Models in Magnetism: Introduction

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Short review:

• basic models describing the magnetic behaviour
• connections between models
General problems

Dimensionality of the system, d:

Moments coupled:
- all space directions \( d = 3 \)
- in a plane \( d = 2 \)
- one direction \( d = 1 \)
- polymer chain \( d = 0 \)

Phase transition:
Existence of a boundary at \( d = 4 \),
spatial dimensionality can be also continous, \( \varepsilon = 4 - d \)

Number of magnetization components, \( n \)
Heisenberg model \( n = 3 \)
X-Y model \( n = 2 \)
Ising model \( n = 1 \)

Phase transitions:
\( n \rightarrow \infty \) spherical model (Stanley, 1968)
\( n = -2 \) Gaussian model
\( n \) can be generalized as continous

For \( d \geq 4 \), for all \( n \) values, critical behaviour can be described by a model of molecular field approximation.
Comparison with experimental data

magnetization versus temperature $M = f(T)$
magnetic susceptibility $\chi = f(T)$
behaviour in critical region

$$\frac{M(T)}{M(O)} \sim t^{\beta}$$
$$\chi \propto t^{-\gamma}$$
$$c_p \propto t^{-\alpha}$$

$$t = \frac{|T_c - T|}{T_c} \leq 10^{-1} - 10^{-2}$$
Transition metals: 3d Fe, Co, Ni

Fe $g = 2.05 - 2.09$
Co $g = 2.18 - 2.23$
Ni $g = 2.17 - 2.22$

Moments due mainly to spin contribution

For 3d metals and alloys

Moments at saturation $\mu = gS_0$,

Effective magnetic moments $\mu_{\text{eff}} = g\sqrt{S_p(S_p+1)}$

generally $r = S_p/S_0 > 1$

Rare-earths: 4f shell presence of spin and orbital contribution

Magnetic insulators: localized moments
Localized moments:

Heisenberg type Hamiltonian: exchange interactions

\[ H = \sum_{i,j} J_{ij} S_i S_j \]

\( J_{ij} \) exchange integral direct

n=3 system

Difficulty in exact computation of magnetic properties: many body problem

Approximations

**Ising model** (Ising 1925)

Exact results in unidimensional and some bidimensional lattices

\[ H = -2J \sum_{i,j} S_{iz} S_{jz} \]

• **Unidimensional**

neglect the spin components \( \perp H \)

strong uniaxial anisotropy
· **Linear Ising lattice**: not ferrromagnetic

\[ \chi \approx \frac{1}{T} \exp \left( \frac{2J}{k_B T} \right) \]

· **Square bidimensional** lattice, \( J_1, J_2 \)

\[ M = [1 - (\sinh 2k_1 \sinh 2k_2)^{-2}]^{1/2} \]

\[ k_1 = \frac{J_1}{k_B T}; \quad k_2 = \frac{J_2}{k_B T} \]

Onsager (1948)

Yang (1952)

· **Tridimensional** lattice: series development method

· **Spherical Ising model** (Berlin-Kac, 1951)

\[ \sum_i S_i^2 = c t \]

arbitrary values for spins but can be solved exactly in the presence of an external field

\( d \geq 4 \); critical exponents are independent of \( d \) and of the geometry of the system
Molecular field models:

Methods which analyse exactly the interactions in a small part of crystal, and the interactions with remaining part are described by an effective field, $H_m$, self consistently determined:

small portion $\rightarrow$ atom (molecular field approach Weiss (1907))

- Magnetic domains
- Molecular field: aligned magnetic moments in the domains

\[ H_m = N_{ii} M \]

Total field $H_T = H + H_m$: $M = \chi_0 H \rightarrow M = \chi_0 (H + N_{ii} M)$

\[ M = \frac{\chi_0 H}{1 - N_{ii} \chi_0} \]
Self consistency:

\[ M = \chi_0 H + N_{ii} \chi_0 M = \chi_0 H + N_{ii} \chi_0 (\chi_0 H + N_{ii} \chi_0 M) = \]

\[ = \chi_0 H (1 + N_{ii} \chi_0) + (N_{ii} \chi_0)^2 M = \]

\[ = \chi_0 H [1 + (N_{ii} \chi_0) + (N_{ii} \chi_0)^2 + (N_{ii} \chi_0)^3 + ...] = \]

\[ = \frac{\chi_0 H}{1 - N_{ii} \chi_0} = \chi H \]

Reverse reaction: corrections are time distributed: n correction after n-1 one

Molecular field:

act at the level of each particle
\[ H_m = -2J_{ij} S_i \sum_{j=1}^{z} S_j \]
\[ H_m = -g\mu_0\mu_B S_i H_m \]

\[ S \rightarrow J \]

\[ M(T) = M(0)B_j(x) \]

\[ x = \frac{\mu_0\mu_B g J H_T}{k_B T} \]

Low temperatures

\[ \frac{M(T)}{M(0)} = 1 - \frac{1}{J} \exp\left(\frac{-3T_C}{J+1T}\right) + \ldots \]

Experimental

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

\[ T < T_C, \text{ close to } T_C \]

\[ \frac{M(T)}{M(0)} \propto T^{\beta} \]

\[ \beta = 1/2 \]

\[ \beta = 1/3 \text{ exp.} \]
\[ T > T_c \]

\textbf{MF:} \( \chi^{-1} \propto T \) \text{ in all temperature range}

\text{experimental around } T_c:

\[ \chi \propto t^{-\gamma} \quad \gamma = 4/3 \]

\textbf{MF:} \( \theta = T_c \)

\[
\frac{\theta - T_c}{T_c} \approx (2.4 - 4.8)\% \\
\text{for Fe, Co, Ni}
\]
Interactions between a finite number of spins +molecular field

Oguchi method (1955); Constant coupling approximation (Kastelijn-Kranendonk, 1956); Bethe-Peierls-Weiss method (Weiss 1948)

Oguchi:

pair of spins

\[ H_0 = -2J_{ij} S_i S_j - g \mu_B \mu_B (S_{iz} + S_{jz}) H_T \]

\[ H_T \rightarrow \text{molecular field for } z-1 \text{ neighbours} \]

\[ T_c \neq 0 \quad \theta / T_c = 1.05 \ (\text{cubic lattice}) \]

\[ \chi^{-1} \text{ nonlinear variation around } T_c \]
Spin Waves

Slater (1954): exact solution for Heisenberg Hamiltonian: all spins (except one) are parallelly aligned

\[
S_t = \sum S_i; \quad S_t = NS, \quad S'_t = NS - 1
\]

\[N \rightarrow \text{number of atoms}\]

\[H = -g\mu_B B \sum S_{iz} - 2J \sum_{\text{neigh.}} S_j S_l\]

Many spin deviations: additivity law \(\Delta E(n) \approx n\Delta E(1)\)

(non rigorous, corrections)

repulsion of spin deviations: atoms with \(S\), no more \(2S\) deviations

attraction: total exchange energy is lower when two spin deviations are localized on neighbouring atoms
• Semiclassical description of spin wave: Bloch (1930) (Heller-Kramers 1934, Herring-Kittel 1951, Van Kranendonk-Van Vleck, 1958)

• Holstein-Primakoff formalism (1940)

\[ M = M(0) (1 - AT^{3/2}) \quad T/T_c \leq 0.3 \]

• Renormalization of spin waves (M. Bloch, 1962)

Keffer-London: effective field proportional with mean magnetization of atoms in the first coordination sphere (1961)

replaced by an effective spin at \( T \), proportional with the angle between two neighbouring spins

\[ \downarrow \]

The system is equivalent, at a given temperature, with a system of independent spin wave, having excitation energy (renormalized energy) equal with the energy of spin wave in harmonic approximation, multiplied by a self consistent term which depends on temperature

The model describe the temperature dependence of the magnetization in higher \( T \) range
The magnetic properties of the system described by Heisenberg hamiltonian, can be analysed around $T_c$, by series development method in $T^{-1}$

$T>T_c$

$\chi \propto (T-T_c)^{-\gamma}$; $\gamma=4/3$; For $S=1/2$ $k_B T_c/J=1.8-1.9$ ($z=6$)

=2.70 ($z=8$)

**Green function method** (Bogolyubov-Tyablikov, 1959)

Bitemporal Green function for a ferromagnet ($S=1/2$). Temperature dependence of magnetization obtained by decoupling Green function equation. The analysis has been made in lowest decoupling order (random phase approximation)

$$M = M(0)(a T^{3/2} + b T^{5/2} + c T^{7/2})$$

$\beta=1/2$; $\gamma=2$

Analysis in the second order of Green function decoupling (Callen, 1963)

$k_B T_c/J$ values only little higher than those obtained by series development method.
Antisymmetric exchange interactions:

(Dzialoshinski 1958)

General form of bilinear spin-spin interaction

\[ H = \sum_{\alpha \beta} J_{\alpha \beta} S_{i\alpha} S_{j\beta} \quad \alpha \beta = x, y, z \]

\[ J_{\alpha \beta} \]

\[ J_{\alpha \beta}^S = J_{\beta \alpha}^S \]

\[ J_{\alpha \beta}^A = -J_{\beta \alpha}^A \]

\[ H_{ij}^a = d_{ij} (S_i \times S_j) \quad d_{ij} = -d_{ji} \]

\[ H_{ij}^s = J_{ij} S_i S_j \]

Explain weak ferromagnetism in \( \alpha \)-Fe\(_2\)O\(_3\)
Indirect exchange interactions through conduction electrons (RKKY) (Ruderman-Kittel Kasuya, Yoshida (1954-1956))

4f shell: small spatial extension

La  Ce  Pr  Nd  Pm  Sm  Eu  Gd  Tb  Dy  Ho  Er  Tm  Yb  Lu

4f⁰  4f⁷  4f¹⁴

3d dilute alloys in nonmagnetic host

\[ H_{s-d(f)} = J s S \]

\[ H = H_{s-d} + H_{\text{cond.el}} + H_{zz} \]

First order perturbation theory

↓

Uniform polarization of conduction electrons
Second order

\[ J(R_{nm}) \propto J^2 F(x) \]

\[ F(x) = \frac{xcosx-sinx}{x^4}; \quad x = 2k_F R_{nm} \]

Oscillatory polarization: decrease as \( R_{nm}^{-3} \)

Example: Stearns 1972: Polarization of s and d itinerant 3d electrons: iron \( T>T_C \)

\[ \Theta \propto (g_J-1)^2 J(J+1) F(x) \]

Rare earths \( F(x) \) are similar
Exchange interactions 4f-5d-3d:

R-M compounds

R = rare-earth

M = 3d metal

\( M_{5d} = M_{5d}(0) + \alpha G \)

\( G = (g_J - 1)^2 J(J+1) \)

\( M_{5d}(0) \propto \sum n_i M_i \)

\( n_i \) number of 3d atoms in the first coordination shell, having \( M_i \) moment
Band models

• non integer number of $\mu_B$
  $M_{Fe}=2.21 \ \mu_B$
  $M_{Co}=1.73 \ \mu_B$
  $M_{Ni}=0.61 \ \mu_B$

• presence of 3d bands: widths of $\approx 1 \text{ eV}$

• difference between the number of spins determined from saturation magnetization and Curie constant
Stoner model
s,d electrons in band description

$$\Delta E = \Delta E_{\text{ex}} + \Delta E_{\text{kin}}$$

Spontaneous splitting 3d band
$$J_{\text{eff}} \eta(E_F) \geq 1$$

Stoner criterion for ferromagnetism
Sc,Ti,V, 3d band large, strongly hybridized with (4s,4p) band→ small density of states at $E_F$: $J_{\text{eff}}$ close to that of free electron gas

↓

no magnetic moments and magnetic order

Cr,Mn,Fe,Co,Ni: 3d band narrow (high density of states around $E_F$)

$J_{\text{eff}}$, more close to values in isolated atom

↓

magnetic moments and magnetic ordering

Many models based on the band concept were developed

$ZrZn_2 \quad M^2(T) = M^2(0)[1 - T^2/T_C^2]$
Hubbard model (Hubbard, 1963, 1964)

Hamiltonian: a kinetic term allowing for tunneling (“hopping”) of particles between sites of the lattice and a potential term consisting of on site interaction

Particles: fermions (Hubbard original work)

    bosons (boson Hubbard model)

Good approximation: particles in periodic potential at low T (particles are in the lowest Bloch band), as long range interactions can be neglected.

Extended Hubbard model: interactions between particles on different sites are included.

Based: tight binding approximation, electrons occupy the standard orbitals of atoms and “hopping” between atoms.

\[ H = \sum_{i,f} \sum_{\sigma} T_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + J \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \]

\[ J \rightarrow \infty, \text{ exact fundamental state} \]

\[ J=0, \text{ band description} \]

\[ \frac{T_{ij}}{J} \text{ ratio} \]

\[ \uparrow \text{ intermediate state} \]

\[ \text{delocalized moments} \]

Metal-Insulator transition
Models considering both band and localized features

• Friedel (1962), Lederer-Blandin (1966)

Starting from band model+features of Heisenberg model

Local polarization \( J_{\text{ef}} \eta(E_F) \geq 1 \)+ oscillatory exchange interactions

• Zener modified model (Herring) lattice of atoms having \( x \) and \( x+1 \) d electrons, respectively

The additional electron (Zener) is itinerant “hopping” from a lattice site to another

• Stearns model

Indirect coupling of localized d electrons through d itinerant electrons. 95% d electrons are in narrow band (localized) and 5% of d electrons are itinerant (Fe).
Approximation based on ionic configurations

coexistence of different ionic configurations \(3d^9, 3d^8, 3d^7\)

there is a possibility for impurity to have another fundamental state of an excited configuration by virtual transition.

\[\rightarrow\]

an effective coupling between impurity and conduction electrons

In zones situated between stable configurations there are regions characterized by fluctuations between configurations

\[\rightarrow\]

both localized and itinerant magnetic behaviour
Spin fluctuations:

Stoner model: itinerant electrons treated as a free electron gas; even the molecular field concept was introduced do not describe the properties of 3d metals at finite temperature.

Spin fluctuations: abandoned the concept of single particle excitation; introduced thermally induced collective excitations.

Deviations (fluctuation) from their average probability distribution of these fluctuations.

\[
\chi_k = \frac{\chi_k^0}{1 - \chi_k^0 \frac{U_{ef}}{\mu_0 \mu_B^2}}
\]

The system is paramagnetic

\[
\chi_k^{-1} > 0
\]

For some k value \( J \eta(E_F) = 1 \rightarrow \) magnetic moments having a life time \( \tau \)

\[
\tau \propto \frac{\eta_d(E_p)}{1 - J \eta_d(E_F)}
\]
Exchange enhanced paramagnet

$s$-Stoner exchange enhancement factor $s \approx 10$
Self consistent theory of spin fluctuations

Wave number dependent susceptibility, $\chi_q$, for a nearly ferromagnetic alloy has a large enhancement for small $q$ values

$$\chi_q = \frac{\bar{\chi}_q}{1 - J\bar{\chi}_q (\mu_0 \mu_B)}$$

Frequency of longitudinal spin fluctuations $\omega^* \propto \frac{1}{\tau}$

$\tau$-lifetime of LSF

Low temperature $\frac{k_B T}{\hbar}$

$\omega^* \frac{k_B T}{\hbar}$ (thermal fluctuations-transversal slow)

$$\chi = s\chi_p \left[ 1 + \frac{\pi^2}{6} \left( 2 \frac{\eta'}{\eta} - 1.2 \frac{\eta'^2}{\eta^2} \right) s^2 T^2 \right]_{E_F}$$
Approximation for nonmagnetic state

\[ \chi \propto T^2 \]

\[ \chi(T) \uparrow \text{ as } T \uparrow \]

\[ \eta'' > 0 \text{ (necessary condition, not sufficient)} \]
High temperature

Average mean amplitude of LSF is temperature dependent

\[ \langle S_{loc}^2 \rangle = 3k_B T \sum_q \chi_q \]

\[ S_{loc} \quad \text{as } T \uparrow \text{ up to } T^* \quad \langle S_{loc} \rangle \]

\[ S_{loc} \quad \text{determined by charge neutrality condition} \]

The system behaves as having local moments for temperatures \( T > T^* \) where the frequency of spin fluctuations

\[ \omega^* < \frac{k_B T}{\hbar} \]

\[ S_{loc} \]
Crossover between low T regime governed by spin fluctuations and high T classical regime
A system can be magnetic or nonmagnetic depending on the temperature (Schrieffer 1967).
Dilute magnetic alloys

Small number of magnetic atoms (3d) in nonmagnetic metallic matrix

3d moments as Fe, dependent on metallic matrix (Clogston 1962)
**Friedel model**: virtual bound state (level)

Resonance phenomena between d states and k states of conduction electrons

Package of waves centered on impurity atom (virtual bond level)

Prediction concerning the appearance of magnetic moment on impurity and experimental data

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**Wolff model:**

Considers scattering of conduction electrons by the potential of impurity atom.

The virtual level can be evidenced by a maximum in scattering section of the conduction electron.

When the virtual level is rather narrow and close to $E_F$, the impurity develops an exchange potential which polarizes the electrons in their neighbor.
Anderson model:
Magnetic impurity,
Bands: \( \uparrow\) (full) \( \downarrow\) (empty)
s or s-p state of conduction band
U d-d interaction
\( V_{dk} \) covalent mixing of conduction band with d states
\[ H = H_0 + H_{sd} \]
\[ H_0 = H_{0k} + H_{0\alpha} + H_{cor} \]
Coulomb interaction between electrons with spin \( \uparrow\) and \( \downarrow\) nonperturbed states
electrons in conduction band
Density of mixing states, \( \eta_{d\alpha} \) has half width \( \Gamma/2 \)
For \( S=1/2 \)
\[ S \approx \frac{1}{2} \left( 1 - \frac{1}{\pi xy(1-x)} \right) \]
\[ x = \frac{E_F - E_0}{U} \]
\[ y = U/(\Gamma/2); \]
Kondo model:

Anomalous temperature dependence of the electrical resistivity

↓

Interaction between the localized magnetic impurities and the itinerant electrons.

Extended to lattice of magnetic impurities, the Kondo effect is belied to underlay the formation of heavy fermions in intermetallic compounds based particularly on rare-earth.
Schrieffer-Wolff (1966): Anderson Hamiltonian can be of a similar form as the Kondo one, considering an antiferromagnetic interaction $J(k, k')$ energy dependent.
Spin glass, Mictomagnets:

Dilute alloy with random distribution of 3d atoms

Oscillatory polarization can direct the moments in different directions.

At low T, the moments are frozen in the direction corresponding to polarization (H=0)-spin glass
At higher concentration of magnetic atoms there are:
- random distributed magnetic atoms
- clusters of atoms

↓

mictomagnetism

Difference in the zero field cooled and field cooled magnetization.

*Insulators*: magnetic atoms in glasses

perovskites
Dynamical Mean Filed Theory (DMFT):  

DMFT, a step to develop methods for describing electronic correlations. Depending on the strength of the electronic correlations, the non-perturbative DMFT correctly yields:

- weakly correlated metal
- strongly correlated metal
- Mott insulator

DMFT+LDA allows a realistic calculation of materials having strong electronic correlations:

- transition metal oxides
- heavy fermion systems

Theory of everything: kinetic energy, lattice potential, Coulomb interactions between electrons
Superexchange Interactions (Van-Vleck 1951)

Two ions $T_1, T_2$ separated by a diamagnetic ion ($O^{2-}$)

Two $p$ electrons of $O^{2-}$ occupy the same $p$ orbital

$T_1, T_2$ have each one $d$ electron

$p$ orbitals axis coincides with $T_1$-$T_2$ axis

↓

Singlet state (no magnetic coupling between $T_1$ and $T_2$

one $p$ electron transferred as $d_1'$: coupling between $d$ and $d_1'$ on $T_1$ atom

the second $p$ electron of $O^{2-}$ can couple with the $d$ electron of $T_2$ atom.

Since of opposite spins of the two $O^{2-}$ electrons will appear an indirect exchange between...
Anderson: a more complex model
The resultant interaction is given as a sum of two competitive effects having opposite signs:
  potential superexchange (Coulomb repulse energy between two magnetic ions) which lead to ferromagnetic coupling
  kinetic superexchange (negative)