Lecture 7
“Magnetic excitations”

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LECTURE 7:  
“Magnetic excitations”

- Phase transitions and the Landau mean-field theory.
- Heisenberg and Ising models.
- Magnetic excitations.
External parameter, as for example the temperature, can drive a **symmetry-breaking transition**, in which a symmetry element of the system is lost.

**Broken rotational and translational symmetry**
The liquid phase is invariant under any arbitrary translation and rotation.
The ordered phase have only a reduced set of symmetry operations

**Broken the full rotational symmetry**
The paramagnetic state possesses complete rotational symmetry.
The ferromagnetic state have a reduced rotational symmetry about the magnetization axis

The ordered phase possesses a lower symmetry with respect to the disordered phase!
Symmetry group:
Collection of elements and a set of operations that combines them:
closure, associativity, existence of an inverse and the identity

A physical system possesses a particular symmetry if the Hamiltonian is invariant with respect to the transformations associated with the element of symmetry group.

Discrete symmetry groups: symmetry group with countable elements
(Ex.: point groups, lattice groups, space groups)

Continuous symmetry groups: uncountable continuum of elements
(Ex.: rotational symmetry group of a sphere O(3), Lie groups)

Global symmetry: the system is invariant under the symmetry elements of the group applied globally to the entire system.

Local symmetry: Hamiltonian is unchanged when the symmetry operations are applied differently to different point in the space.
- Phase transitions occur when an internal symmetry is broken by an external force.
- Consequences of broken symmetry are:

PHASE TRANSITION
sharp change in behaviour at the critical temperature and the region near the PT is called critical region

RIGIDITY or STIFFNESS
resistance of the system against any attempt to change its state

DEFECTS
Symmetry broken differently in two adjacent part of the system (grain boundary or magnetic domain wall)

EXCITATIONS
At \( T \neq 0 \) the dynamic excitations of the order parameter tend to remove or to weakens the ordered state
- **Magnetic phases**: Phase transitions occur between different magnetic phases as a function of the thermodinamical parameters: Pressure, Magnetic field, Temperature

- **Stability of a magnetic structure**: $k_B T \ll J_{ij}$ (exchange constant)

- **Phase Transitions**: from a long-range magnetic ordered state (low $T$) to a paramagnetic state (high $T$)

- **Critical temperature**: $T_C = \text{Curie temperature (ferromagnets)}$  
  $T_N = \text{Néel temperature (antiferromagnets)}$

- **Critical fluctuations**: the magnetic moments fluctuate in space and time

Free energy: $F = E - TS$

Energy (Low $T$)  
Entropy (High $T$)
The order parameter $\eta$ saturate at low temperature and vanishes above the critical temperature $T_c$.

- The order parameter can vanishes continuously (second order transition) or discontinuously (first order transition).

The free energy $F(T, \eta)$ of a $2^{nd}$ order magnetic phase transition can be expanded near $T_c$ as:

$$F(T, \eta) = F_0(T) + \alpha_2(T)\eta^2 + \alpha_4(T)\eta^4 + \ldots$$

where the order parameter $\eta=0$ for $T>T_c$

The thermal equilibrium condition at any $T<T_c$ require that $F(T, \eta)$ have a minimum:

$$\frac{\partial F}{\partial \eta} \bigg|_T = 0 \quad \text{and} \quad \frac{\partial^2 F}{\partial^2 \eta} \bigg|_T > 0$$
Order parameter: Magnetization $\eta = M$

$$F(T, M) = F_0 + a(T)M^2 + bM^4 + \ldots$$

$$a(T) = a_0(T - T_C)$$

$b > 0$

Notice that odd power terms are null because:

$$F(M) = F(-M)$$

Condition for thermal stability:

$$\frac{\partial F(M)}{\partial M} = 2M \left[ a_0(T - T_C) + 2nM^2 \right] = 0$$

Solutions:

$$M = 0$$ and

$$M = \pm \left[ \frac{a_0(T - T_C)}{2b} \right]^{1/2}$$

$T > T_C$  Valid only if $T < T_C$

Mean-field Magnetization

$$M \propto |T_C - T|^{\beta} \quad \beta = \frac{1}{2}$$
In the presence of a magnetic field $H$

$$F(M, H) = F(M) - \mu_0 MH$$  \hspace{1cm} \mu_0 = 1$$

**Condition for stability:**

$$\frac{\partial F(M, H)}{\partial M} = \frac{\partial F(M)}{\partial M} - H = 0$$

$$\frac{\partial^2 F(M, H)}{\partial M^2} = \frac{\partial H}{\partial M} > 0$$

Magnetic susceptibility

$$\chi = \frac{\partial M}{\partial H} = \left(\frac{\partial^2 F(M, H)}{\partial M^2}\right)^{-1}$$

$$2M[a_0(T - T_C + 2bM^2)] = H$$

$$T = T_C \rightarrow M \propto H^{1/\delta} \hspace{1cm} \delta = 3$$

**Mean-field Susceptibility**

$$\chi = \begin{cases} 
\frac{1}{2a_0(T - T_C)} & T > T_C \\
\frac{1}{4a_0(T - T_C)} & T < T_C 
\end{cases}$$

$$\chi \propto |T - T_C|^{-\gamma} \hspace{1cm} \gamma = 1$$
Mean field theories fail in describing the systems near $T_c$ because they ignore correlations and fluctuations.

Independently of the precise nature of the interactions considered, near $T_c$ the phase transitions show an **Universal behaviour**.

\[ \tau = \frac{T - T_c}{T_c} \]

**Reduced temperature**

- specific heat $c_H \propto \tau^{-\alpha}$
- magnetic moment $m \propto (-\tau)^\beta$
- susceptibility $\chi \propto \tau^{-\gamma}$
- correlation length $\xi \propto \tau^{-\nu}$
The microscopic models of magnetic interactions are classified in terms of:
- Dimensionality of the order parameter \( D \)
- Space dimensionality \( d \)

\( D (=1, 2, 3) \) depends on the number of components of \( S_x \), \( S_y \), and \( S_z \) of the spin operator \( S \).

**Heisenberg model: \( D=3 \)**
Spins are 3D vectors
The lattice dimensionality \( d=1, 2, 3 \ldots \)

\[
\hat{H}_{\text{Heisenberg}} = - \sum_{\langle ij \rangle} J S_i \cdot S_j
\]

**Ising model: \( D=1 \)**
Spins are 1D vectors \( (S=S_z) \)
The lattice dimensionality can be \( d=1, 2, 3 \ldots \)

\[
\hat{H}_{\text{Ising}} = - \sum_{\langle ij \rangle} J S_i^z S_j^z
\]
The universality classes are defined in terms of:
- Order parameter dimensionality $D$
- System dimensionality $d$
- Short or long range interaction (e.g., covalent or metallic bonding)

*Within a given universality class the value of the critical exponents are the same and do not depend on the detailed nature of the system.*

<table>
<thead>
<tr>
<th>Model</th>
<th>Mean-field</th>
<th>Ising</th>
<th>Ising</th>
<th>Heisenberg</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>any</td>
<td>1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>$d$</td>
<td>any</td>
<td>2</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Specific heat</td>
<td>$\alpha$</td>
<td>0</td>
<td>0.106</td>
<td>-0.121</td>
</tr>
<tr>
<td>Magnetization</td>
<td>$\beta$</td>
<td>1/8</td>
<td>0.326</td>
<td>0.367</td>
</tr>
<tr>
<td>Susceptibility</td>
<td>$\gamma$</td>
<td>7/4</td>
<td>1.2378(6)</td>
<td>1.388(3)</td>
</tr>
<tr>
<td>Correlation length</td>
<td>$\nu$</td>
<td>1</td>
<td>0.636</td>
<td>0.707</td>
</tr>
</tbody>
</table>
1-D lattice of $N+1$ atoms
-All spin ferromagnetically aligned

Ground state energy:
$$E_0 = -N \frac{J}{2}$$

Energy cost to flip the chain:
$$E = J$$
+J/2 because is already in favourable state
+J/2 because cost energy in the new state

Entropy gain: $S = k_B \ln N$
because we can put the defect in any position

For a long chain: $N \to \infty$, $S \to \infty$, $F \to -\infty$
and as far as $T>0$, the long range order is never reached because just the presence of one defect break the long range order in $d=1$
- Phonons and magnons are quasi-particle associated to the lattice and spin excitations
- They are characterized by a frequency $\omega$ and a wavevector $q$
- Dispersion relationship between energy $\hbar \omega$ and momentum $\hbar q$
- Magnons and phonons are BOSONS, and they are described by symmetric wavefunction with respect to the exchange of particle positions

Lattice waves $\Rightarrow$ Phonons
collective acoustic and optic lattice vibrations

Spin-waves $\Rightarrow$ Magnons
collective magnetic excitations
associated to the in-phase precession of the spin moments
- Semi-classical derivation
- Linear chain of aligned spins \((S=S_z, S_x=S_y=0)\)

\[ \hat{\mathcal{H}} = -2J \sum_i \hat{S}_i \cdot \hat{S}_{i+1} \]

\[
\frac{d\langle \hat{S}_j \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{S}_j, \hat{\mathcal{H}}] \rangle \\
= -\frac{2J}{i\hbar} \langle [\hat{S}_j, \hat{S}_{j-1} \hat{S}_j + \hat{S}_j \hat{S}_{j+1} + \cdots] \rangle \\
= -\frac{2J}{i\hbar} \langle [\hat{S}_j, \hat{S}_{j-1} \hat{S}_j] + [\hat{S}_j, \hat{S}_j \hat{S}_{j+1}] \rangle \\
= \frac{2J}{\hbar} \langle \hat{S}_j \times (\hat{S}_{j-1} + \hat{S}_{j+1}) \rangle.
\]

Small perturbation \(S_z \sim S, S_x, S_y \ll S\)

Spins treated as classical vectors

\[
\begin{align*}
\frac{dS_j^x}{dt} &\approx \frac{2JS}{\hbar} (2S_j^y - S_{j-1}^y - S_{j+1}^y) \\
\frac{dS_j^y}{dt} &\approx -\frac{2JS}{\hbar} (2S_j^x - S_{j-1}^x - S_{j+1}^x) \\
\frac{dS_j^z}{dt} &\approx 0.
\end{align*}
\]

\[
S_j^x = Ae^{i(qJa - \omega t)} \\
S_j^y = Be^{i(qJa - \omega t)}
\]
Raising and lowering operators are defined as:

\[
\hat{S}^+ = \hat{S}^x + i\hat{S}^y \\
\hat{S}^- = \hat{S}^x - i\hat{S}^y
\]

\[
\hat{S}^+ |\uparrow_z\rangle = 0 \\
\hat{S}^+ |\downarrow_z\rangle = |\uparrow_z\rangle \\
\hat{S}^- |\uparrow_z\rangle = |\downarrow_z\rangle \\
\hat{S}^- |\downarrow_z\rangle = 0
\]

Commutation relations

\[
\left[\hat{S}^+, \hat{S}^-\right] = 2\hat{S}^z \\
\left[\hat{S}^z, \hat{S}^{\pm}\right] = \pm\hat{S}^{\pm} \\
\left[\hat{S}^2, \hat{S}^{\pm}\right] = 0
\]

\[
\hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+ = 2 \left[ (\hat{S}^x)^2 + (\hat{S}^z)^2 \right]
\]

\[
\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \hat{S}_z^2 + \frac{1}{2} \left( \hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+ \right)
\]
- Quantum mechanical derivation
- Heisenberg Hamiltonian for a linear chain of spins

\[
\hat{H} = -2J \sum_j \left[ \hat{S}_j^z \hat{S}_{j+1}^z + \frac{1}{2} \left( \hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+ \right) \right]
\]

\[|\Psi> = \cdots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \cdots\]

Ground state \(|\Psi>\)

\[\hat{H}|\Psi> = -NS^2J|\Psi>\]

\[E_0 = NS^2J\] eigenvalue of the ground state \(|\Psi>\)

\[|j> \text{ excited state: spin flip at site } j\]

\[|j> = \hat{S}_j^-|\Psi>\]

\[|j> = \cdots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \cdots\]

\[\hat{H}|j> = 2 \left[ \left( -NS^2J + 2SJ \right)|j> - SJ|j+1> - SJ|j-1> \right]\]

\[\Delta S = 1 \text{ total change of the spin}\]

Magnons are Bosons!

Notice that \(|j>\) is not an eigenstate of the Hamiltonian because:

\[\hat{H}|j> \neq c|j>\]
Plane waves solution in form of a spin-flip excitation propagating along the 1D-dimensional chain

\[ |q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqR_j} |j\rangle \]

Flipped spin state \(|j\rangle\) delocalized along the chain

- Total spin of the perturbed state \(|j\rangle\) is: \(NS - \Delta S = NS - 1\)
- The total energy solution of \(H|j\rangle = E(q)|j\rangle\) is:

\[ E(q) = -2NS^2J + 4JS [1 - \cos(qa)] \]

- Magnon dispersion relation:

\[ \hbar \omega = E(q) - E_0 = 4JS [1 - \cos(qa)] \]

- If \((qa) << 1\) => parabolic dispersion:

\[ \hbar \omega \approx 4JSa^2q^2 \]
- At low temperature the density of states is \( g(q) \, dq \sim q^2 \) and then \( g(\omega) \, d\omega \sim \sqrt{\omega} \, d\omega \).

- In order to calculate the number of magnons at finite temperature \( T \) we need to integrate over all frequencies the magnon density of states multiplied by the Bose factor:

\[
\frac{n_{magn.}}{M_s} = \int_0^\infty \frac{g(\omega) \, d\omega}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1} = \left(\frac{k_B T}{\hbar}\right)^{3/2} \int_0^\infty \frac{x^{1/2} \, dx}{e^x - 1} \propto T^{3/2}
\]

Reduced magnetization at low \( T \) due to the magnon excitations:

\[
\frac{M(0) - M(T)}{M(0)} \propto T^{3/2}
\]

Block law \( T^{3/2} \)
Electron with momentum k+q and spin down is excited in the state k with spin up

\[ \hbar \omega = E_{k+q} - E_k + \Delta \]

\( \Delta = \) exchange splitting

- Electron-hole excitations between filled and empty spin-split bands
- Broadening of energy => Short timescale fluctuations
- Single electron excitation

In paramagnetic state the spin wave excitations are overdamped and are called paramagnons.
The triple axis spectrometer (TAS) (Brockhouse 1952)

\[ k = \frac{\pi}{d_M \sin \theta_M} \quad E_i = \frac{\hbar^2 k^2}{2m_n} \]

\[ k' = \frac{\pi}{d_A \sin \theta_A} \quad E_f = \frac{\hbar^2 k'^2}{2m_n} \]

Energy conservation

\[ E_i - E_f = \pm \hbar \omega \]

Kinematical condition

\[ Q^2 = k^2 + k'^2 - 2k_i k_f \cos \phi \]

\[ Q = G_{222} + q \]
Different possibilities to cross the dispersion surface $S(Q, \omega)$ in 4D space

- In general, 3 parameters are varied between $(\theta_M, \theta_A, \phi \Omega)$
- Different choices for the same scattering point

**Constant-Q scans:**
We scan the energy axis when $Q$ is constant
- $\theta_M$ (or $\theta_A$) is kept fixed
- $\theta_A$ (or $\theta_M$) and $\phi \Omega$ are varied in order to keep $Q$ constant

**Constant-E scans:**
We scan one of the Q axis when $(E_i - E_f)$ is kept constant
- Both $\theta_M$ and $\theta_A$ are kept fixed
- $Q$ is varied along a particular trajectory by varying $\phi \Omega$
Inelastic structure factor

Bose-Einstein Thermal population factor

Phonon Polarization factor
Reciprocal lattice
Transverse scan <111>
Constant-Q

Longitudinal scan <111>
Constant-Q

Phonon polarization
Transverse phonons (TA)

Longitudinal phonons (LA)

S(q, ω)

Observed intensity
de-focusing region
focusing region

neutron energy loss
neutron energy gain
Magnons (or spin waves) are collective magnetic excitations associated to the precession of the spin moments.

\[
\frac{d^2 \sigma}{d\Omega dE}(Q, \omega)^{\text{Magn}} = (\gamma r_0^2) \frac{k'}{k} \frac{2\pi^3}{2v_0} \frac{1}{2} S(1+Q^2) \left[ \frac{1}{2} g f(Q) \right]^2 \left( n_q + \frac{1}{2} \pm \frac{1}{2} \right) \left[ \delta(\omega - \omega_s) \delta(Q - q_{ph} - \tau) \right]
\]

Iron Spin wave in YFe₂

\[
E = E_{gap} + Dq^2 + Gq^4
\]

Magnon stiffness constant related to the exchange interaction

\[ D \propto JS^2 \]
ErFe$_2$

T = 295K

Reduced wave vector coordinate $\zeta = \frac{aq}{2\pi}$

Spin wave in metals (Band like model)
Broadening of energy => Short timescale fluctuations
Stoner excitations => single electron excitation