \)

\( U \) favors magnetic state

Hartree-Fock approximation:

\[
H = \sum_{k,\sigma} (\varepsilon_k + V_\sigma) n_{k,\sigma}
\]

with:

\[
V_{i\sigma} = -\sigma U / 2 \langle n_{i\uparrow} - n_{i\downarrow} \rangle
\]

\[
E_M = U n_{\uparrow} n_{\downarrow} = U \left( \frac{N}{2} + \rho(\varepsilon_F) \delta \varepsilon \right) \left( \frac{N}{2} - \rho(\varepsilon_F) \delta \varepsilon \right)
\]

\[
= U \frac{N^2}{4} - U \left( \rho(\varepsilon_F) \delta \varepsilon \right)^2
\]

\[
\Delta E_c = \rho(\varepsilon_F) (\delta \varepsilon)^2
\]
Total energy variation:

$$\Delta E_t = \Delta E_M + \Delta E_c = \rho(\varepsilon_F) \delta \varepsilon^2 (1 - U \rho(\varepsilon_F))$$

⇒ Stoner criterion:

- If $1 - U \rho(\varepsilon_F) < 0$: magnetic state is stable (ferromagnetism)
- If $1 - U \rho(\varepsilon_F) > 0$: paramagnetic state

Magnetic moments are non-integer

For pure transition metals:
- Fe $\rightarrow m_0 \approx 2.2 \ \mu_B / \text{atom}$
- Co $\rightarrow m_0 \approx 1.8 \ \mu_B / \text{atom}$
- Ni $\rightarrow m_0 \approx 0.64 \ \mu_B / \text{atom}$
Weak vs strong ferromagnets

W.F: both spin directions at $E_F$ (Fe)

SF: only 1 spin directions at $E_F$
Gap in the spin flip excitations
(Co and Ni)
Itinerant systems: Stoner theory at finite temperature:

Order of magnitudes for $T_c$:
- Fe: 1040 (Stoner: 4400-6000)
- Co: 1400 (Stoner: 3300-4800)
- Ni: 630 (Stoner: 1700-2900)

More on Hubbard model and itinerant magnetism: next talk! (M. Lavagna)
There are few exact results for the Hubbard model:

\[ H = \sum_{k,\sigma} \varepsilon_k \, n_{k,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Stoner criterion for ferromagnetism: \( 1 - U \rho(\varepsilon_F) < 0 \) ?

- \( U \) cannot be too large (screening effects)
- But almost all these exact results do not give a ferromagnetic ground state, even for large \( U \) (see also the arguments given by T. Dietl)

Orbital degeneracy (Hund’s coupling) and s-d interactions are very important for stabilizing ferromagnetism
Why is mean field not good for large U?

If the number of electrons is small: uniform potential on all sites

\[ V_{i\sigma} = -\sigma U/2\langle n_{i\uparrow} - n_{i\downarrow} \rangle \]

and the electrons density is the same on all sites.

However it could be more favorable to « maintain » the electrons far from each other, so that they almost not interact. This is not described by mean field.

In mean field: small moments everywhere

Large U: large moments, well separated
Magnetism at finite temperature: molecular field, phase transitions

- The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  - critical exponents
  - spin waves
  Dimensionality effects: absence of phase transition in 1D and 2D models
Landau expansion for 2nd order phase transition

Free energy near Tc can be expanded in powers of M:

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

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

- They depend on the microscopic parameters: \( J_{ij} \) or \( U \) and band structure

- They depend on temperature

\( \Rightarrow \) magnetization, specific heat, susceptibility above \( T_c \) can be obtained from \( F(M,H,T) \)
Different situations as a function of the sign of coefficients (c > 0)

Magnetization is determined by: \( aM + bM^3 + cM^5 = H \)

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

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

Usually \( T_c \) 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 \( T_c \): \( M/H = 1/a = 1/a_0 (T-T_c) \) \( \Rightarrow \) Curie Weiss law

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

This may occur if the Fermi level is located in a minimum of DOS
- 1st order transition at $T_c$: discontinuity of $M(T)$

- Expansion of $F$ in powers of $M$ is not justified if $\Delta M$ is large

- No critical phenomena
1st order transition under magnetic field: **metamagnetism**

Occurs if \( a > 0 \) and \( b^2 - 4ac > 0 \)
Advantages and limitations of mean field approximations

- Simplicity (localized and itinerant systems)
- Simple calculations of thermodynamic properties
- Physical origin of the magnetic order
- 1st step to investigate a model.
- Extension to antiferromagnetism, itinerant models, …..

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 not described: absence of magnetism for $d=1$, $T_c = 0$
  for $d=2$ (Heisenberg case)
- Size effect: MF predicts magnetic order in finite systems
Estimation of $T_C$

**Mean field:** $k_B T_C = zJ$

Real $T_C$ is always smaller (event 0 for some models)

**$T_C$ for the Ising model:**

<table>
<thead>
<tr>
<th>lattice</th>
<th>$d$</th>
<th>$z$</th>
<th>mean-field</th>
<th>Oguchi</th>
<th>exact</th>
</tr>
</thead>
<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!
Magnetism at finite temperature: molecular field, phase transitions

- The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  critical exponents
  spin waves
  Dimensionality effects: absence of phase transition in 1D and 2D models
Improving the mean field approximation

- Phenomenological fit of Landau expansion
- Low T: spin waves
- Spin fluctuations theories
- Description of critical phenomena

Mean field results can be tested with

- numerical results (Monte Carlo),
- or expansions…
- exact results in a few cases
Improving the mean field approximation

- Phenomenological fit of Landau expansion

- Low T: spin waves

- Spin fluctuations theories

- Description of critical phenomena

- Short range correlations

Mean field results can be tested with

- numerical results (Monte Carlo),
- or expansions…
- exact results in a few cases
At low temperature: thermal variation is dominated by spin waves

Collective excitations of magnetic moments:

Ground state:

Spin wave: linear combination of:

This is not an eigenstate: $S^+_i S^-_j$ induces correlated spin flips

Energy of spin waves: $E(k) = \hbar \omega(k) = 2S(I(0) - I(k))$

$$I(k) = \sum_{ij} I(r_i - r_j) e^{ik(r_i - r_j)}$$

Spin waves excitations: low energy cost
At low $k$: $E(k) \approx 2zJ \left(1 - \frac{(ka)^2}{2}\right)$

In antiferromagnets: spin wave energies $E(k) \propto \sin(ka)$

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

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

$\Rightarrow$ in a ferromagnet: magnetization $M(T)/M_0 = 1 - AT^{3/2}$

in antiferromagnet: $1 - AT^2$

If gap in the spin wave spectrum (i.e. anisotropy), behavior is different: $\exp(-\Delta/T)$
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 $\Delta_0$ at $q=0$; continuum at $q \neq 0$
- Collective excitations: spin waves

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

Spin waves: talk by W. Wulfheckel on Monday 7th
Improving the mean field approximation

- Phenomenological fit of Landau expansion
- Low T: spin waves
- Spin fluctuations theories
- Description of critical phenomena

Mean field results can be tested with

- numerical results (Monte Carlo),
- or expansions…
- exact results in a few cases
Spatial spin fluctuations in Landau–Ginzburg model

Near $T_c$: large fluctuations of $M$.

$$F = \int dr \left[ \frac{1}{2} a M(r)^2 + \frac{g}{2} \left( \nabla M(r) \right)^2 - M(r) \cdot H_{\text{ext}} \right]$$

$$M(r) = M_0 + m(r)$$

Small fluctuations can be included in the free energy:

$$\langle |m(q)|^2 \rangle \sim k_B T / \left( g q^2 + a + 3bM_0^2 \right)$$

Fluctuations of small $q$ are large

Above $T_c$: $M_0 = 0$; characteristic length $\zeta \sim q^{-1} \sim (g/a)^{1/2} \sim (T_c - T)^{-1/2}$

$$\langle |m(q)|^2 \rangle \sim k_B T / (q/\zeta)^2 + 1$$

Characteristic length diverges at $T_c$: critical fluctuations
Why a \((\nabla M(r))^2\) contribution?

If variations 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:

\[ J(R_i - R_j)S^2/2 \ (\theta_i - \theta_j)^2 \approx A (d\theta/dr)^2 \text{ in the continuum limit} \]

If \(S_i = S(\cos\theta_i, \sin\theta_i, 0)\), then

\[ (\nabla M(r))^2 = S^2 \left(\frac{d\theta}{dr}\right)^2 \]

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

Fourier transform:

\[ M(r) = \sum_q M(q)e^{iqr} \Rightarrow \nabla M(r) = \sum_q qM(q)e^{iqr} \]

\[ |\nabla M(r)|^2 = \sum_{q,q'} qq' M(q)M^*(q')e^{i(q-q')r} \]

Integration over \(r\): only \(q=q'\)
Correlation length can be observed with neutron scattering:

\[ \chi(q) \sim \frac{<|m(q)|^2>}{kT} \] through the fluctuation-dissipation theorem

\[ <|m(q)|^2> \sim k_B T/(q/\zeta)^2 + 1 \]

Above \( T_c \): width of \( \chi(q) \) is \( \approx \zeta^{-1} \) ⇒ measure of the correlation length \( \zeta \) : direct access to \( \zeta(T) \)
Validity of Landau Ginzburg expansion

\[ F = \int dr \left( \frac{1}{2} a M(r)^2 + \frac{g}{2} (\nabla M(r))^2 - M(r) \cdot H_{\text{ext}} \right) \]

The \( \frac{1}{4} b M^4 \) is neglected. This is valid as long as

\[ \frac{1}{2} a M^2 \gg \frac{1}{4} b M^4 \]

If \( \langle |m(q)|^2 \rangle \sim k_B T / (gq^2 + a + 3bM_0^2) \), \( M^2 = \sum_q \langle |m(q)|^2 \rangle \)

This leads to the Landau- Ginzburg criterion for the validity of Landau expansion:

\[ \frac{b^2 (kT_c)^2}{2a_0 g^3} \ll \left| \frac{T - T_c}{T_c} \right| \ll 1 \]

If \( T_c \) is small, Landau expansion is not valid. Quantum fluctuations become more important than thermal fluctuations

\( \Rightarrow \) Quantum critical point (QCP)
Improving the mean field approximation

- Phenomenological fit of Landau expansion
- Low T: spin waves
- Spin fluctuations theories
- Description of critical phenomena

Mean field results can be tested with

- numerical results (Monte Carlo),
- or expansions…
- exact results in a few cases
Some generalities on phase transitions and critical phenomena

-Liquid-solid transition: spontaneous symmetry breaking at $T_c$
-Order parameter (spatial)
-A liquid has more symmetries as 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>phonons</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>$S = \langle \frac{1}{2} (3 \cos^2 \theta - 1) \rangle$</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>
</tr>
</tbody>
</table>
2nd order phase transitions:

- Order parameter below \( T_c \)
- divergence of some thermodynamics quantities

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

values in M. F. approximation

\[
\begin{align*}
M(T) & \sim t^\beta \quad (h=0) & \beta = 1/2 \\
M(h) & \sim h^{1/\delta} \quad (t=0) & \delta = 3 \\
\chi(T) & \sim t^{-\gamma} & \gamma = 1 \\
\zeta(T) & \sim t^{-\nu} & \nu = 1/2 \\
C(T) & \sim t^{-\alpha} & \alpha = 0 \\
S(k) & \sim k^{-2+\eta} \quad (t=0)
\end{align*}
\]
**Critical exponents**

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

\[ M(T) \propto (T_c - T)^\beta \quad \chi(T) \propto (T - T_c)^{-\gamma} \]

<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></td>
<td></td>
<td>( \beta = 0.36 )</td>
<td>( \gamma = 1.39 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( \gamma = \infty )</td>
<td>( \beta = 0.35 )</td>
</tr>
<tr>
<td>X-Y</td>
<td></td>
<td>( \gamma = \infty )</td>
<td>( \beta = 0.35 )</td>
<td>( \gamma = 1/2 )</td>
</tr>
<tr>
<td></td>
<td>( T_c = 0 )</td>
<td>( \beta = 1/8 )</td>
<td>( \beta = 0.32 )</td>
<td>( \gamma = 1 )</td>
</tr>
<tr>
<td>Ising</td>
<td>( \chi \sim \exp(-2J/T) )</td>
<td>( \gamma = 7/4 )</td>
<td>( \gamma = 1.24 )</td>
<td></td>
</tr>
</tbody>
</table>

Several relations between the critical exponents:

\( \alpha + 2 \beta + \gamma = 2 \), \( \gamma = \beta(\delta - 1) \)
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

(K. Baberschke)
Magnetism at finite temperature: molecular field, phase transitions

- The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  critical exponents
  spin waves

  Dimensionality effects: absence of phase transition in 1D and 2D models
Phase transitions and low dimensionality

\[
\begin{align*}
\text{Sr}_2\text{CuO}_3 & \quad \text{SrCuO}_2 \\
\text{Li}_2\text{VO(Si,Ge)O}_4 & \quad \text{NaV}_2\text{O}_5
\end{align*}
\]
Magnetic properties of 1-dimensional and 2-dimensional spin systems (⇒ workshop Tuesday 8th)

- Models calculations

- Heisenberg spins: no magnetic order in 1D and 2D and T > 0 (Mermin-Wagner theorem)

Spin waves argument:

Magnetization at T ≠ 0: \( M(T) = M(0) - N_{SW} \), with \( N_{SW} \) = number of excited spin waves

\[
N_{SW} \propto \int \frac{k^{d-1}}{\exp(\varepsilon/T) - 1} dk
\]

If \( \varepsilon(k) = ck^2 \): integral is divergent for d=1 and d=2 (for d=3: \( T^{3/2} \))

No long range magnetic ordering for Heisenberg spins with short range interactions in 1-D and 2-D at T>0
Qualitative argument for the absence of ordering in 1D and 2D

Fluctuations in Landau theory:

\[ M(r)^2 = (M_0 + m(r))^2 \]

\[ \Rightarrow < M(r)^2 > = M_0^2 + < m(r)^2 > \]

\[ = - \frac{a(T)}{b} + \sum_q < |m(q)|^2 > \]

\[ = \frac{a(T)}{b} + A \sum_q \frac{kT}{\Gamma q^2 + a(T) + 3bM_0^2} \]

In 1D and 2D the integral is divergent near \( T_C \): fluctuations become larger than \( M_0 \). No long range magnetic ordering at \( T \neq 0 \)

(Mermin-Wagner theorem)
Heisenberg spins with anisotropy

Uniaxial anisotropy: \(-K S_i z^2\)

**easy axis: \(K > 0\):** spin wave gap \(\propto K\)

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

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 → surfaces and thin films
Examples of 2D systems:

- Compounds with in-plane interactions >> interplane interactions
  examples: $\text{La}_2\text{CuO}_4$….

- 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
Reduction of Curie temperature

In 2D: 
- no order if no anisotropy (spin waves divergence)
- with anisotropy: reduced $T_c$ (reduction of nb of nearest neighbors $T_c \propto zJS(S+1)$ + spin wave effects)
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

- Problems for low dimension systems