Condensed Matter Physics I

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Last time

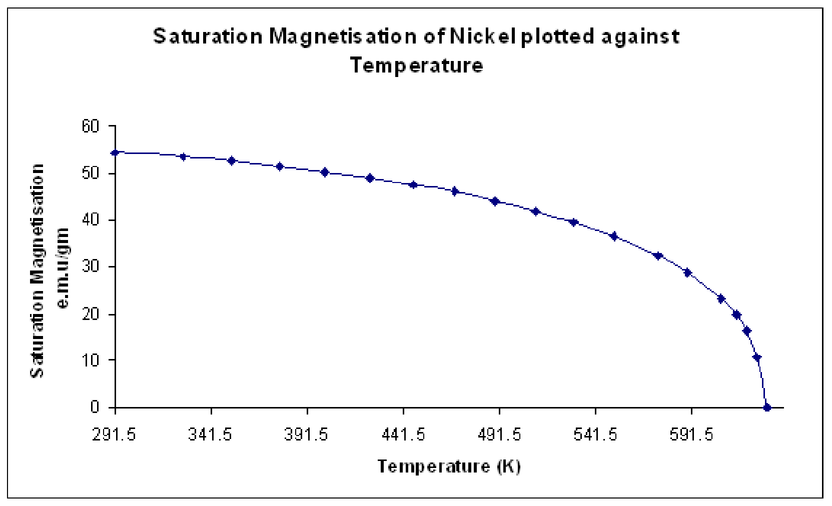
Paramagnetism

- Curie paramagnetism
- van Vleck magnetism
- Pauli paramagnetism

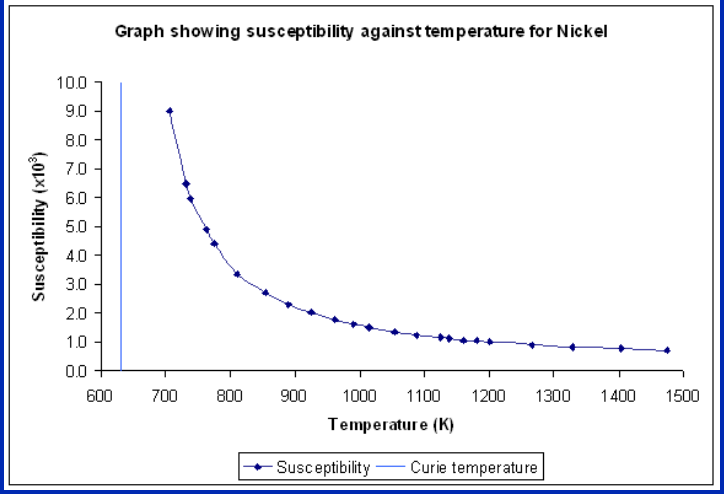
Ordered magnetism

- Curie-Weiss law
- Spontaneous magnetization
- Mean field approach

Magnetization in Ni



Variation of saturation magnetisation with temperature for Nickel. (Data from Weiss and Forrer, 1926)



Variation of susceptibility with temperature for Nickel (Sucksmith and Pearce, 1938)

Magnetic interaction

$$H_{i,j} = -2J_{i,j}\vec{S}_i \cdot \vec{S}_j$$

$$E_i = \sum_j -2J\, S_i \cdot S_j = -2Jz\langle S\rangle \cdot S_i \equiv -m_i \cdot H_{mf} = -g_o\mu_B S_i \cdot H_{mf}$$

$$\left.\begin{aligned} H_{mf} &= \frac{2Jz}{g_o\mu_B}\langle S\rangle \\ \langle S\rangle &= \frac{M}{n\, g_o\mu_B} \end{aligned}\right\}$$

$$H_{mf} \equiv \lambda M = \frac{2Jz}{(g_o\mu_B)^2 n} M$$

$$\left.\begin{aligned} T_c &= \lambda C \\ C &= \frac{n(p\mu_B)^2}{3k_B} \end{aligned}\right\}$$

$$T_c = \frac{Jzp^2}{6k_B}$$

$$J = \frac{6}{zp^2} k_B T_c$$

Iron: $T_c \sim 1000$ K

Dipole-dipole interaction

Dipole-dipole interaction is an anisotropic interaction

$$E = \frac{\mu_0}{4\pi} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \vec{e}_{12})(\vec{\mu}_2 \cdot \vec{e}_{12})}{r_{12}^3}$$

$$E \approx 10^{-23}\ \mathrm{J} \sim 1\mathrm{K}\ \text{ for } r = 2\,\mathrm{\mathring{A}} \text{ and } \mu = \mu_B$$

In real materials: $T_c \sim 10^2 – 10^3$ K !!

→ Dipole-dipole interaction hardly ever dominates

Magnetic parameters

	z	n [10^{22} cm^{-3}]	g	p	C [K]	T_c [K]	J [meV]	λ
Fe	8	8.5	2	5.4	0.51	1043	2.3	2045
Co	12	9	2	4.8	0.43	1388	2.3	3228
Ni	12	9.1	2	3.2	0.19	627	0.6	3300
Gd	12	3	2	8.0	0.40	293	0.2	733

	M(0) [gauss]	**M(0)/Nμ_B**	**H_{mf} [10^6 gauss]**
Fe	1740	2.22	3.6
Co	1446	1.72	4.7
Ni	510	0.606	1.7
Gd	2060	7.63	1.5

- spin-orbit
- canted, ferri
- conduction electrons

Interactions

- Dipole – Dipole
- Direct exchange (H_2 molecule)
- Indirect exchange
- Double exchange
- Anisotropic exchange
- Rudeman Kittel Kasuya Yoshida (RKKY)
- Stoner ("spontaneous Pauli")

H_2 molecule

- LCAO gives wrong solution (e.g. triplet ground state)
- Correlated picture (Heitler-London approach) is better
  - Starting point: two electron orbitals $\left|\phi_a(1)\phi_b(2)\right\rangle$ and $\left|\phi_a(2)\phi_b(1)\right\rangle$
  - Wavefunctions (anti-symmetric under particle exchange)

$$\Psi_S = \frac{1}{\sqrt{2}}\left[\phi_a(1)\phi_b(2) + \phi_a(2)\phi_b(1)\right]\chi_S$$

$$\Psi_T = \frac{1}{\sqrt{2}}\left[\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)\right]\chi_T$$

  - Spin parts: $\chi_S = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

$$\chi_T = \begin{cases} \left|\uparrow\uparrow\right\rangle \\ \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right) \\ \left|\downarrow\downarrow\right\rangle \end{cases}$$

H_2 molecule

- Singlet ground state
- Exchange energy: Pauli + Coulomb

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1{}^2 + \nabla_2{}^2\right) + V_c(1,2)$$

$$V_c(1,2) = \frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|R_1 - R_2|} - \frac{e^2}{|r_1 - R_2|} - \frac{e^2}{|r_2 - R_2|}$$

$$E_S - E_T = 2\left\langle \phi_a(1)\phi_b(2)\middle| V_c \middle| \phi_a(2)\phi_b(1)\right\rangle := 2J$$

$$H = -2J\vec{S}_1 \cdot \vec{S}_2 = \begin{cases} -2J \cdot -\frac{3}{4} & \text{for the spin singlet} \\ -2J \cdot \frac{1}{4} & \text{for the spin singlet} \end{cases}$$

Exchange interaction

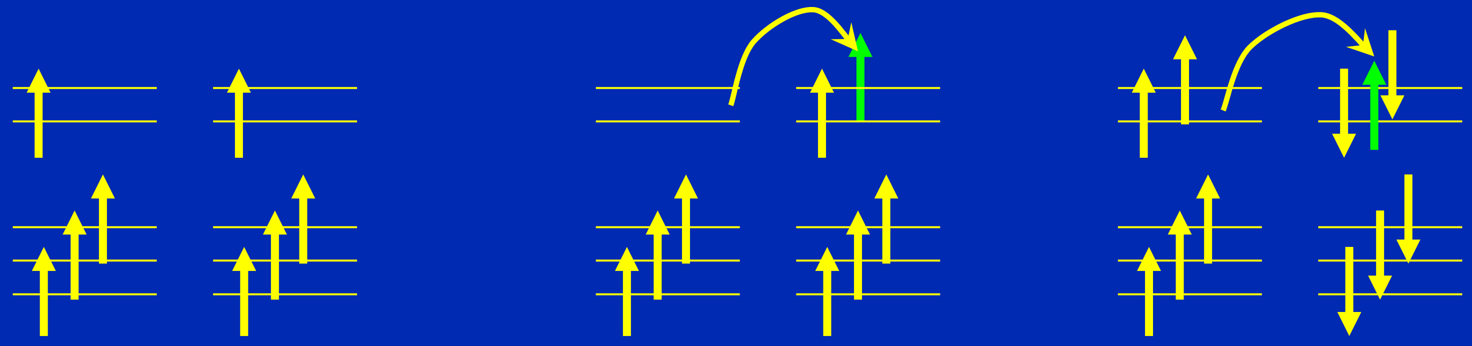
- Heisenberg Hamiltonian

$$H = -2\sum_{i,j}{}' J_{ij}\vec{S}_i \cdot \vec{S}_j$$

- J>0: Ferro
- J<0: Antiferro

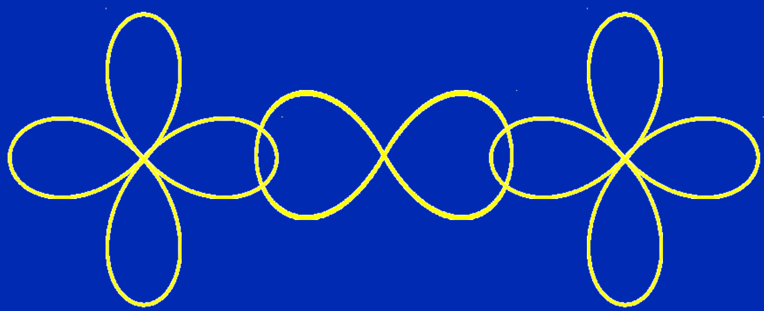
Direct exchange

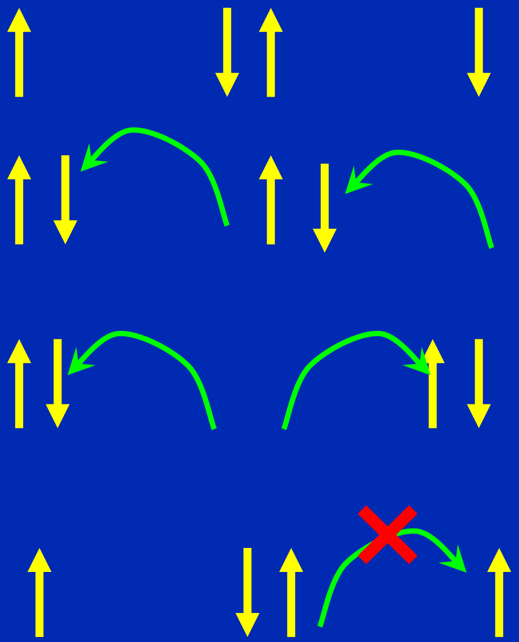
- Need direct wave function overlap
  - Ferromagnetic
  - Small in 4f, 5f elements
  - Can be important in 3d oxides (but see indirect!)
  - In 3d metals: electron delocalization



- Relatively small (but remember TiOX)
- Depends on orbital occupation and geometry

Indirect exchange





Ground state antiferro

‘2*hopping’

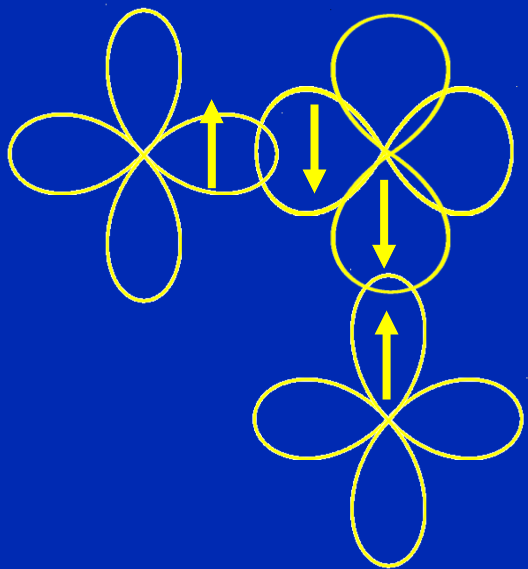
Pauli forbidden

Hopping →
delocalization →
energy gain

Energy: 2 hops = 2t; cost=U
➔ $J \sim -t^2/U$

Examples: High Tc’s; MnO; MnF_2

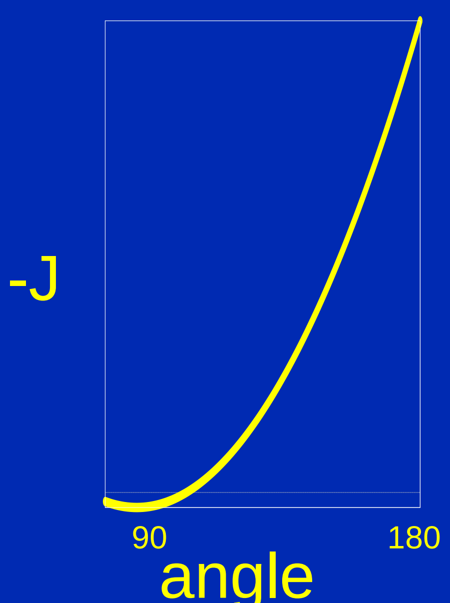
Indirect exchange



Hopping → delocalization → energy gain
Energy: 2 hops = 2t; cost=U

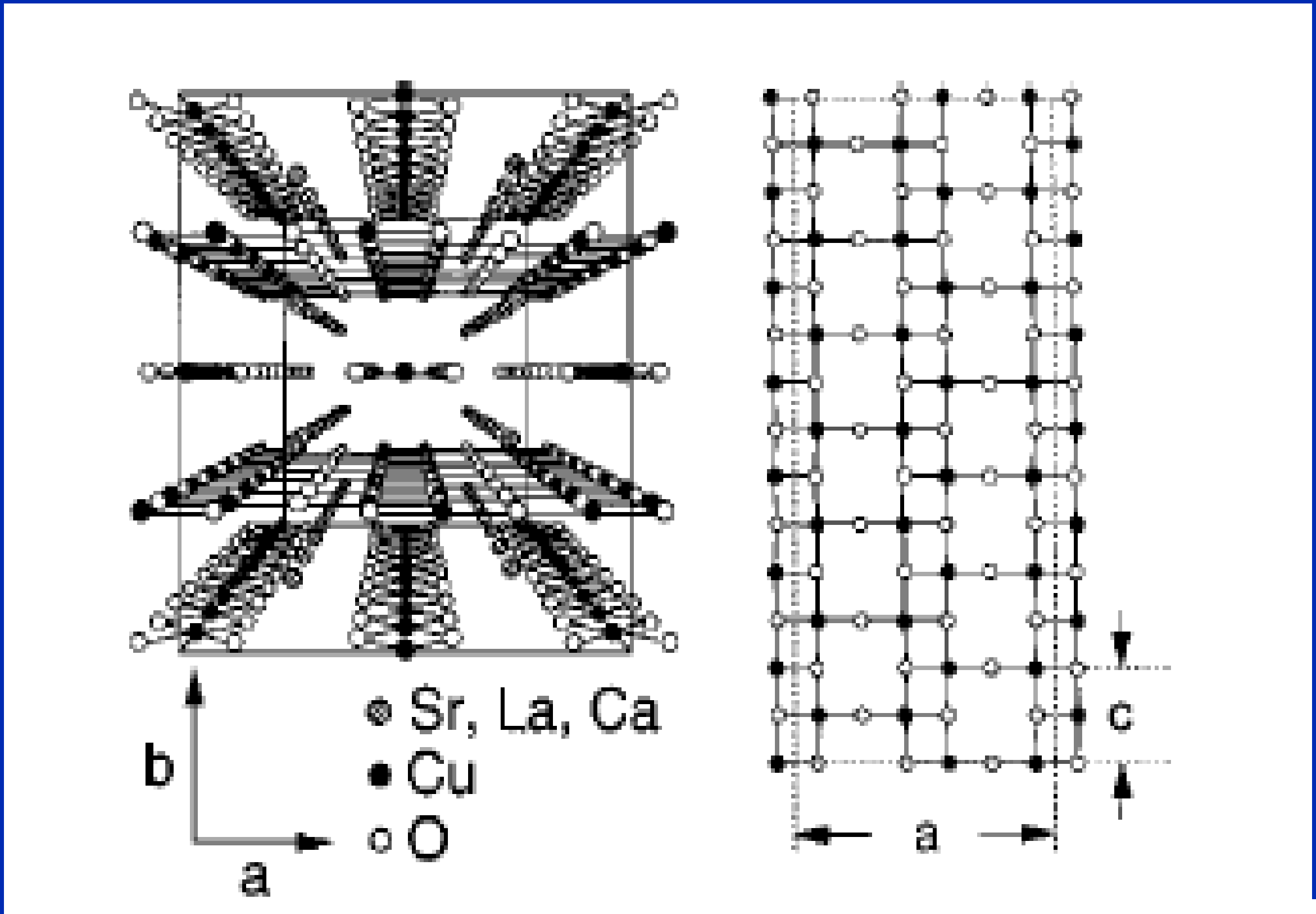
→ $J \sim -t^2/U$

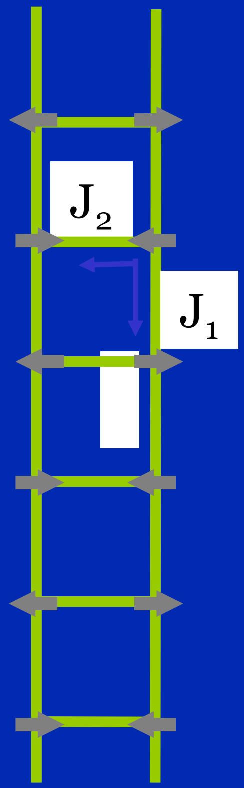
Examples: High Tc's; MnO; MnF_2;
telephone number compound



Relatively strong (depends on U)
Usually AF (F when not same 3d, e.g.d^3-d^5)
Strongly dependent on angle of bonding
at 180^0 strongly AF
at zero weakly F
(goodenough kanamouri rules

$(Sr,La,Ca)_{14}Cu_{24}O_{41}$





Eccleston *et al.*, PRL **81**, 1702 (1998)

J_1=130 meV
J_2= 70 meV
Δ=32 meV

$La_9Ca_5Cu_{24}O_{41}$