Lecture 1-3

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PHYSICS OF EXCHANGE INTERACTIONS

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PHYSICS OF EXCHANGE (SPIN DEPENDENT) INTERACTIONS

between:

- band (itinerant) carriers
- band carriers and localised spins
- localised spins

OUTLINE

0. Preliminaries
1. Why one-electron approximation is often valid
2. Source of electron correlation
   -- Coulomb repulsion
   -- statistical forces
3. Correlation energy
4. Potential exchange
   -- localised states
   -- extended states

Bloch vs. Stoner models of itinerant ferromagnetism

5. Kinetic exchange

Kondo hamiltonian

6. Experimental example: DMS

7. Double exchange

8. Indirect exchange between localised spins

-- *via* carrier spin polarisation

Zener model, RKKY

-- *via* valence bands'/*d* orbitals' spin polarisation

Blombergen-Rowland mechanism, superexchange

Literature

➔ general

- *Y. Yoshida, Theory of Magnetism (Springer 1998)*
- *R.M. White, Quantum Theory of Magnetism (McGrown-Hill 1970)*
- *J.B. Goodenough, Magnetism and chemical bond (Wiley 1963)*

➔ DMS

- *TD, in: Handbook on Semiconductors, vol. 3B ed. T.S. Moss (Elsevier, Amsterdam 1994) p. 1251.*
- *P. Kacman, Semicond.Sci.Technol., 2001, 16, R25-R39.*

➔ ferromagnetic DMS

- *F. Matsukura, H. Ohno, TD, in: Handbook of Magnetic Materials, vol. 14, Ed. K.H.J. Buschow, (Elsevier, Amsterdam 2002) p. 1*
- *„Spintronics" vol. 82 of Semiconductors and Semimetals eds. T. Dietl, D. D. Awschalom, M. Kaminska, H. Ohno (Elsevier 2008)*

Preliminaries

Dipole-dipole interactions

(classical int. between magnetic moments)

$\mu = - g_{\mathrm{eff}} \mu_B S, \qquad H_{ab} = \mu_a \mu_b / r_{ab}^3 - 3(\mu_a \mathbf{r}_{ab})(\mu_a \mathbf{r}_{ab}) / r_{ab}^5$

for $S = 1/2$, $r_{ab} = 0.15$ nm =>

$E_{dd} = 2\mu_a \mu_b / r_{ab}^3 = 0.5 \text{ K} = 0.4 \text{ T}$

$(E = k_B T \text{ or } E = g \mu_B B)$

⇒ **non-scalar**

=> **long range** => remanence, demagnetization, domain structure, EPR linewidth, fringing fields in hybrid structures, …

⇒ **too weak to explain magnitude of spin-spin interactions**

➔ ***quantum effects: Pauli exclusion principle + Coulomb int.***

Exchange interaction

$$H_{ab} = - \boldsymbol{S}_a \mathcal{J}(\boldsymbol{r}_a, \boldsymbol{r}_b) \boldsymbol{S}_b$$

potential energy depends on spins' directions

potential exchange

kinetic energy depends on spins' directions

kinetic exchange

One electron approximation

Why one electron approximation is often valid?

- Quasi-particle concept: $m^* \rightarrow m^{**}$ -

  -- one-electron theory can be used (interaction renormalizes only the parameters of the spectrum)
- Correlation energy of e-e interaction is the same in initial and finite state

  -- center mass motion only affected by the probe (Kohn theorem)

  -- z-component of total spin affected (Yafet theorem)

- Momentum and (for spherical Fermi surface) velocity is conserved in e-e collisions

- Total Coulomb energy of neutral solid with randomly distributed charges is zero

Electrostatic Coulomb interactions in solids

- Two energies
  => **positive**: repulsion between positive charges
  => **negative**: attraction between negative and positive charges

- Neutrality => number of positive and negative charges equal

- Partial cancellation between the two energies

$$E_C = \tfrac{1}{2}\int d\,\boldsymbol{r}_1\,\rho_p(\boldsymbol{r}_1)\int d\,\boldsymbol{r}_2\,\rho_p(\boldsymbol{r}_2)\,e^2/|\boldsymbol{r}_1-\boldsymbol{r}_2| + \tfrac{1}{2}\int d\,\boldsymbol{r}_1\,\rho_n(\boldsymbol{r}_1)\int d\,\boldsymbol{r}_2\,\rho_n(\boldsymbol{r}_2)\,e^2/|\boldsymbol{r}_1-\boldsymbol{r}_2| - \int d\,\boldsymbol{r}_1\,\rho_p(\boldsymbol{r}_1)\int d\,\boldsymbol{r}_2\,\rho_n(\boldsymbol{r}_2)\,e^2/|\boldsymbol{r}_1-\boldsymbol{r}_2|$$

… the number of pairs of the like charges is $N(N-1)/2$

Pair correlation function $g(\boldsymbol{r})$

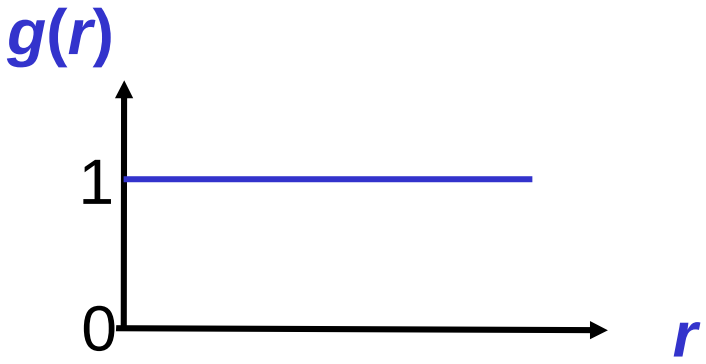
- $g(\boldsymbol{r})$ probability of finding another particle at distance $\boldsymbol{r}$ in the volume d$\boldsymbol{r}$

pair correlation function

- normalization: $\int d\boldsymbol{r}\, \rho\, g(\boldsymbol{r}) = N - 1$

- an example:

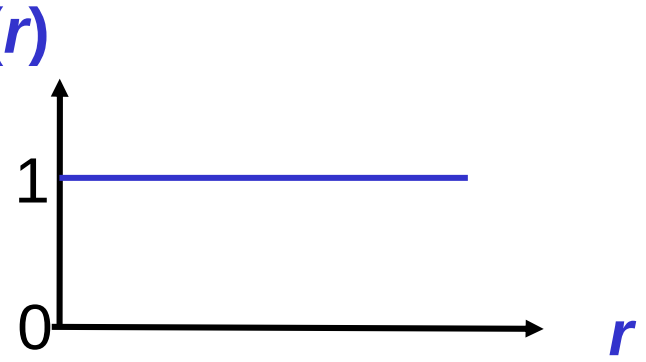
random (uncorrelated distribution):



Total Coulomb energy for random distribution of charges

- For random distribution of charges, $\rho = N_p/V = N_n/V$

pair correlation function



$$E_C = \tfrac{1}{2}\int d\,\boldsymbol{r}_1\,\rho_p(\boldsymbol{r}_1)\int d\,\boldsymbol{r}_2\,\rho_p(\boldsymbol{r}_2)\,e^2/|\,\boldsymbol{r}_1 - \boldsymbol{r}_2\,| + \tfrac{1}{2}\int d\,\boldsymbol{r}_1\,\rho_n(\boldsymbol{r}_1)\int d\,\boldsymbol{r}_2\,\rho_n(\boldsymbol{r}_2)\,e^2/|\,\boldsymbol{r}_1 - \boldsymbol{r}_2\,| + - \int d\,\boldsymbol{r}_1\,\rho_p(\boldsymbol{r}_1)\int d\,\boldsymbol{r}_2\,\rho_n(\boldsymbol{r}_2)\,e^2/|\,\boldsymbol{r}_1 - \boldsymbol{r}_2\,| = 0!$$

=> Coulomb energy contributes to the total energy of the system and one-electron approximation ceases to be valid if the motion of charges is **correlated**

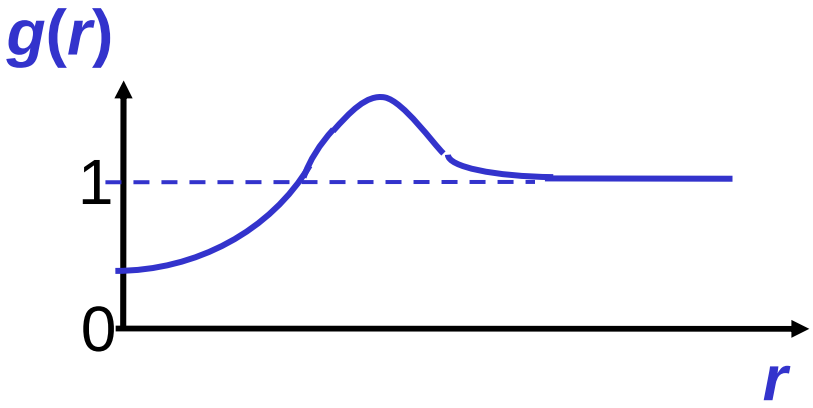
Origin of correlations

Sources of correlation

(why motion and distribution of charges may not be independent)

- Coulomb interaction itself:
  - -- H^-
  - -- exciton
  - -- ionic crystals
  - -- Wigner crystals
  - -- Laughlin liquid
  - -- ….

Coulomb gap in g(r)



Spin and statistics in quantum mechanics

The core of quantum mechanics:

- principle of linear superposition of wave functions, also of a **single** particle => interference
  (Young experiment works with a single photon, electron, …)

- not all the solutions of a given Schroedinger equation (wave functions) represents states: *initial and boundary conditions*

- wave function of a system of many **identical** particle is (must be):
  -- symmetric against permutation of two particles if their spin is muliple of $h/2\pi$
  - bosons ➔ superconductivity, superfluidity, B-E condensation, ...

  -- antisymmetric otherwise
  - fermions ➔ nucleus, chemistry, magnetism, …..

Statistical transmutation, fractional statistics, ...

Many-fermion wave function

- $H = \Sigma_{l=1 \text{ to } N} H_i + V(\boldsymbol{r}^{(1)},.., \boldsymbol{r}^{(N)})$

Since $\Psi_A(\boldsymbol{r}^{(1)},.., \boldsymbol{r}_1^{(k)},...,\boldsymbol{r}_2^{(m)},..., \boldsymbol{r}^{(N)}) = -\Psi_A(\boldsymbol{r}^{(1)},.., \boldsymbol{r}_2^{(k)},...,\boldsymbol{r}_1^{(m)},..., \boldsymbol{r}^{(N)})$

=> the probability of finding two fermions in the same place is zero

Correlation:

Fermions (with the same spin) avoid each other

Sources of correlation

(why motion and distribution of charges may not be independent)

- Coulomb interaction itself:

  -- H^-

  -- exciton

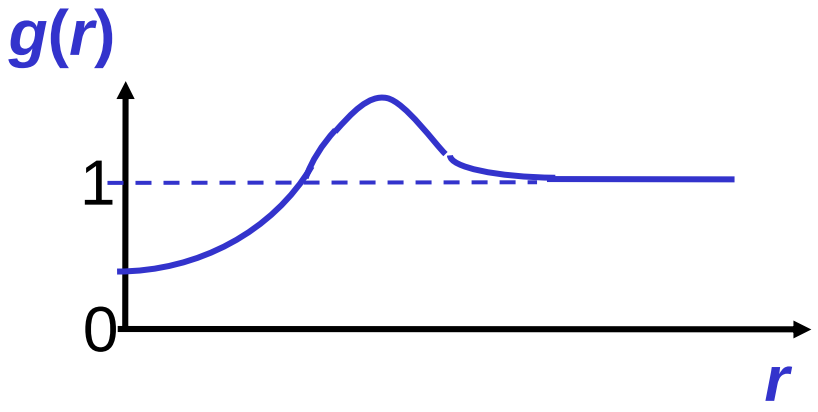
  -- ionic crystals

  -- Wigner crystals

  -- Laughlin liquid

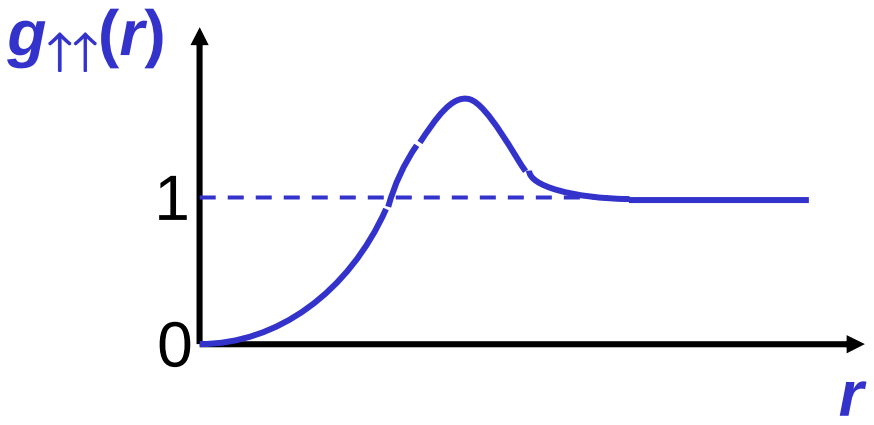
  -- ….

  Coulomb gap in g(r)



- Pauli exclusion principle

  Exchange gap in g(r)



Construction of many body wave function

- ***principle of linear superposition***
- **not all the solutions of a given Schroedinger equation (wave functions) represent a state: *initial and boundary conditions***
- **wave function of a system of many fermion system is (must be) *antisymmetric***

In the spirit of perturbation theory (Hartree-Fock approximation):

=> energy calculated from wave functions of noniteracting electrons, i.e.:

$H = \Sigma_i H_i$; $H_i = H_i(\boldsymbol{r}^{(i)})$ and thus:

- one-electron states are identical for all electrons
- many-electron wave function: the product of one-electron wave functions

consider a state *A* of *N* electrons distributed over α_N states

$$\Psi_A(\boldsymbol{r}^{(1)},.., \boldsymbol{r}^{(k)},..., \boldsymbol{r}^{(m)},..., \boldsymbol{r}^{(N)}) = \psi_{a1}(\boldsymbol{r}^{(1)})\ldots\psi_{ak}(\boldsymbol{r}^{(k)})\ldots\psi_{am}(\boldsymbol{r}^{(m)})\ldots\psi_{aN}(\boldsymbol{r}^{(N)})$$

also $\Psi_{A'}(\boldsymbol{r}^{(1)},.., \boldsymbol{r}^{(m)},..., \boldsymbol{r}^{(k)},..., \boldsymbol{r}^{(N)}) = \psi_{a1}(\boldsymbol{r}^{(1)})\ldots\psi_{am}(\boldsymbol{r}^{(k)})\ldots\psi_{ak}(\boldsymbol{r}^{(m)})\ldots\psi_{aN}(\boldsymbol{r}^{(N)}),$

and all such wave functions **and** their linear superpositions correspond to the situation *A* (<u>all electrons are identical</u>!) and fulfilled Schroedinger equation giving the same eigenvalue (total energy)

Which of those wave functions represent a many electron state?

The wave function has to be antisymmetric =>

Slater determinant

$$\Psi_A = 1/\sqrt{N!} \begin{vmatrix} \psi_{a1}(\boldsymbol{r}^{(1)}) & \dots & \psi_{a1}(\boldsymbol{r}^{(k)}) & \dots & \psi_{a1}(\boldsymbol{r}^{(m)}) & \dots & \psi_{a1}(\boldsymbol{r}^{(N)}) \\ \dots & & & & & & \\ \psi_{ak}(\boldsymbol{r}^{(1)}) & \dots & \psi_{ak}(\boldsymbol{r}^{(k)}) & \dots & \psi_{ak}(\boldsymbol{r}^{(m)}) & \dots & \psi_{a1}(\boldsymbol{r}^{(N)}) \\ \dots & & & & & & \\ \psi_{am}(\boldsymbol{r}^{(1)}) & \dots & \psi_{am}(\boldsymbol{r}^{(k)}) & \dots & \psi_{am}(\boldsymbol{r}^{(m)}) & \dots & \psi_{am}(\boldsymbol{r}^{(N)}) \\ \dots & & & & & & \\ \psi_{aN}(\boldsymbol{r}^{(1)}) & \dots & \psi_{aN}(\boldsymbol{r}^{(k)}) & \dots & \psi_{aN}(\boldsymbol{r}^{(m)}) & \dots & \psi_{aN}(\boldsymbol{r}^{(N)}) \end{vmatrix}$$

$\Psi_A(.., \boldsymbol{r_1}^{(k)},..., \boldsymbol{r_2}^{(m)},...) = -\Psi_A(.., \boldsymbol{r_2}^{(k)},..., \boldsymbol{r_1}^{(m)},...)$ -- OK

$\Psi_A(.., \boldsymbol{r}^{(k)},..., \boldsymbol{r}^{(m)},...) = 0$ if $\alpha_i = \alpha_j$: Pauli exclusion principle

Slater determinant is an approximate wave function… (takes only the presence of exchange gap into account)

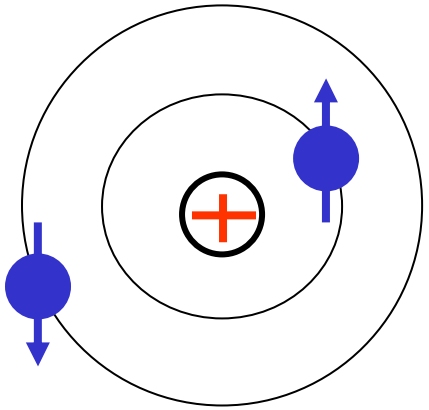
improvements:

- combination of Slater determinants (configuration mixing)
- variational wave function, e.g., Laughlin wave function in FQHE
- ….

Correlation effects for localised states

Energy of two electrons in quantum dots, atoms,...

$$H = H_1 + H_2 + V_{12}$$



Ground state - singlet $1s^2$ (or ^1S)

$$\Psi_s(\mathbf{r}^{(1)},\mathbf{r}^{(2)}) = (\exp[-ar_1-br_2] + \exp[-br_1-ar_2])\,(1+c|\mathbf{r}_2-\mathbf{r}_1|)\,[\downarrow\uparrow - \uparrow\downarrow]/\sqrt{2}$$

a, b, c – variational parameters

For H^- ionisation energy ~0.7 eV

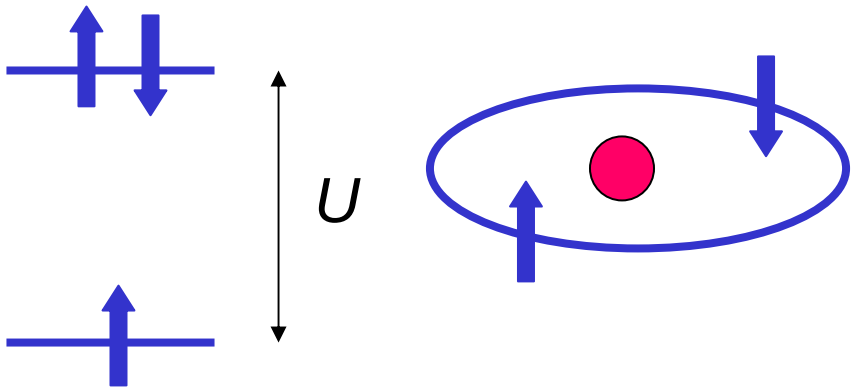
Correlation energy – Hubbard *U*

hydrogen ion H^-

$H = H_1 + H_2 + V_{12}$ for Coulomb interaction $V_{12} = e^2/(\varepsilon|\mathbf{r}_1 - \mathbf{r}_2|)$

$E_1 = E_2 = -1$ Ry

$E_b \approx -0.05$ Ry



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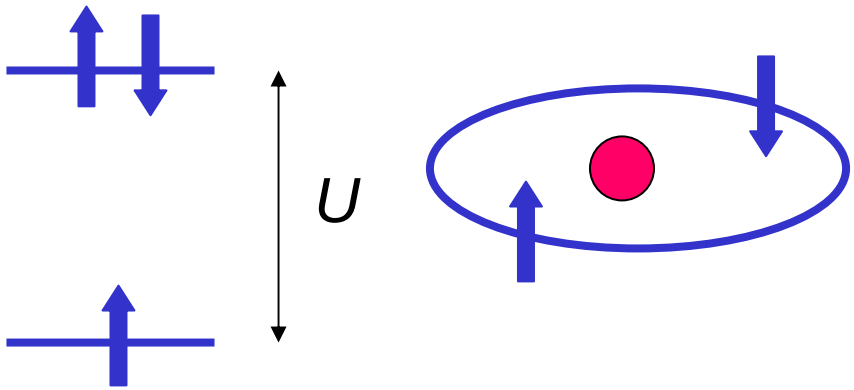
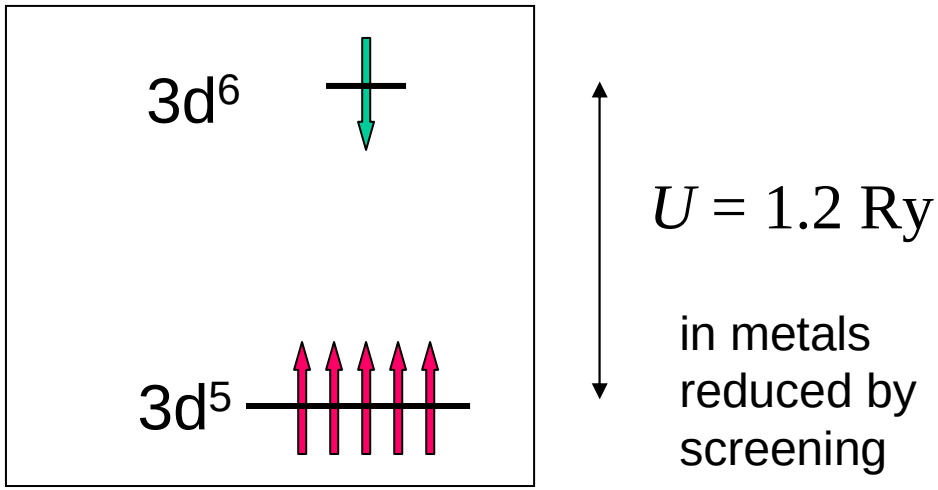


Mn atom



Potential exchange – localised states

Wave function for two electrons in states α and β

e.g., $1s^1 2p^1$ configuration in He

$$\mathrm{H} = H_1 + H_2 + V_{12}$$

Perturbation theory – effect of V_{12} calculated with unperturbed wave functions; antisymmetric combination is chosen

$$\Psi_A(\mathbf{r}^{(1)},\mathbf{r}^{(2)}) = [\,\psi_\alpha(\mathbf{r}^{(1)})\;\psi_\beta(\mathbf{r}^{(2)}) - \psi_\beta(\mathbf{r}^{(1)})\;\psi_\alpha(\mathbf{r}^{(2)})\,]/\sqrt{2}$$

Entangled wave function for two electrons in orbital states α and β taking spin into account:

singlet state: $\Psi_s(\mathbf{r}^{(1)},\mathbf{r}^{(2)}) = [\,\psi_\alpha(\mathbf{r}^{(1)})\;\psi_\beta(\mathbf{r}^{(2)}) + \psi_\beta(\mathbf{r}^{(1)})\;\psi_2(\mathbf{r}^{(2)})]\;[\downarrow\uparrow - \uparrow\downarrow]/2$

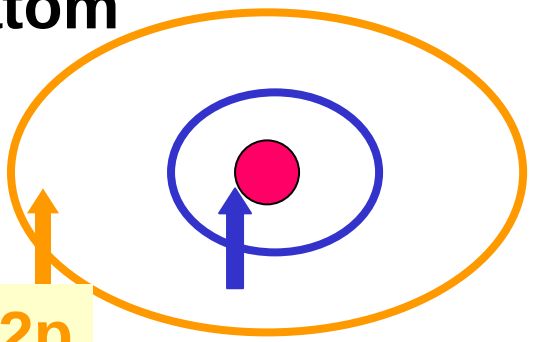
triplet states $\Psi_t(\mathbf{r}^{(1)},\mathbf{r}^{(2)})$ $= [\,\psi_\alpha(\mathbf{r}^{(1)})\;\psi_\beta(\mathbf{r}^{(2)}) - \psi_\beta(\mathbf{r}^{(1)})\;\psi_2(\mathbf{r}^{(2)})]\;\uparrow\uparrow/\sqrt{2}$

$= [\,\psi_\alpha(\mathbf{r}^{(1)})\;\psi_\beta(\mathbf{r}^{(2)}) - \psi_\beta(\mathbf{r}^{(1)})\;\psi_2(\mathbf{r}^{(2)})]\;\downarrow\downarrow/\sqrt{2}$

$= [\,\psi_\alpha(\mathbf{r}^{(1)})\;\psi_\beta(\mathbf{r}^{(2)}) - \psi_\beta(\mathbf{r}^{(1)})\;\psi_2(\mathbf{r}^{(2)})]\;\;[\downarrow\uparrow + \uparrow\downarrow]/2$

Energy for two electrons in states α and β

He atom



$\mathrm{H} = H_1 + H_2 + V_{12}$ ← *Coulomb interaction*

Perturbation theory – effect of V_{12} is calculated with antisymmetric wave functions

singlet state: $E_s = \langle\Psi_s | \mathrm{H} | \Psi_s\rangle = E_\alpha + E_\beta + U + J/2$

triplet states: $E_t = \langle\Psi_t | \mathrm{H} | \Psi_t\rangle = E_\alpha + E_\beta + U - J/2$

$U = \int dr^{(1)}\, dr^{(2)}\, V_{12}(r^{(1)}, r^{(2)}) |\psi_\alpha(r^{(1)})|^2 |\psi_\beta(r^{(2)})|^2$ -- *Hartree term*

$J = 2\int dr^{(1)}\, dr^{(2)}\, V_{12}(r^{(1)}, r^{(2)})\, \psi_\alpha(r^{(1)})\, \psi_\beta^*(r^{(1)})\, \psi_\alpha^*(r^{(2)})\, \psi_\beta(r^{(2)}) > 0$ -- *Fock term*

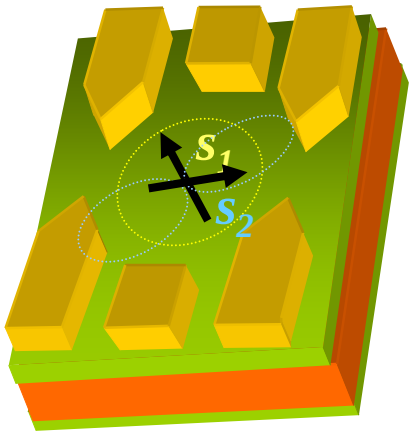
Heisenberg hamiltonian

$E_{s(t)} = E_\alpha + E_\beta + U - J/4 - J\mathbf{s}_1\mathbf{s}_2,$

ferromagnetic ground state (potential exchange)

Properties of exchange interactions

$$H_{ex} = - J s_1 s_2$$



two electrons
in a quantum dot

potential exchange

$$J = 2\int dr^{(1)}\, dr^{(2)}\, e^2/(|(r^{(1)} - r^{(2)}|\varepsilon)\, \psi_\alpha(r^{(1)})\psi^*_\beta(r^{(1)})\psi_\alpha{}^*(r^{(2)})\psi_\beta(r^{(2)})$$

$$= 2\sum_k [4\pi e^2/\varepsilon k^2\,]|\int dr\, \psi_\alpha(r)\psi^*_\beta(r)e^{ikr}|^2 > 0$$

- ferromagnetic
- short range – determined by overlap of wave functions (contrary to U)

Transition metals – free atoms

- **Electronic configuration of TM atoms: $3d^n4s^2$**

  $1 \le n \le 10$: Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn

- **Important role of electron correlation for open d shells**

  - intra site correlation energy $U = E_{n+1} - E_n$

  for $n = 5$, $U \approx 15$ eV

  - intra-site exchange interaction: *ferromagnetic*

  Hund's rule: *S* the highest possible

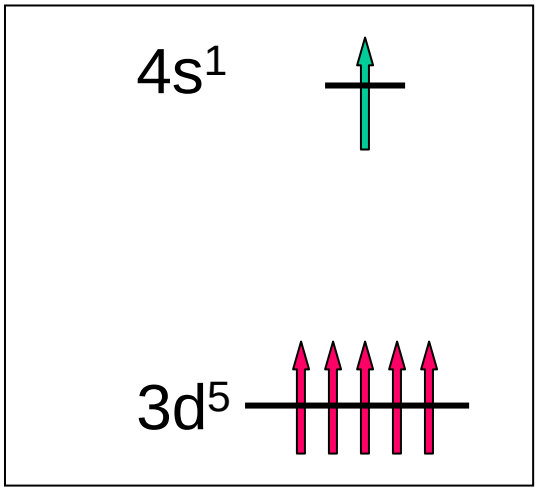
  for $n = 5$, $E_{S=3/2} - E_{S=5/2} \approx 2$ eV

  - TM atoms, $3d^n4s^1$, e.g., Mn:

  $E_{S=2} - E_{S=3} \approx 1.2$ eV ➔ $J_{s\text{-}d} \approx 0.4$ eV *ferromagnetic*

  $[H = -J_{sd}\mathbf{sS}]$

  despite of screening and hybridization these effects survive in solids



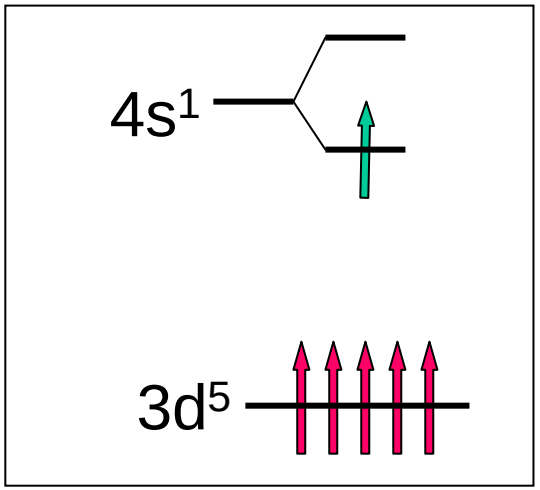
Potential s-d exchange interaction

for singly ionised Mn atom

$J_{4s\text{-}3d}$ = 0.40 eV, $J_{4p\text{-}3d}$ = 0.20 eV

or singly ionised Eu atom

$J_{6s\text{-}4f}$ = 0.052 eV, $J_{5d\text{-}4f}$ = 0.22 eV



in metals/semiconductors with delocalised s band and localised d spins

J_{sd} only slightly reduced by screening:

$$H_{sd} = -\sum_i J_{sd}\boldsymbol{s}(\boldsymbol{r}_i)\boldsymbol{S}_i$$

➔ exchange splitting of c. b., e.g., $Cd_{1-x}Mn_xTe$

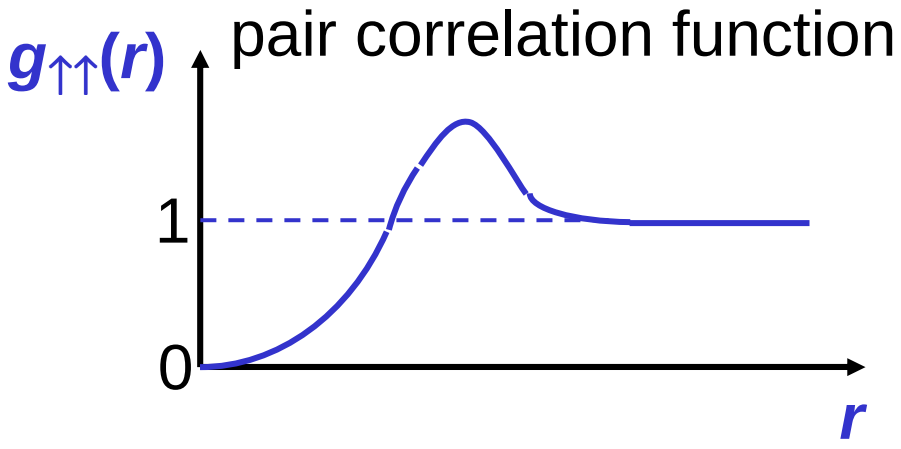
$$\Delta = |x\alpha N_0 <\boldsymbol{S}_i>|; \qquad \alpha N_0 \equiv J_{sd}\,; \quad N_0 \text{ – cation concentration}$$

Potential exchange – extended states

Ferromagnetism of late TM

Exchange energy of electron gas

$$E_{ex} = \int d\boldsymbol{r}\, [g_{\uparrow\uparrow}(\boldsymbol{r})-1] e^2/\varepsilon r$$



Probability (triplet):

$$P_{kk'}(\boldsymbol{r}^{(1)},\boldsymbol{r}^{(2)}) = |\varphi_k(\boldsymbol{r}^{(1)})\, \varphi_{k'}(\boldsymbol{r}^{(2)}) - \varphi_{k'}(\boldsymbol{r}^{(1)})\, \varphi_k(\boldsymbol{r}^{(2)})|^2/2$$

$$P(y) = \int dx P(x) \delta(y - y(x))$$

$$g_{\uparrow\uparrow}(\boldsymbol{r}) = \int d\boldsymbol{r}^{(1)} d\boldsymbol{r}^{(2)} \delta(\boldsymbol{r} - \boldsymbol{r}^{(1)} - d\boldsymbol{r}^{(2)}) \times$$

$$\sum_{kk', < kF} \{|\varphi_k(\boldsymbol{r}^{(1)})\, \varphi_{k'}(\boldsymbol{r}^{(2)})|^2 - \varphi_k(\boldsymbol{r}^{(1)}) \varphi_{k'}^{*}(\boldsymbol{r}^{(1)}) \varphi_{k'}(\boldsymbol{r}^{(2)}) \varphi_k^{*}(\boldsymbol{r}^{(2)})\}$$

$$\varphi_k(\boldsymbol{r}) = \exp(i\boldsymbol{k}\boldsymbol{r})/\sqrt{V}$$

- **exchange energy of electron gas**
  E_{ex} = - 0.916 Ry/(r_s /a_B)

Consequences of fermionic correlation - metals

- **Exchange interaction within the electron gas**

  since the electron with the same spins avoid each other
  the energy of electron-electron repulsion is reduced

$\Rightarrow$ cohesion energy of metals

- kinetic energy of electron gas
  $E_k = (3/5)E_F = 2.2\ \mathrm{Ry}/(r_s/a_B)^2$
- exchange energy of electron gas
  $E_{ex} = -0.916\ \mathrm{Ry}/(r_s/a_B)$

Minimum E_{tot} ➔ $r_s/a_B \approx 1.6$; real metals $2 < r_s/a_B < 6$

=> band-gap narrowing in doped semiconductors

$\Delta E\ [\mathrm{eV}] \approx -e^2/\varepsilon r_s = -1.9\ 10^{-8}\ (p[\mathrm{cm}^{-3}])^{1/3}$

=> enhancement of tendency towards ferromagnetism

tendency towards ferromagnetism

Experimental facts on Fe, Co, Ni

- both *s* and *d* electrons contribute to the Fermi sphere

  -- no localised spins

  ➔ itinerant magnetism

- robust ferromagnetism T_c = 1390 K for Co

Two time honoured models:

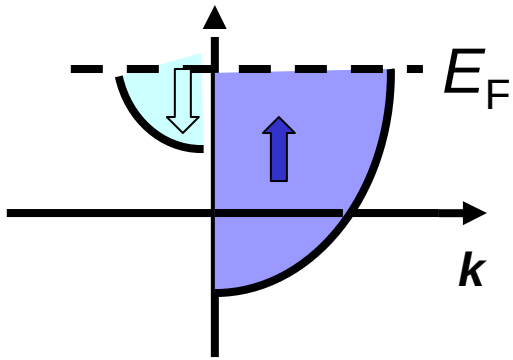
-- Bloch model

-- Stoner model

Bloch model of ferromagnetism

- kinetic energy of electron gas

$$E_k = 2.2\ \mathrm{Ry}/(r_s/a_B)^2[n_\uparrow^{5/3} + n_\downarrow^{5/3}]/[2(n/2)^{5/3}]$$



- exchange energy of electron gas

$$E_{ex} = \int d\boldsymbol{r}\,[g_{\uparrow\uparrow}(\boldsymbol{r})-1]e^2/\varepsilon r + \int d\boldsymbol{r}\,[g_{\downarrow\downarrow}(\boldsymbol{r})-1]e^2/\varepsilon r$$

$$E_{ex} = -\,0.916\ \mathrm{Ry}/(r_s/a_B)[n_\uparrow^{4/3} + n_\downarrow^{4/3}]/[2(n/2)^{4/3}]$$

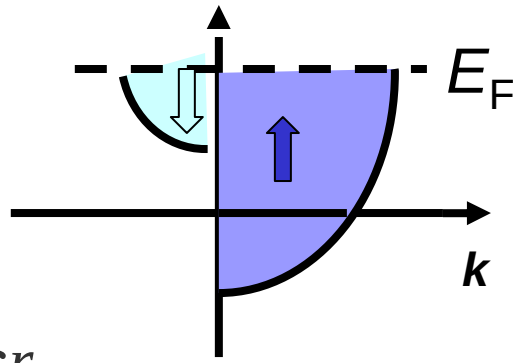
Minimising in respect to $n_\uparrow - n_\downarrow$ at given $n = n_\uparrow + n_\downarrow$

=> ferromagnetism at $r_s/a_B > 5.4$

Stoner model of ferromagnetism

- kinetic energy of electron gas

$$E_k = 2.2\ \mathrm{Ry}/(r_s/a_B)^2[n_\uparrow^{5/3} + n_\downarrow^{5/3}]/[2(n/2)^{5/3}]$$



- exchange energy of electron gas

$$E_{ex} = \int d\boldsymbol{r}\,[g_{\uparrow\uparrow}(\boldsymbol{r}) - 1]e^2/\varepsilon r + \int d\boldsymbol{r}\,[g_{\downarrow\downarrow}(\boldsymbol{r}) - 1]e^2/\varepsilon r$$

$4\pi e^2/[\varepsilon|k_1 - k_2|^2] \rightarrow I/N_0$ [screening]; I - a parameter

$$E_{ex} = -0.69\ \mathrm{Ry}/(r_s/a_B)^2 I[n_\uparrow^2 + n_\downarrow^2]/(nN_0)$$

Minimizing in respect to $n_\uparrow - n_\downarrow$ at given $n = n_\uparrow + n_\downarrow$

=> ferromagnetism at $A_F = \rho(E_F)I/N_0 > 1$

Why these models are not correct?

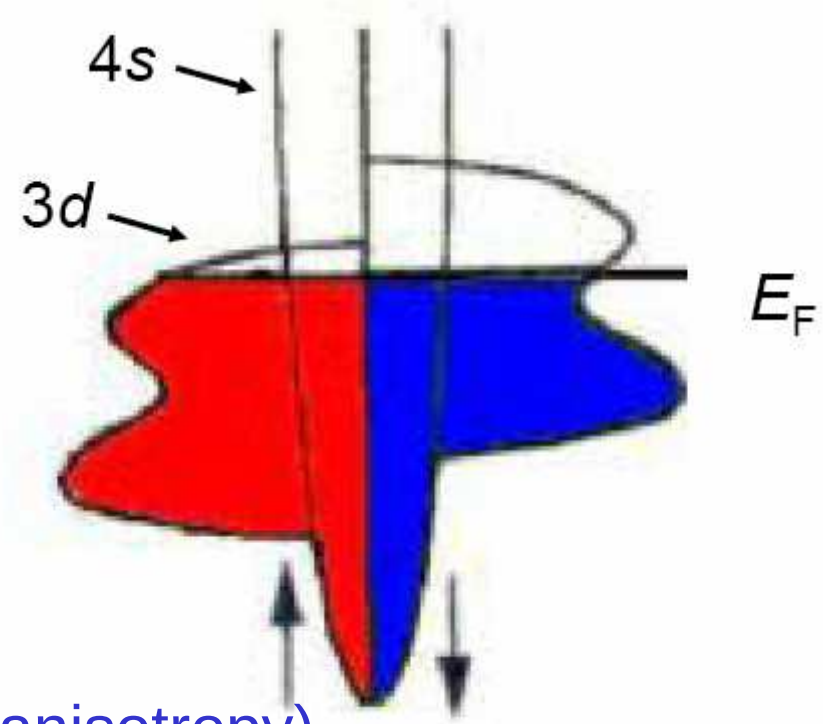
- theory: higher order terms wash out ferromagnetism

- experiment: no ferromagnetism observed in modulation doped heterostructures

Failure of free electron model

ferromagnetism is not expected in TM metals!

➔ band structure effects crucial:

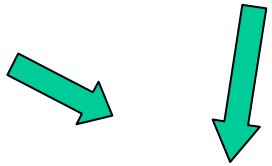


- orbital character (*s*, *d*)
- multi bands' effects
  -- narrow plus wide band
- *s-d* exchange coupling
- spin-orbit interaction (magnetic anisotropy)
- ….

Kinetic exchange

Direct exchange interactions

$$H_{12} = -J\boldsymbol{s}_1\boldsymbol{s}_2$$



potential energy depends on spins' directions

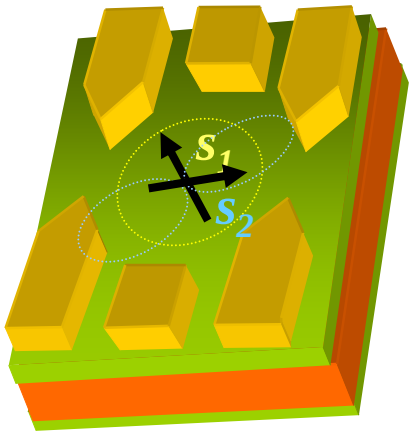
potential exchange

kinetic energy depends on spins' directions

kinetic exchange

Direct exchange interactions

$$H_{ex} = - J s_1 s_2$$



two electrons in one quantum dot

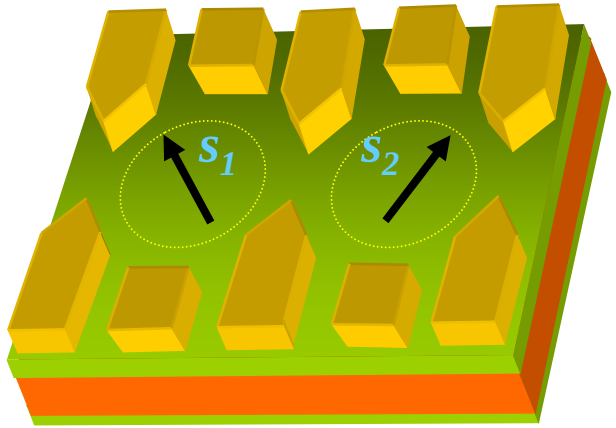
potential exchange

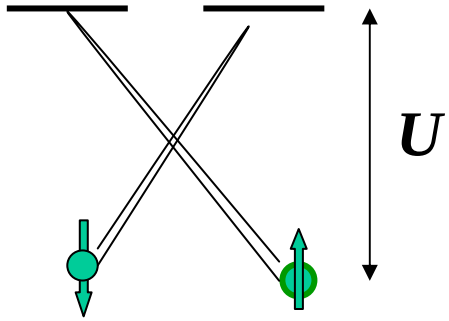
$$J = 2\int dr^{(1)}\, dr^{(2)}\, V_{12}(r^{(1)},r^{(2)})\, \psi_a(r^{(1)})\psi^*_b(r^{(1)})\psi_a{}^*(r^{(2)})\psi_b(r^{(2)}) > 0$$

Kinetic exchange

$$J = -2<\psi_1|H|\psi_2>|^2/U < 0$$

also H_2





two electrons in two quantum dots

Kinetic exchange in metals – Kondo hamiltonian

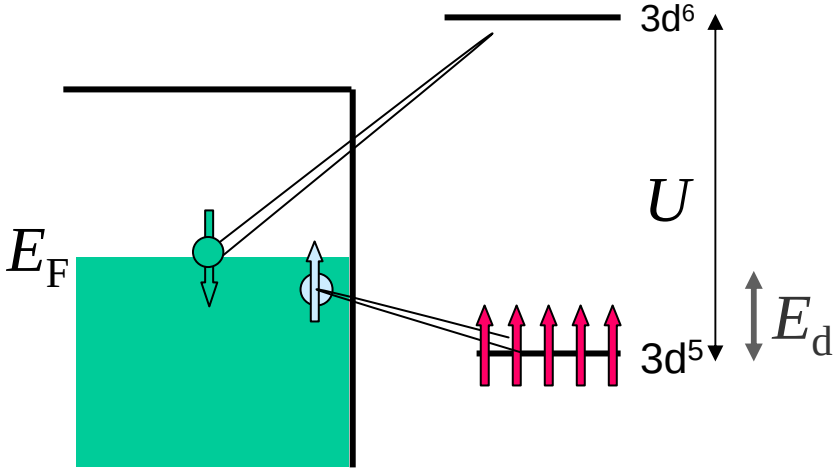
Lowering of kinetic energy due to symmetry allowed hybridization

- **quantum hopping of electrons to the *d* level**

[e^{ikr} contains all point symmetries]

- **quantum hopping of electrons from the *d* level to the hole state**

➔ ***H_i = - JsS$_i$ (Schriffer-Wolff)***
kinetic exchange



$$J_{kin} = -\langle\psi_k|H|\psi_d\rangle|^2[1/E_d + 1/(U - E_d)]$$

$$|J_{kin}| > J_{potential}$$

exchange splitting of the band: $\Delta = x|J_{kin} - J_{potential}|\langle S_i\rangle$

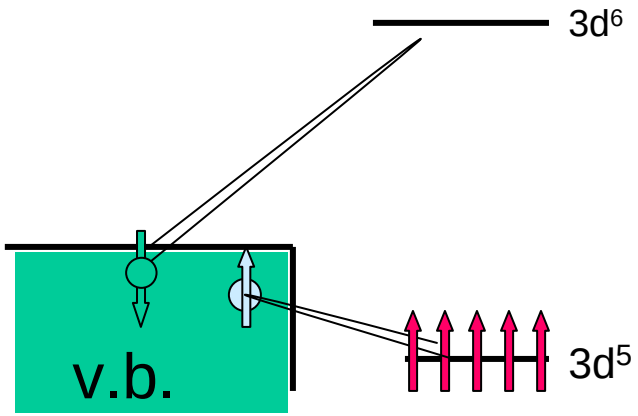
[in the weak coupling limit – no Kondo screening]

Kinetic exchange in DMS

$$\langle\psi_s|H|\psi_d\rangle = 0$$

$$\langle\psi_p|H|\psi_d\rangle \neq 0$$

- **quantum hopping of electrons from the v.b. to the d level**
- **quantum hopping of electrons from the d level to the empty v.b. states**



e.g., Mn in CdTe
Fe in GaN

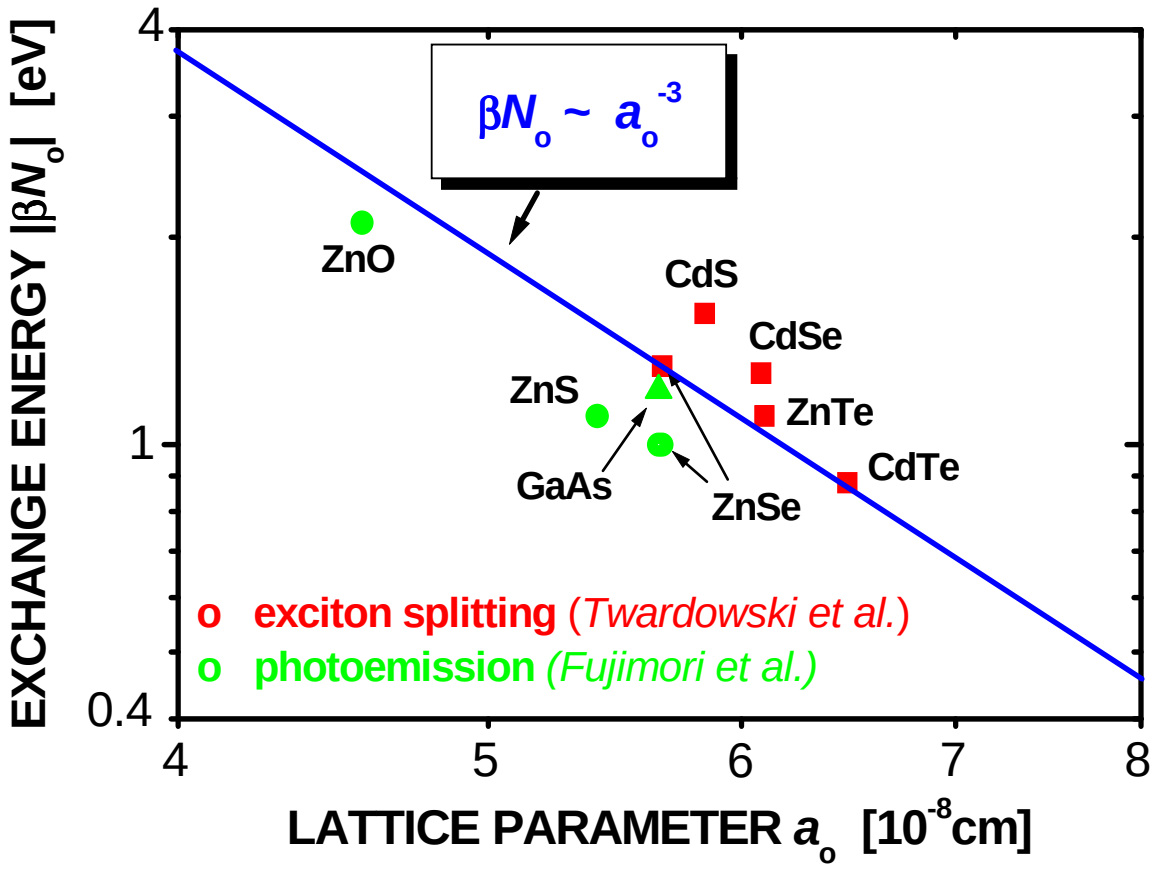
$$J_{kin} \equiv \beta N_o = -|\langle\psi_p|H|\psi_d\rangle|^2[1/E_d + 1/(U - E_d)]$$

exchange splitting of v.b., e.g., $Ga_{1-x}Mn_xAs$: $\Delta = x|\beta N_0|\langle S\rangle$

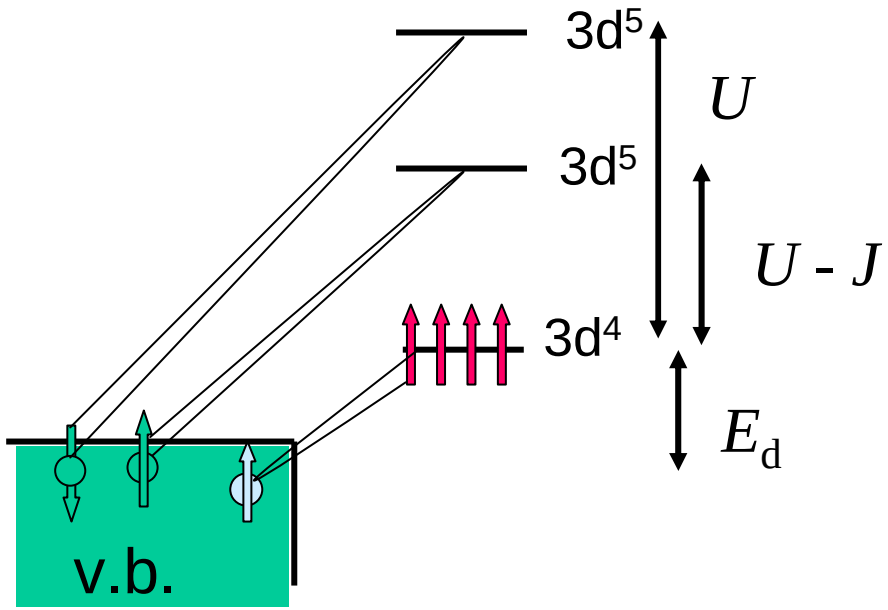
[in the weak coupling limit – TM does not bind a hole]

Exchange energy βN_o in Mn-based DMS

- **Antiferromagnetic (Kondo-like)**
- **Magnitude increases with decreasing lattice constant**



Ferromagnetic kinetic exchange in Cr-based DMS



d state in the gap

$$\beta N_o = -|\langle\psi_p|H|\psi_d\rangle|^2[1/(U+E_d) - 1/(U+E_d-J) - 1/E_d] > 0$$

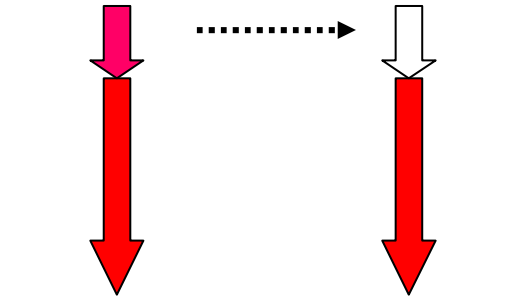
attention: in thermal equillibrium Cr d electrons neutralize holes but ferromagnetic βNo was determined by exciton reflectivity

Mac et al., PRL'93

Double exchange

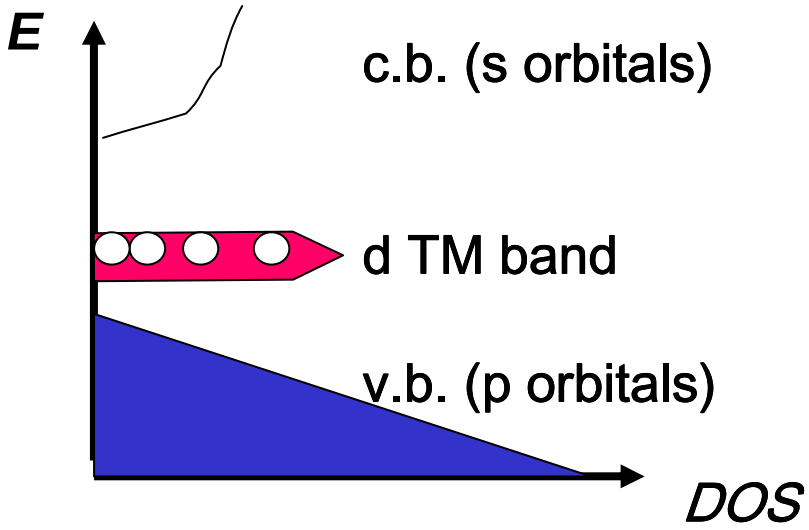
Zener double exchange

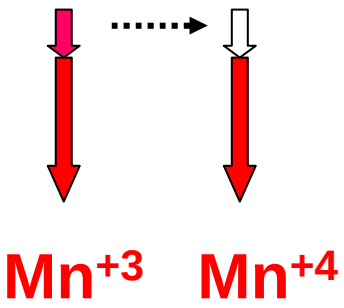
- two centres with different spin states



- because of intra-centre exchange hopping (lowering of kinetic energy) for the same orientations of two spins ➔ ferro

Doped manganites: (La,Sr)MnO_3





- *d* -states in the gap
- Sr acceptors take electrons from Mn ions

  ➔ mixed valence ➔ two spin states
- Ferromagnetic arrangement promots hopping

  ➔ Anderson-Mott insulator-to-metal transition at x ≅ 0.2
- narrow band for AFM, wide band for FM $T_C \approx 300$ K

Indirect exchange interaction between localised spins

Overlap of wave functions necessary for the exchange interaction

➔ weak for

-- diluted spins

-- spin separated by, e.g, anions

but … *sp-d* interaction $J_{\text{sp-d}} \equiv I$ can help!

Localised spin polarises band electrons ➔

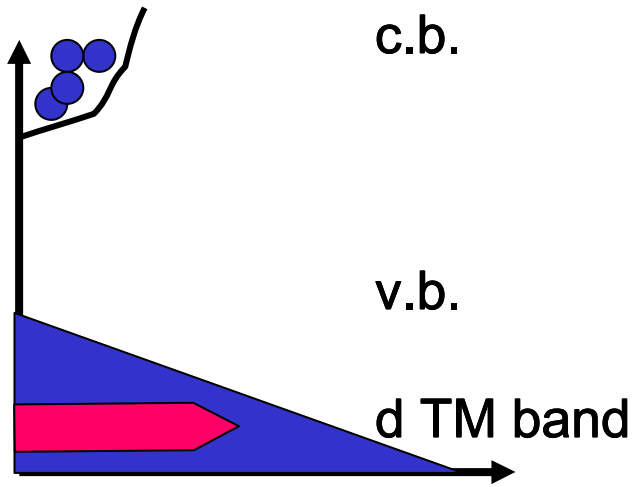
spin polarised band electrons polarise other localised spins

s-d Zener model

s-d Zener model

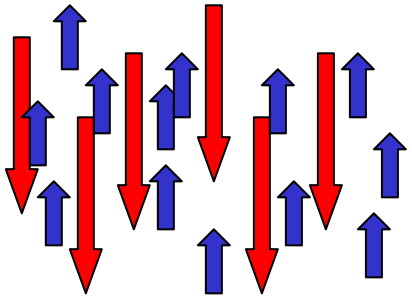
- METALS

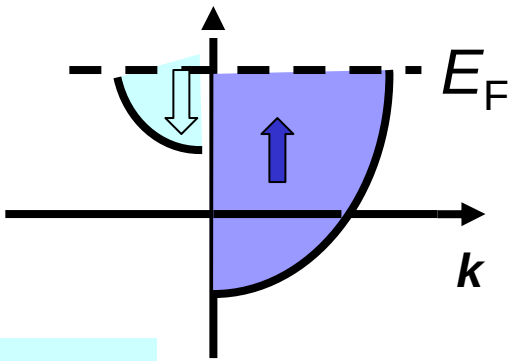
(heavily doped semiconductors)



Zener exchange mediated by free carriers

redistribution of carriers between spin subbands lowers energy





$$\Delta = x|I|\langle \boldsymbol{S} \rangle$$

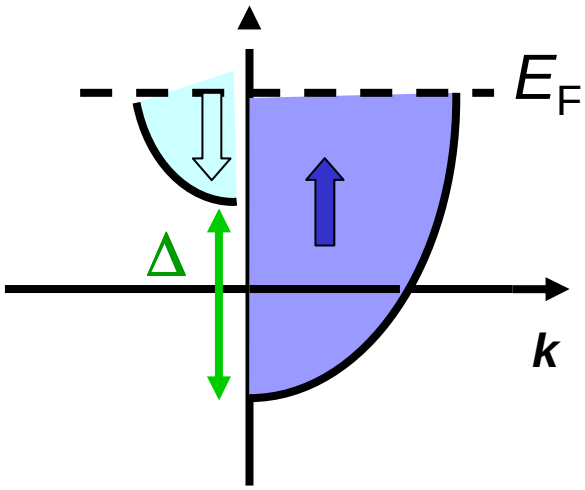
long range, ferromagnetic

Landau free energy functional of carriers

$$F_{\text{carriers}}[M] = \frac{1}{2}\int_0^\infty dE E\rho(E) f_\downarrow(E) + \frac{1}{2}\int_0^\infty dE E\rho(E) f_\uparrow(E) -$$

$$-\int_0^\infty dE E\rho(E) f(E) = -\frac{1}{8}\rho(E_F)\Delta^2 = -\frac{1}{8}\rho(E_F)\left(\frac{IM}{g\mu_B}\right)^2$$

for $\Delta, kT << E_F$



Ground state always FM if no competing AF interactions

Mean-field Zener model

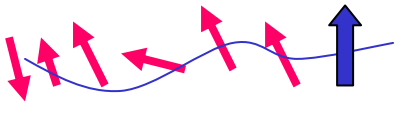
Which form of magnetization minimizes *F[**M(r)**]* ?

$F = F_{\text{carriers}}[\boldsymbol{M(r)}] + F_{\text{Spins}}[\boldsymbol{M(r)}]$

F_{carriers} <= VCA, Mol.F.A, *kp*, empirical tight-binding

F_{spins} <= from *M(H)* for undoped DMS

M(r) $\neq 0$ for $H = 0$ at $T < T_C$

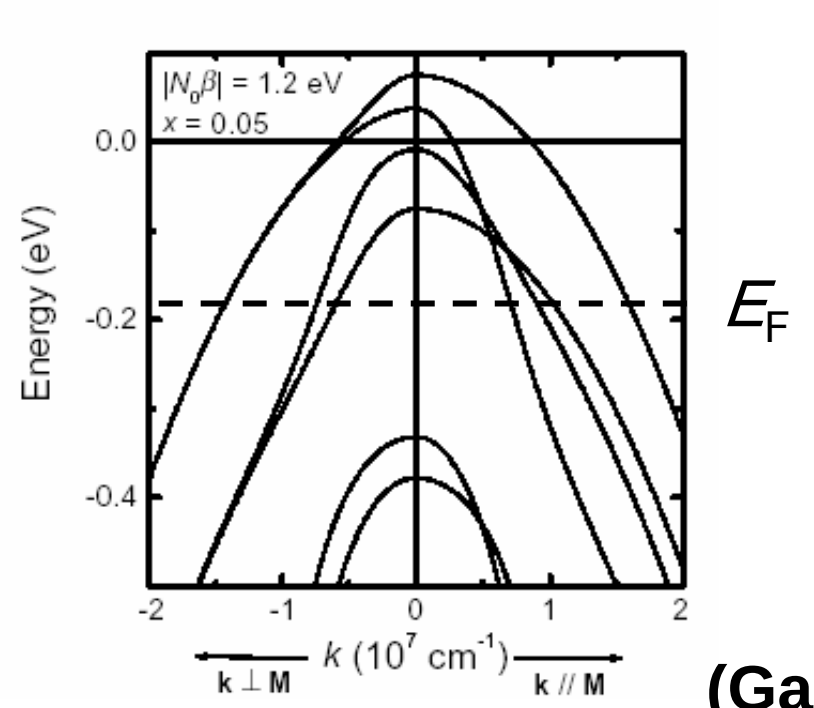


if ***M(r)*** uniform => ferromagnetic order

otherwise => modulated magnetic structure

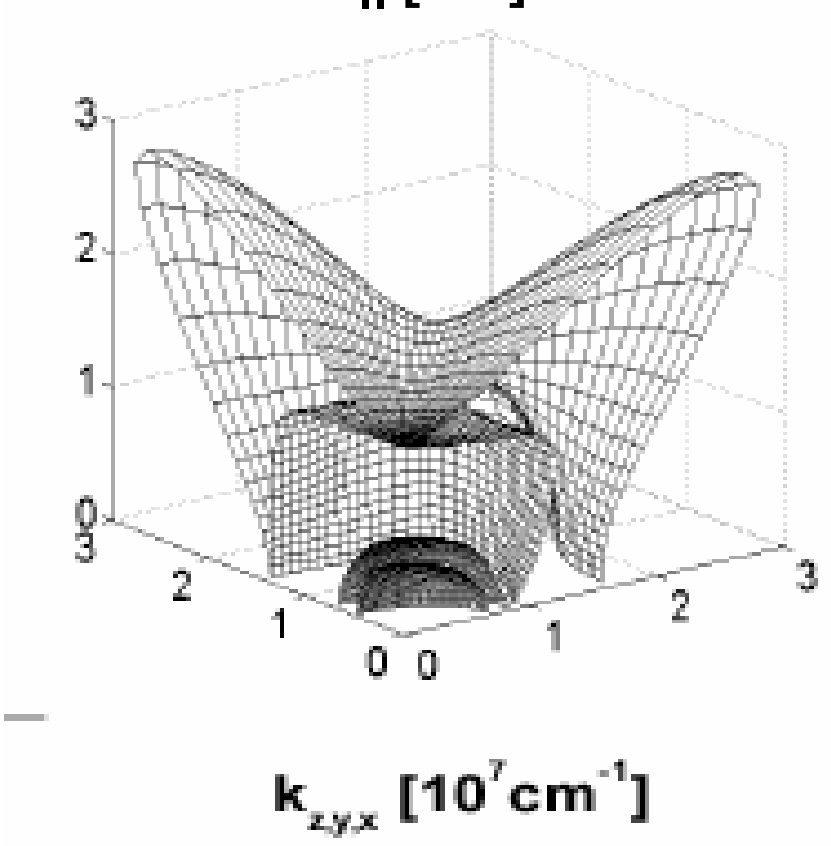
How to describe valence band structure?

Essential features:
- spin-orbit coupling
- anisotropy
- multiband character



E_F

Cross-section of the Fermi surface
M **|| [100]**



(Ga,Mn)As

Zener/RKKY MF model of p-type DMS

Competition between entropy, AF interactions, and lowering of carrier energy owing to spin-splitting

Curie temperature $T_C = T_{CW} = T_F - T_{AF}$ ⟸ **superexchange**

$$T_F = S(S+1)x_{eff}N_o A_F \rho^{(s)}(E_F)\beta^2/12L_c^{d-3}$$

$A_F > 1$ Stoner enhancement factor

($A_F = 1$ if no carrier-carrier interaction)

$\rho^{(s)}(E_F) \sim m^* k_F^{d-2}$

(if no spin-orbit coupling, parabolic band)

L_c – quantum well width ($d = 2$), wire cross section ($d = 1$)

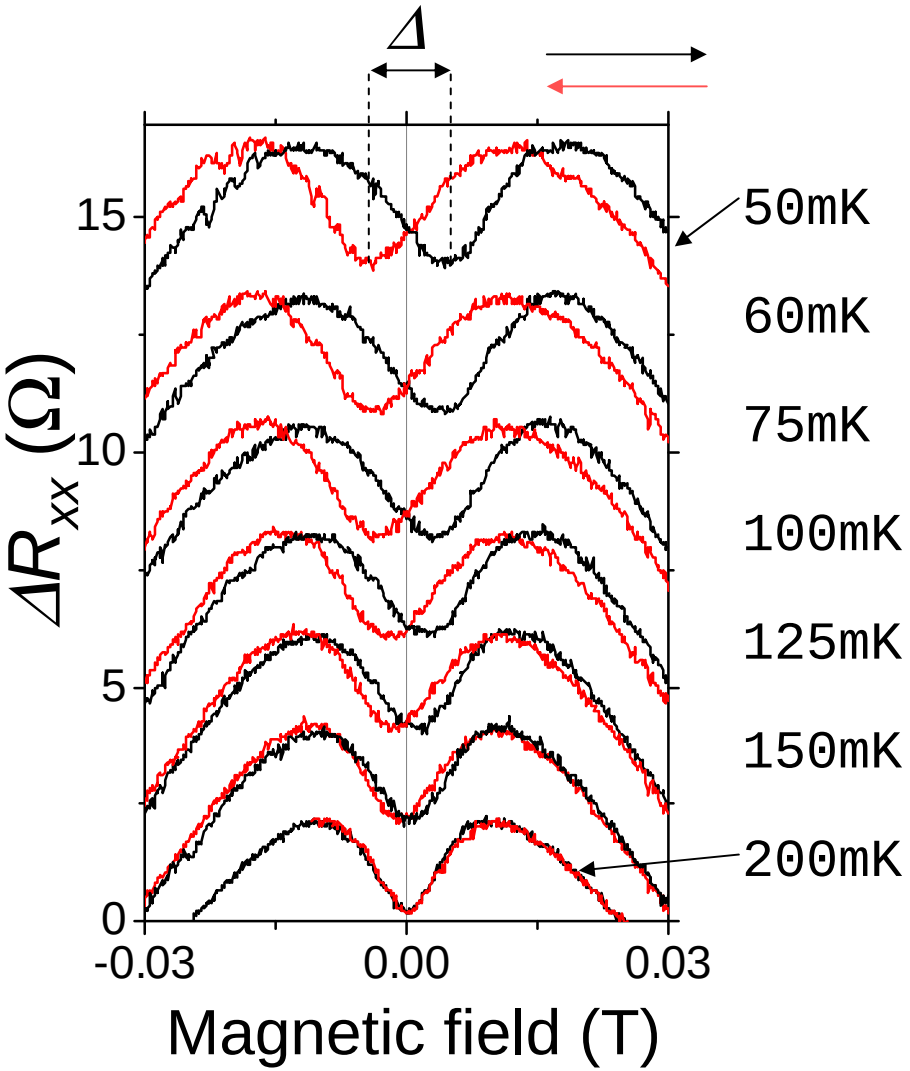
=> T_C ~ 50 times greater for the holes

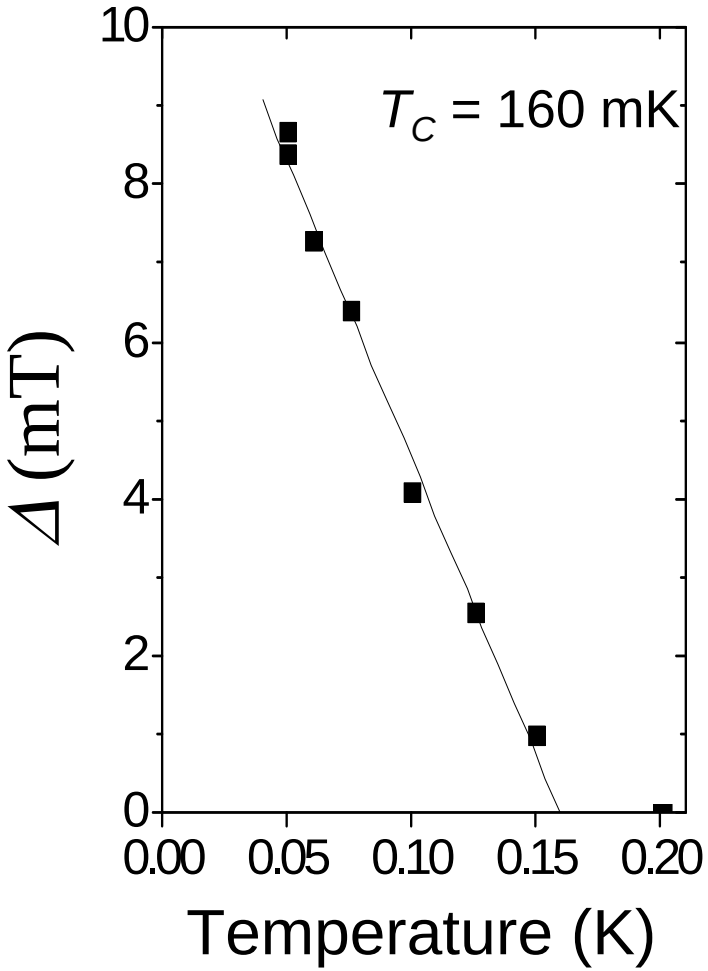
large m*

large β

T.D. et al. PRB'97,'01,'02, Science '00

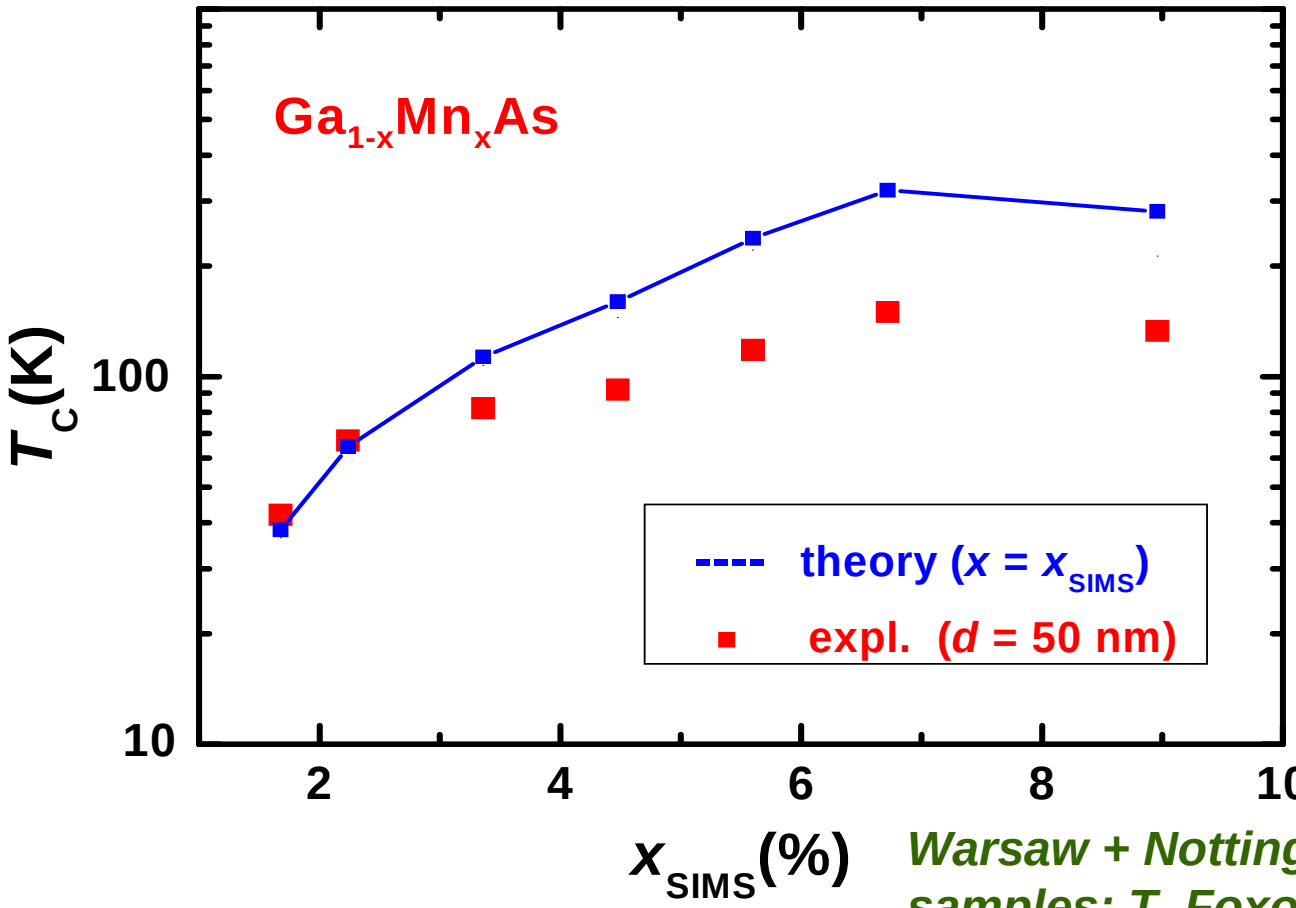
Magnetoresistance hysteresis
n-$Zn_{1-x}Mn_xO$:Al, x = 0.03





M. Sawicki, ..., M. Kawasaki, T.D., ICPS'00

Curie temperature in p-$Ga_{1-x}Mn_xAs$ theory and experiment

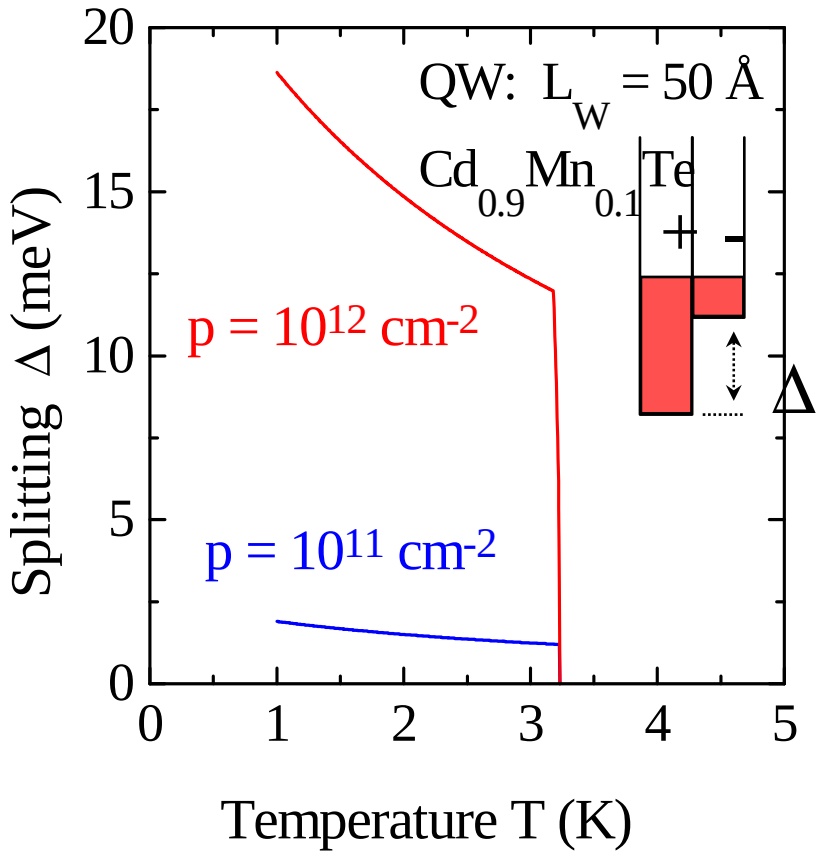


Warsaw + Nottingham'03
samples: T. Foxon et al.
expl. M. Sawicki i K. Wu
theory: Zener model, T.D. et al.

Effect of dimensionality
-- magnetic quantum wells (theory)

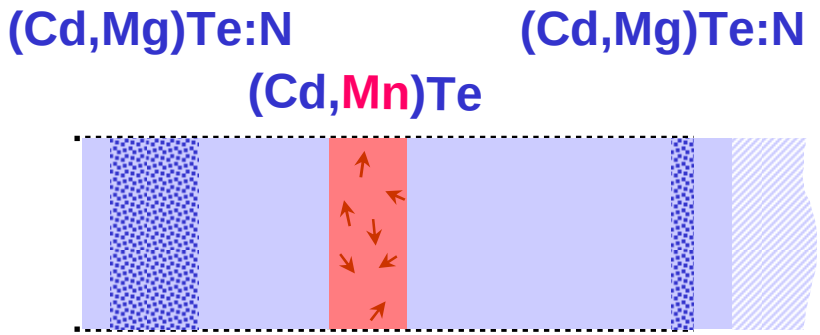
- T_C independent of hole concentration p
- T_C inversely proportional to L_W
- spontaneous splitting proportional to p

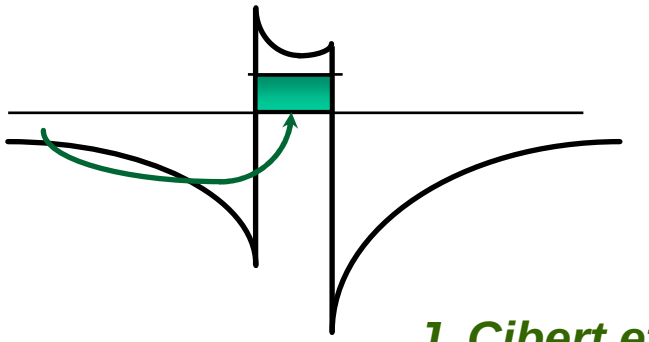
spontaneous splitting of the valence band subband



T.D. et al. PRB'97

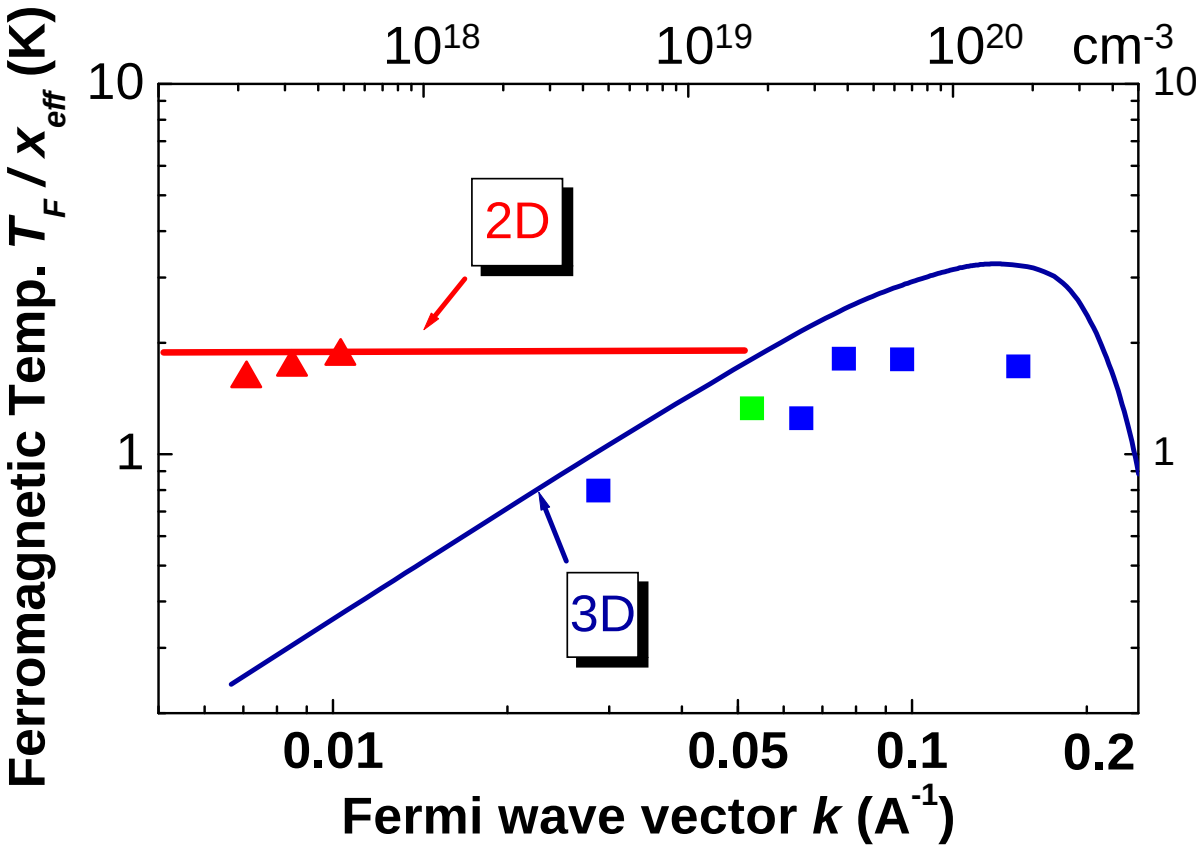
Modulation doped (Cd,Mn)Te QW





J. Cibert et al. (Grenoble)

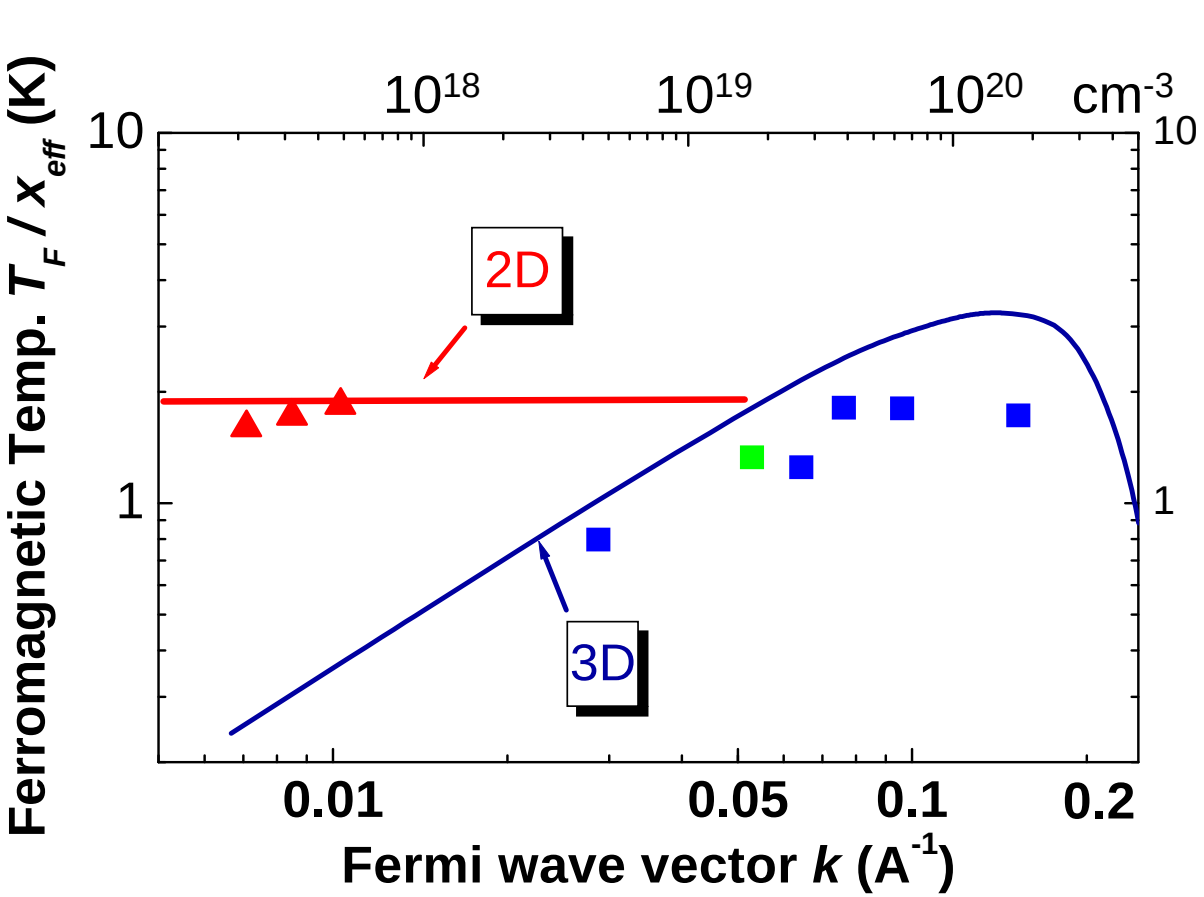
Ferromagnetic temperature in 2D p-$Cd_{1-x}Mn_xTe$ QW and 3D $Zn_{1-x}Mn_xTe$:N

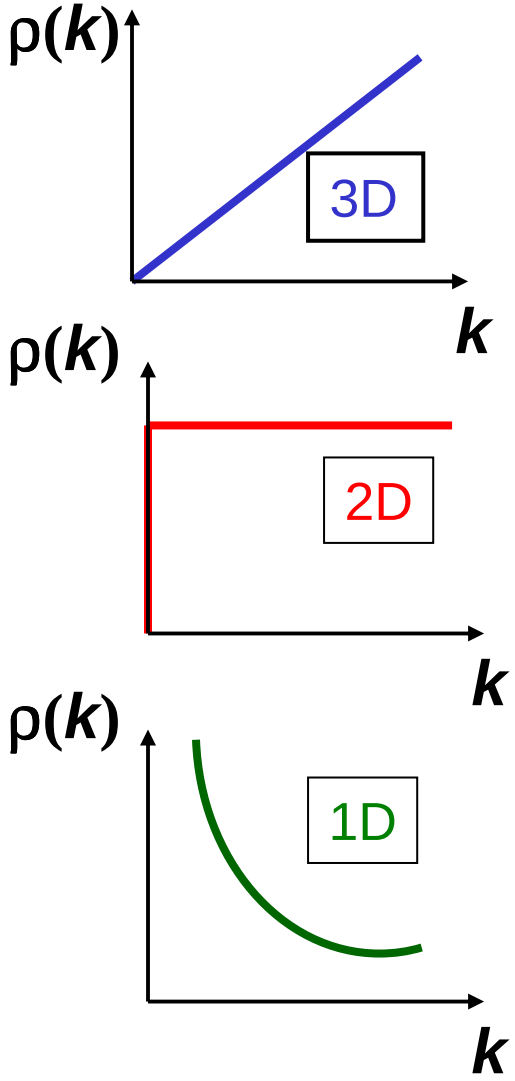


H. Boukari, ..., T.D., PRL'02

D. Ferrand, ... T.D., ... PRB'01

Ferromagnetic temperature in 2D p-$Cd_{1-x}Mn_xTe$ QW and 3D $Zn_{1-x}Mn_xTe$:N





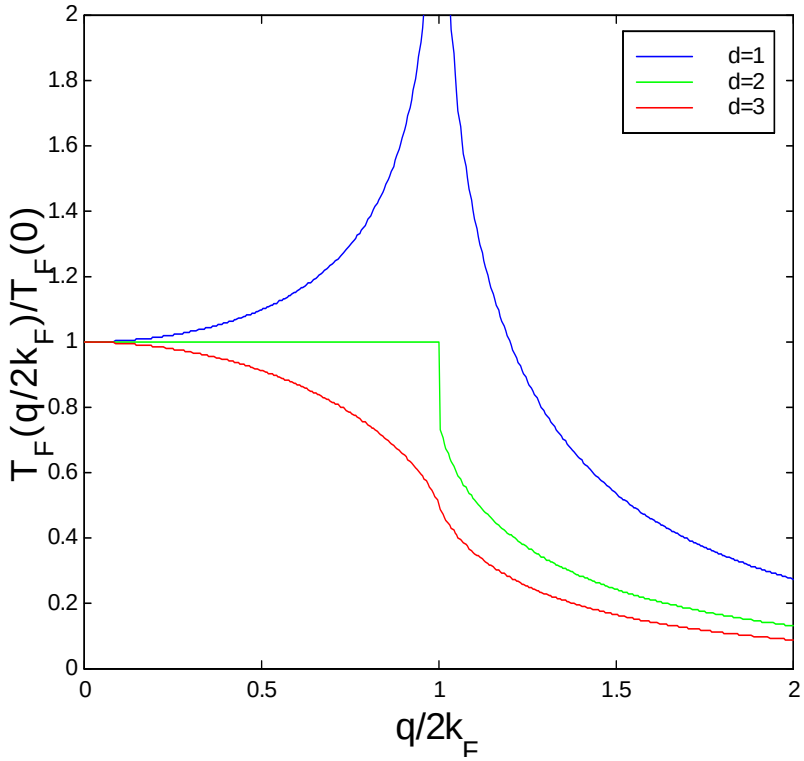
H. Boukari, ..., T.D., PRL'02

D. Ferrand, ... T.D., ... PRB'01

Effects of confinement magnetic quantum wires - expectations

1D: $T_F(q)$ has maximum at $2k_F$

➔ spin-Peierls instability ➔ SDW

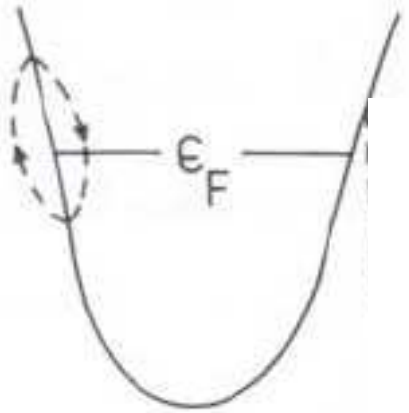


***$T_F(q)/T_F$ (0)* for s-electrons neglecting e-e interactions and disorder**

RKKY model

RKKY – metals/doped semiconductors

How energy of carriers depends on relative orientation of two spins $\boldsymbol{S}_i$ and $\boldsymbol{S}_j$ in the presence of $\mathcal{H}_{sp\text{-}d} = -\mathcal{I}(\boldsymbol{r}-\boldsymbol{R}_i)s\boldsymbol{S}_i$

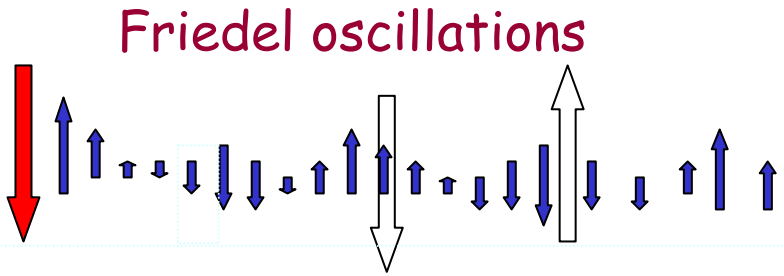


$$H_{ij} = \sum_{nk\sigma}\sum_{n'k'\sigma'}\left[\frac{\langle\psi_{nk\sigma}|I(\boldsymbol{r}-\boldsymbol{R}_i)\boldsymbol{s}\cdot\boldsymbol{S}_i|\psi_{n'k'\sigma'}\rangle\langle\psi_{n'k'\sigma'}|I(\boldsymbol{r}-\boldsymbol{R}_j)\boldsymbol{s}\cdot\boldsymbol{S}_j|\psi_{nk\sigma}\rangle}{\varepsilon_{nk\sigma}-\varepsilon_{n'k'\sigma'}}+i\leftrightarrow j\right]$$
$$\times f_{nk\sigma}(1-f_{nk'\sigma'}),$$

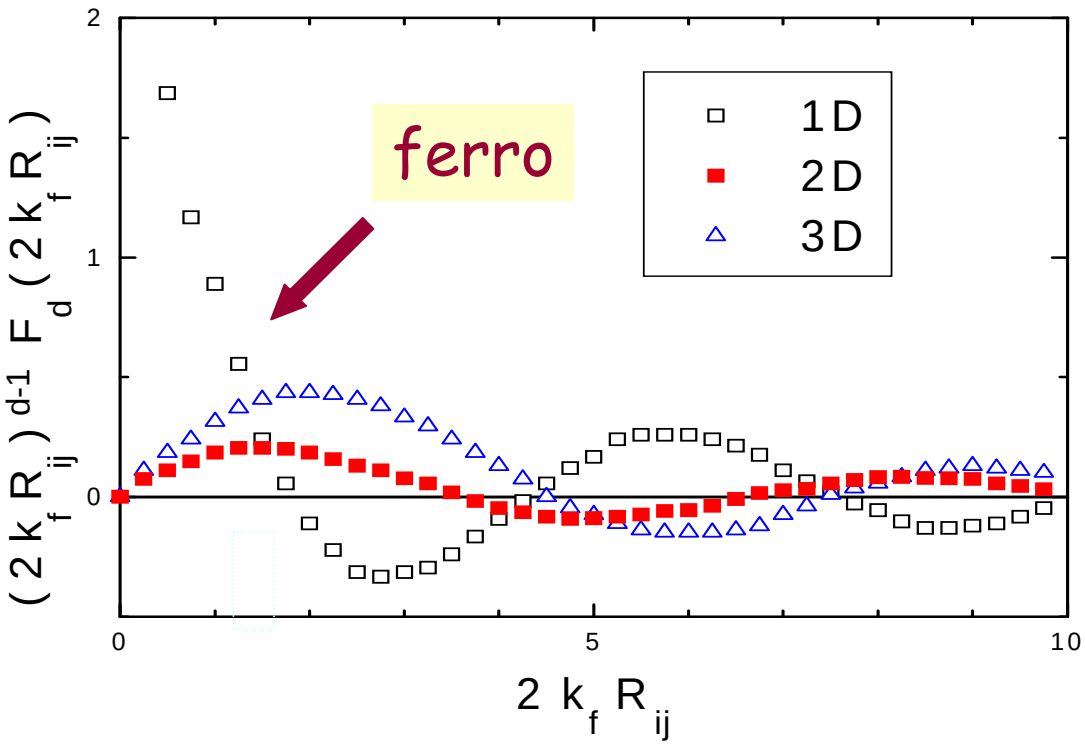
➔ $H_{ij} = -J(\boldsymbol{R}_i - \boldsymbol{R}_j)\boldsymbol{S}_i\boldsymbol{S}_j$

Ruderman-Kittel-Kasuya-Yosida interaction

Spin polarisation of free carriers induced by a localised spin:

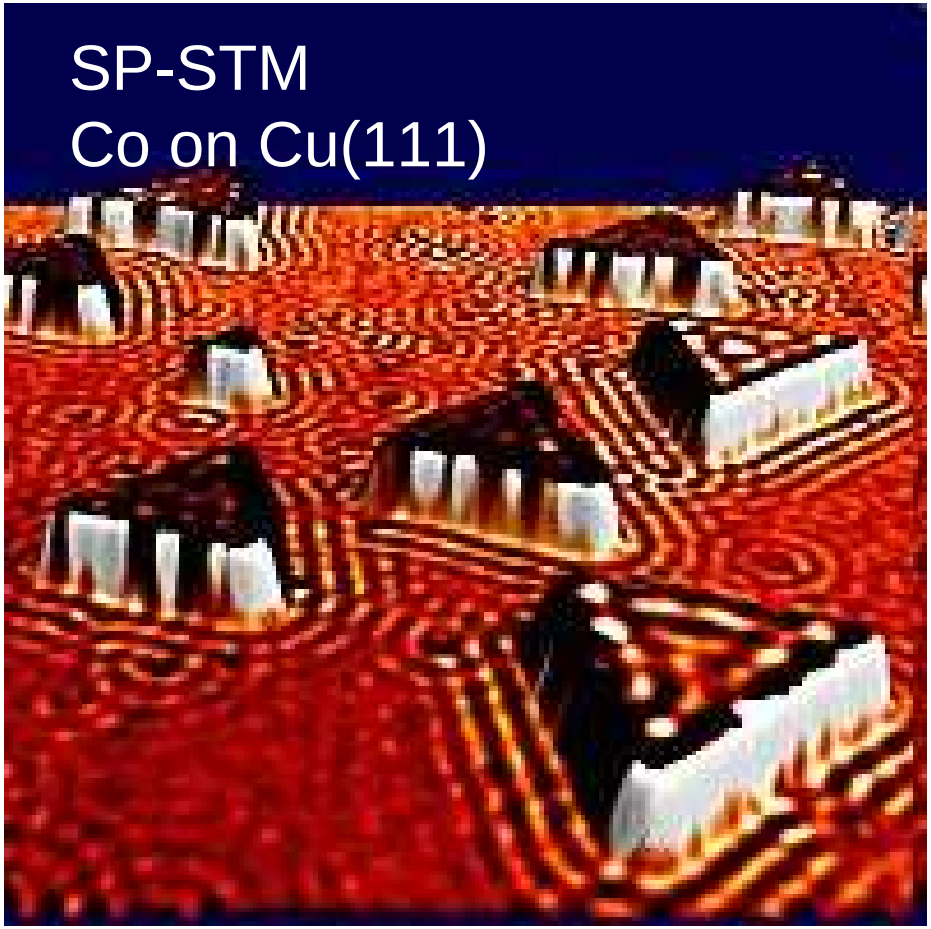


$$H_{ij} = -J(R_i - R_j)S_iS_j$$



- long range
- sign oscillates with k_FR_{ij}
- FM at small distances

Spin density oscillations



R. Wiesendanger et al., PRL'04

Magnetic order induced by RKKY

$$H_{ij} = -J(\boldsymbol{R}_i - \boldsymbol{R}_j)\boldsymbol{S}_i\boldsymbol{S}_j$$

in the MFA T_C (RKKY) = T_C(s-d Zener)

- MFA valid when $n < xN_0$ (semiconductors)

  interaction merely FM

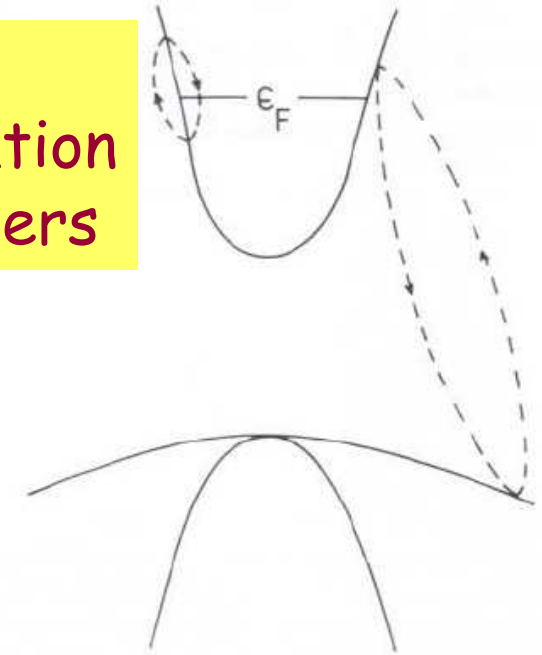
- MFA not valid when $n > xN_0$

  both FM and AFM important ➔ spin glass

Blomberg-Rowland and superexchange

RKKY and Blomberg-Rowland mechanism

spin polarisation of carriers

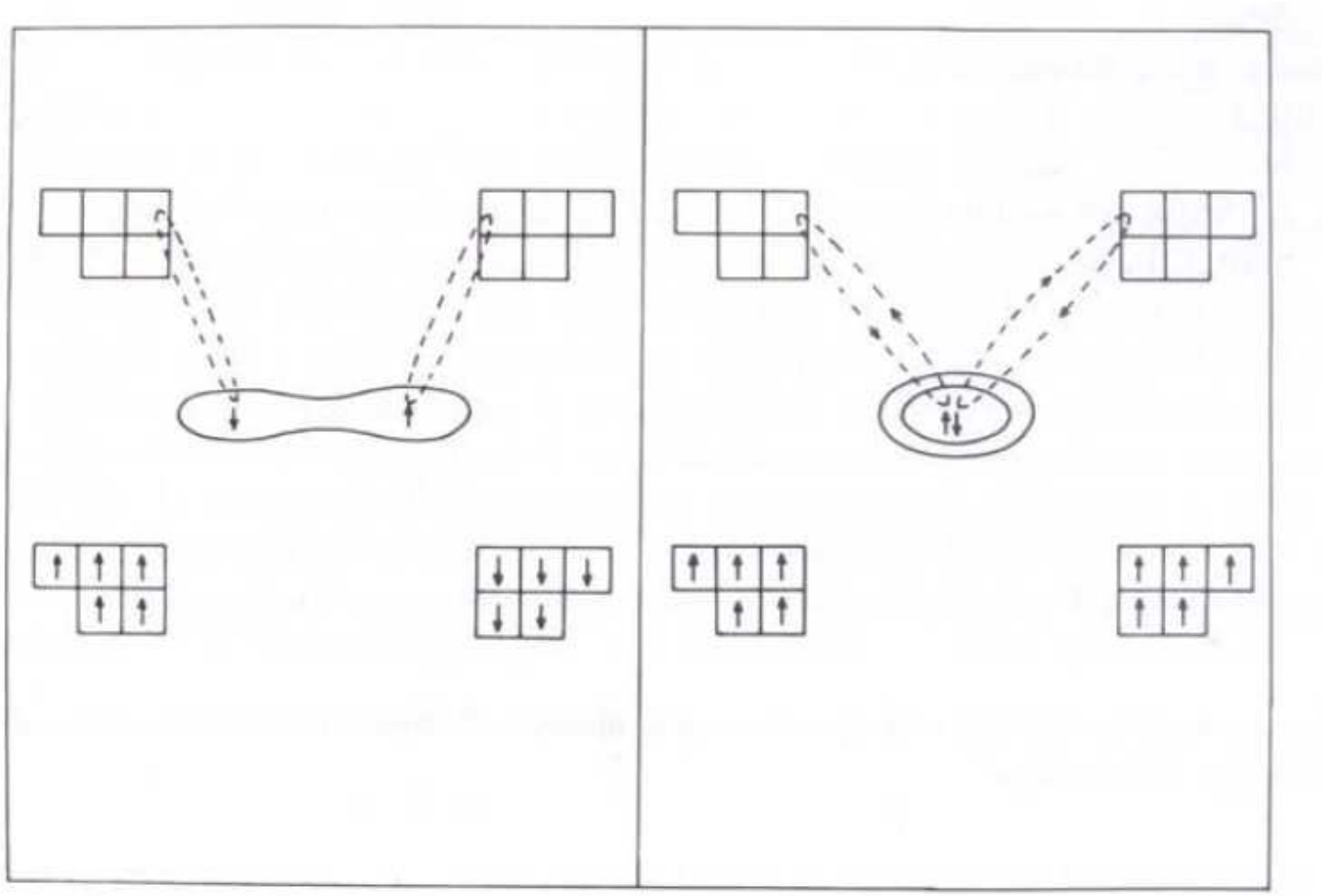


spin polarisation of valence electrons

$$H_{ij} = \sum_{nk\sigma} \sum_{n'k'\sigma'} \left[\frac{\langle \psi_{nk\sigma} | I(\boldsymbol{r} - \boldsymbol{R}_i) \boldsymbol{s} \cdot \boldsymbol{S}_i | \psi_{n'k'\sigma'} \rangle \langle \psi_{n'k'\sigma'} | I(\boldsymbol{r} - \boldsymbol{R}_j) \boldsymbol{s} \cdot \boldsymbol{S}_j | \psi_{nk\sigma} \rangle}{\varepsilon_{nk\sigma} - \varepsilon_{n'k'\sigma'}} + i \leftrightarrow j \right]$$
$$\times f_{nk\sigma}(1 - f_{nk'\sigma'}),$$

4th order process in hybridisation $<\psi_{\boldsymbol{k}}|H|\psi_{\mathrm{d}}>$

Example: hopping to *d*-orbitals



Superexchange

- Derivation of $J(\boldsymbol{R}_i - \boldsymbol{R}_j)$ in spin hamiltonian $H_{ij} = - J(\boldsymbol{R}_i - \boldsymbol{R}_j)\boldsymbol{S}_i\boldsymbol{S}_j$

taking systematically into account hybridisation terms

$\langle\psi_{\boldsymbol{k}}|H|\psi_d\rangle$ up to at least 4th order

- merely AFM, if FM – small value – Goodenogh-Kanamori rules

END