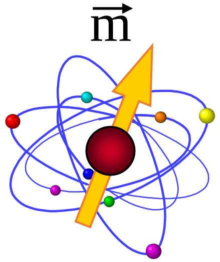
Lecture 3

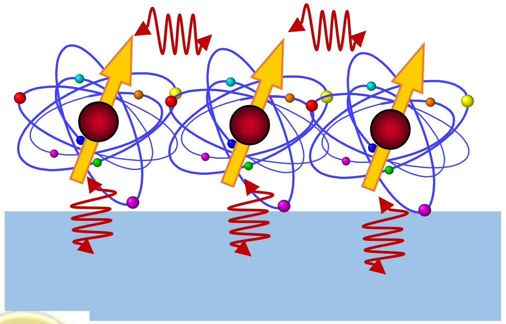
Exchange interactions

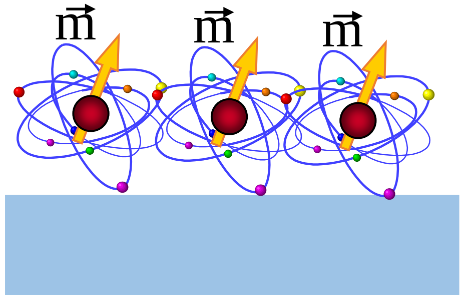
The spintronics "goose game"

Atom magnetism

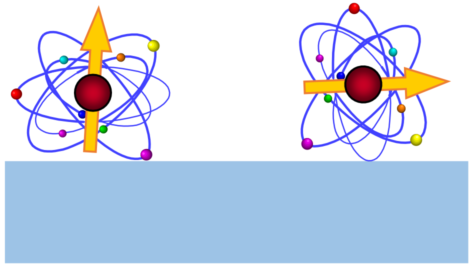


interactions between spins and with the supporting substrate



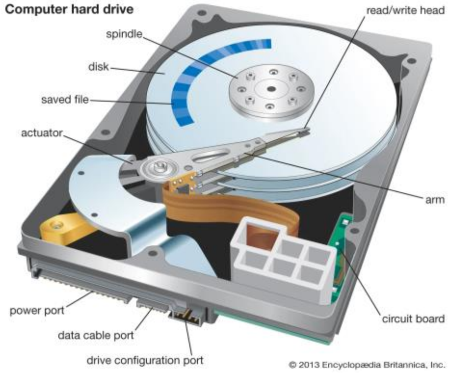


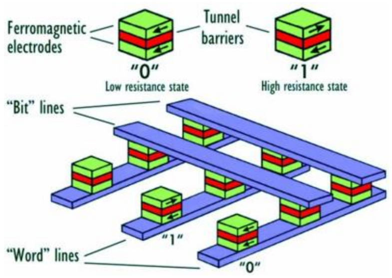
magnetic moment in a cluster and/or on a support



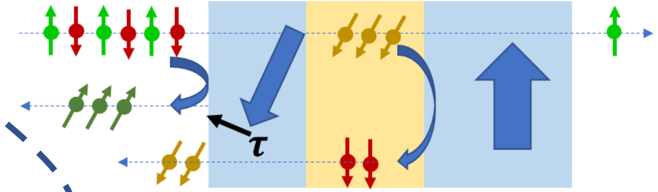
Magnetization easy axis

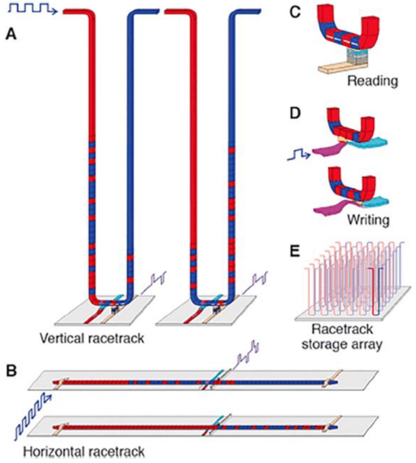
applications



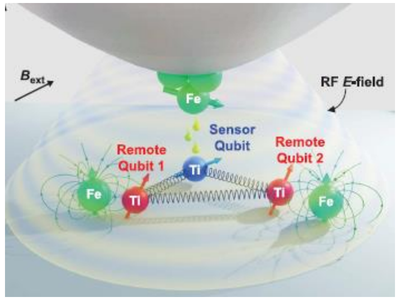


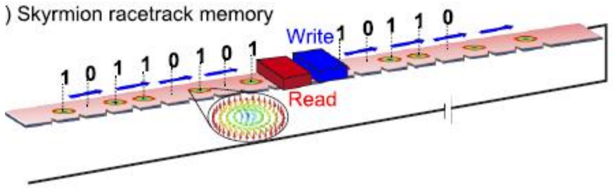
STT - SOT





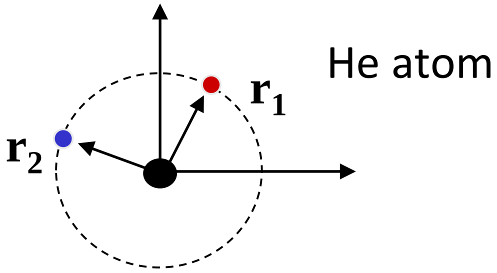
Future





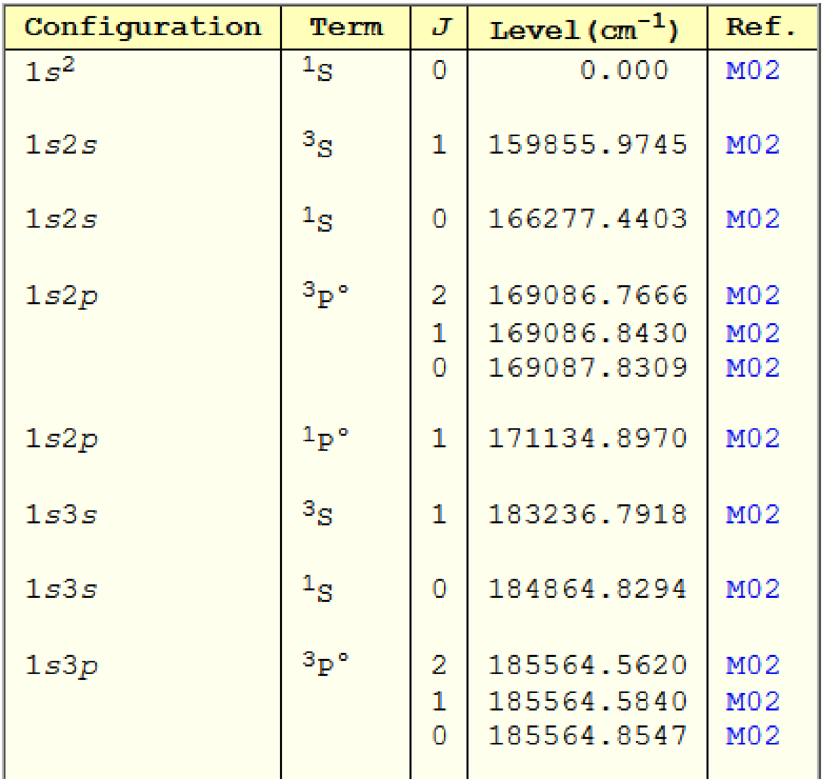
The He atom: intra-atomic exchange

$$H_{He}=\sum_{i=1}^{2}\frac{p_i^2}{2m}-\frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{2}\frac{Ze^2}{r_i}+\frac{1}{4\pi\varepsilon_0}\frac{e^2}{|r_2-r_1|}=H_0+V_{ee}$$



Ground state -> the two electrons occupy the 1s orbital
-> the spatial part of the wavefunction is symmetric (electrons have identical quantum numbers *nlm*=100)
-> because electrons are fermions, the spin part must be antisymmetric (change sign) upon particle exchange

$$\Psi_{\text{ground}}=\Psi_{\text{sym}}(\mathrm{r}_1,\mathrm{r}_2)\chi_{\text{antisym}}(\mathrm{s}_1,\mathrm{s}_2)=\frac{1}{2}[\Psi_{100}(\mathrm{r}_1)\Psi_{100}(\mathrm{r}_2)+\Psi_{100}(\mathrm{r}_1)\Psi_{100}(\mathrm{r}_2)][\alpha\beta-\beta\alpha]$$



Configuration	Term	J	Level (cm^{-1})	Ref.
$1s^2$	^1S	0	0.000	M02
$1s2s$	^3S	1	159855.9745	M02
$1s2s$	^1S	0	166277.4403	M02
$1s2p$	$^3P°$	2	169086.7666	M02
		1	169086.8430	M02
		0	169087.8309	M02
$1s2p$	$^1P°$	1	171134.8970	M02
$1s3s$	^3S	1	183236.7918	M02
$1s3s$	^1S	0	184864.8294	M02
$1s3p$	$^3P°$	2	185564.5620	M02
		1	185564.5840	M02
		0	185564.8547	M02

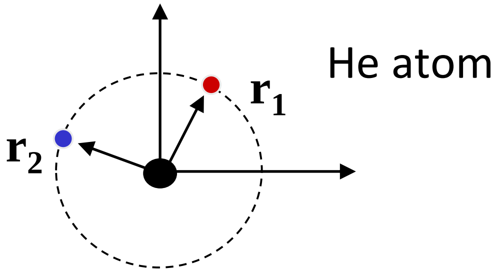
Energy levels of neutral He

1 eV = 8066 cm^-1

https://physics.nist.gov/PhysRefData/Handbook/Tables/heliumtable5.htm

The He atom: intra-atomic exchange

$$H_{He} = \sum_{i=1}^{2} \frac{p_i^2}{2m} - \frac{1}{4\pi\varepsilon_0} \sum_{i=1}^{2} \frac{Ze^2}{r_i} + \frac{1}{4\pi\varepsilon_0} \frac{e^2}{|r_2 - r_1|} = H_0 + V_{ee}$$



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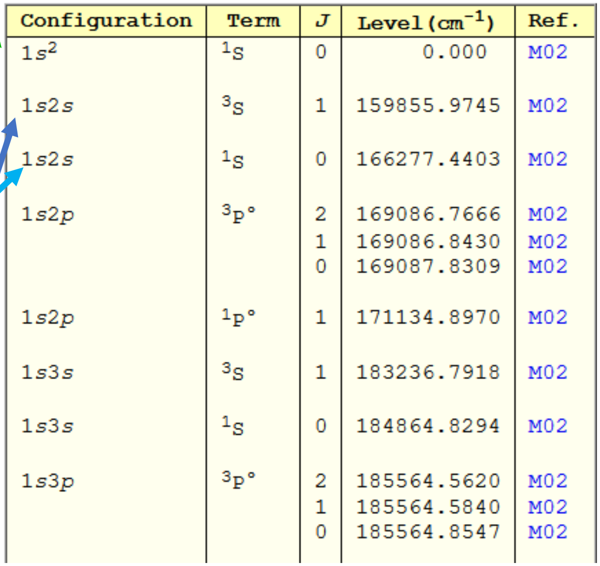
Singlet S=0

$1\ eV \approx 8000\ cm^{-1}$



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		1	185564.5840	M02
		0	185564.8547	M02

Excited state -> one electron in the 1s orbital (*nlm*=100); the second electron in an excited state *nlm:*
1) the spatial part of the wavefunction is symmetric and the spin part is antisymmetric

$$\Psi^{S}_{\text{exci}} = \Psi_{\text{sym}}(\mathrm{r}_1,\mathrm{r}_2)\chi_{\text{antisym}}(\mathrm{s}_1,\mathrm{s}_2) = \frac{1}{2}[\Psi_{100}(\mathrm{r}_1)\Psi_{\text{nlm}}(\mathrm{r}_2) + \Psi_{\text{nlm}}(\mathrm{r}_1)\Psi_{100}(\mathrm{r}_2)][\alpha\beta - \beta\alpha]$$

Singlet S=0

2) the spatial part of the wavefunction is antisymmetric and the spin part is symmetric

$$\Psi^{T}_{\text{exci}} = \Psi_{\text{antisym}}(\mathrm{r}_1,\mathrm{r}_2)\chi_{\text{sym}}(\mathrm{s}_1,\mathrm{s}_2) = \frac{1}{2}[\Psi_{100}(\mathrm{r}_1)\Psi_{\text{nlm}}(\mathrm{r}_2) - \Psi_{\text{nlm}}(\mathrm{r}_1)\Psi_{100}(\mathrm{r}_2)]\chi_{\text{sym}}(\mathrm{s}_1,\mathrm{s}_2)$$

Triplet S=1

$$\alpha = \frac{1}{2};\ \beta = -\frac{1}{2} \qquad \chi_{\text{sym}}(\mathrm{s}_1,\mathrm{s}_2) = \alpha\alpha;\ \beta\beta;\ \frac{1}{\sqrt{2}}(\alpha\beta + \beta\alpha)$$

The exchange interaction

H_0 applied to the singlet and triplet wavefunctions give the same energy; the V_{ee} contribution can be calculated with the perturbation theory

$$I = \int\int |\Psi_{100}(r_1)|^2 \frac{e^2}{4\pi\varepsilon_0|r_1 - r_2|} |\Psi_{nlm}(r_2)|^2 dr_1 dr_2$$

$$J = \int\int \Psi_{100}^*(r_1)\Psi_{nlm}^*(r_2) \frac{e^2}{4\pi\varepsilon_0|r_1 - r_2|} \Psi_{100}(r_2)\Psi_{nlm}(r_1)\, dr_1 dr_2$$

$$\mathrm{E}_{\mathrm{e-e}}^{\mathrm{S}} = \mathrm{I} + \mathrm{J}$$

$$\mathrm{E}_{\mathrm{e-e}}^{\mathrm{T}} = \mathrm{I} - \mathrm{J}$$

I is the Coulomb integral -> electrostatic repulsion between the electrons ($|\Psi(r)|^2$ -> electron density)
J is the exchange integral -> energy associated with a exchange of electron quantum states (e1 exchanged with e2)

The energy difference between the singlet and triplet state is $\Delta E = 2J$

Origin of Exchange interaction: -> Coulomb repulsion between electrons
-> total anti-symmetric wave function (Pauli exclusion principle)

J is positive	-> triplet ground state S=1	-> parallel spins
J is negative	-> singlet ground state S=0	-> antiparallel spins

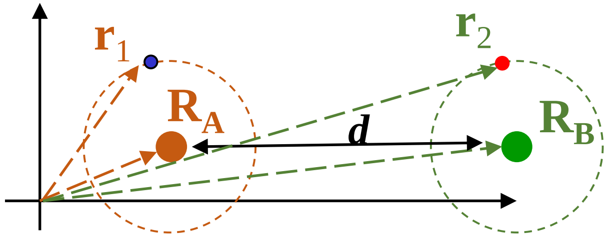
Note: we get the exchange energy from an Hamiltonian not including (explicit) spin terms !!!!!

H_2 molecule: inter-atomic exchange

H^2_{1s}

$$H = \boxed{-\frac{\hbar^2\nabla_1^2}{2m}} \boxed{-\frac{\hbar^2\nabla_2^2}{2m}} + \frac{e^2}{4\pi\epsilon_0}\left\{\boxed{-\frac{1}{|\mathbf{R}_A-\mathbf{r}_1|}}\boxed{-\frac{1}{|\mathbf{R}_B-\mathbf{r}_2|}} + \overbrace{\frac{1}{d} + \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} - \frac{1}{|\mathbf{R}_A-\mathbf{r}_2|} - \frac{1}{|\mathbf{R}_B-\mathbf{r}_1|}}^{\text{interaction terms } U}\right\}$$

H^1_{1s}



Atom A with electron 1, atom B with electron 2, at distance d

Because electrons are fermions, the total wavefunction (orbital x spin) must be antisymmetric (change sign) upon particle exchange

Spin wavefunctions are generated by linear combinations of the 4 spin states: $|m_{s1}, m_{s2}\rangle$: $|\uparrow\uparrow\rangle,\quad |\uparrow\downarrow\rangle,\quad |\downarrow\uparrow\rangle,\quad |\downarrow\downarrow\rangle$

$|S, m_S\rangle$

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left[\,|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$$

→ singlet, antisymmetric upon particle exchange

$$\left.\begin{aligned}|1,+1\rangle &= |\uparrow\uparrow\rangle \\ |1,0\rangle &= \frac{1}{\sqrt{2}}\left[\,|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right] \\ |1,-1\rangle &= |\downarrow\downarrow\rangle\end{aligned}\right\}$$

→ triplet, symmetric upon particle exchange

H_2 molecule: inter-atomic exchange

Orbital wavefunction associated with the singlet (triplet) must be symmetric (antisymmetric);
such orbital wavefunctions are obtained by different linear combinations of the products of the atomic orbitals $\phi(\boldsymbol{r})$:

$$\psi_{\text{sym}}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_A(\mathbf{r}_1)\phi_B(\mathbf{r}_2) + \phi_A(\mathbf{r}_2)\phi_B(\mathbf{r}_1)\right]$$

$$\psi_{\text{asym}}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_A(\mathbf{r}_1)\phi_B(\mathbf{r}_2) - \phi_A(\mathbf{r}_2)\phi_B(\mathbf{r}_1)\right]$$

Combining orbital and spin wavefunctions in the appropriate way, antisymmetric total wavefunctions are obtained:

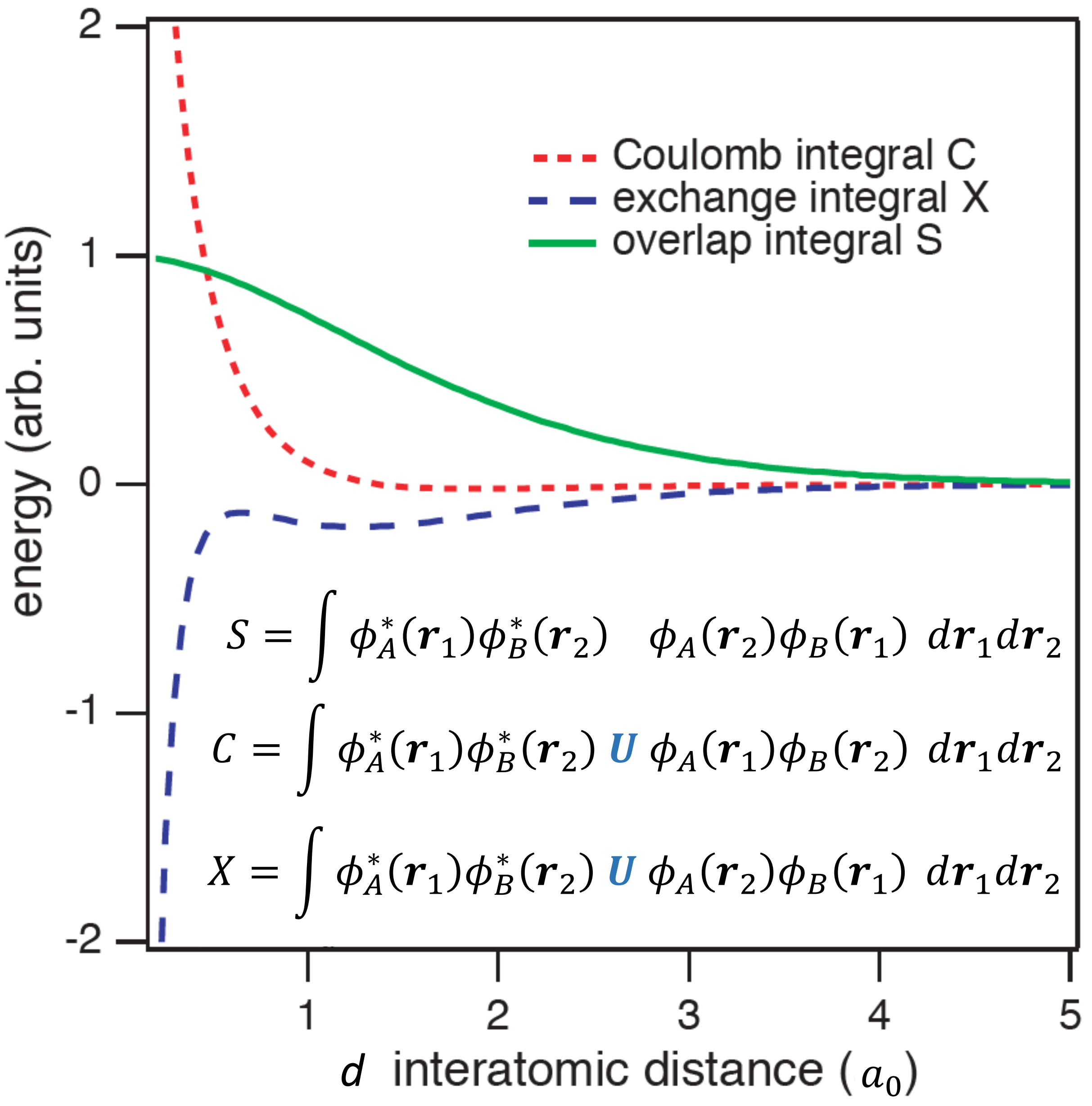
$$\Psi_{singlet} = \psi_{sym}(\boldsymbol{r}_1,\boldsymbol{r}_2)\,|0,0\rangle$$

$$\Psi_{triplet} = \psi_{asym}(\boldsymbol{r}_1,\boldsymbol{r}_2)\,|1,m_S\rangle \qquad m_S = -1,0,1$$

Heitler - London
Calculate the molecular energy levels
for the two orbital wavefunctions:

$$E = \frac{\int \psi^*(\mathbf{r}_1,\mathbf{r}_2)\,H\,\psi(\mathbf{r}_1,\mathbf{r}_2)\,d\mathbf{r}_1 d\mathbf{r}_2}{\int \psi^*(\mathbf{r}_1,\mathbf{r}_2)\,\psi(\mathbf{r}_1,\mathbf{r}_2)\,d\mathbf{r}_1 d\mathbf{r}_2}$$

H_2 molecule: inter-atomic exchange



$$S = \int \phi_A^*(\boldsymbol{r}_1)\phi_B^*(\boldsymbol{r}_2)\quad \phi_A(\boldsymbol{r}_2)\phi_B(\boldsymbol{r}_1)\ d\boldsymbol{r}_1 d\boldsymbol{r}_2$$

$$C = \int \phi_A^*(\boldsymbol{r}_1)\phi_B^*(\boldsymbol{r}_2)\ \boldsymbol{U}\ \phi_A(\boldsymbol{r}_1)\phi_B(\boldsymbol{r}_2)\ d\boldsymbol{r}_1 d\boldsymbol{r}_2$$

$$X = \int \phi_A^*(\boldsymbol{r}_1)\phi_B^*(\boldsymbol{r}_2)\ \boldsymbol{U}\ \phi_A(\boldsymbol{r}_2)\phi_B(\boldsymbol{r}_1)\ d\boldsymbol{r}_1 d\boldsymbol{r}_2$$

$$E = 2E_{H,1s} + \Delta E_{sing/trip}$$

$$E_{H_{1s}} = \int \phi_A^*(\boldsymbol{r}_1) H_{1s}^1 \phi_A(\boldsymbol{r}_1)\ d\boldsymbol{r}_1 = \int \phi_B^*(\boldsymbol{r}_2) H_{1s}^2 \phi_B(\boldsymbol{r}_2)\ d\boldsymbol{r}_1$$

$$\Delta E_{trip} = \frac{C(d) - X(d)}{1 - S(d)}$$

$$E_{trip} > E_{sing}$$

$$\Delta E_{sing} = \frac{C(d) + X(d)}{1 + S(d)}$$

At long distances $S(d) \approx 0 \Rightarrow E = 2E_{H,1s} + C \pm X$

The energy of the system depends on the spin of the electrons, despite of the fact that the spin does not enter the calculation directly ($E_{sing} - E_{trip} = 2X$)

The H_2 molecule can be described by an *effective* Hamiltonian given by:

$$H_{eff} = 2H_{H,1s} + H_{Coul} + H_{exch}$$

The Heisenberg Hamiltonian for the H_2 molecule

Total spin $\boldsymbol{S} = \boldsymbol{\sigma_1} + \boldsymbol{\sigma_2}$ One electron $\Rightarrow$ $\sigma = \frac{1}{2}$ $\boldsymbol{\sigma}^2 = \hbar^2\sigma(\sigma+1)$

$\boldsymbol{S}^2 = \boldsymbol{\sigma}_1^2 + \boldsymbol{\sigma}_2^2 + 2\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$ ($\mathbf{S}^2 = \hbar^2 S(S+1)$)

$2\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = \boldsymbol{S}^2 - \boldsymbol{\sigma}_1^2 - \boldsymbol{\sigma}_2^2 = \boldsymbol{S}^2 - \frac{3}{4} - \frac{3}{4}$

$S = 0 \rightarrow \boldsymbol{S}^2 = 0 \rightarrow 2\,\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = -3/2$ singlet

$S = 1 \rightarrow \boldsymbol{S}^2 = 2 \rightarrow 2\,\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = +1/2$ triplet

$$H_{eff} = 2H_{H,1s} + H_{Coul} + H_{exch}$$

$$E_{sing} = \int \Psi^*_{sing}\, H\, \Psi_{sing}\, dr_1 dr_2$$

$$E_{trip} = \int \Psi^*_{trip}\, H\, \Psi_{trip}\, dr_1 dr_2$$

$$\Delta E_{ST} = E_S - E_T = 2X$$

$J_{ex} = X$

$$H_{Heisenberg} = \frac{1}{4}(E_S + 3E_T) - \Delta E_{ST}\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = \frac{1}{4}(E_S + 3ET) - 2\,J_{ex}\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

$S = \sigma_1 + \sigma_2 = 1$ $E = (E_S + 3E_T)/4 - 1/2\, J_{ex}$

$S = \sigma_1 + \sigma_2 = 0$ $E = (E_S + 3E_T)/4 + 3/2\, J_{ex}$

The energy depends on the relative orientation of the two spins and on the sign of J_{ex}

Origin of Exchange interaction:

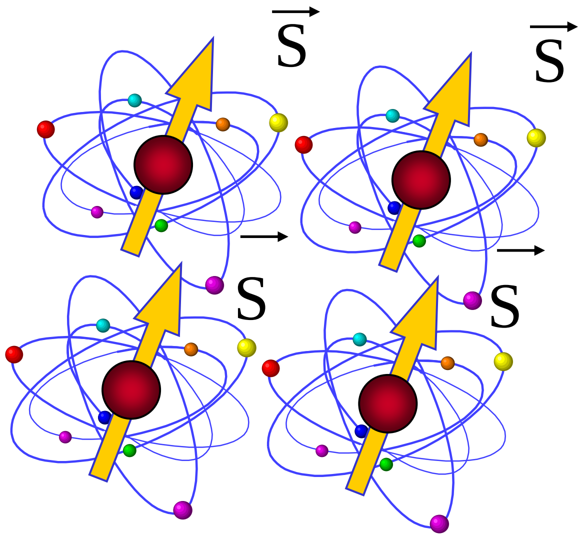
→ Coulomb repulsion between electrons

→ total anti-symmetric wave function (Pauli exclusion principle)

$$H_{exch} = -2J_{ex}\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

Inter-atomic exchange in solids: Heisenberg model

atoms with any spin ***S***



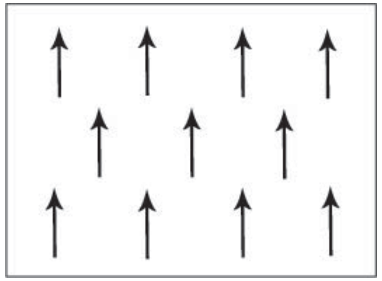
Orbital overlapping between adjacent atoms (similarly to the H_2 molecule)

We can describe the interaction via an effective Hamiltonian similar to the one developed for the H_2 molecule

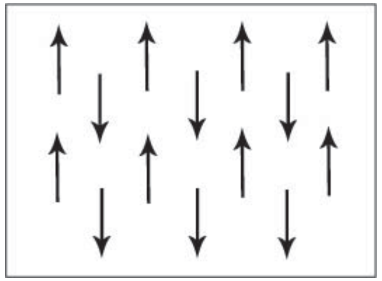
Heisenberg Hamiltonian

$$H = -2J_{ex}\,\boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

$J_{ex} > 0$ Ferromagnetic coupling



$J_{ex} < 0$ Antiferromagnetic coupling



The strength of the interaction depends on the orbital overlap between neighboring atoms $\Rightarrow$ decreases exponentially with distance $\Rightarrow$ short-range interaction

Note that the exchange integral mainly depends on the radial part of the electron wave function but it also depends on the angular part: $\phi(r) = \Psi_{nlm}(r) = R_{nl}(r)Y_l^m$

H.S. Li *et al*. J.Phys.: Condens Matter **3**, 7277 (1991)

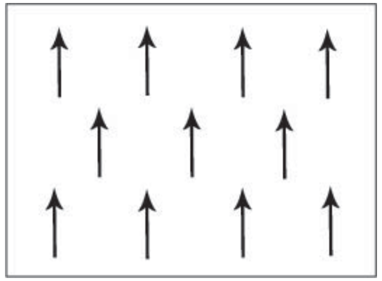
Where the exchange gets into play

$J\,\boldsymbol{S}\cdot\boldsymbol{S}$ type	Curie (Néel) temperature	⇒	magnetic order in a ferromagnetic (antiferromagnetic) nanostructure
	Super-exchange	⇒	mediated interaction between magnetic atoms
	Bias exchange	⇒	interaction at the interface of FM – AFM structures
SOC + $J\,\boldsymbol{S}\cdot\boldsymbol{S}$ type	Dzyaloshinskii-Moriya Interaction (DMI)	⇒	Antisymmetric exchange
$J\,\boldsymbol{S}\cdot\boldsymbol{\sigma}$ type	Stoner exchange	⇒	Spontaneous magnetization
	s-d model	⇒	interaction *between* a *magnetic impurity* and the *conduction band electrons*
	Kondo effect	⇒	interaction *between* a *magnetic impurity* and the *conduction band electrons*
	RKKY interaction	⇒	interaction *between magnetic impurities* mediated by the conduction band electrons

Ordering temperature

See exercise: 3.1-3.2

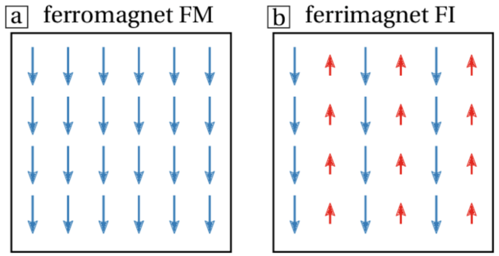
Ferromagnet



$T<T_C$

(T_C is the Curie temperature)

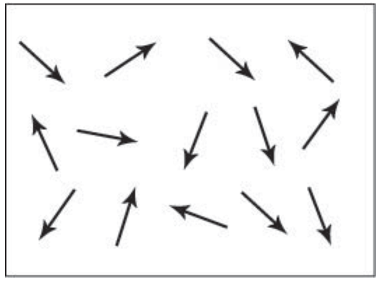
$T>T_C$



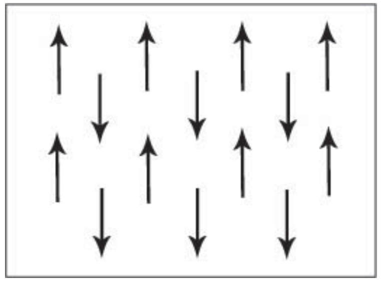
Magnetic moments oppose but do not cancel below TC

Paramagnet

the magnetic moments are randomly oriented due to thermal fluctuations



Antiferromagnet



$T<T_N$

(T_N is the Néel temperature)

$T>T_N$

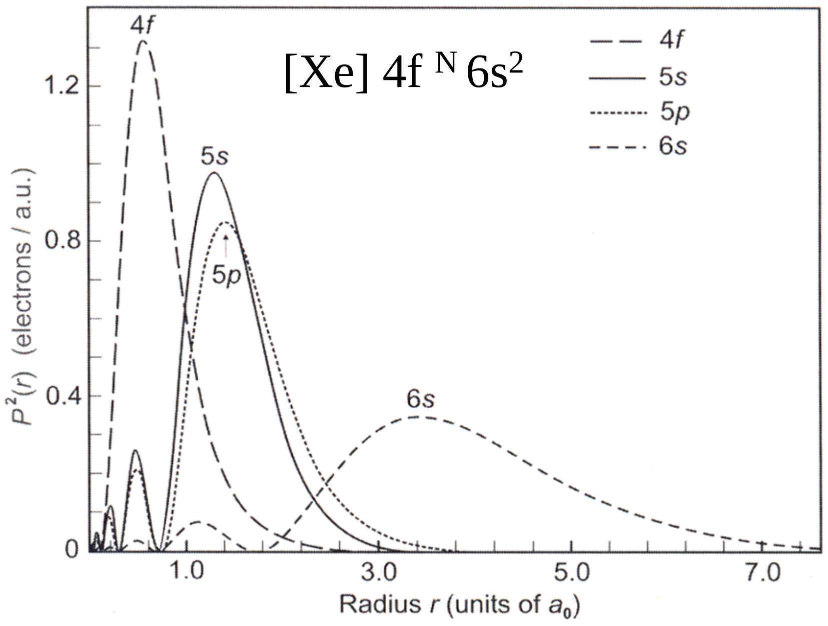
The Curie (Néel) temperature depends on the exchange coupling and on the number of nearest neighbors N

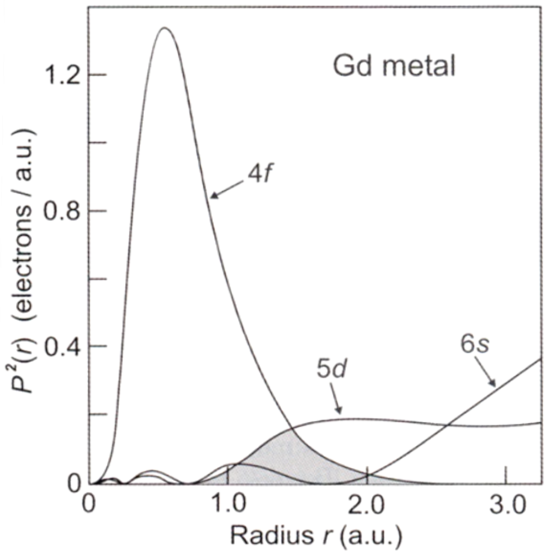
$$T_{C(N)} = \frac{2\,S(S+1)\,N\,J_{ex}}{3\,k_B}$$

Valence orbitals in rare earth and consequences for the exchange

Electronic configuration in atomic case: [Xe] $4f^N\,6s^2$
(exception for Gd: [Xe] $4f^7\,5d^1\,6s^2$)

In rare earth, magnetism originates from 4f states





Radial distribution of the different orbitals

4f states are strongly localized →
do not overlap with wave functions of
neighbouring atoms
but
overlap with 5d and 6s states

How collective magnetism is possible in rare earth compounds ?

Inter-atomic + intra-atomic exchange: 4f-3d strong magnets ($SmCo_5$, Nd_2Fe_{14})

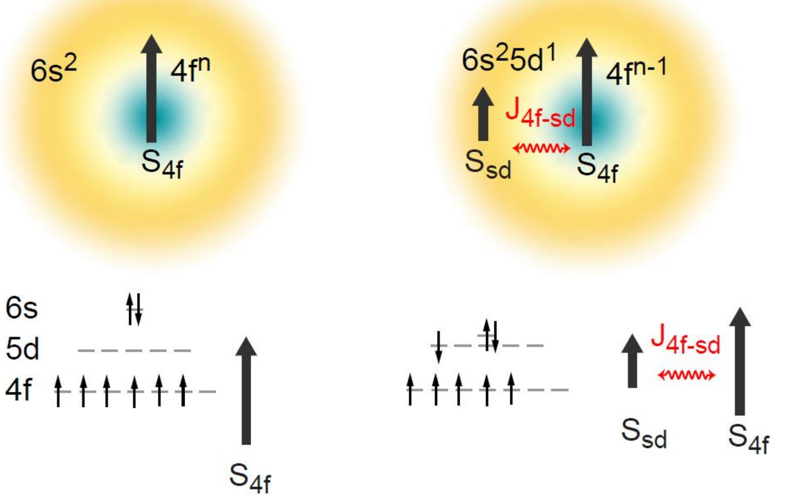
Gas phase

Bulk phase

Rare earths (RE)

$Xe\ 4f^{N}\ 6s^2$

$S_{6s} = 0$



$Xe\ 4f^{N-1}\ 6s^2\ 5d^1$

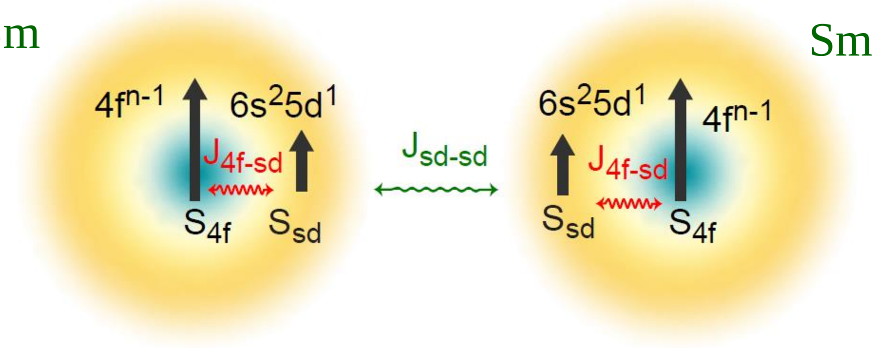
$S_{6s5d} \neq 0$

S_{sd} and S_{4f} are coupled by the intra-atomic exchange interaction $J_{4f\text{-}sd}$

Pure Sm

Sm

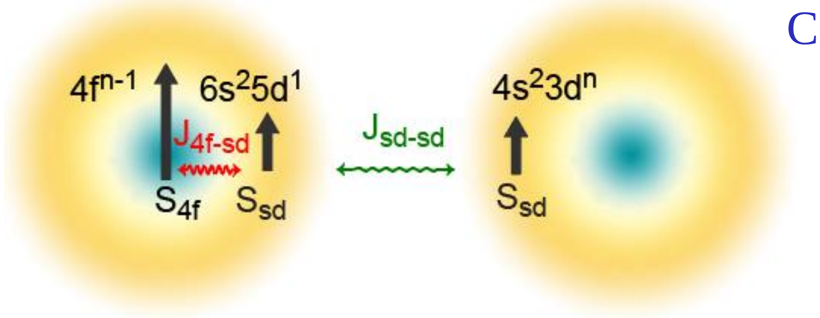
Sm



$SmCo_5$

Sm

Co



$H_{ex} = -2\, J^{Sm\text{-}Sm}_{sd\text{-}sd}\, S^{Sm}_{sd}\, S^{Sm}_{sd}$

T_C (T_N) < 300 K

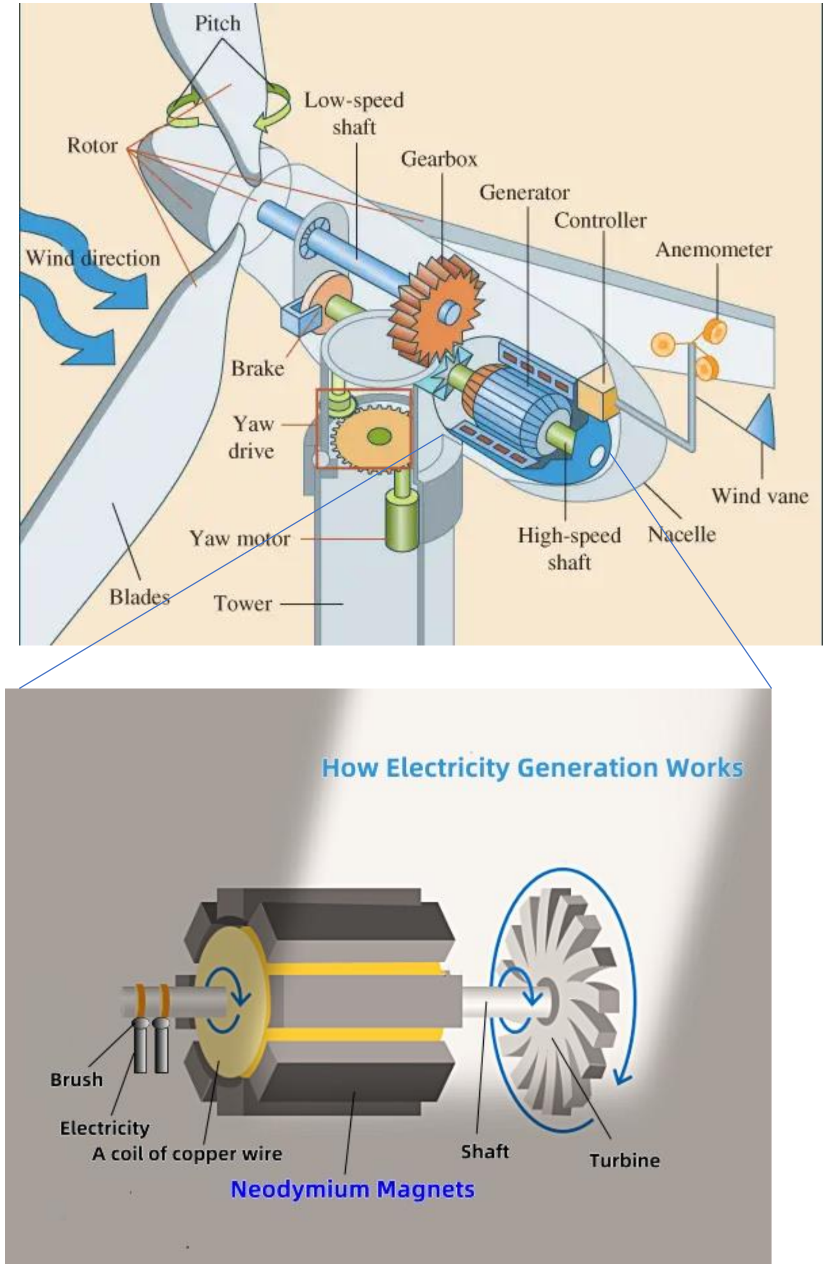
Highest T_C for Gd T_C = 292 K

$H_{ex} = -2\, J^{Sm\text{-}Co}_{sd\text{-}sd}\, S^{Co}_{sd}\, S^{Sm}_{sd}$

The 3d element (having large $\boldsymbol{S}_{sd}$) increases the strength of the exchange interaction thus increasing T_C

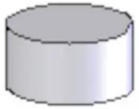
$SmCo_5$ -> T_C = 800°C

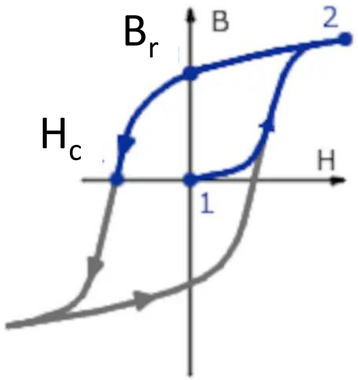
Strong magnet



Magnet Type	Max Energy Product (MGOe)
Neodymium	35-52
SmCo 26	26
Alnico 5/8	5.4
Ceramic	3.4
Flexible	0.6-1.2

B_r x H_c

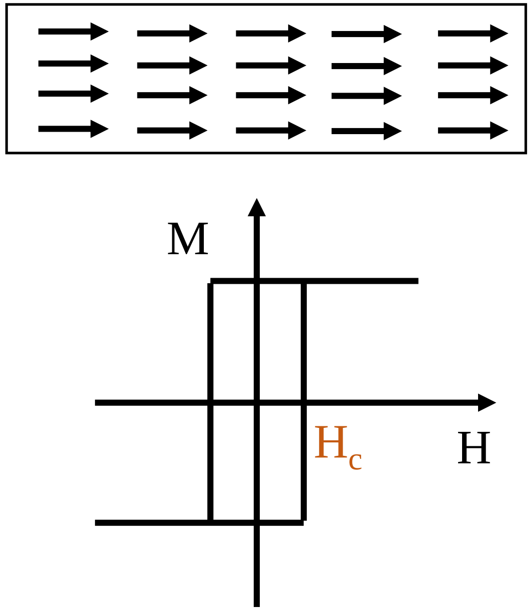




The energy product is the magnetic energy stored in the magnet i.e. the energy one needs to provide to reverse the magnetization of the magnet

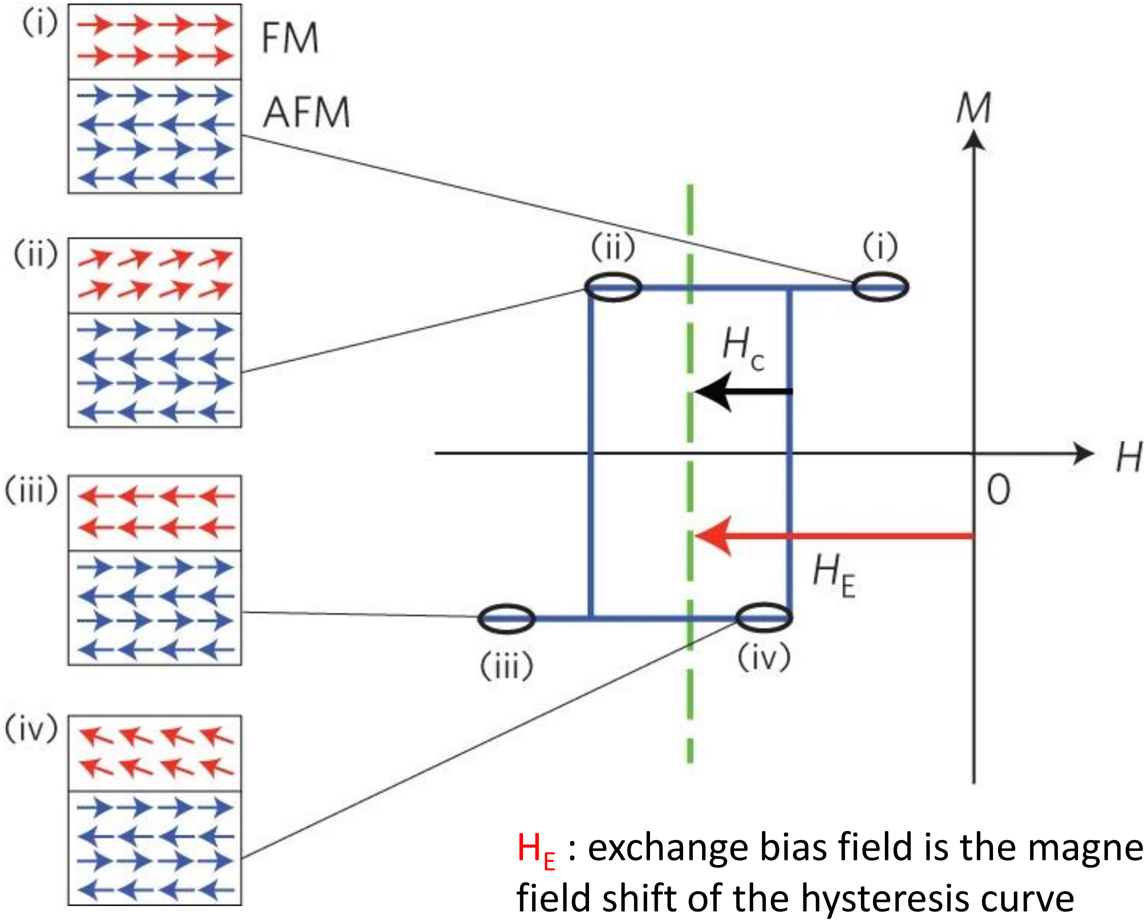
Exchange bias

FM: ferromagnetic material; AFM: antiferromagnetic material



In a FM layer the magnetization reverses at a field H_c (reversal or coercive field)

Due to the exchange interaction at the FM-AFM interface, the field necessary to orient the FM layer parallel to the direction of the surface AFM spins is reduced compared to the field necessary to force the anti-parallel alignment by an amount equal to H_E

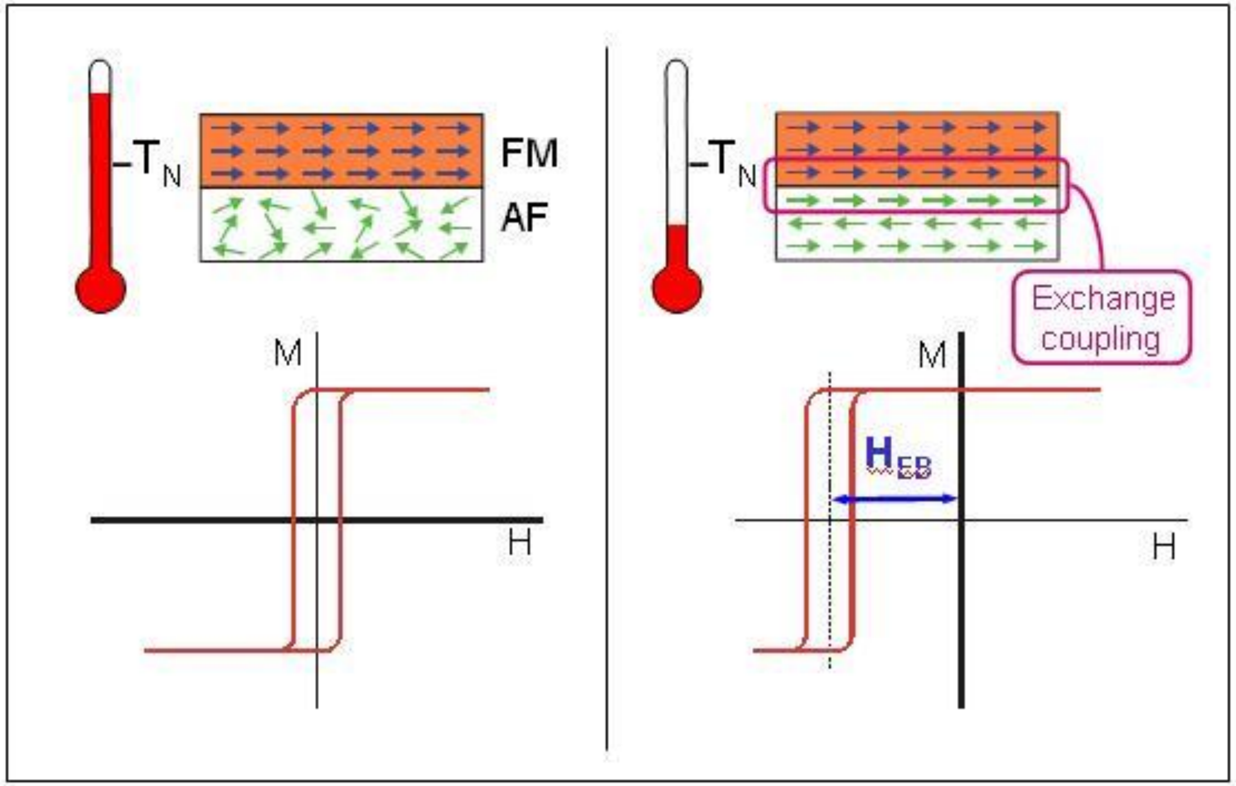


H_E : exchange bias field is the magnetic field shift of the hysteresis curve

The magnetic field required to reverse the pinned layer becomes $H_c + H_E$

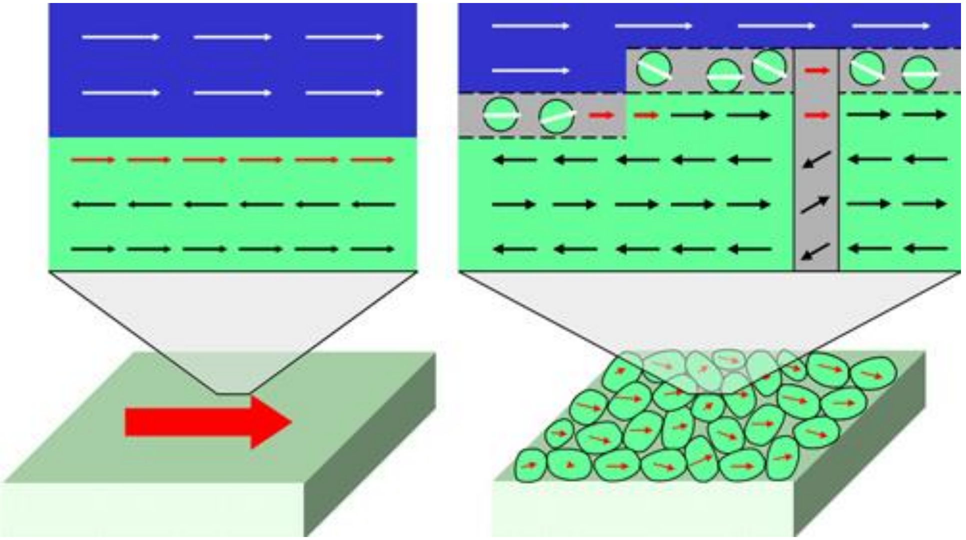
J. Magn. Magn. Mater. **192**, 203 (1999)

Exchange bias *vs* T



Above the Néel temperature of the AF all its spins are disordered. Below T$_N$ they become ordered and the exchange coupling between FM and AF spins leads to the shift of the hysteresis loop.

Exchange bias: a real case



$$H_E = \frac{\sigma}{M_{FM} t_{FM}} = J \frac{S_{AFM} S_{FM}}{a_{AFM}^2 M_{FM} t_{FM}}$$

σ -> interface energy (theoretic value)

σ_{eff} -> experimental value deduced from H_E

J -> exchange energy at the AFM – FM interface

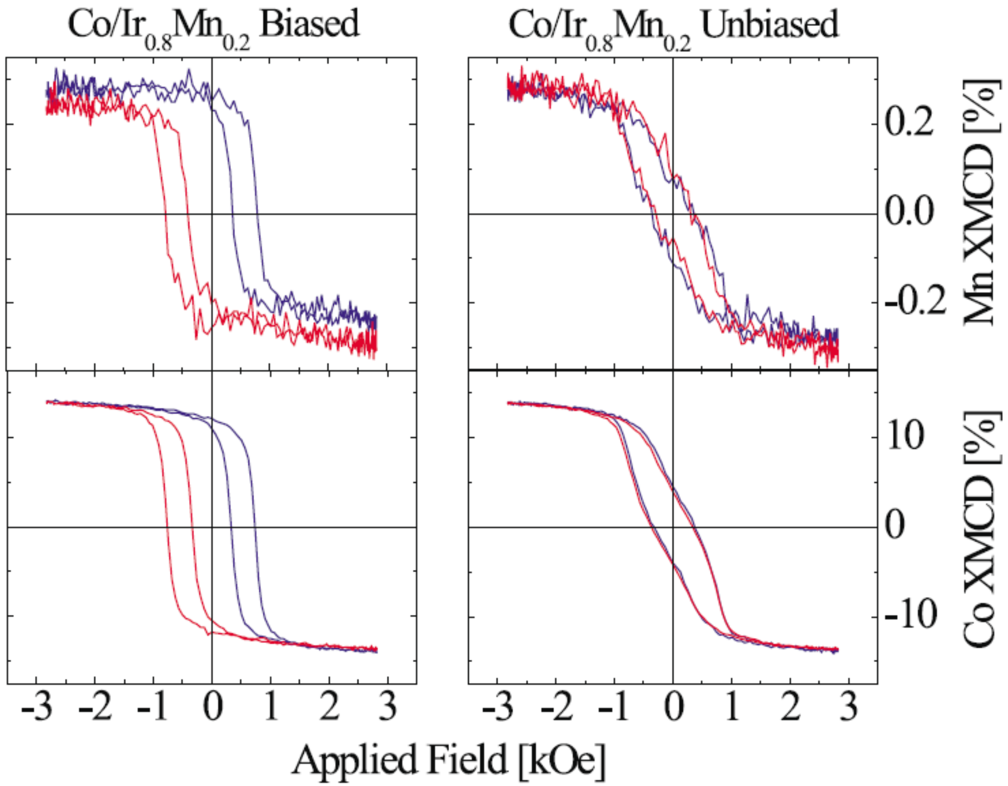
S_{AFM} (S_{FM}) -> Spin of AFM (FM) layer

a_{AFM} -> lattice parameter

only a small fraction ($\rho = \sigma_{eff}/\sigma \cong 5\%$) of interfacial spins is pinned, and these cause the horizontal hysteresis loop shifts.

TABLE I. Effective and corrected interface energies σ calculated from the macroscopic loop shift and the coverage with pinned spins ρ.

Sample	ρ (ML)	σ_{eff} (mJ/m^2)	σ (mJ/m^2)
A 3 nm Co/NiO	0.04 ± 0.01	0.052 ± 0.005	1.3 ± 0.5
B 2 nm Co/IrMn	0.04 ± 0.01	0.168 ± 0.020	4.1 ± 1.4
C 1 nm CoFe/PtMn	0.03 ± 0.01	0.124 ± 0.014	3.9 ± 1.4
D 2 nm CoFe/PtMn	0.04 ± 0.01	0.188 ± 0.015	4.8 ± 1.7
E 3 nm CoFe/PtMn	0.04 ± 0.01	0.229 ± 0.027	5.7 ± 2.0



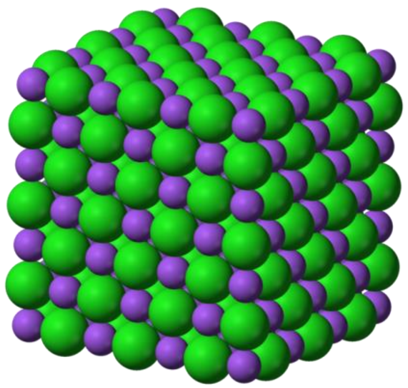
H. Ohldag *et al*., Phys. Rev. Lett. **91**, 017203 (2003)

Super-exchange

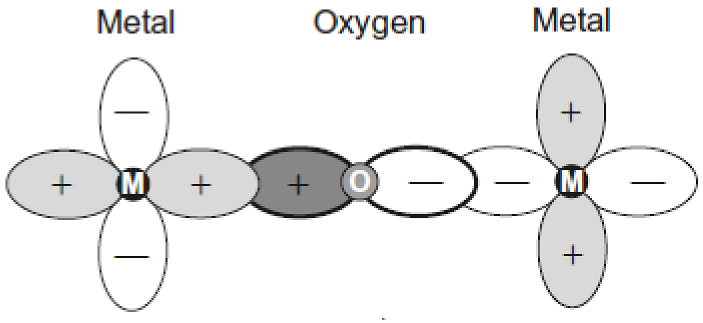
● oxigen

● metal

(ex: MnO)



in many materials (oxides), magnetic atoms are separated by non-magnetic ions (oxygen)



Indirect interactions through oxygen atoms

In the antiferromagnetic configuration, 3d-electrons of atoms A and B can both hybridize with 1p-electron of Oxygen

energy depends on the relative spin orientation

Dzyaloshinskii-Moriya interaction (DMI)

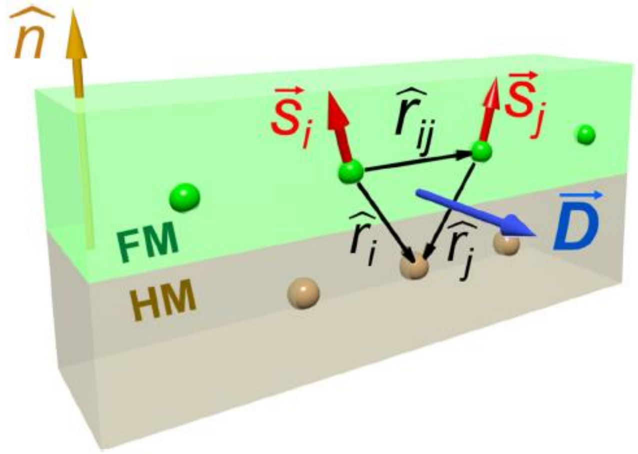
See exercise: 3.3

Consequence of:
- super-exchange
- spin-orbit interaction

$$\delta E = \sum_m \left[\frac{\langle n|\lambda \hat{\mathbf{L}}_i \cdot \hat{\mathbf{S}}_i|m\rangle 2J(mn'nn')\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j}{E_n - E_m} + \frac{2J(nn'mn')\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \langle m|\lambda \hat{\mathbf{L}}_i \cdot \hat{\mathbf{S}}_i|n\rangle}{E_n - E_m} \right] + \sum_{m'} \left[\frac{\langle m'|\lambda \hat{\mathbf{L}}_j \cdot \hat{\mathbf{S}}_j|m\rangle 2J(m'nn'n)\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j}{E_{n'} - E_{m'}} + \frac{2J(n'nm'n)\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \langle m'|\lambda \hat{\mathbf{L}}_j \cdot \hat{\mathbf{S}}_j|n'\rangle}{E_{n'} - E_{m'}} \right]$$

Effective Hamiltonian

$$H_{DMI} = \sum_{ij} \vec{D}_{ij} \cdot (\vec{S}_i \wedge \vec{S}_j)$$



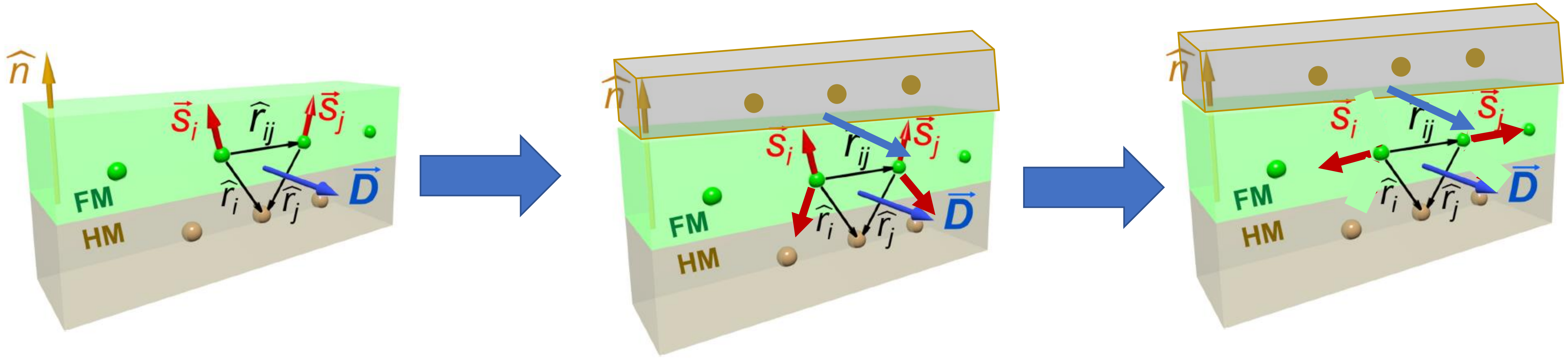
Contrary to the Heisenberg-type exchange, which favors collinear alignment, the DMI promotes an orthogonal arrangement between $\vec{S}_i$ and $\vec{S}_j$, with a **chirality imposed by the direction of $\vec{D}_{ij}$**.

DMI at interfaces.
Broken symmetry at the interface. The exchange coupling between the spins $\vec{S}_i$ and $\vec{S}_j$ in a ferromagnetic (FM) layer is mediated by a heavy metal (HM) atom with large SOC. In this case, the local DMI vector $\vec{D}_{ij}$ is perpendicular to the plane formed by the two atoms of the ferromagnetic layer and the one of the heavy metal layer. Because a large SOC exists only in the bottom HM layer, this DMI is not compensated by a DMI coming from a top layer

DOI: 10.1103/RevModPhys.95.015003 I. Dzyaloshinskii, J. Phys. Chem. Sol. **4**, 241 (1958); T. Moriya, Phys. Rev. **120**, 91 (1960)

Dzyaloshinskii-Moriya interaction (DMI): need of breaking symmetry

The DMI has a net contribution only in systems without a center of inversion (Moriya rules)



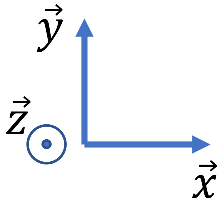
$\vec{S}_i \wedge \vec{S}_j = 0$ because parallel

Adapted from DOI: 10.1103/RevModPhys.95.015003

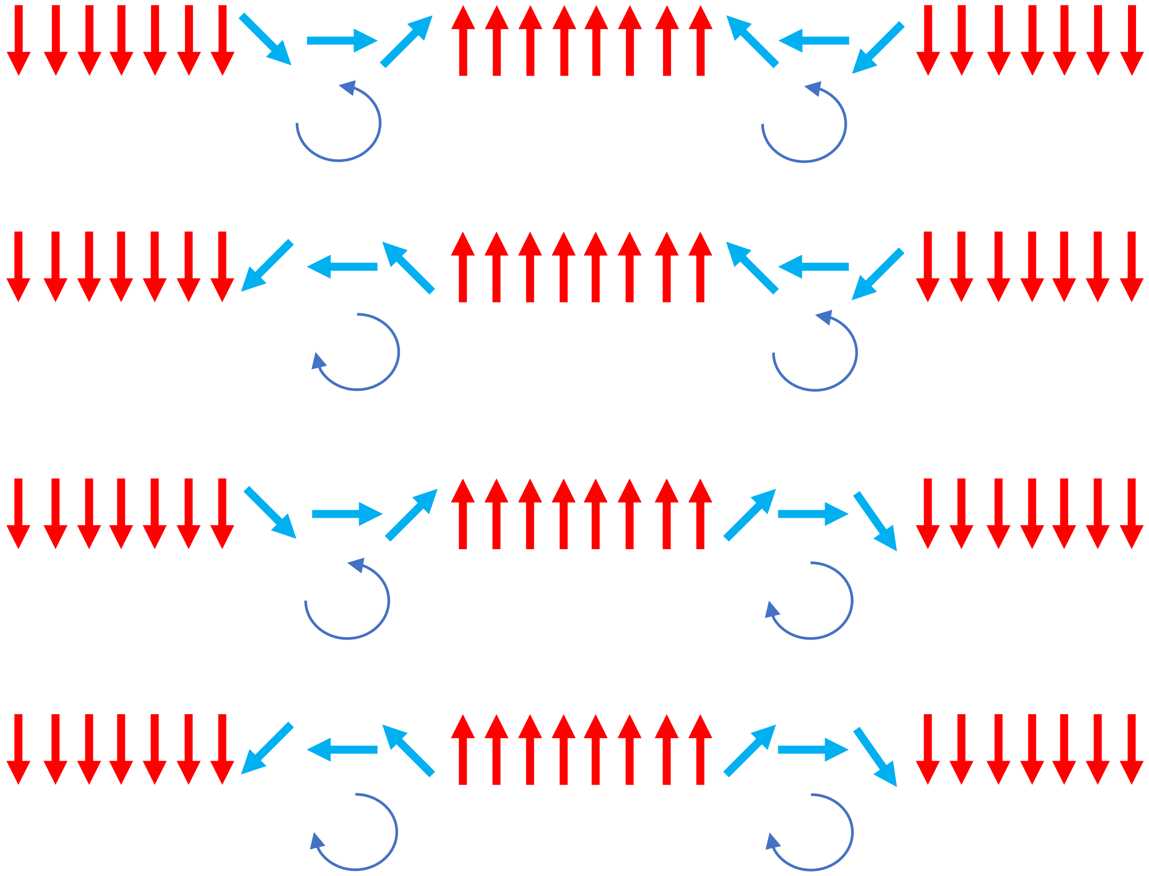
DMI induces chiral spin structures

See exercise: 3.4

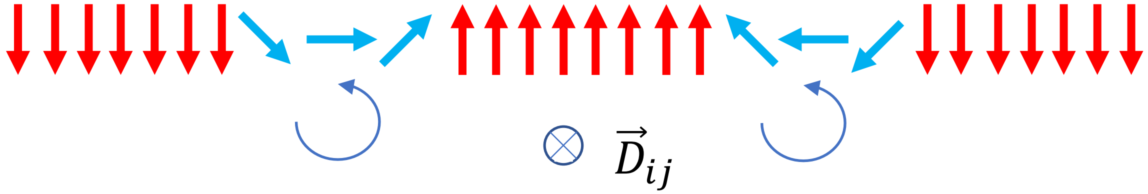
2 domain walls in a 1D chain of spin forced (by anisotropy) in the xy plane



Exchange interaction:
4 degenerate configurations



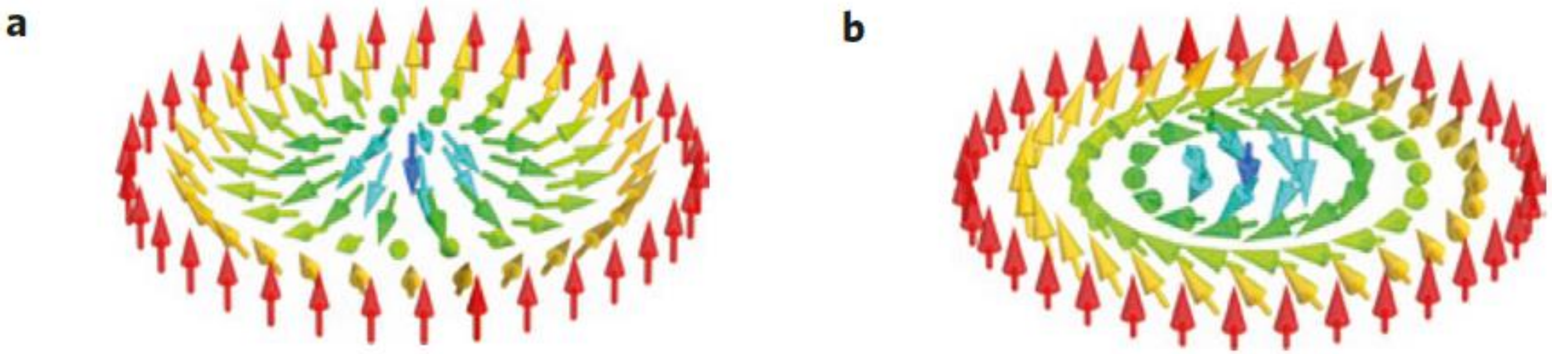
DMI interaction:
1 configuration



$$H_{DMI} = \sum_{ij} \vec{D}_{ij} \cdot (\vec{S}_i \wedge \vec{S}_j)$$

DMI generates skyrmions

$\vec{D}_{ij} \perp \vec{r}_{ij}$ $\vec{D}_{ij} \parallel \vec{r}_{ij}$

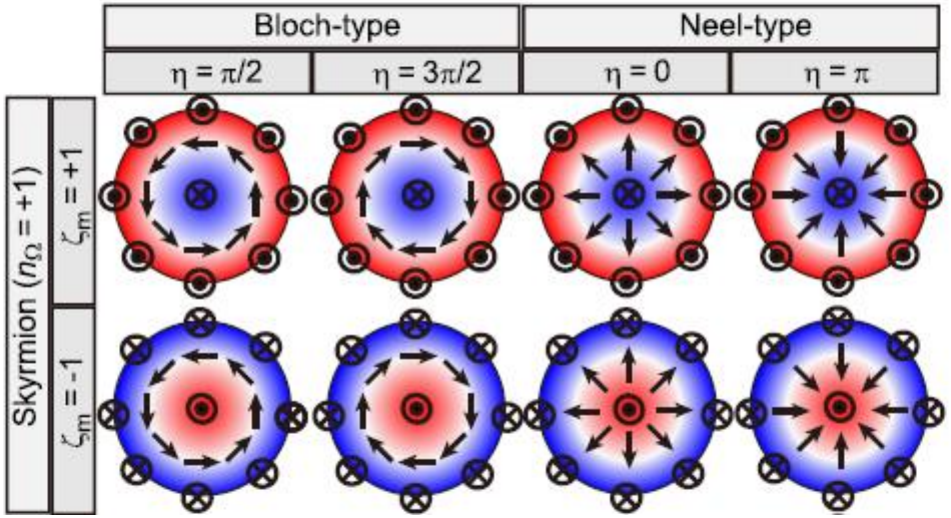


Néel-type Bloch-type

Spins in a skyrmion.
Skyrmions in a 2D ferromagnet with uniaxial magnetic anisotropy along the vertical axis. The magnetization is pointing up on the edges and pointing down in the center. Moving along a diameter, the magnetization rotates by 2π around an axis perpendicular to the diameter (**a**) and by 2π around the diameter (**b**), which corresponds to different orientations of the Dzyaloshinskii–Moriya vector.

In a Neel-type skyrmion, the spins rotate in the radial planes from the core to the periphery.
In a Bloch-type skyrmion, the spins rotate perpendicular to the radial directions, when moving from the core to the periphery.

Starting from a ferromagnetic state with $\vec{S}_i$ parallel to $\vec{S}_j$, the DMI tilts $\vec{S}_i$ with respect to $\vec{S}_j$ by a rotation around $\vec{D}_{ij}$. In a 2D ferromagnet with uniaxial anisotropy and a non-negligible DMI compared with the exchange interaction, the energy is minimized by the skyrmion structure. $\vec{r}_{ij}$ is the vector joining the site of $\vec{S}_i$ to the site of $\vec{S}_j$

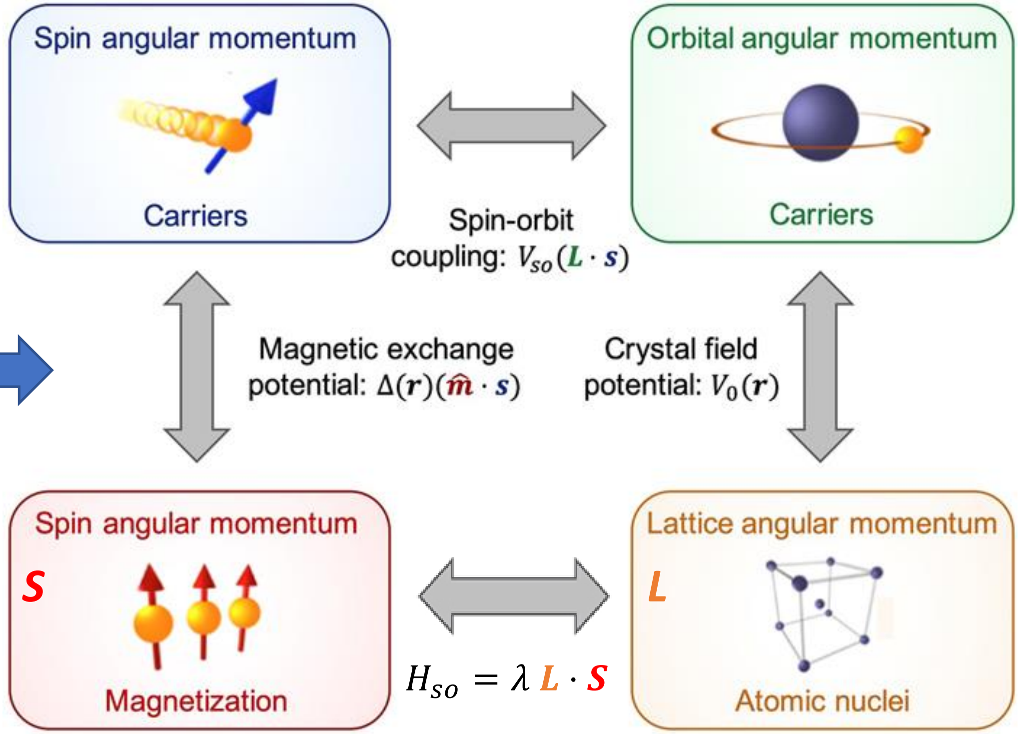


https://doi.org/10.1038/nnano.2013.29

https://doi.org/10.1088/1361-648X/ad861b

The Anderson and s-d model

Interactions between
carrier spins and localized spins



Spin angular momentum

Carriers

Orbital angular momentum

Carriers

Spin-orbit coupling: $V_{so}(\boldsymbol{L}\cdot\boldsymbol{s})$

Magnetic exchange potential: $\Delta(\boldsymbol{r})(\hat{\boldsymbol{m}}\cdot\boldsymbol{s})$

Crystal field potential: $V_0(\boldsymbol{r})$

Spin angular momentum

$\boldsymbol{S}$

Magnetization

$H_{so} = \lambda\,\boldsymbol{L}\cdot\boldsymbol{S}$

Lattice angular momentum

$\boldsymbol{L}$

Atomic nuclei

The Anderson impurity model describes a localized state, the 3d-state (or 4f-state), interacting with delocalized electrons in a valence band

Let introduce:

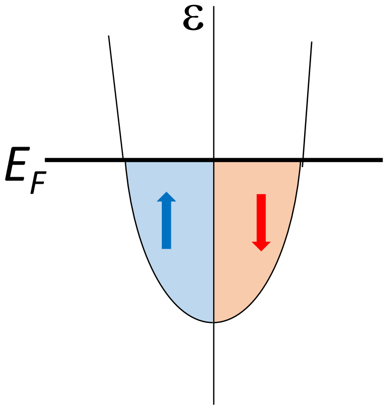
$\tilde{a}_{k,\sigma}$ and $a_{k,\sigma}$ are the operators corresponding to the annihilation and creation of an electron with wave vector *k* and spin σ

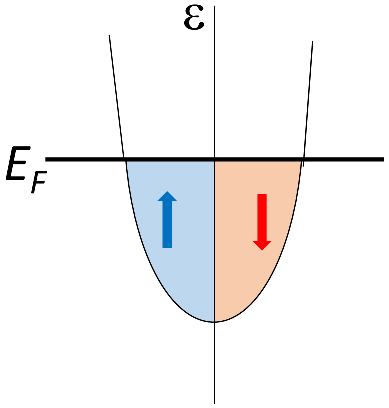
$n_{k,\sigma} = \tilde{a}_{k,\sigma} a_{k,\sigma}$ is the number of electrons with wave vector *k* and spin σ

The Anderson and s-d model

s states

$$H_s = \sum_{k,\sigma} \epsilon_k n_{k,\sigma}$$





$$H_s + U_{ss} =$$

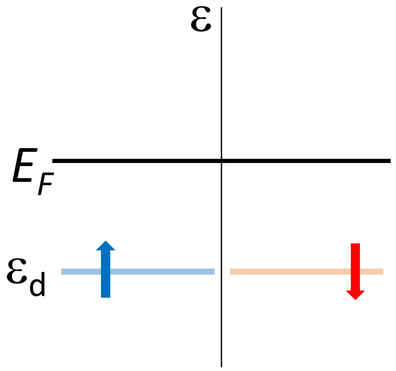
$$= \sum_{k,\sigma} \epsilon_k n_{k,\sigma} + \sum_{d} U_s n_{d,\uparrow}\, n_{d,\downarrow} \approx H_s$$

V_{ee} between delocalized states is negligible

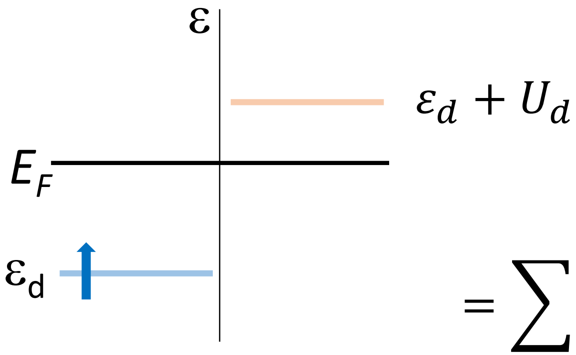
$$\boldsymbol{V_{ee} = 0}$$

$$\boldsymbol{V_{ee} \neq 0}$$

d states



$$H_d = \sum_{d,\sigma} \epsilon_d n_{d,\sigma}$$

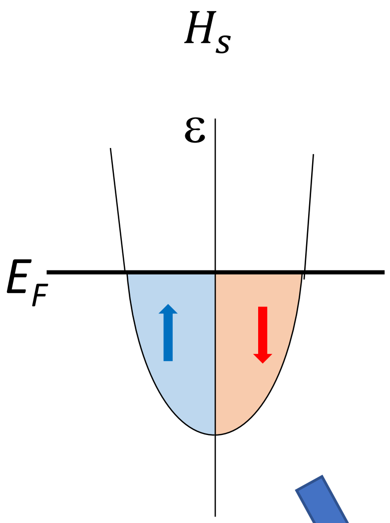


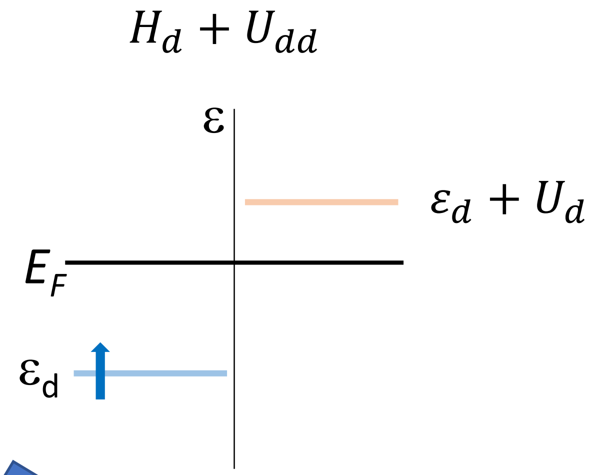
$$H_d + U_{dd} =$$

$$= \sum_{d,\sigma} \epsilon_d n_{d,\sigma} + \sum_{d} U_d n_{d,\uparrow}\, n_{d,\downarrow}$$

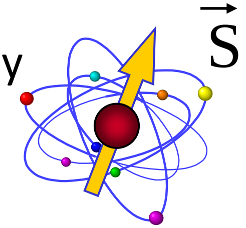
The Anderson and s-d model

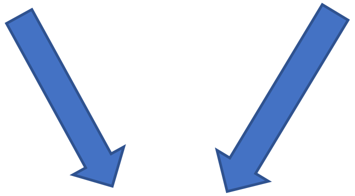
Non magnetic host





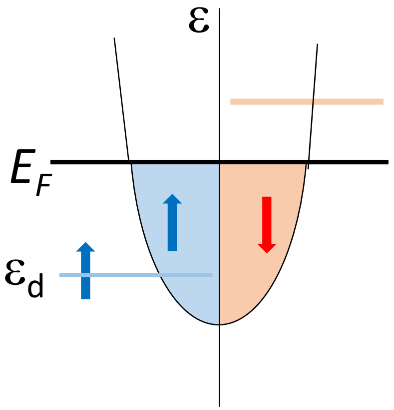
Spin impurity

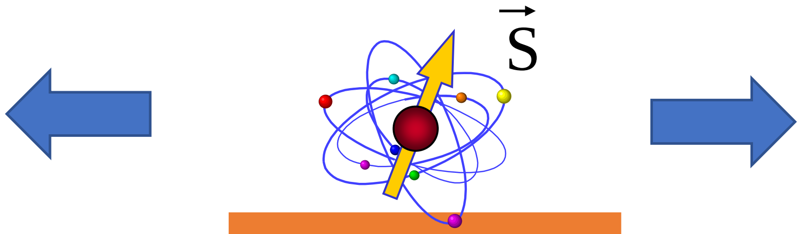




without s-d hybridization

$H_s + H_d + U_{dd}$

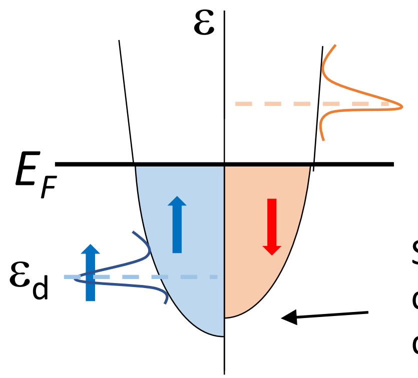




Non magnetic host

With s-d hybridization

$$H_s + H_d + U_{dd} + t_{sd} \sum_{k,\sigma} \tilde{a}_{k,\sigma} a_{d,\sigma} + \tilde{a}_{d,\sigma} a_{k,\sigma}$$



Energy spread due to finite lifetime $\approx \frac{\hbar}{t_{sd}}$

Some spin polarization can also appear in the delocalized states

t_{sd} is the hopping integral (energy)

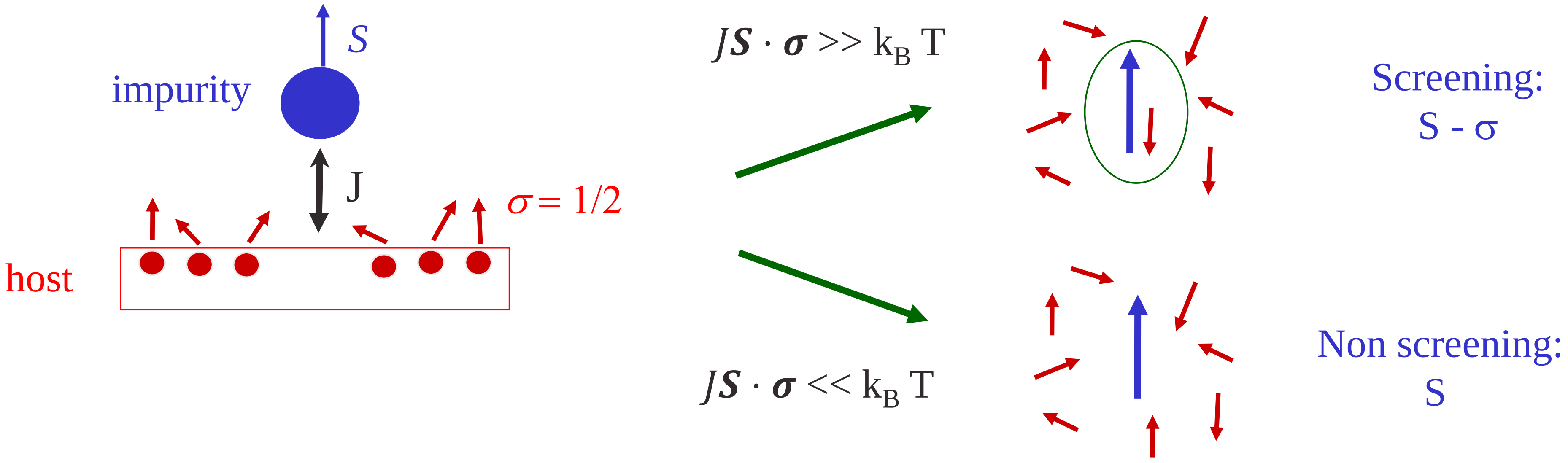
The Anderson and s-d model

Anderson Hamiltonian: $H = H_s + H_d + U_{dd} + t_{sd} \sum_{k,\sigma} \tilde{a}_{k,\sigma} a_{d,\sigma} + \tilde{a}_{d,\sigma} a_{k,\sigma} = H_0 + H_{hop}$

If $t_{sd} \ll U_{dd}$, we can use perturbation theory to evaluate H_{hop}

s-d model (effective) Hamiltonian: $H_{hop} \approx -J\boldsymbol{S} \cdot \boldsymbol{\sigma}$

Kondo effect



S

impurity

J

$\sigma = 1/2$

host

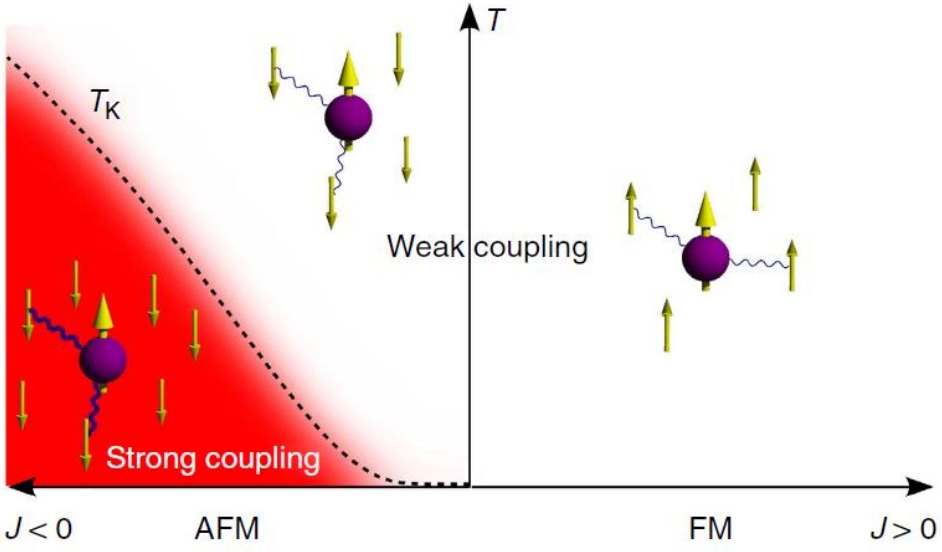
$J\boldsymbol{S} \cdot \boldsymbol{\sigma} >> k_B\ T$

Screening:
S - σ

$J\boldsymbol{S} \cdot \boldsymbol{\sigma} << k_B\ T$

Non screening:
S

The Kondo interaction $J\boldsymbol{S} \cdot \boldsymbol{\sigma}$ couples itinerant electrons of the host with spin σ = 1/2 to a magnetic impurity with spin S. For exchange interaction $J < 0$, antiferromagnetic (AFM) coupling of the spins of the conduction electrons screens the impurity spin. The ground state at temperatures T below the Kondo temperature T_K is a spin $\boldsymbol{S}_{tot} = \boldsymbol{S} - \boldsymbol{\sigma}$ (red area).
For J > 0, the ferromagnetic (FM) coupling tends to create a cloud of spins aligned parallel to the impurity spin, which becomes asymptotically free at high temperatures.



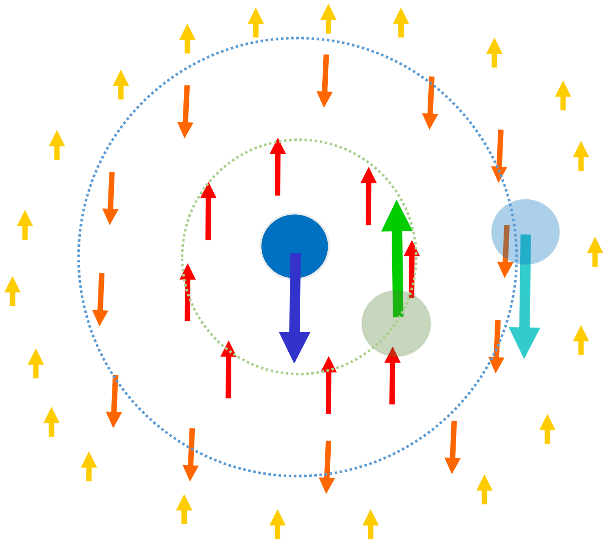
For S = ½ complete screening
For S > 1 under-screening Kondo

NATURE COMMUNICATIONS | 4:2110 | DOI: 10.1038/ncomms3110

RKKY interaction

See exercise: 3.4

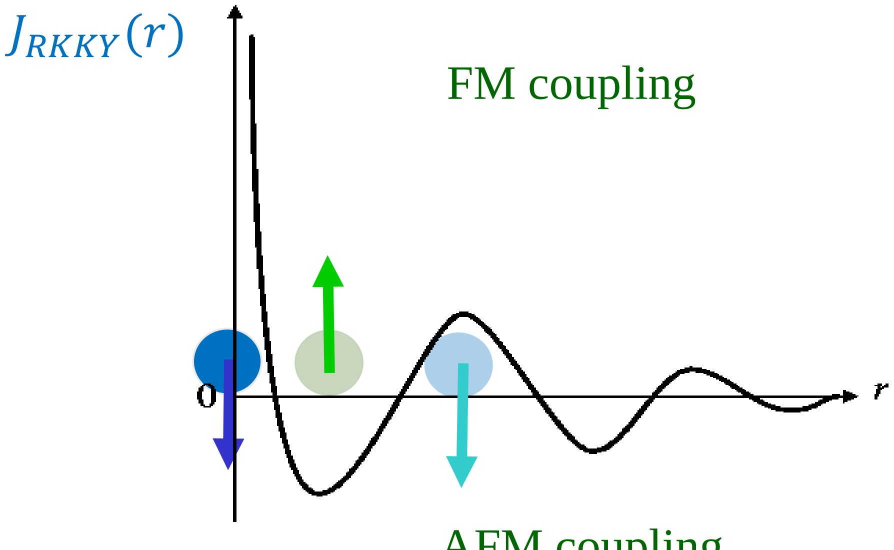
Indirect exchange couples moments (in impurities or magnetic layers) over relatively large distances



● Impurity (“shell” 1)

● Impurity (“shell” 2)

The electron gas is spin polarized by an impurity spin. Due to the interference between electronic waves scattered from the impurity, the spin polarization oscillates with a period set by the Fermi wave vector. A second spin is subject to an indirect exchange interaction that oscillates in sign with the spin polarization of the electron gas.



Effective Hamiltonian: $H_{RKKY} = J_{RKKY}(r)\boldsymbol{S}_0 \cdot \boldsymbol{S}_i$

$$J_{RKKY}(r) = J_0 \frac{x\cos x - \sin x}{x^{D+1}} \underset{x\to\infty}{\rightarrow} J_0 \frac{\cos x}{x^D}$$

$$x = 2k_F r$$

D represent the system dimensionality

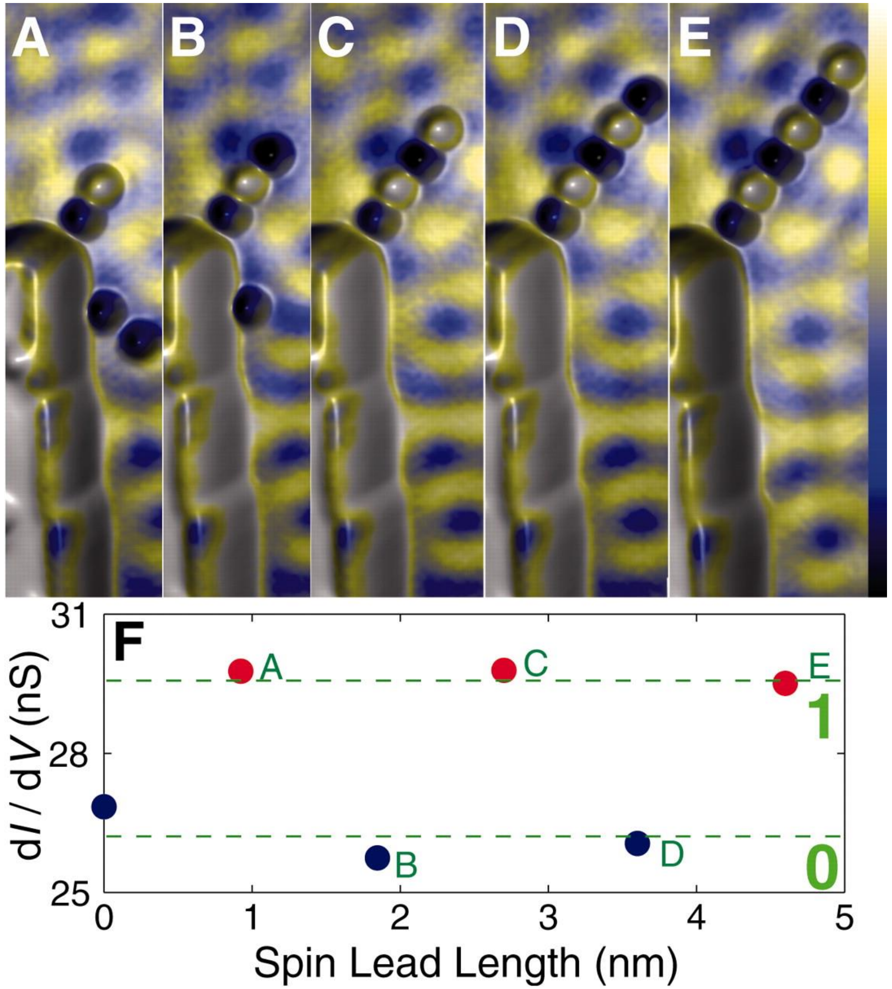
$\lambda_F = 2\pi/k_F$ Fermi wave length

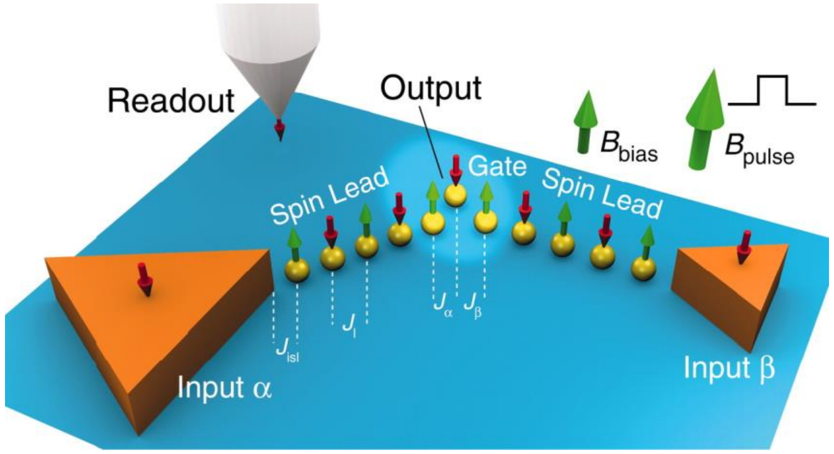
(in metal is of the order of a few nm)

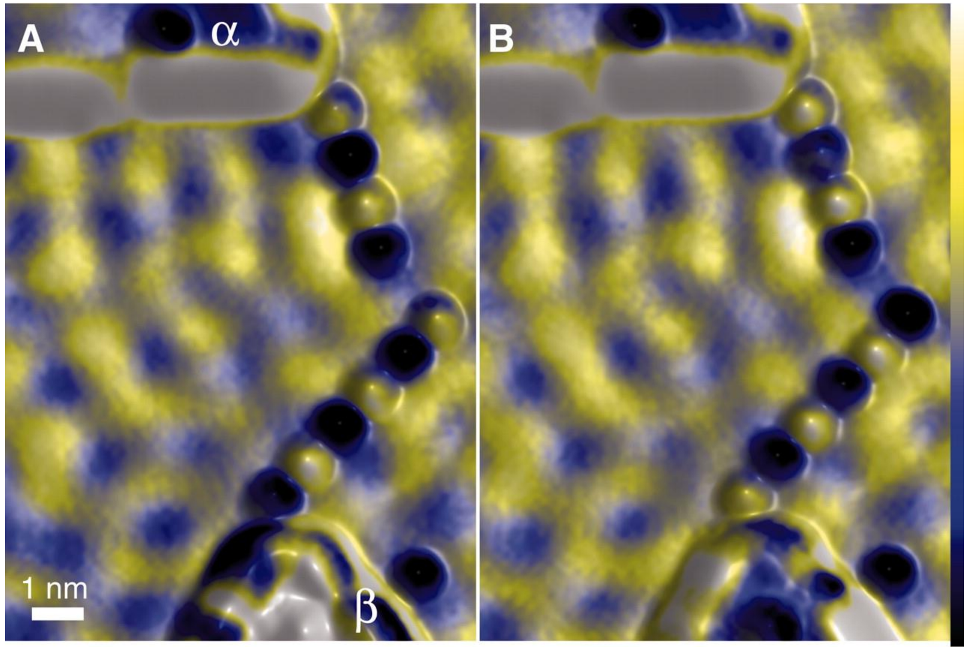
RKKY interaction visualized with SP-STM

SP-STM: spin polarized scanning tunneling microscope

The adatoms interact with the spin polarized gas







DOI: 10.1126/science.1201725

RKKY coupling between magnetic layers mediated by non magnetic spacer

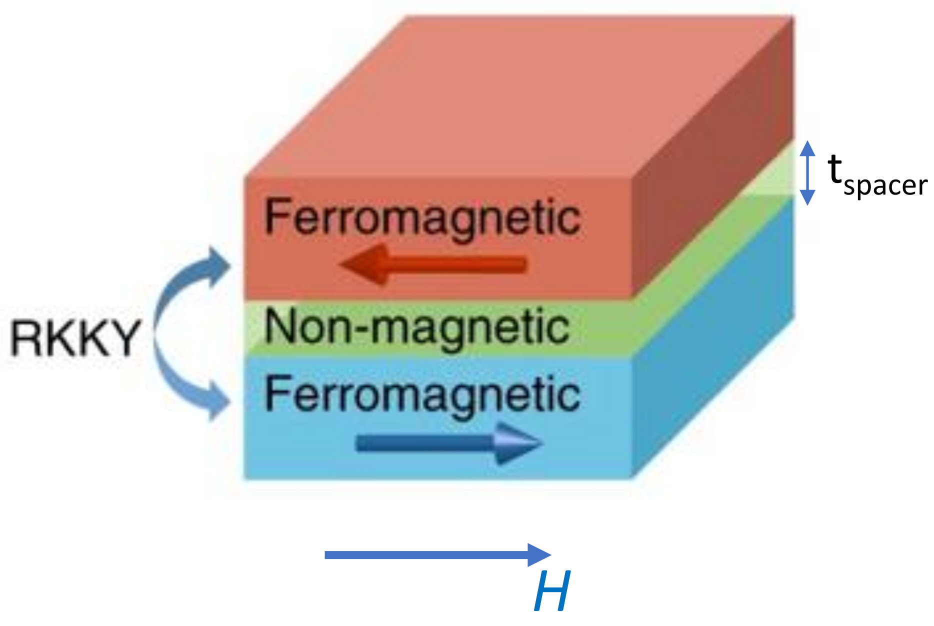
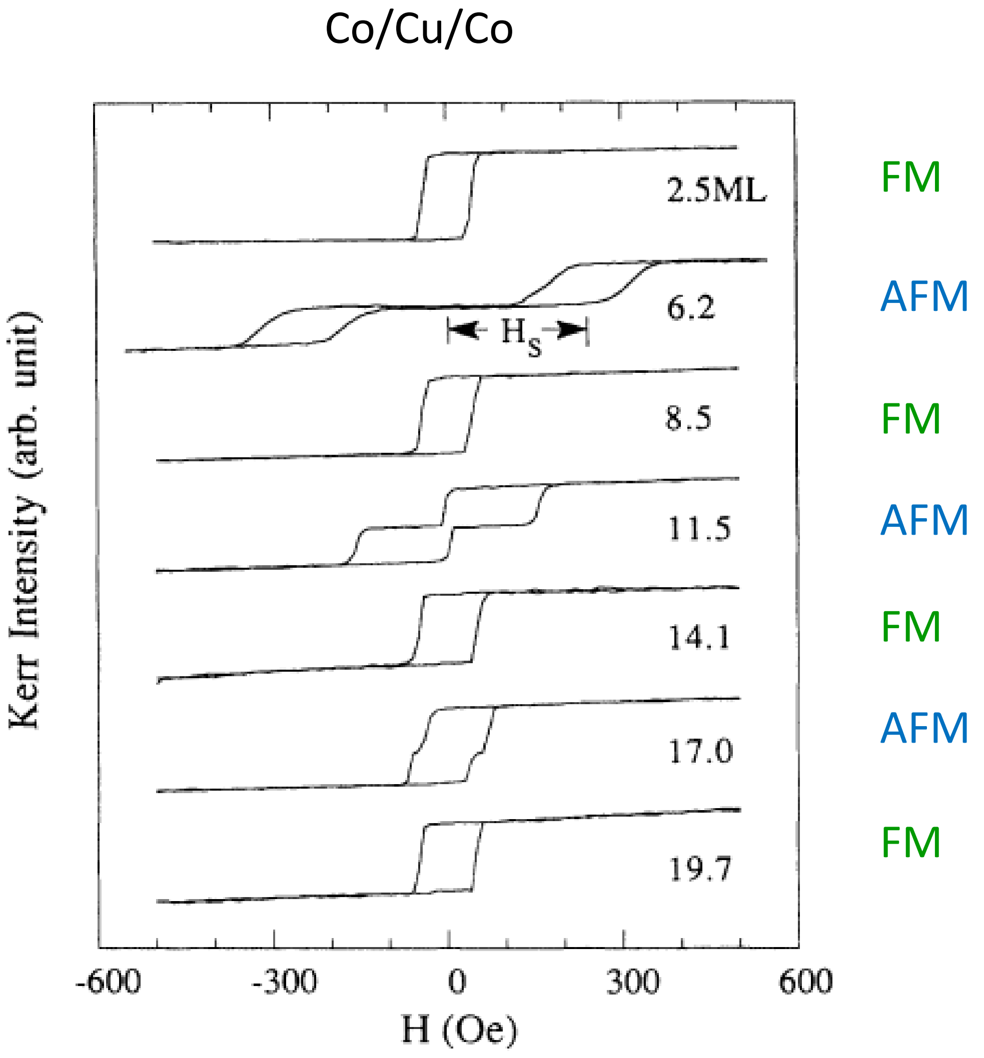


Table 15.1. coupling strength $-J$ in mJ/m^2 at an interlayer thickness z in nm and oscillation periods in monolayers (and nm) of various systems

System	$-J$	z	Oscillation periods
Co / Cu / Co(100)	0.4	1.2	2.6 (0.47), 8 (1.45)
Co / Cu / Co(110)	0.7	0.85	9.8 (1.25)
Co / Cu / Co(111)	1.1	0.85	5.5 (1.15)
Fe / Au / Fe(100)	0.85	0.82	2.5 (0.51), 8.6 (1.75)
Fe / Cr / Fe(100)	>1.5	1.3	2.1 (0.3); 12 (1.73)
Fe / Mn / Fe(100)	0.14	1.32	2 (0.33)
Co / Rh / Co(111)	34	0.48	2.7 (0.6)

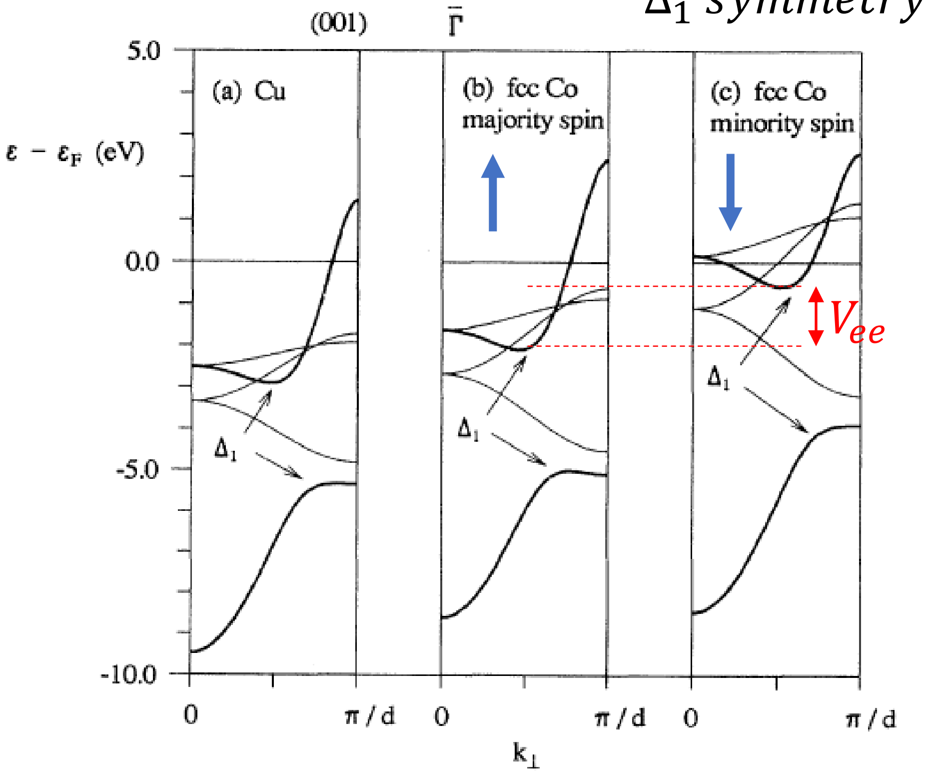


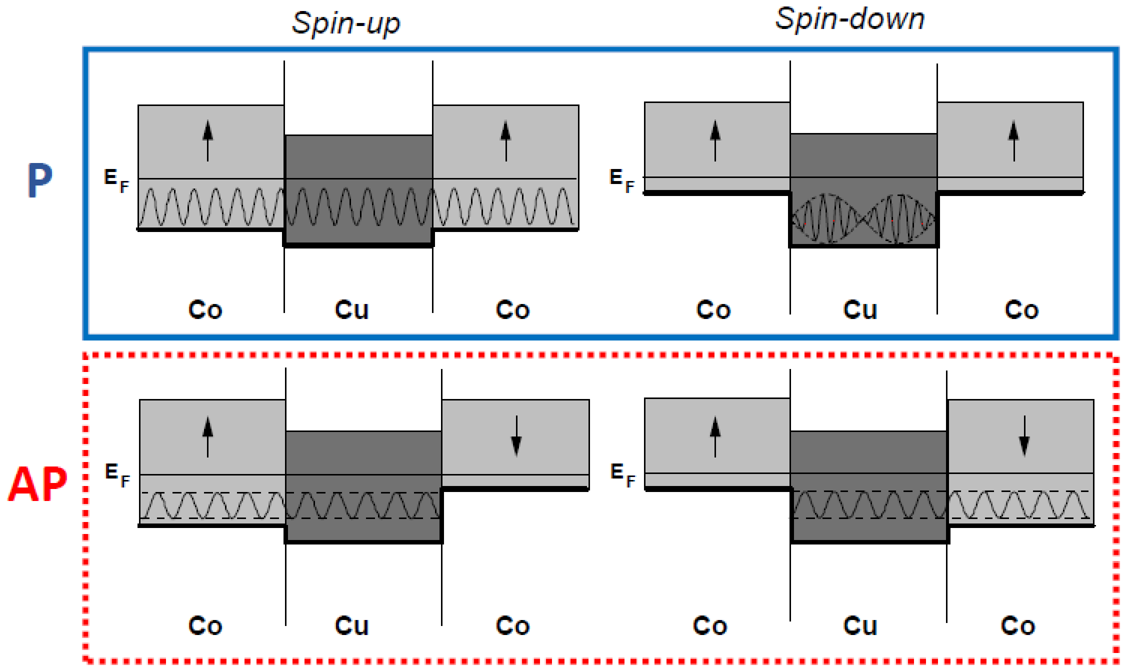
Hysteresis loops for Co(20-ML)/Cu/Co(20-ML) sandwiches for different thicknesses of the Cu spacer layer.

DOI: https://doi.org/10.1103/PhysRevB.46.8659

Origin of RKKY interaction in multilayers

Δ_1 *symmetry* $\rightarrow d_{z^2}$





Courtesy: P. Gambardella

The majority (↑) and minority (↓) states of Co are split by the exchange interaction (V_{ee})

The majority and minority states of Cu are degenerate (Cu is nonmagnetic)

The dispersion of the majority states of Co is very similar to that of Cu → weak reflection ($R_\uparrow \approx 0$)

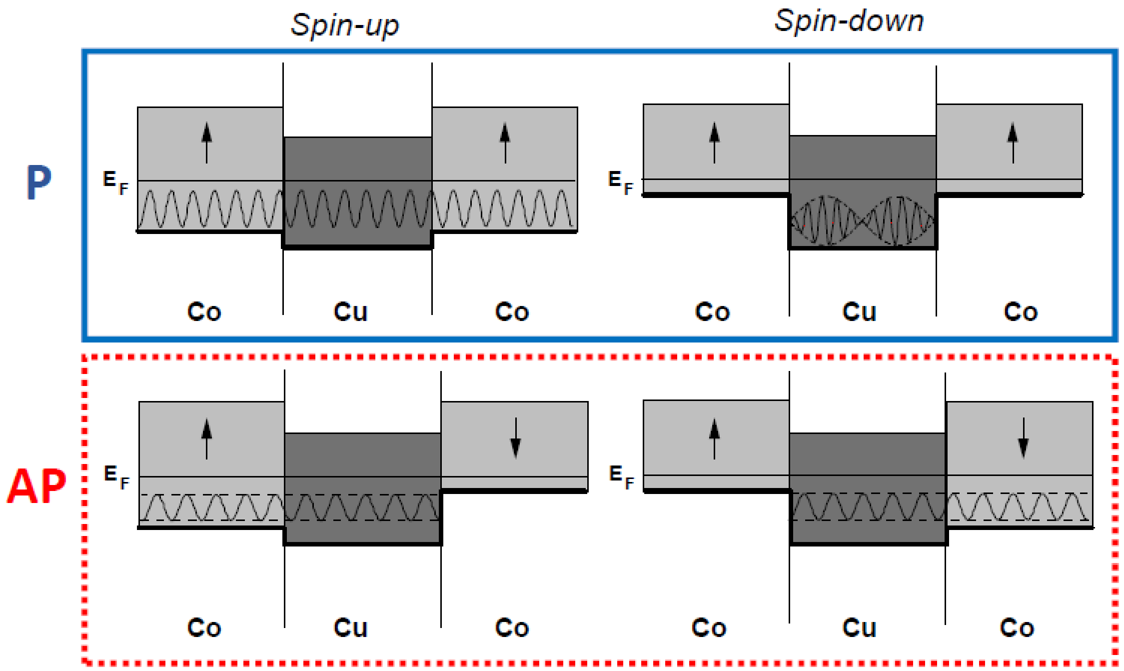
The minority states of Co are mismatched with respect to the Cu states → strong reflection ($R_\downarrow \approx 1$)

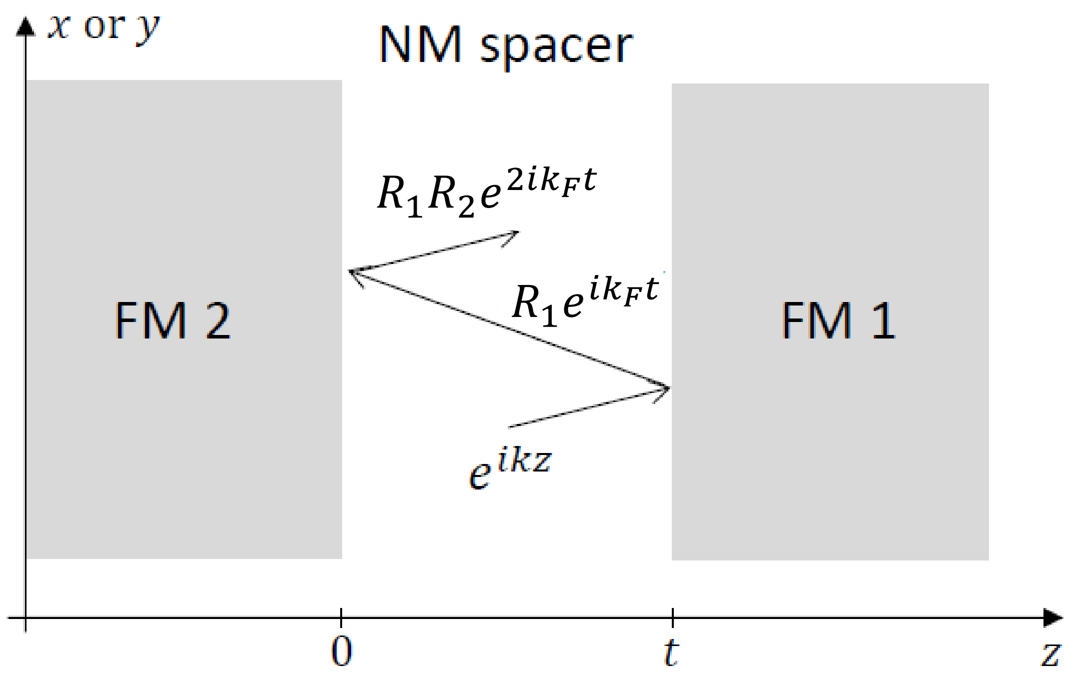
Electron confinement is spin-dependent: the formation of QWs occurs mostly for minority electrons

J. Mathon, *et al.*, Phys. Rev. let. **74**, 3696 (1995); P. Bruno https://doi.org/10.1103/PhysRevB.52.411; M.D. Stiles https://doi.org/10.1103/PhysRevB.48.7238

Origin of RKKY interaction in multilayers

Courtesy: P. Gambardella





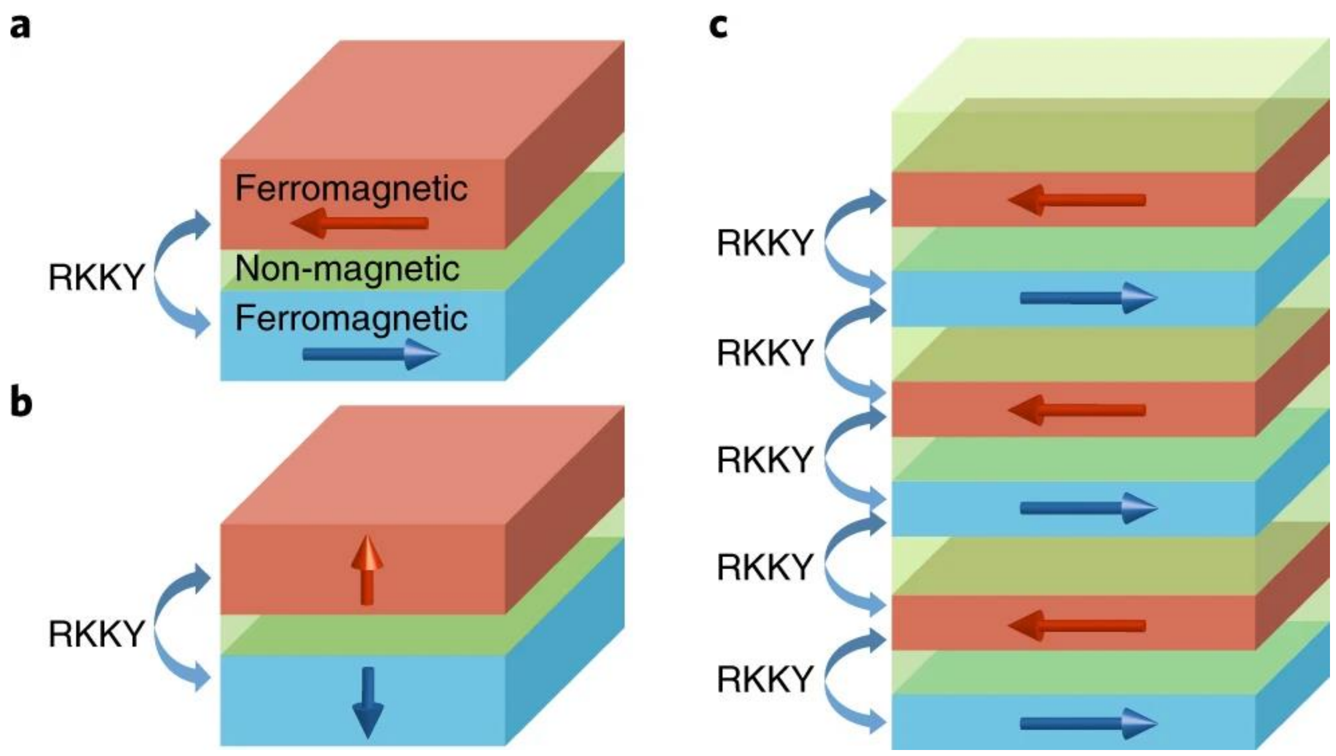
The interlayer exchange coupling is the sum of the energy differences (with respect to the absence of quantum well) for the four different cases:

The amplitude for one round trip in a spacer layer of thickness t is $R_1e^{ik_Ft}R_2e^{ik_Ft}$, where e^{ikk_Ft} is the phase accumulated on one traversal of the spacer and $R_{1,2}$ are the reflection amplitudes from the right and left interfaces

$$J = -\frac{\hbar k_F v_F}{8\pi^2} R_1 R_2 \frac{1}{t^2}\left[\cos(2k_F t) - \frac{\sin(2k_F t)}{(2k_F t)}\right]$$

J. Mathon, *et al.*, Phys. Rev. let. **74**, 3696 (1995); P. Bruno https://doi.org/10.1103/PhysRevB.52.411; M.D. Stiles https://doi.org/10.1103/PhysRevB.48.7238

Synthetic antiferromagnets with tuned properties



a, Bilayers with in-plane magnetization. **b**, Bilayers with out-of-plane magnetizations. **c**, Multilayers. The arrows within each ferromagnetic layer indicate the direction of magnetization. Depending on the magnetic configurations the RKKY coupling and dipolar fields add (**a**) or subtract (**b**), leading in part to the large degree of tunability of multilayers.

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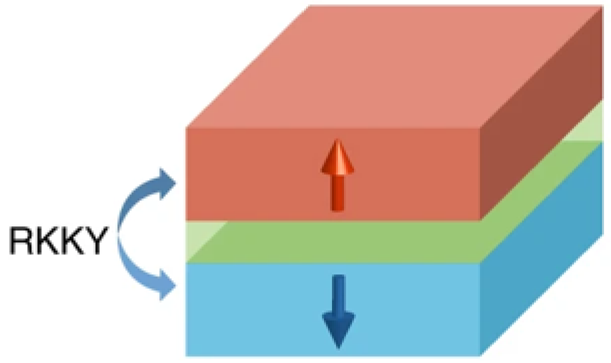
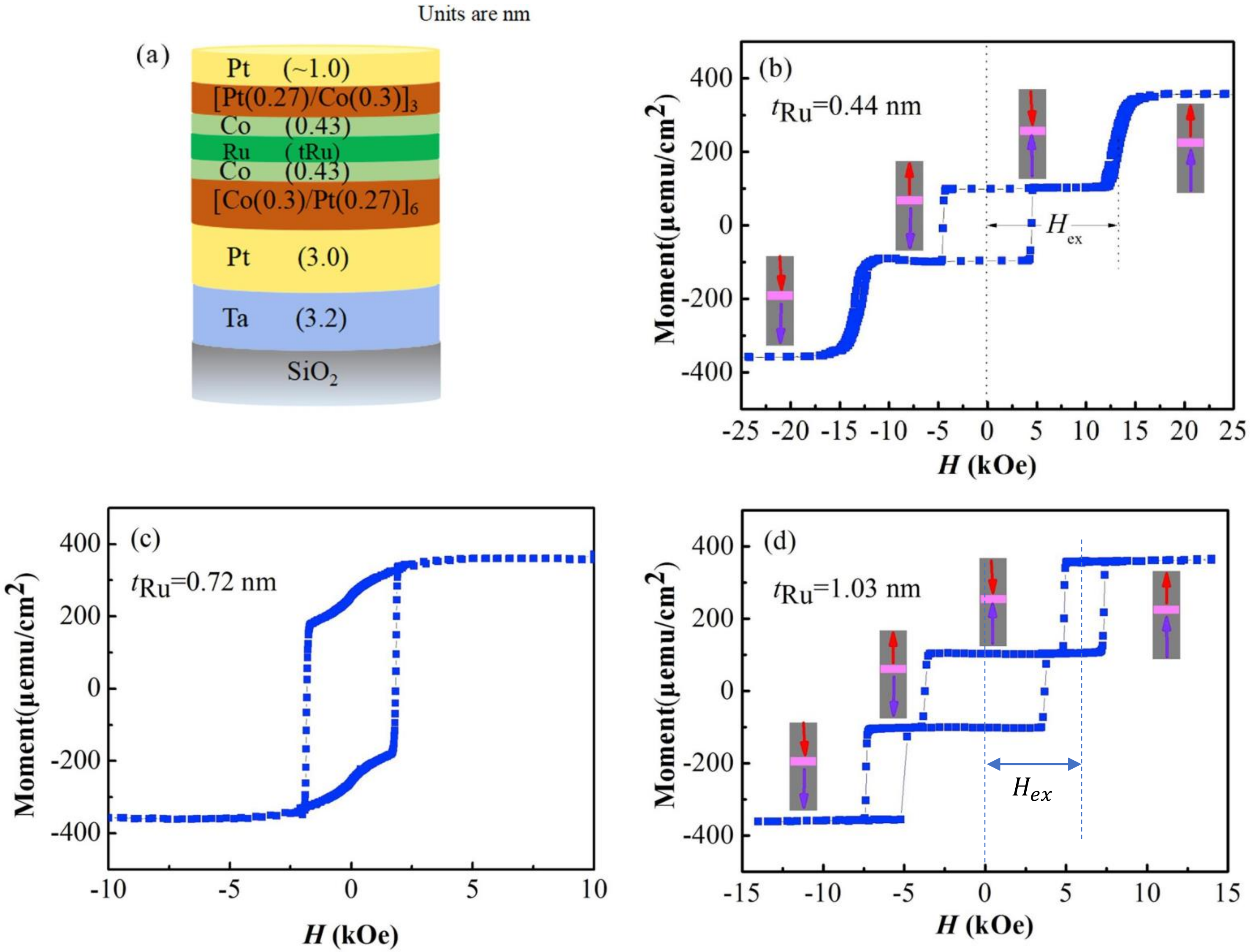
Ex.: Synthetic antiferromagnets with PMA



P-SAF (perpendicular synthetic AFM)



(a) Schematic of p-SAF structure based on [Co/Pt] superlattice. The out-of-plane magnetic hysteresis loops for the as-deposited Ta(3.2)/Pt(3)/[Co(0.30)/Pt(0.27)]$_6$/Co(0.43)/Ru(t_{Ru})/Co(0.43)[Pt(0.27)/Co(0.30)]$_3$/Pt(1) samples of t_{Ru} = (b) 0.44 nm, (c) 0.72 nm, and (d) 1.03 nm, respectively.

https://doi.org/10.1016/j.jmmm.2018.10.090

Better choice of the non-magnetic spacer

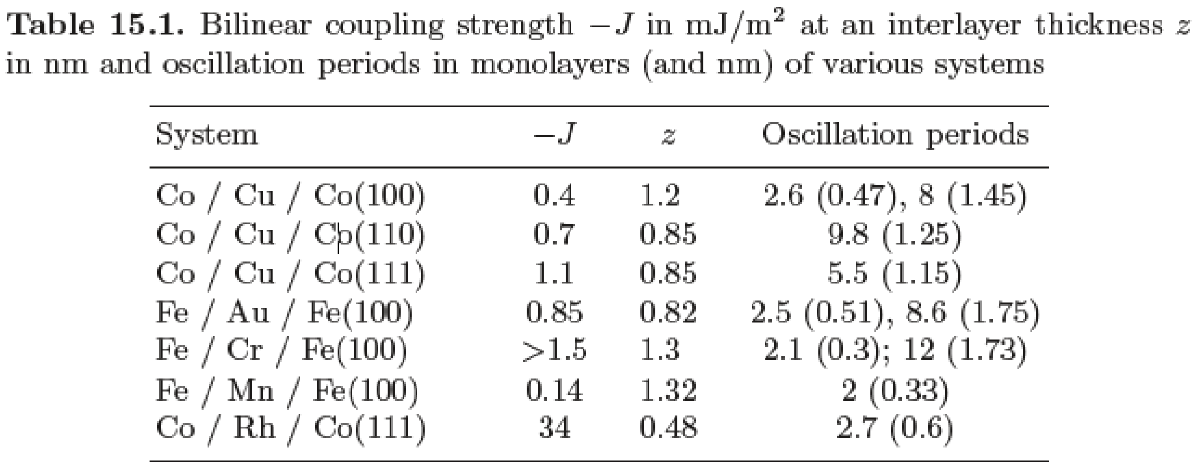
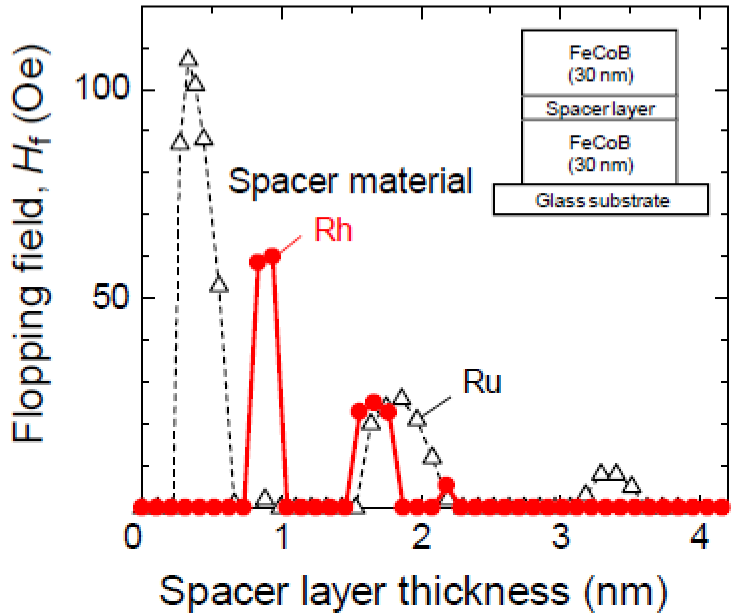


Table 15.1. Bilinear coupling strength $-J$ in mJ/m^2 at an interlayer thickness z in nm and oscillation periods in monolayers (and nm) of various systems

System	$-J$	z	Oscillation periods
Co / Cu / Co(100)	0.4	1.2	2.6 (0.47), 8 (1.45)
Co / Cu / Co(110)	0.7	0.85	9.8 (1.25)
Co / Cu / Co(111)	1.1	0.85	5.5 (1.15)
Fe / Au / Fe(100)	0.85	0.82	2.5 (0.51), 8.6 (1.75)
Fe / Cr / Fe(100)	>1.5	1.3	2.1 (0.3); 12 (1.73)
Fe / Mn / Fe(100)	0.14	1.32	2 (0.33)
Co / Rh / Co(111)	34	0.48	2.7 (0.6)

Higher *J* and smaller *z* for 4d spacers compared to 3d ones

Flopping field = exchange field



Comparison between 4d transition metals: Ru provides higher exchange and smaller thickness compared to Rh

W X Xia et al 2011 J. Phys.: Conf. Ser. 266 012064