Condensed Matter Physics I

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Last time

Heitler-London
Pauli + Coulomb
Exchange interactions

Interactions

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

Exchange interaction

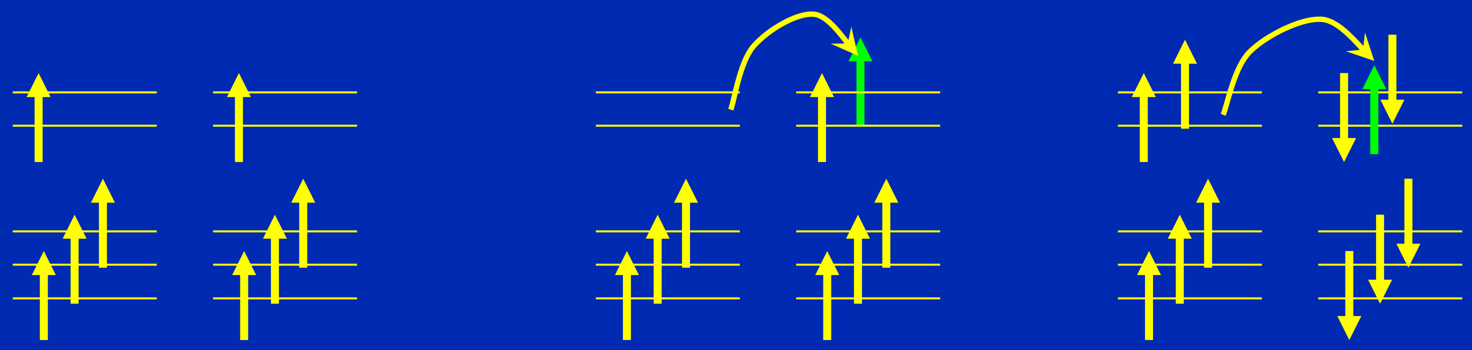
- Heisenberg Hamiltonian

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

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

Direct exchange

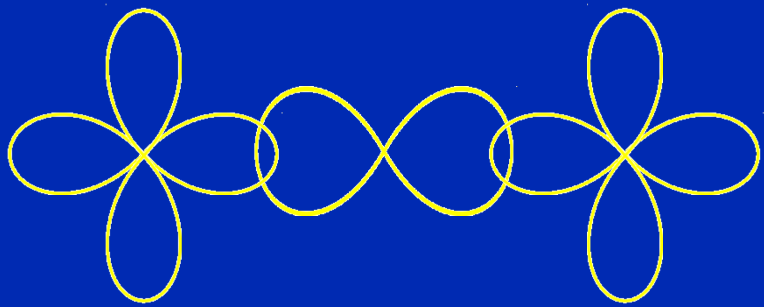
- Need direct wave function overlap
  - Ferromagnetic
  - Small in 4f, 5f elements
  - Can be important in 3d oxides (but see indirect!)
  - In 3d metals: electron delocalization

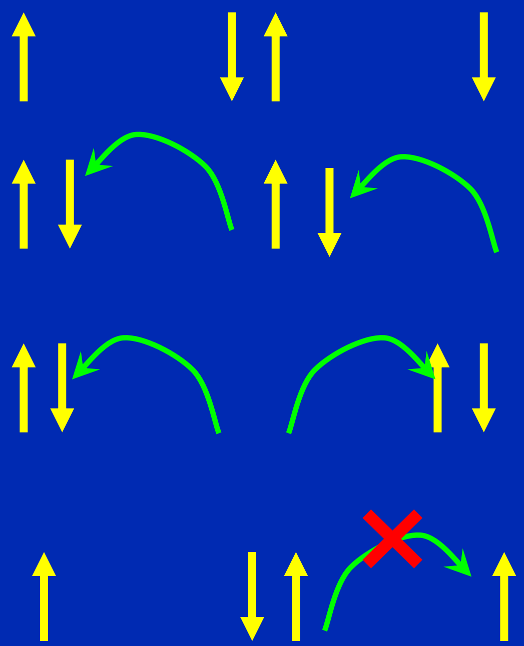


Oxide: ferro　　‘hopping’: ferro　　‘hopping’: antiferro

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

Indirect exchange





Ground state antiferro

‘2*hopping’

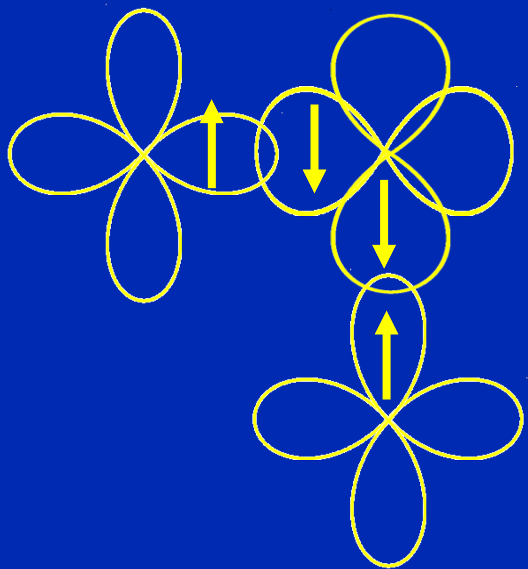
Pauli forbidden

Hopping →
delocalization →
energy gain

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

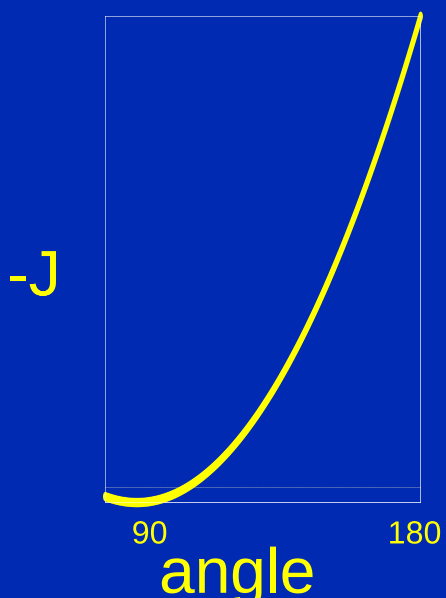
Examples: High Tc’s; MnO; MnF_2

Indirect exchange



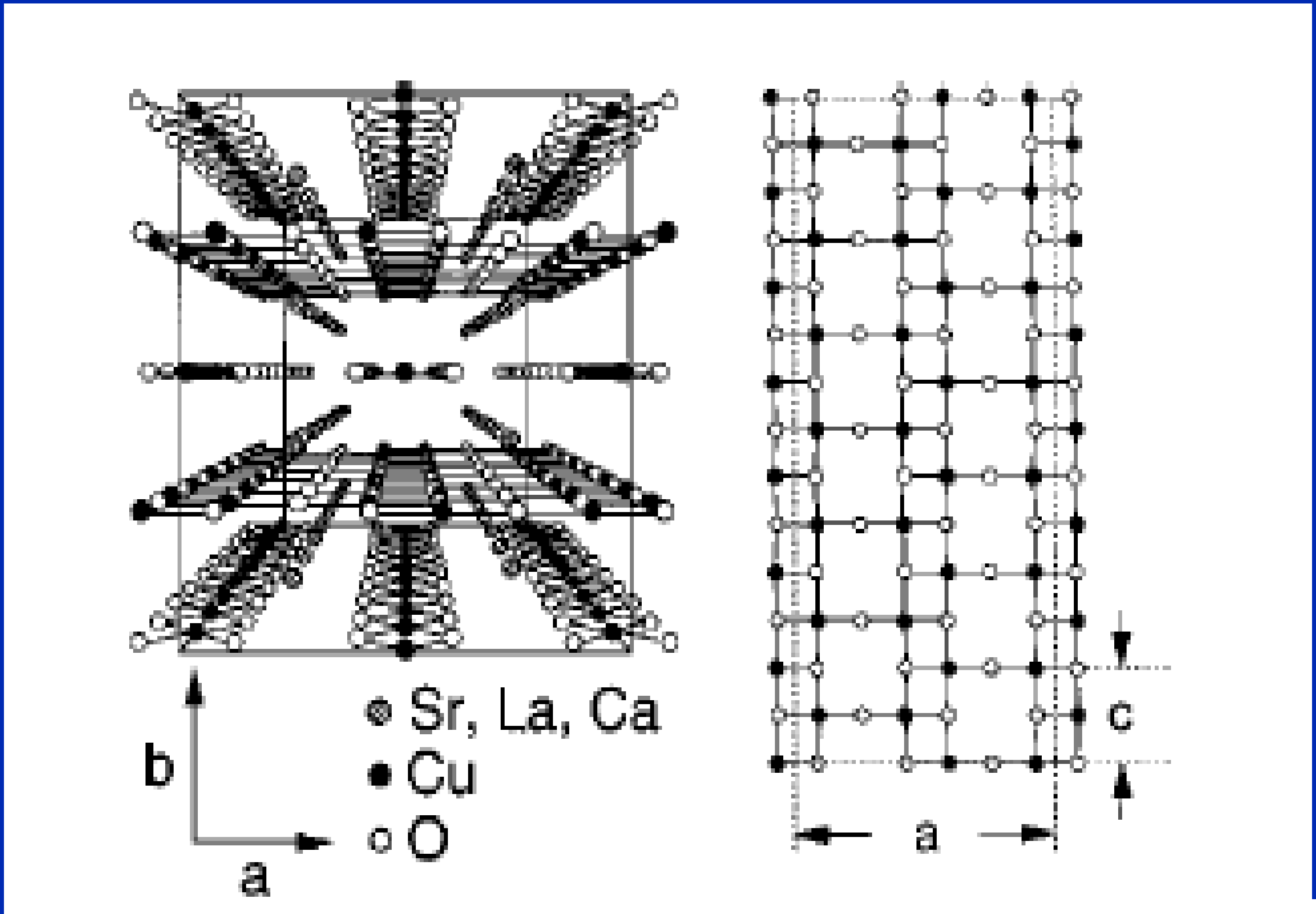
Hopping → delocalization → energy gain
Energy: 2 hops = 2t; cost=U
→ $J \sim -t^2/U$

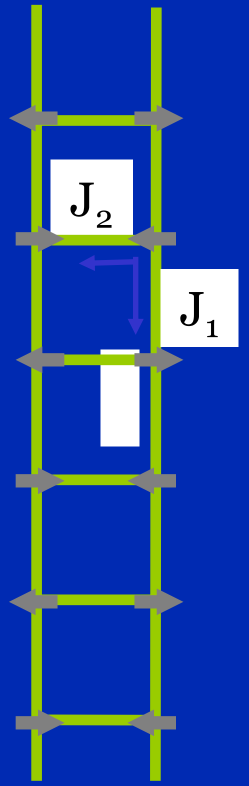
Examples: High Tc's; MnO; MnF_2;
telephone number compound



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

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

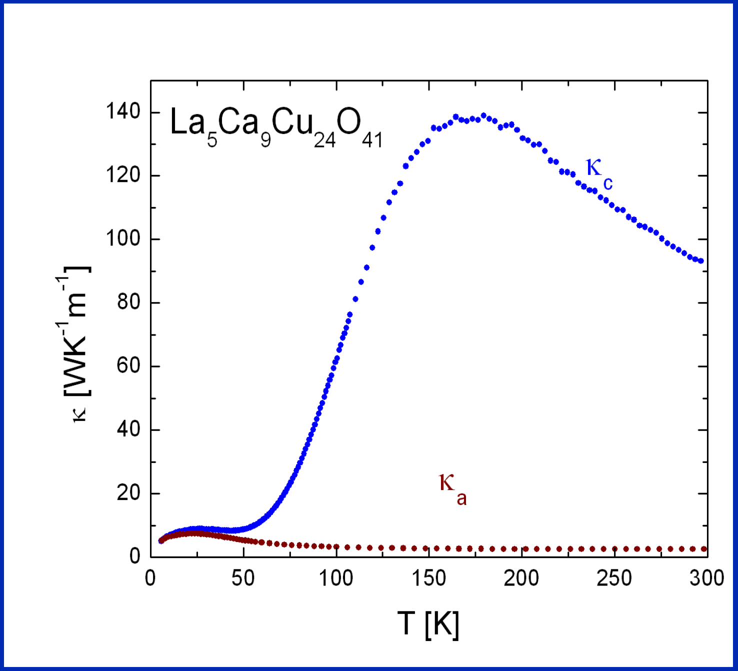


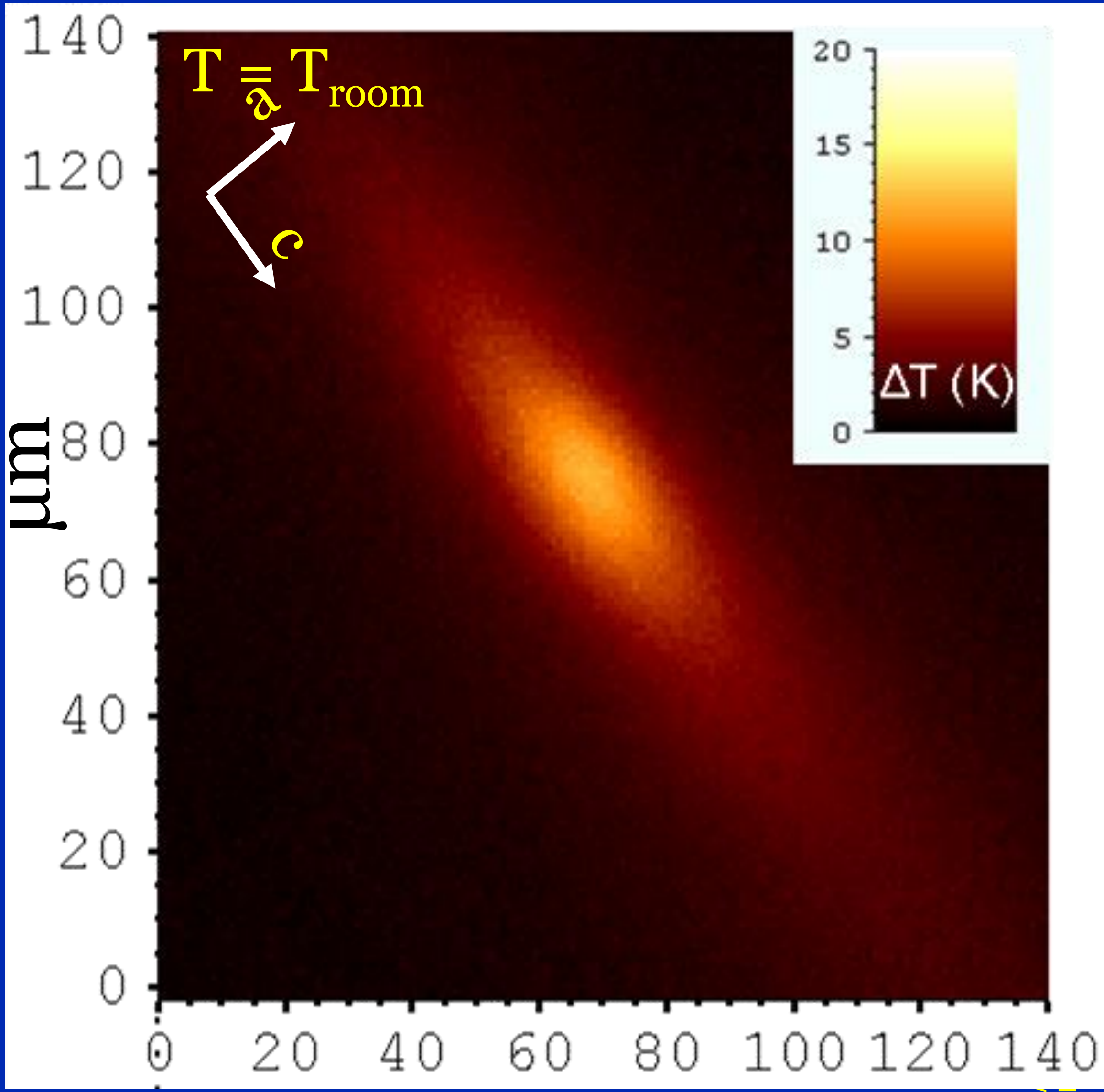


J_1=130 meV
J_2= 70 meV
Δ=32 meV

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

$La_9Ca_5Cu_{24}O_{41}$

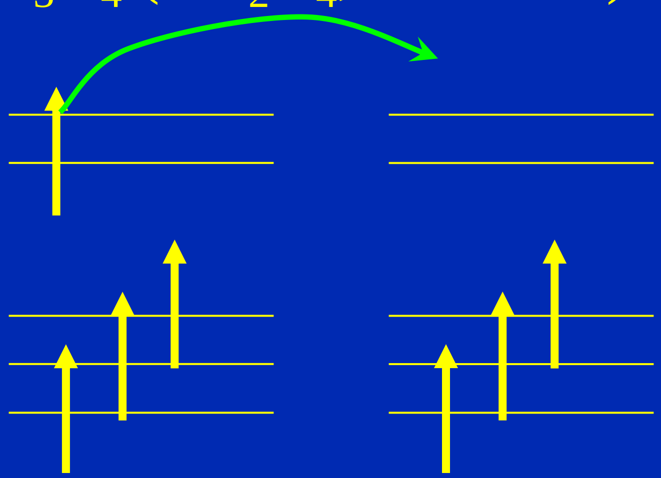




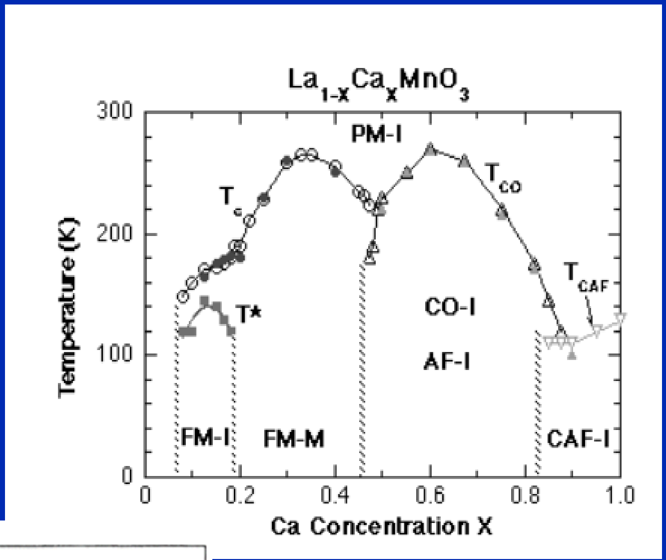
OCMP 2008

Double exchange

- Mixed valency
- Usually ferro metal
- Relatively strong
- $La_{1-x}Sr_xMnO_3$ (Mn^{3+}/Mn^{4+})
  Fe_3O_4 (AB_2O_4, Fe^{2+}/Fe^{3+})



Mn^{3+} Mn^{4+}



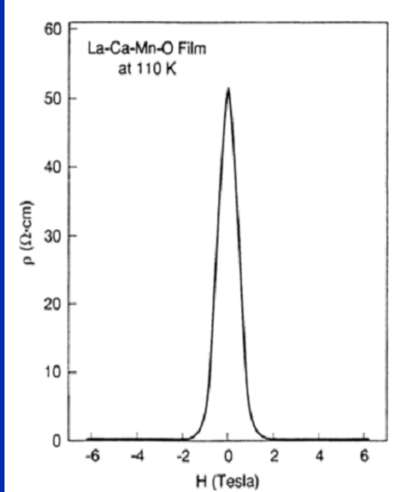


Figure 1. Resistivity versus field curve for the La-Ca-Mn-O film at 110 K.

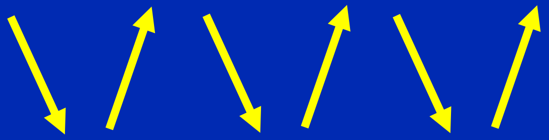
PM-I paramagnetic insulator
FM-M ferromagnetic metal
FM-I ferromagnetic insulator
CO-I charge-ordered insulator
CAF-I canted antiferromagnetic insulator

Fujishiro and co-workers

CMR in para phase close to T_{curie}

Anisotropic exchange

- Dzyaloshinsky-Moriya interaction
- Mixing in of excited d-states
- LS coupling in excited state
- If spins inversion symm. related then 0
- From different from Heisenberg: $\vec{D} \cdot \vec{S}_i \times \vec{S}_j$
- Favors perpendicular alignment
- Examples: α-Fe_2O_3, $MnCO_3$
- In AF's leads to net moment → weak ferro



Multiferroics

nature materials | VOL 6 | JANUARY 2007 |

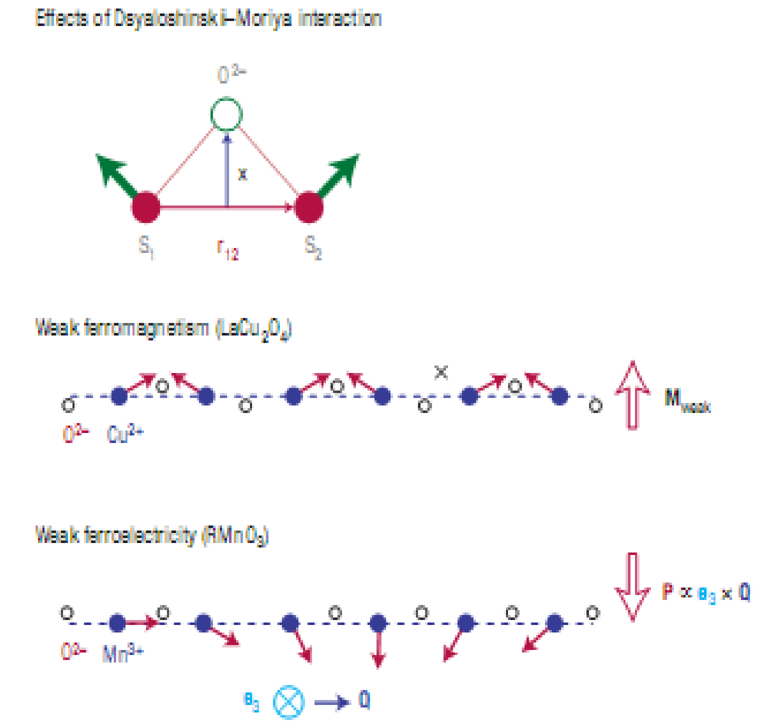
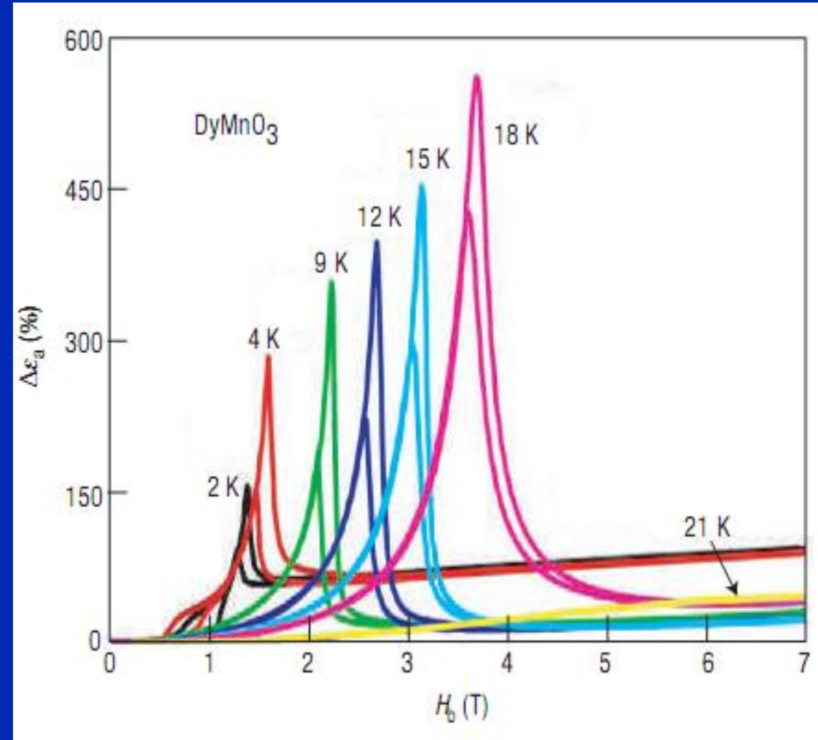


Figure 5 Effects of the antisymmetric Dzyaloshinskii–Moriya interaction. The interaction $H_{DM} = \mathbf{D}_{12} \cdot [\mathbf{S}_1 \times \mathbf{S}_2]$. The Dzyaloshinskii vector $\mathbf{D}_{12}$ is proportional to spin-orbit coupling constant λ, and depends on the position of the oxygen ion (open circle) between two magnetic transition metal ions (filled circles), $\mathbf{D}_{12} \propto \lambda \mathbf{x} \times \hat{\mathbf{r}}_{12}$. Weak ferromagnetism in antiferromagnets (for example, $LaCu_2O_4$ layers) results from the alternating Dzyaloshinskii vector, whereas (weak) ferroelectricity can be induced by the exchange striction in a magnetic spiral state, which pushes negative oxygen ions in one direction transverse to the spin chain formed by positive transition metal ions.



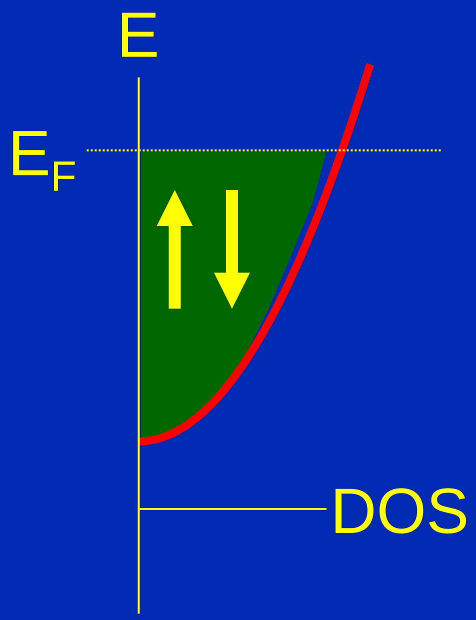
$$\mathbf{P} \propto [(\mathbf{M} \cdot \partial)\mathbf{M} - \mathbf{M}(\partial \cdot \mathbf{M})] .$$

Mostovoy & Cheong

Magnetism in metals

Free electron gas

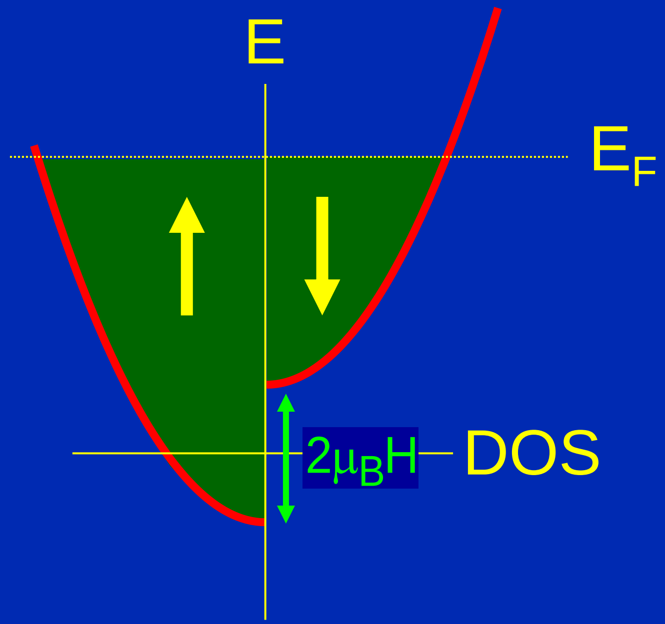
No field: $E = \frac{\hbar^2 k^2}{2m^*}$ $\qquad E_F = \frac{\hbar^2}{2m^*}\left(3\pi^2 n\right)^{2/3}$ $\qquad D(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}$



- Pauli paramagnetism, Landau diamagnetism
- Curie-like (E_F~kT)
- Spontaneous spin polarization (Stoner)
- RKKY

Pauli paramagnetism

$\mathrm{H} \neq 0:$ $\quad E = \dfrac{\hbar^2 k^2}{2m^*} \pm \dfrac{1}{2} g_0 \mu_B H$



$$N_\uparrow = \frac{1}{2} \int_{-\mu_B}^{E_F} D(E + \mu_B H)\, dE$$

$$\approx \frac{1}{2} \left(\int_0^{E_F} D(E)\, dE + \mu_B H \cdot D(E_F) \right)$$

$$N_\downarrow \approx \frac{1}{2} \left(\int_0^{E_F} D(E)\, dE - \mu_B H \cdot D(E_F) \right)$$

Pauli: $M = \mu_B (N_\uparrow - N_\downarrow)$

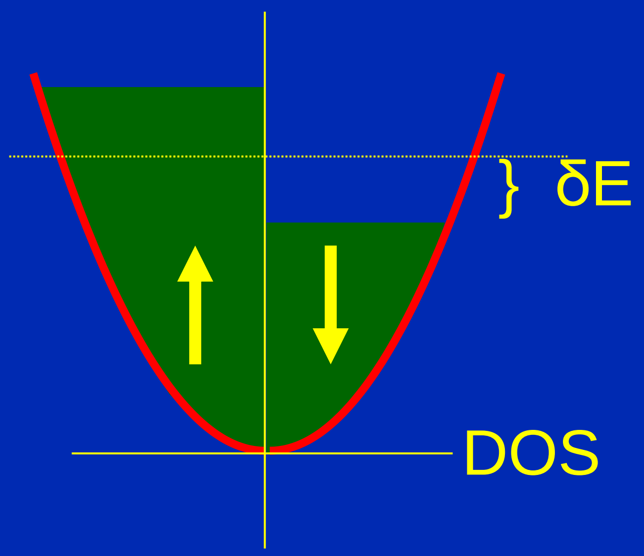
$$= \mu_B^2 D(E_F) H = \frac{3n\mu_B^2}{2kT_F} H$$

Landau (dia): $M = -\dfrac{n\mu_B^2}{2kT_F} H$

$\Rightarrow$ $$\chi_e = \frac{n\mu_B^2}{kT_F}$$

Stoner magnetism

Spontaneous spin polarization



If spin split then 'internal' field $H = \lambda M$

Cost in kinetic energy : $\Delta E_k = \frac{1}{2}\left[D(E_F)\cdot\delta E\right]\cdot\delta E$

Magnetization :

$$n_\uparrow = \frac{1}{2}\left(n + D(E_F)\cdot\delta E\right); \qquad n_\downarrow = \frac{1}{2}\left(n - D(E_F)\cdot\delta E\right)$$

$$M = \mu_B(n_\uparrow - n_\downarrow) = \mu_B D(E_F)\cdot\delta E$$

Field energy

$$\Delta E_p = -\int_0^M B\,dM' = -\int_0^M \mu_0(\lambda M')\,dM' = -\frac{1}{2}\mu_0\lambda M^2$$

$$= -\frac{1}{2}\mu_0\mu_B^2\lambda(n_\uparrow - n_\downarrow)^2 = -\frac{1}{2}U(n_\uparrow - n_\downarrow)^2 = -\frac{1}{2}U\left[D(E_F)\cdot\delta E\right]^2$$

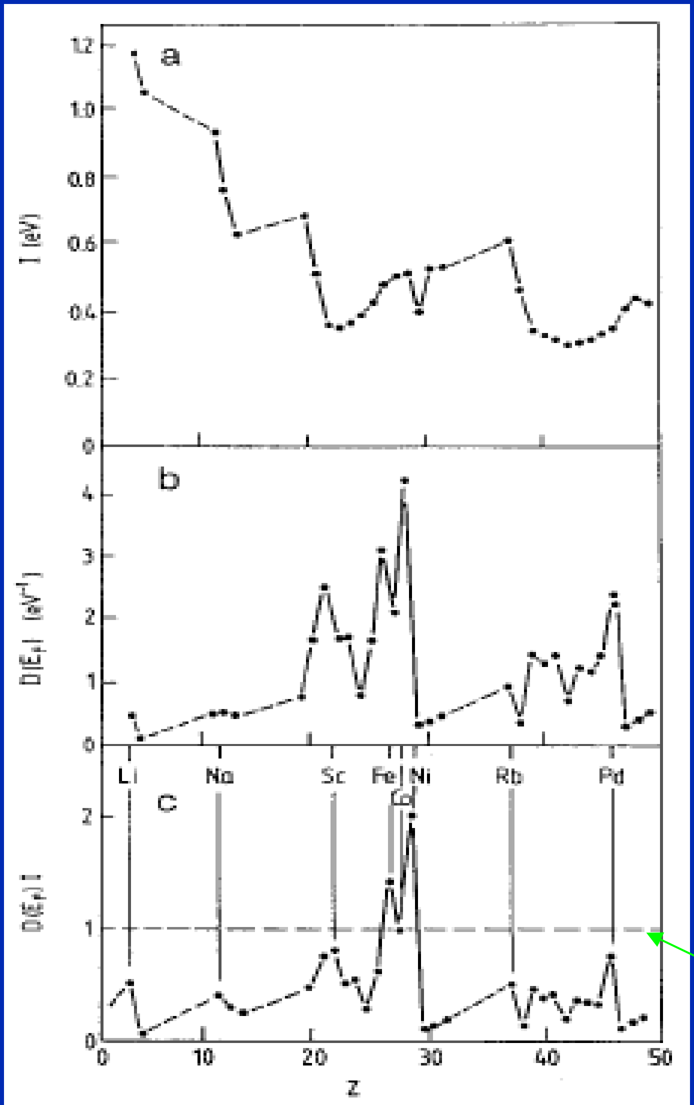
Total energy $\Delta E_{tot} = \Delta E_k + \Delta E_p$

$$\Delta E_{tot} = \frac{1}{2}D(E_F)\cdot\delta E^2\left[1 - UD(E_F)\right]$$

If $\left[1 - UD(E_F)\right] < 0$ then $\Delta E_{tot} < 0 \Rightarrow$ Magnetic ground state

Happens for strong Coulomb and high D.O.S.

Stoner criterium



Exchange interaction

Density of States at E_F

Product

In agreement with
Fe, Ni, Co ferromagnets

Stoner criterium

Stoner magnetism

- If $UD(E_F)<1$ then still change in susceptibility

$$\text{Total energy } \Delta E_{tot} = \Delta E_k + \Delta E_p - MB$$

$$M = \mu_B (n_\uparrow - n_\downarrow) = \mu_B D(E_F) \cdot \delta E$$

$$\Delta E_{tot} = \frac{1}{2} \frac{M^2}{\mu_B^2 D(E_F)} \left[1 - UD(E_F)\right] - M \cdot B$$

Minimizati on w.r.t. M leads to

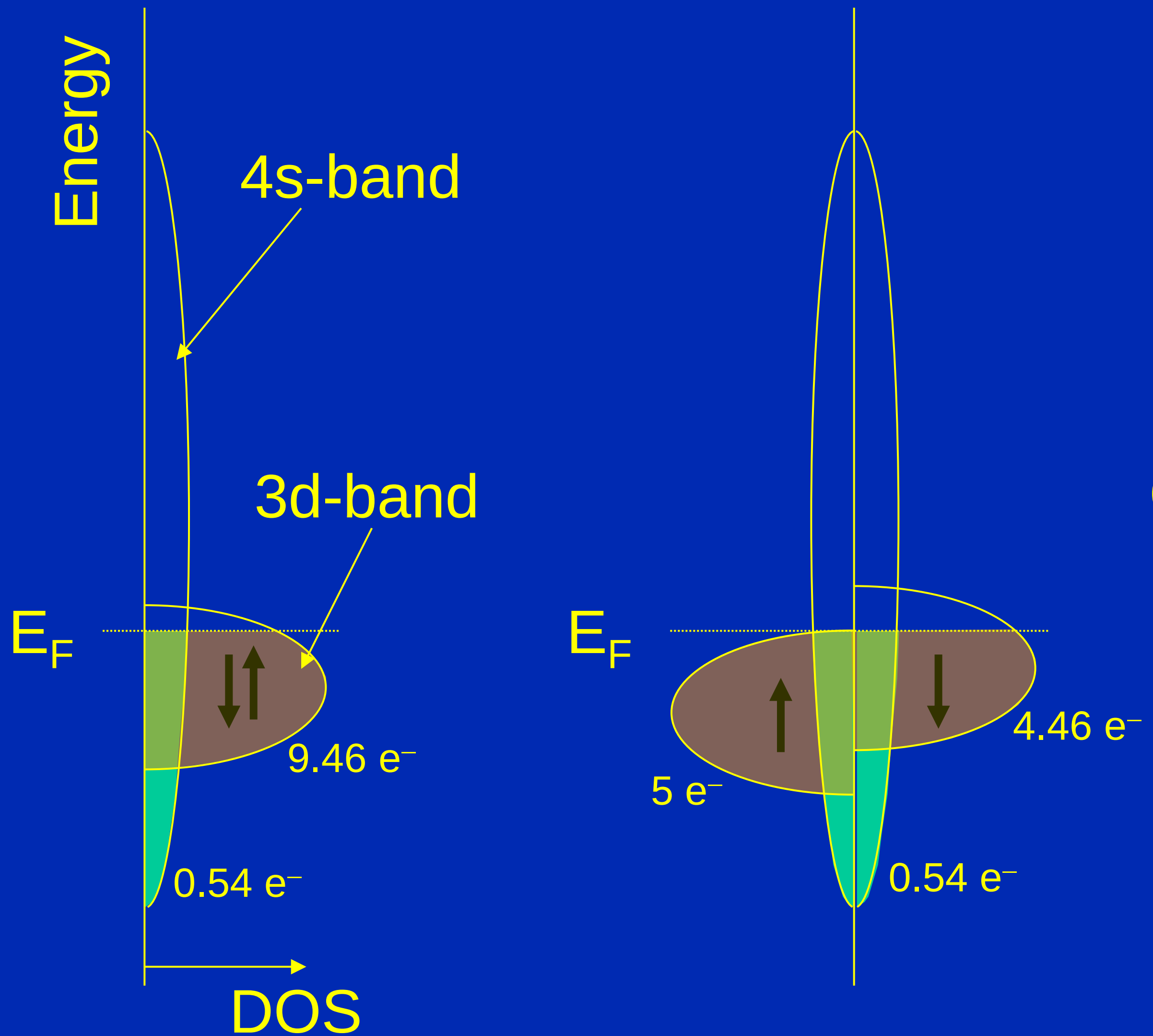
$$M = \frac{\mu_B^2 D(E_F)}{\left[1 - UD(E_F)\right]} B$$

Susceptibi lity $\chi = M/H = M/(B/\mu_0)$

$$\chi = \frac{\mu_0 \mu_B^2 D(E_F)}{\left[1 - UD(E_F)\right]} = \frac{\chi_{Pauli}}{\left[1 - UD(E_F)\right]}$$

$\Rightarrow$ Enhanced susceptibi lity

Conduction electrons

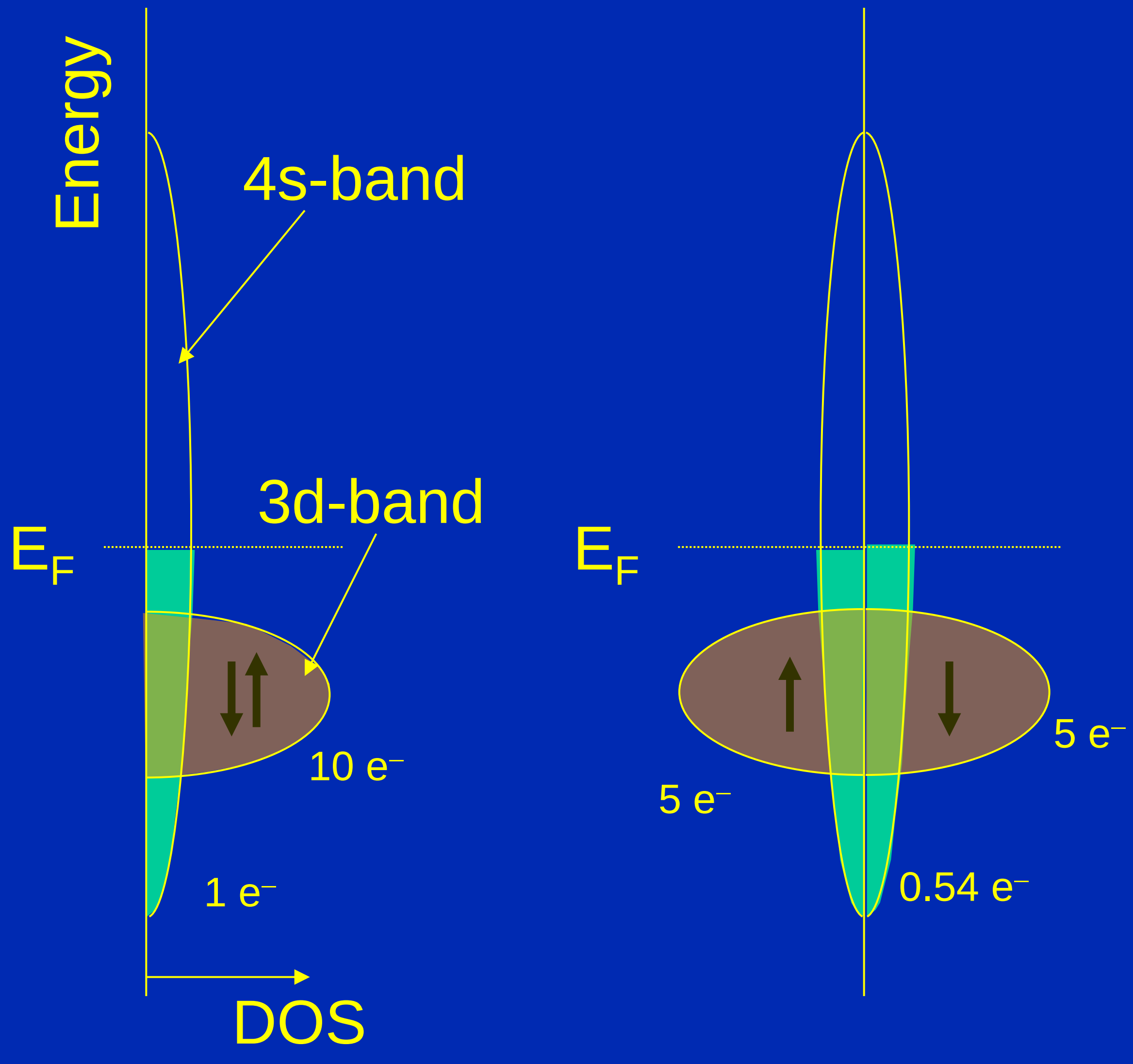


Ni $3d^8 4s^2$

Net magnetization due to d-band:

$$(5-4.46)\mu_B = 0.54\mu_B$$

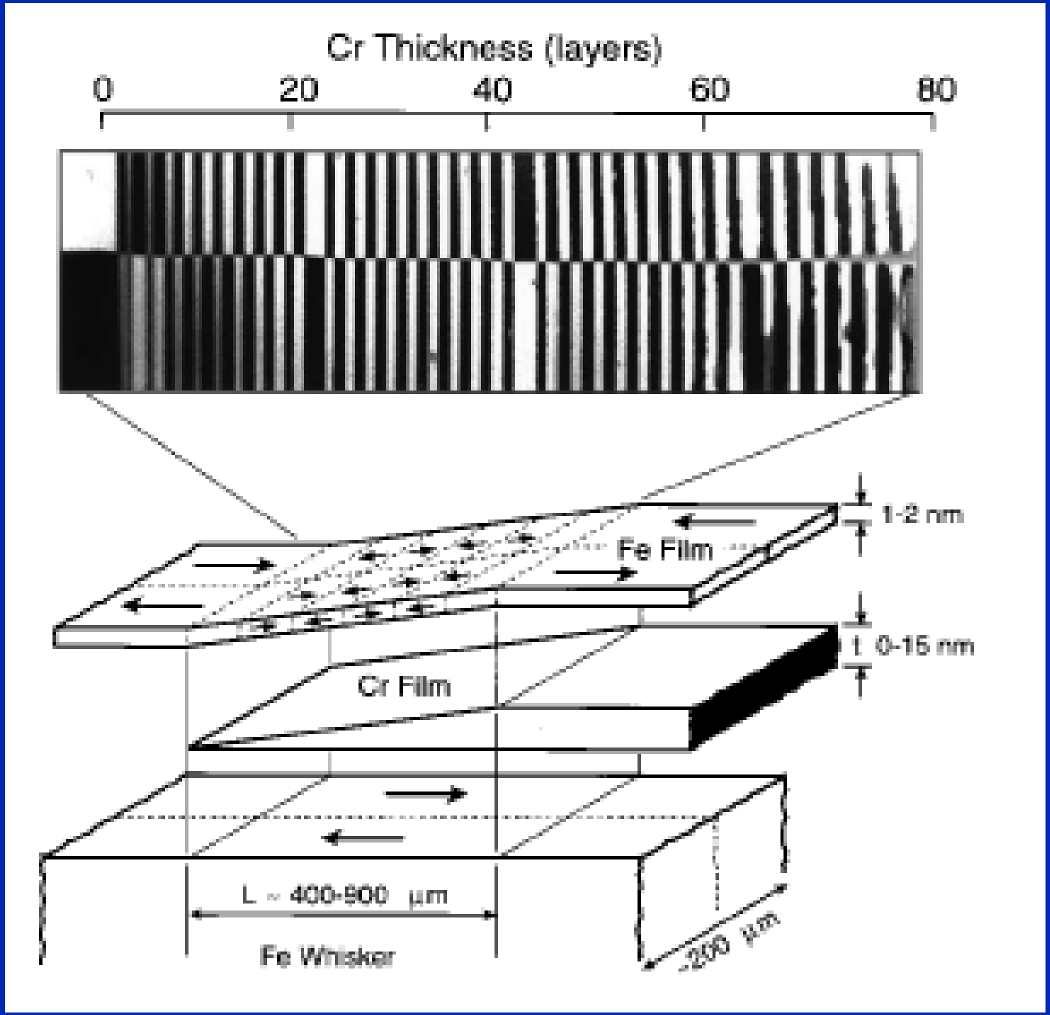
Conduction electrons

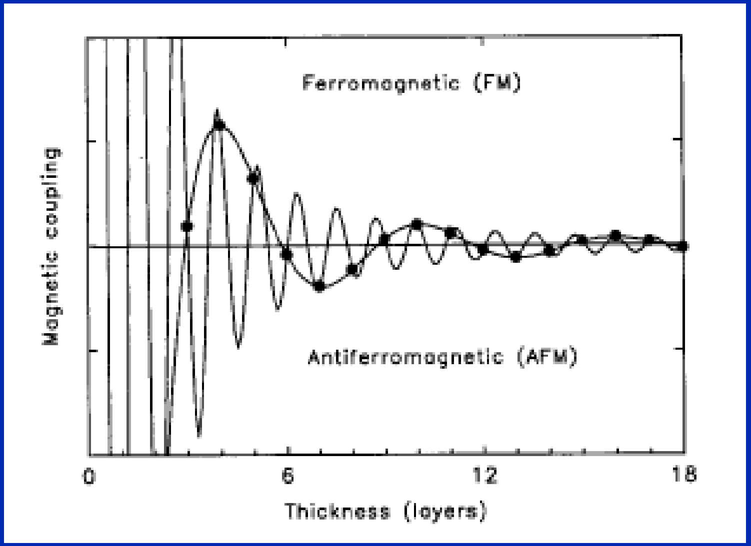


Cu $3d^{10}4s^{1}$

d-DOS at E_F is zero
No net magnetization

RKKY interaction





RKKY interaction

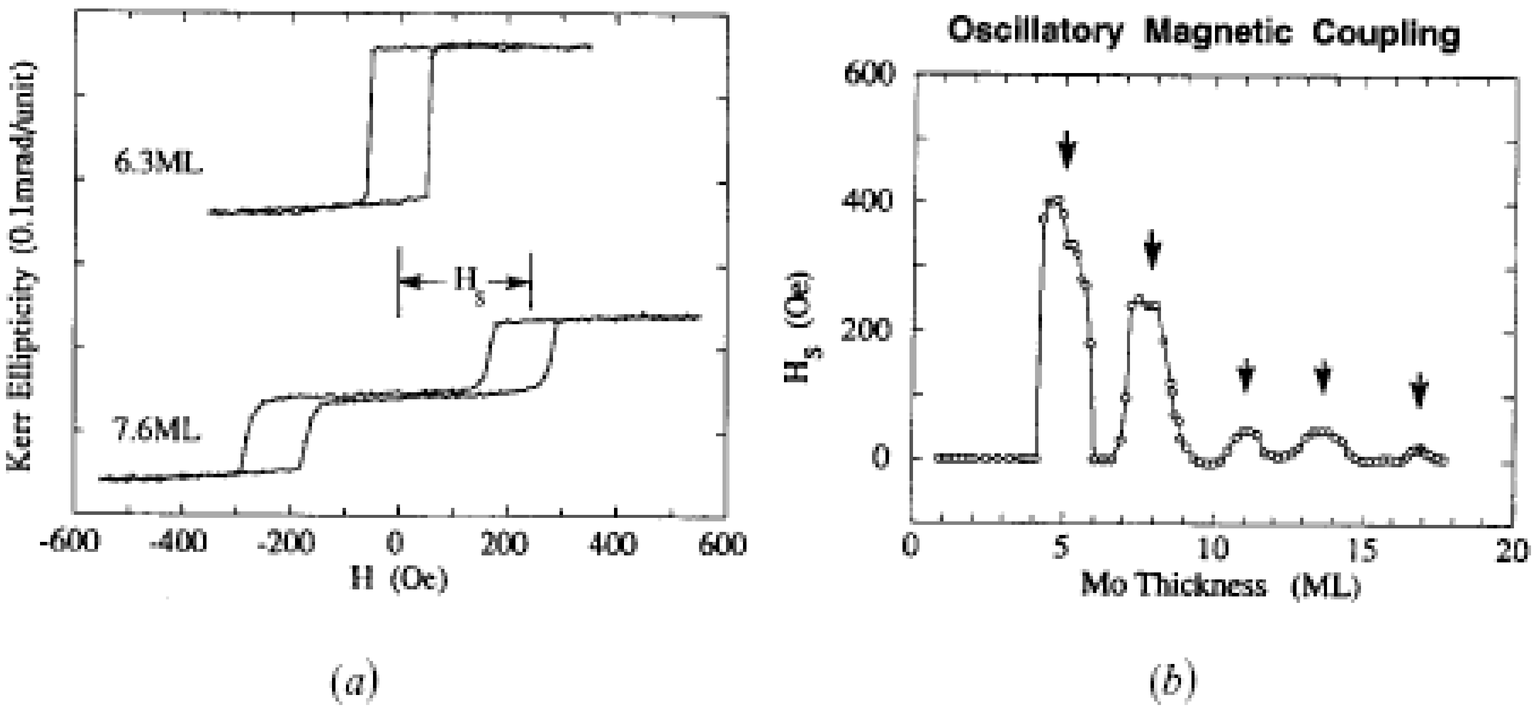
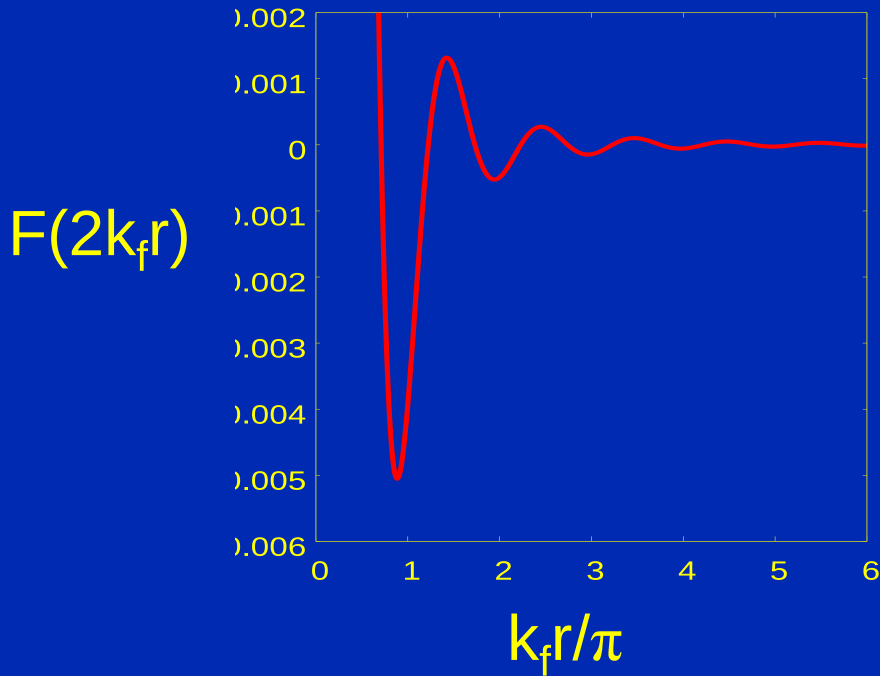


Figure 38. Magnetic oscillations at Fe/Mo/Fe(100) trilayers determined by the SMOKE (Qiu *et al.* 1992b). (*a*) Hysteresis loops characteristic of parallel and antiparallel coupling (top and bottom). H_s is the magnetic field required to force antiparallel layers parallel. Adding just slightly more than a monolayer to the Mo spacer reverses the magnetic orientation. (*b*) Alternating antiparallel and parallel coupling (arrows and baseline respectively).

Spatially varying fields

- RKKY interaction *(Ruderman-Kittel-Kasuya-Yosida)*



$$H(r) = H\,\delta(r)$$

$$\chi(r) = \frac{2}{\pi} k_f^3 \chi_{pauli} F(2k_f r) \overset{x>>1}{=} -\frac{2}{\pi} k_f^3 \chi_{pauli} \frac{\cos(2k_f r)}{\left(2k_f r\right)^3}$$

Ferromagnetic magnons

Magnetic energy (Heisenberg) $U = -2J\sum_{i} \vec{S}_i \cdot \vec{S}_{i+1}$

In groundstate (classical S) ↑↑↑↑↑↑↑↑↑ $U_0 = -2JNS^2$

First excited state ? ↑↑↑↑↓↑↑↑↑ $U = U_0 + 8JS^2$

No !
share spin-flip
with all ⇒ Magnons