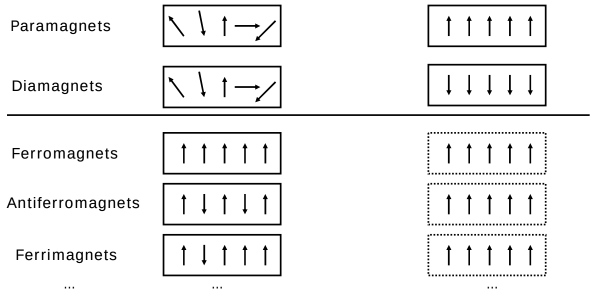
Magnetism

- Types of magnetic systems
- Pauli paramagnetism in metals
- Landau diamagnetism in metals
- Larmor diamagnetism in insulators
- Ferromagnetism of electron gas
- Spin Hamiltonian
- Mean field approach
- Curie transition

Magnets

Zero external field | Finite external field ↑



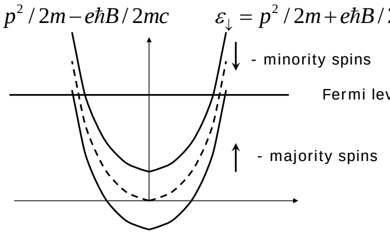
Pauli paramagnetism

Let us first look at magnetic properties of a free electron gas.

Electron are spin-1/2 particles

In external magnetic field ***B*** – Zeeman splitting

$\varepsilon_\uparrow = p^2/2m - e\hbar B/2mc \qquad \varepsilon_\downarrow = p^2/2m + e\hbar B/2mc$



Pauli paramagnetism

$\varepsilon_\uparrow = p^2/2m - e\hbar B/2mc \qquad \varepsilon_\downarrow = p^2/2m + e\hbar B/2mc$

#of majority spins:

#of minority spins:

$$N_{\uparrow,\downarrow} = V\int \frac{d^3\vec{p}}{(2\pi\hbar)^3} f(\varepsilon_{\uparrow,\downarrow})$$

Magnetization (magnetic moment per unit volume):

$$M = \frac{e\hbar}{2Vmc}(N_\uparrow - N_\downarrow)$$

: aligned along the field and proportional to *B* in low fields

$M = \chi B$ $\quad \chi$ - magnetic succeptibility

$\chi > 0$ - paramagnetism

Pauli succeptibility

$\varepsilon_\uparrow = p^2/2m - e\hbar B/2mc \qquad \varepsilon_\downarrow = p^2/2m + e\hbar B/2mc$

$$N_\uparrow - N_\downarrow = \frac{V}{2}\int_{\mu - e\hbar B/2mc}^{\mu + e\hbar B/2mc} g(\varepsilon)d\varepsilon \approx \frac{g}{2}\frac{e\hbar B}{mc}V$$

*B=1*T corresponds to $e\hbar B/mc = 1K \times k_B$ provided *m* is free electrons's mass

For any fields, $e\hbar B/mc \ll \mu$

Magnetic succeptibility:

$$\chi_P = \left(\frac{e\hbar}{2mc}\right)^2 g$$

Landau quantization

A free electron in magnetic field: $\vec{B} \parallel \hat{z}$

Schrödinger equation: $-\frac{\hbar^2}{2m}\left(\vec{\nabla} + \frac{ie\vec{A}}{\hbar c}\right)^2 \psi = \varepsilon\psi \qquad A_y = Bx;\ A_x = A_z = 0$

Solutions: labeled by two indices n, k_z

$$\psi_{nk}(\vec{r}) = \exp(ik_y y + ik_z z)\varphi_n(x - \hbar c k_y/eB)$$

φ_n - wave functions of a harmonic oscillator

Energies: $\varepsilon_{nk} = \hbar^2 k_z^2/2m + (e\hbar B/mc)(n+1/2)$ - strongly degenerate!!

We “quantized” momenta transverse to the field (Landau levels)

Landau diamagnetism

A free electron in magnetic field: moves along spiral trajectories and create magnetic field themselves.
This magnetic field is directed antiparallel to the external one

⇓ Diamagnetism

Energy: $E = 2_s \sum_n \int \frac{dk}{2\pi} \varepsilon_{nk} f(\varepsilon_{nk})$

Magnetization: $M = -V^{-1} \partial E / \partial B$

Result for the succeptibility: $\chi_L = -\frac{1}{3}\left(\frac{e\hbar}{2mc}\right)^2 g = -\frac{1}{3}\chi_P$

Total succeptibility: $\chi = \chi_P + \chi_L = 2\chi_P / 3 > 0$: paramagnetic!

Electrons in metals

We know that there are diamagnetic metals. How can we explain their existence?

Different spectra of electrons in metals and free electrons.
Example: renormalized electron mass m^*

This only affects orbital motion, not Zeeman splitting

⇓

$\chi_P^* = \chi_P;\ \chi_L^* = \chi_L (m/m^*)^2$

We can explain paramagnetic and diamagnetic metals!
But there is no way we can explain ferromagnetic and antiferromagnetic metals in non-interacting electron model.

Try insulators?

Larmor diamagnetism

Consider an ionic insulator with filled shells. Electrons are localized at the ions

Electron Hamiltonian: $\hat{H} = -\frac{\hbar^2}{2m}\left(\vec{\nabla} + \frac{ie\vec{A}}{\hbar c}\right)^2 + \frac{e\hbar}{mc}\vec{B}\vec{S};\ \vec{A} = \vec{B} \times \vec{r}$

r small: consider terms with the field as a perturbation.

Correction to the energy in the ground state: $\Delta E_g = \left\langle g.s \middle| \hat{H} \middle| g.s \right\rangle$

Total spin and total momentum of electrons in a filled shell are zero; only the term with r^2 contributes.

$$\Delta E_g = \frac{e^2}{8mc^2} B^2 \left\langle \sum_i \left(x_i^2 + y_i^2\right) \right\rangle_g = \frac{e^2}{12mc^2} B^2 \left\langle \sum_i r_i^2 \right\rangle_g$$

Larmor diamagnetism

$$\Delta E_g = \frac{e^2}{12mc^2} B^2 \left\langle \sum_i r_i^2 \right\rangle_g = \frac{e^2 ZN}{12mc^2} B^2 \left\langle r^2 \right\rangle_g$$

Susceptibility: $\chi = -\frac{1}{V}\frac{\partial^2 E}{\partial B^2} = -\frac{e^2 Z}{6mc^2} c_A \left\langle r^2 \right\rangle_g$

Z - ionic charge

c_A #of atoms per unit volume

Diamagnetism!

If the ionic shells are not filled – can get paramagnetic contribution due to other terms.

Can explain paramagnetic and diamagnetic insulators, but not ferromagnetic and antiferromagnetic ones!

Exchange interaction

Two electrons: antisymmetric wave function!

Take an electron level ε

Wave function of two electrons:

$\psi(r_1, r_2) = \frac{1}{\sqrt{2}}\left[\varphi_1(r_1)\varphi_2(r_2) \pm \varphi_2(r_1)\varphi_1(r_2)\right]$ for $S = 0,1$

Energy splitting due to interaction: spin-dependent! $\varepsilon \to \varepsilon + C \pm J/2$

$$C = \int dr_1 dr_2 U(r_1 - r_2) \left|\varphi_1(r_1)\right|^2 \left|\varphi_2(r_2)\right|^2$$

$$J = 2\int dr_1 dr_2 U(r_1 - r_2) \varphi_1(r_1)\varphi_1^*(r_2)\varphi_2^*(r_1)\varphi_2(r_2)$$

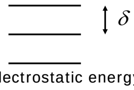
$\hat{H} = const - J\vec{S}_1\vec{S}_2$ Spin Hamiltonian

Ferromagnetism for localized electrons

Try to visualize for localized electrons
(atoms; artificial atoms – quantum dots; defects etc)

The simplest model:

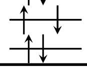
Discrete electron states; spacing δ
(each level is doubly degenerate)



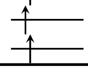
To put an electron into the system costs electrostatic energy U and exchange energy $-J$

Energy to pay: Same spin: $U + \delta - J$ Opposite spin: U

$J < \delta$ Non-magnetic state



$J > \delta$ Ferromagnetic state



Itinerant ferromagnetism

If we can not get ferromagnetism with free electrons, try interacting electrons.

Hartree-Fock approximation:

$$E_{\text{int}} = \langle g | V_{\text{int}} | g \rangle$$
$$\approx \frac{1}{2}\sum_{ij}\int d\vec{r}d\vec{r}\,'\frac{e^2}{|\vec{r}-\vec{r}\,'|}\left[|\psi_i(\vec{r})|^2|\psi_j(\vec{r}\,')|^2 - \psi_i^*(\vec{r})\psi_j^*(\vec{r}\,')\psi_i(\vec{r}\,')\psi_j(\vec{r})\right]$$

Hartree (direct) interaction

Fock (exchange) interaction. Only exists if spin projections are the same in the states *i* and *j*

Itinerant ferromagnetism

Working the interaction terms out for free electrons (see *Advanced Quantum Mechanics, lecture 4*)

Kinetic energy: $E_{kin} = \frac{3}{5}NE_F = \frac{3N}{5}\frac{\hbar^2 k_F^2}{2m}$

Potential energy: $E_{\text{int}} = -\frac{3}{4}Ne^2\frac{k_F}{\pi}$ NB: $N = Vk_F^3/(3\pi^2)$

Try now a spin-polarized ground state: $k_F^\uparrow \neq k_F^\downarrow$

Kinetic energy loss can be compensated by the potential energy gain!

For $k_F a_B < \frac{5}{2\pi}\frac{1}{2^{1/3}+1}$ - spin-polarized ground state (ferromagnetism!!)

$a_B = \hbar^2/me^2$ - Bohr radius

Never occurs in real life.

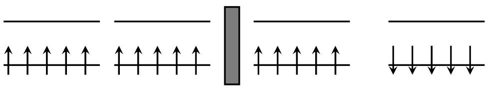
Antiferromagnetic ordering

A different situation: a pair of magnetic atoms in an insulating matrix

Consider d-electrons, 5 electrons per atom

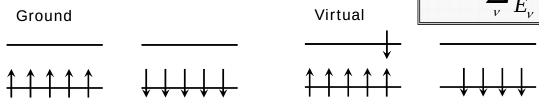
U – ionization energy; *t* – overlap between the atoms $t \ll U$

Unperturbed ground state: either parallel or antiparallel spins.



Antiferromagnetic ordering

2nd order corrections to the ground state: virtual states $\Delta E = -\sum_\nu \frac{|M_{i\nu}|^2}{E_\nu - E_i}$



$\Delta E = -25t^2/U \ll t, U$

Ferromagnetic state: no second-order correction (forbidden by Pauli principle)

Antiferromagnetic state preferential!

Spin Hamiltonian

Does not work for many atoms – but still represents a good model to treat magnetism

$\hat{H} = -\sum_{ij} J_{ij}\hat{\vec{S}}_i\hat{\vec{S}}_j$ *i* and *j* – lattice sites

Common approximation: only nearest neighbours interact; the same exchange integrals for all bonds

Heisenberg model: $\hat{H} = -J\sum_{\langle ij\rangle}\hat{\vec{S}}_i\hat{\vec{S}}_j$

$J > 0\ (J < 0)$ favors ferromagnetism (antiferromagnetism)

Exact solution: only known for 1D chain (Bethe 1931) – no magnetism!

Can also be treated for high spins (classical)

Let us see what we can do with approximate solutions.

Mean field approach

Let us single out one particular spin at *i*.

$\hat{H} = -J\hat{\vec{S}}_i\sum_j\hat{\vec{S}}_j + \text{(all other spins)}$

Approximation: this spin sees the average field (Weiss field) $\vec{h} = -J\left\langle\sum_j\hat{\vec{S}}_j\right\rangle$ $\hat{H} = \vec{h}\hat{\vec{S}}_i$

Now we need to calculate the average field self-consistently.

Each site has N nearest neighbours. For each neighbour,

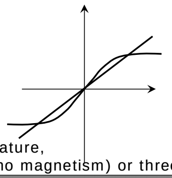
chance to be "up" (parallel to the field) $P_\uparrow \propto \exp(-h/2k_BT)$

chance to be "down" (antiparallel to the field) $P_\downarrow \propto \exp(+h/2k_BT)$

Equation for the field: $h = -\frac{JN}{2}\left(P_\uparrow - P_\downarrow\right) = \frac{JN}{2}\tanh\frac{h}{2k_BT}$

Mean field approach

$$h = \frac{JN}{2}\tanh\frac{h}{2k_B T}$$



Depending on the temperature,
either one solution *h=0* (no magnetism) or three solutions (ferromagnetism)

Three solutions at: $$\frac{JN}{2}\frac{1}{2k_B T} > 1 \Rightarrow k_B T < \frac{JN}{4}$$ Curie's temperature

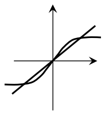
A phase transition between a ferromagnetic and paramagnetic state!

Curie transition

Magnetization close to transition temperature

$$T_c = \frac{JN}{4k_B}$$

$$\tanh x \approx x - x^3/3$$



Solution:

$$h = \sqrt{12k_B^2 T_c (T_c - T)}$$

Square-root singularity

Numerical solutions: give power laws, but not the square root.
Obviously, these are problems of the mean-field approximation.

To describe paramagnetic state: Can add the external field h_0

$$h = h_0 + \frac{JN}{2}\tanh\frac{h}{2k_B T}$$