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Magnetic couplings

MAGNETIC MATERIALS AND HYSTERESIS

Poznań 2019

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4
Magnetic couplings

- Introduction
- Exchange coupling
- Magnetostatic coupling
- Dzyaloshinskii–Moriya interaction
- RKKY coupling

Introduction
Pauli principle – fermions, bosons

In a system composed of indistinguishable particles the exchange of the particles does not change the wave function and related observables (e.g. energy)

$$H\psi(r_1,r_2)=E\psi(r_1,r_2) \qquad H\psi(r_2,r_1)=E\psi(r_2,r_1)$$

The transposition operator T_{12} exchanges two particles:

$$T_{12}\psi(r_1,r_2)=\psi(r_2,r_1)$$

But exchanging the particles twice brings us back to the initial state, so:

$$T_{12}^2=1$$

It follows T_{12}**=±1**

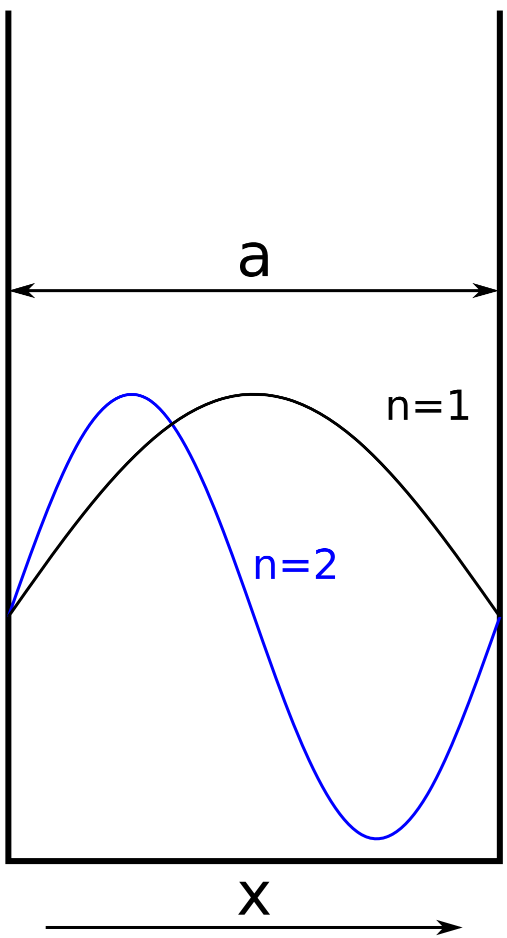
- $\mathbf{T_{12}=1}$ – symmetric wave functions – bosons (spin 1,2,3,….)
- $\mathbf{T_{12}=-1}$ – antisymmetric wave functions – fermions (electrons, protons, neutrons)

*at least some authors [104] **doubt the applicability of indistinguishability** in proving that wave functions must be symmetric or antisymmetric

Introduction Pauli principle – fermions, bosons

Assume that two identical particles are confined to a potential well of the **infinite** depth and width **a**. The normalized 1-D solutions to Schrödinger equation are of the form [9]:

$$\psi(x)=\sqrt{\frac{2}{a}}\sin\left(n\frac{\pi}{a}x\right), \qquad n=\pm1,\pm2,\ldots$$



Depending on whether the particles are distinguishable (classical case) or not and on whether they are bosons or fermions the wave function of two non-interacting particles can be written in one of three ways*:

- distinguishable particles

$$\psi(r_1,r_2)=\psi_{n1}(r_1)\psi_{n2}(r_2)$$

which means that particle no.1 is in state n1 at position r_1 and particle no.2 is in state n2 at position r_2

- bosons (symmetric wave function)

$$\psi(r_1,r_2)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)+\psi_{n1}(r_2)\psi_{n2}(r_1)\right]$$

- fermions (antisymmetric function)

$$\psi(r_1,r_2)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)-\psi_{n1}(r_2)\psi_{n2}(r_1)\right]$$

*see the video lectures 7.1-7.5 of Ron Reifenberger () [26]

Introduction
Pauli principle – fermions, bosons

Symmetric wave function [105]:

$$\psi(r_1,r_2)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)+\psi_{n1}(r_2)\psi_{n2}(r_1)\right]$$

is not changed when we exchange positions of two particles $r_1 \leftrightarrow r_2$:

$$\psi(r_2,r_1)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_2)\psi_{n2}(r_1)+\psi_{n1}(r_1)\psi_{n2}(r_2)\right]=\psi(r_1,r_2)$$

The sign of **antisymmetric** wave function:

$$\psi(r_1,r_2)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)-\psi_{n1}(r_2)\psi_{n2}(r_1)\right]$$

is changed when we exchange positions of two particles $r_1 \leftrightarrow r_2$:

$$\psi(r_2,r_1)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_2)\psi_{n2}(r_1)-\psi_{n1}(r_1)\psi_{n2}(r_2)\right]=-\psi(r_1,r_2)$$

*see the video lectures 7.1-7.5 of Ron Reifenberger () [26]

Introduction

Pauli principle – fermions, bosons

Assume that two identical particles are confined to a potential well of the **infinite** depth and width **a**. The normalized 1-D solutions to Schrödinger equation are of the form [9]:

$$\psi(x)=\sqrt{\frac{2}{a}}\sin\left(n\frac{\pi}{a}x\right), \qquad n=\pm 1,\pm 2,\ldots$$

Depending on whether the particles are distinguishable (classical case) or not and on whether they are bosons or fermions the wave function of two non-interacting particles can be written in one of three ways*:

Both particles in the same quantum state [26] probability density

- distinguishable particles

$$\psi(r_1,r_2)=\psi_{n1}(r_1)\psi_{n2}(r_2)$$

$$P(r_1,r_2)=\psi_n(r_1)\psi_n(r_2)\psi_n(r_1)^*\psi_n(r_2)^*$$

- bosons (symmetric wave function)

$$\psi(r_1,r_2)=\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)+\psi_{n1}(r_2)\psi_{n2}(r_1)\right]$$

$$P(r_1,r_2)=\left(\frac{1}{\sqrt{2}}\left[2\psi_n(r_1)\psi_n(r_2)\right]\right)\left(\frac{1}{\sqrt{2}}\left[2\psi_n(r_1)\psi_n(r_2)\right]\right)^*$$

$$=2\psi_n(r_1)\psi_n(r_2)\psi_n(r_1)^*\psi_n(r_2)^*$$

Bosons have enhanced probability of being in the same quantum state

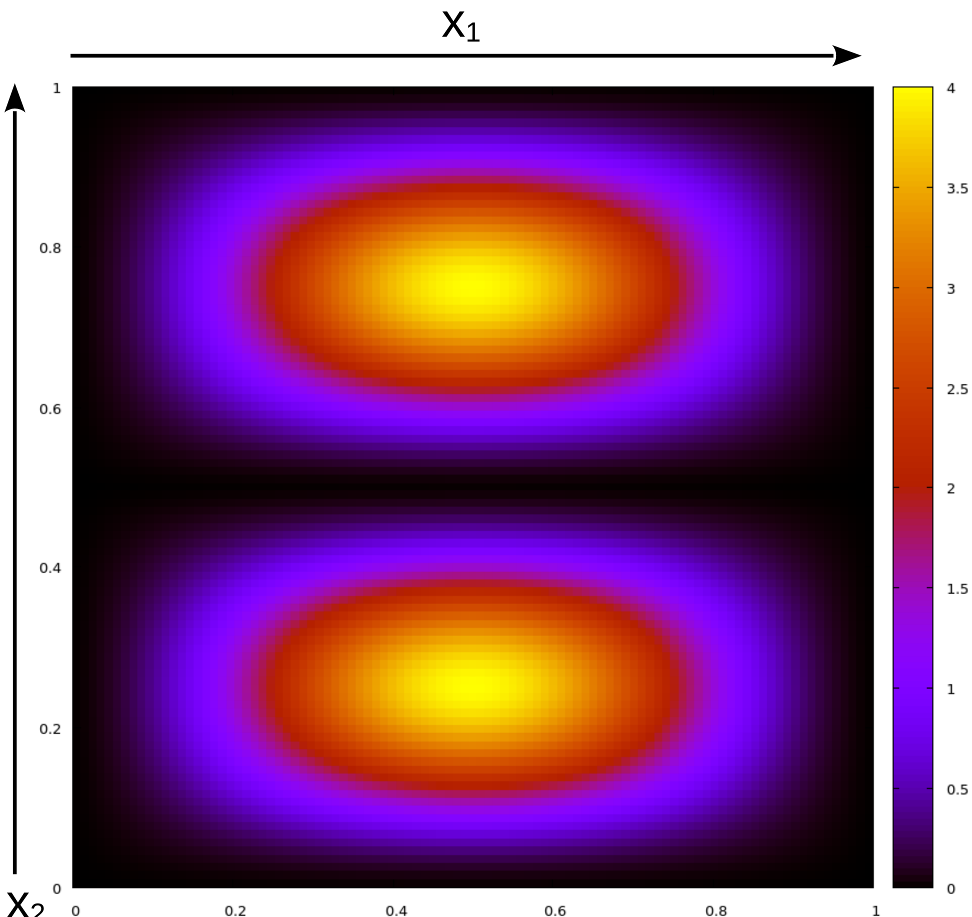
Introduction

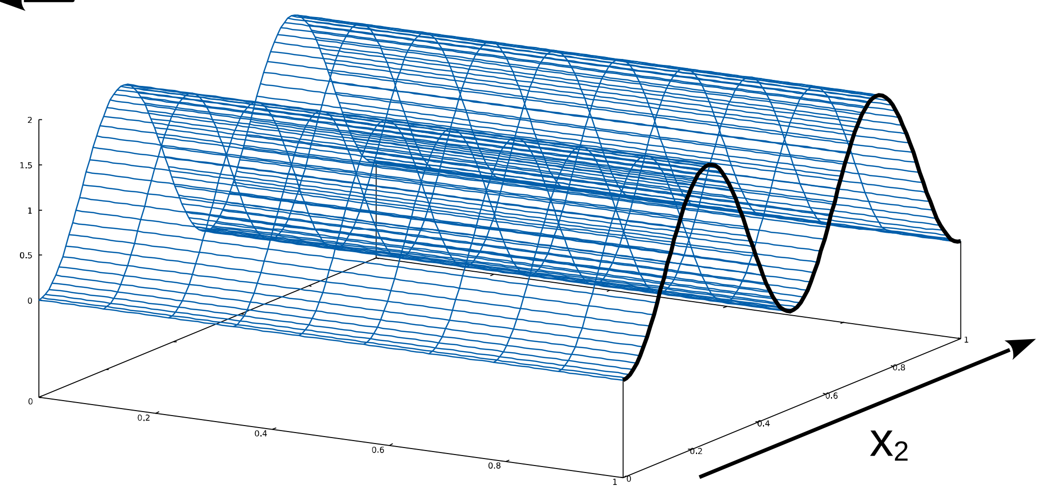
Pauli principle – fermions, bosons

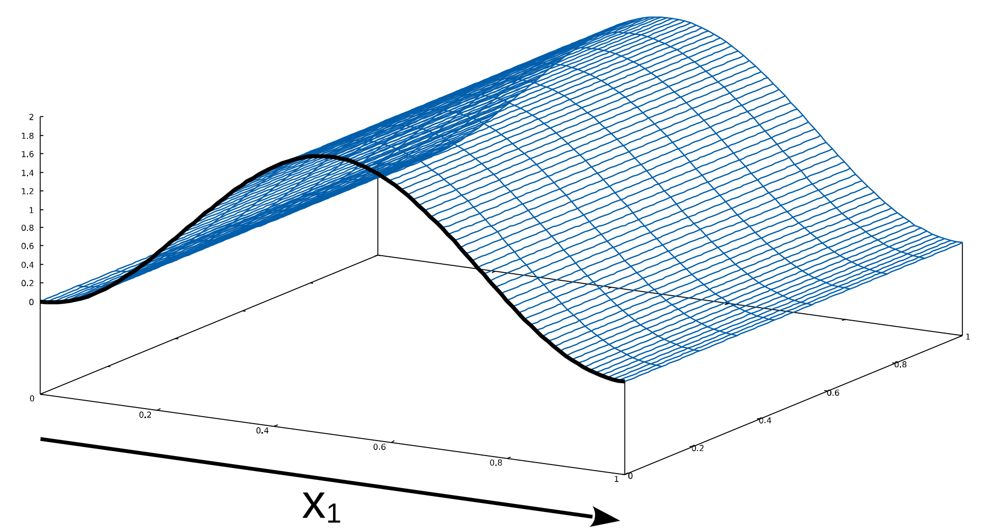
We consider first two levels in a well: one particle in state with n=1 and the other with n=2

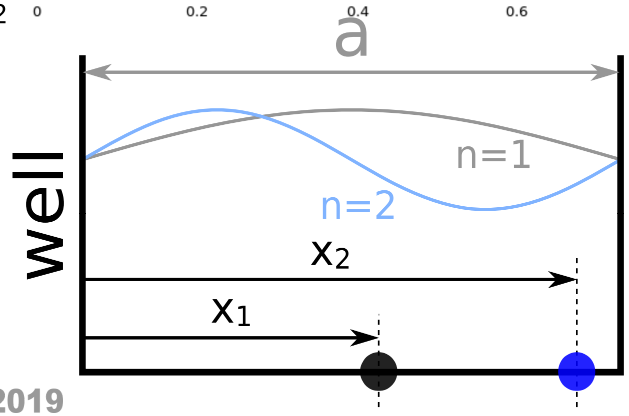
Distinguishable particles – classical description

$$P(x_1,x_2)=\left[\sqrt{\frac{2}{a}}\sin\left(1\,\frac{\pi}{a}\,x_1\right)\sqrt{\frac{2}{a}}\sin\left(2\,\frac{\pi}{a}\,x_2\right)\right]^2$$









x_1 and x_2 denote the positions of particles along x-axis

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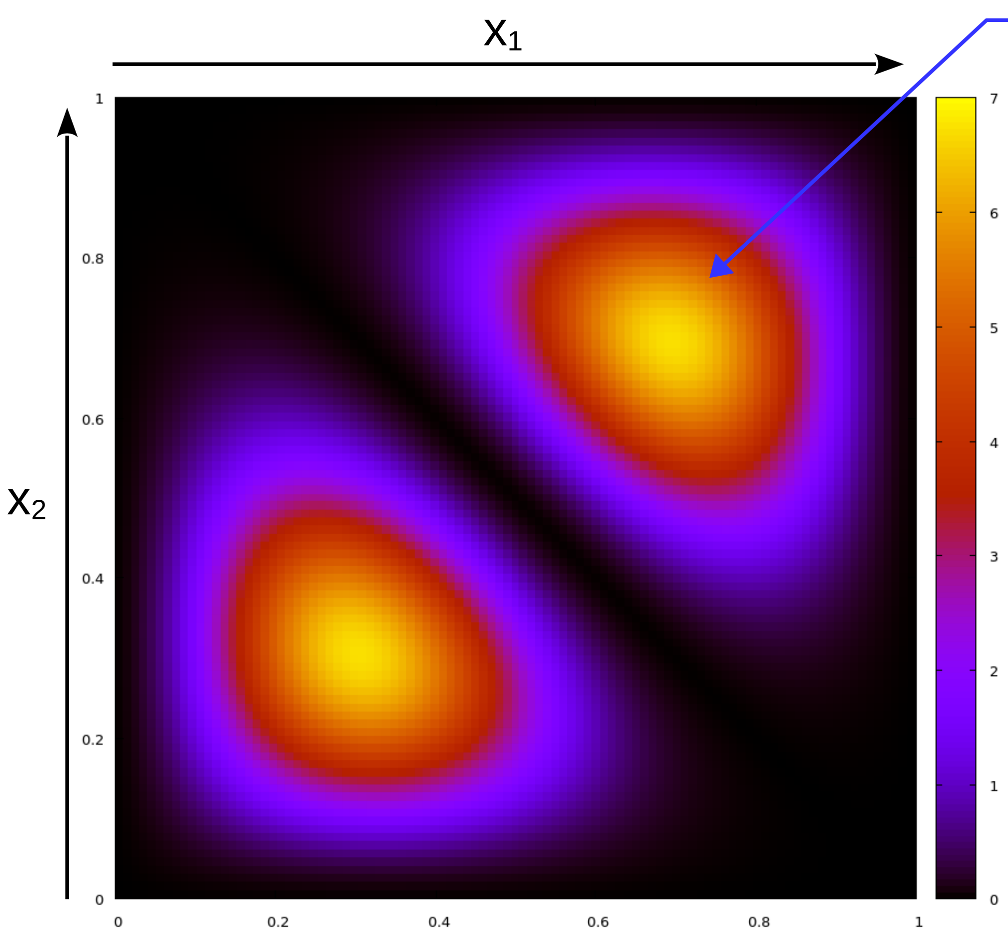
Introduction
Pauli principle – fermions, bosons

We consider first two levels in a well: one particle in state with n=1 and the other with n=2
Indistinguishable boson particles



Probability maxima correspond to both particles being at the same location

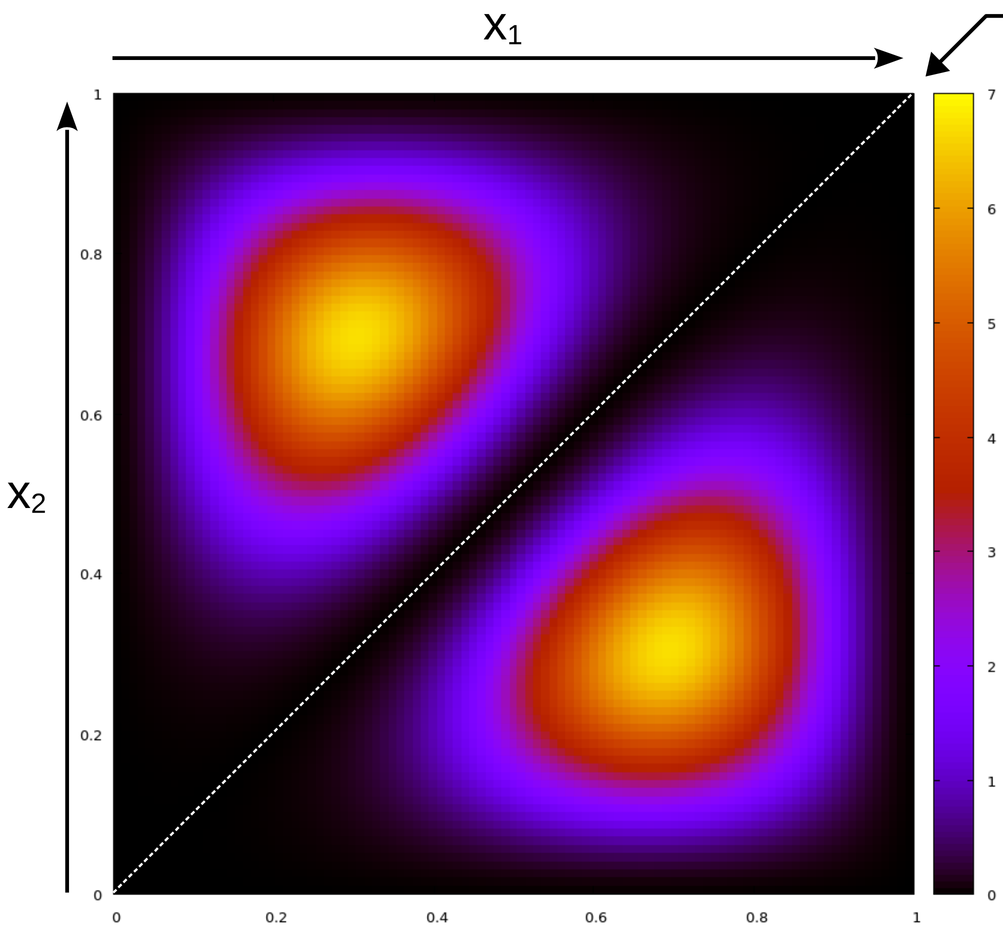
$$x_2 = x_1$$

Bosons, due to the symmetry of the wave function alone, have a tendency to lump [106 p. 57].

$$P(x_1, x_2) = \left[\sqrt{\frac{2}{a}} \sin\left(1 \frac{\pi}{a} x_1\right) \sqrt{\frac{2}{a}} \sin\left(2 \frac{\pi}{a} x_2\right) + \sqrt{\frac{2}{a}} \sin\left(1 \frac{\pi}{a} x_2\right) \sqrt{\frac{2}{a}} \sin\left(2 \frac{\pi}{a} x_1\right) \right]^2$$

Introduction

We consider first two levels in a well: one particle in state with n=1 and the other with n=2
Indistinguishable fermions (with the same spin- see next slides)



Probability of finding both particles in the same location is zero

$$P(x_1, x_2 = x_1) = 0$$

"Non interacting" Fermions with the same spin, due to the symmetry of the wave function alone, have a tendency to avoid each other* [106, p. 36].

$$P(x_1, x_2) = \left[\sqrt{\frac{2}{a}}\sin\left(1\,\frac{\pi}{a}\,x_1\right)\sqrt{\frac{2}{a}}\sin\left(2\,\frac{\pi}{a}\,x_2\right) - \sqrt{\frac{2}{a}}\sin\left(1\,\frac{\pi}{a}\,x_2\right)\sqrt{\frac{2}{a}}\sin\left(2\,\frac{\pi}{a}\,x_1\right)\right]^2$$

*in case of electrons the Coulomb repulsion amplifies this tendency [106]

Exchange coupling

Consider a system composed of two particles with spin ½. For one spin we have a set of matrices

z-component of spin

$$S_x = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli matrices $\sigma_1,\ \sigma_2,\ \sigma_3$

with eigenvalues $\pm\frac{1}{2}\hbar$ and corresponding eigenvectors $\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ for $S_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

With 2 spins we should work in 4-dimensional representation. Each spin has two eigenvectors so there are 4 possibilities:

spin1/spin2	↑↑	↑↓	↓↑	↓↓
traditional notation	α(1)α(2)	α(1)β(2)	β(1)α(2)	β(1)α(2)

meaning first spin down, second spin up

α and β traditionally mean up and down, respectively

Exchange coupling

From single spin vectors we can construct symmetric and antisymmetric functions (with respect to spin exchange) [B. Średniawa, 39 p..233]:

$$\alpha(1)\alpha(2),\quad \beta(1)\beta(2),\quad \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)+\beta(1)\alpha(2)\right],$$

$$\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)-\beta(1)\alpha(2)\right] = -\left[\frac{1}{\sqrt{2}}\left[\alpha(2)\beta(1)-\beta(2)\alpha(1)\right]\right]$$

1→2

2→1

note the minus sign

antisymmetric combination

Combining Pauli matrices into vector we get:

$$\vec{\sigma}=\hat{x}\,\sigma_x+\hat{y}\,\sigma_y+\hat{z}\,\sigma_z=\hat{x}\begin{pmatrix}0&1\\1&0\end{pmatrix}+\hat{y}\begin{pmatrix}0&-i\\i&0\end{pmatrix}+\hat{z}\begin{pmatrix}1&0\\0&-1\end{pmatrix}=\begin{pmatrix}\hat{z}&\hat{x}-i\,\hat{y}\\\hat{x}+i\,\hat{y}&-\hat{z}\end{pmatrix}$$

and for a resultant spin momentum of two spins

$$\vec{J}=\frac{\hbar}{2}\left(\vec{\sigma}(1)+\vec{\sigma}(2)\right)$$

each operator acts on its "own " spin

For a square of the momentum we have

$$J^2=\frac{\hbar^2}{4}\left[\left(\sigma_x(1)+\sigma_x(2)\right)^2+\left(\sigma_y(1)+\sigma_y(2)\right)^2+\left(\sigma_z(1)+\sigma_z(2)\right)^2\right]=\frac{\hbar^2}{2}\left[3+\vec{\sigma}(1)\cdot\vec{\sigma}(2)\right]$$

We act now with the operator $\vec{\sigma}(1)\cdot\vec{\sigma}(2)$ on constructed spin functions (using explicit forms of Pauli matrices):

$$\left[\vec{\sigma}(1)\cdot\vec{\sigma}(2)\right]\alpha(1)\alpha(2)=\left[\sigma_x(1)\sigma_x(2)+\sigma_y(1)\sigma_y(2)+\sigma_z(1)\sigma_z(2)\right]\alpha(1)\alpha(2)$$
$$=\beta(1)\beta(2)+i\beta(1)\,i\beta(2)+\alpha(1)\alpha(2)=1\cdot\alpha(1)\alpha(2)$$

Introduction Exchange coupling

Which means that eigenvalue of $\vec{\sigma}(1)\cdot\vec{\sigma}(2)$ for $\alpha(1)\alpha(2)$ function is **1**:

$$[\vec{\sigma}(1)\cdot\vec{\sigma}(2)]\alpha(1)\alpha(2)=1\cdot\alpha(1)\alpha(2)$$

Inserting this "1" into the expression for the square of the momentum yields:

$$J^2=\frac{\hbar^2}{2}[3+\vec{\sigma}(1)\cdot\vec{\sigma}(2)]=\frac{\hbar^2}{2}4 \quad \rightarrow \quad J=\hbar\sqrt{2}$$

From the expression of the momentum corresponding to a spin ($L_S=\sqrt{S(S+1)}\hbar$) we see that:

$S=1$: $L_S=\sqrt{1(1+1)}\hbar=\hbar\sqrt{2}$

- this value of momentum ($\hbar\sqrt{2}$) corresponds to resultant **spin 1**
- and consequently the function $\alpha(1)\alpha(2)$ corresponds to **spin 1**

Analogous calculations show that all three symmetric two spin functions correspond to **spin 1** (each of them corresponds to different component of momentum along z-axis)

$\alpha(1)\alpha(2)$, $\frac{1}{\sqrt{2}}[\alpha(1)\beta(2)+\beta(1)\alpha(2)]$, $\beta(1)\beta(2)$

S_z: $+\hbar$ $\quad 0 \quad$ $-\hbar$

resultant spin S=1 **triplet**

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2)-\beta(1)\alpha(2)]$

resultant spin S=0 **singlet**

Exchange coupling

When we are dealing **with fermions the total wave function must be asymmetric**.
If Hamiltonian has no terms dependent on spin we can write the total wave function as a product of spatial and spin wave functions. We can have thus two cases [105]:

- spatial function is asymmetric, spin function is symmetric (triplet)

$$\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)-\psi_{n1}(r_2)\psi_{n2}(r_1)\right] \times \alpha(1)\alpha(2)$$

$$\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)-\psi_{n1}(r_2)\psi_{n2}(r_1)\right] \times \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)+\beta(1)\alpha(2)\right]$$

$$\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)-\psi_{n1}(r_2)\psi_{n2}(r_1)\right] \times \beta(1)\beta(2)$$

- spatial function is symmetric, spin function is asymmetric (singlet)

$$\frac{1}{\sqrt{2}}\left[\psi_{n1}(r_1)\psi_{n2}(r_2)-\psi_{n1}(r_2)\psi_{n2}(r_1)\right] \times \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)-\beta(1)\alpha(2)\right]$$

spin functions

Exchange coupling

Assume now that the two particles (electrons with a spin) interact via Coulomb electrostatic interactions.
If the interaction is weak we can us a non-degenerate perturbation method for which we have

$$E_m^{(1)} = V_{mm} = \int \psi_m^{(0)*} \hat{V} \psi_m^{(0)} dV \qquad E_m = E_m^{(0)} + \lambda V_{mm} \qquad E_m = E_0 + \langle 0\ \mathrm{m}| H^{(1)} |0\ \mathrm{m}\rangle$$

The correction to the eigenvalues in the first order approximation is the equal to the average energy of the perturbation in the unperturbed state

Depending on the spin state (triplet, singlet) the spatial wave function is either symmetric or antisymmetric, and because the spin function is not acted upon by a the perturbation we get [39]

$$E^{(1)} = \int \frac{1}{\sqrt{2}} \left[\psi_{n1}(r_1)\psi_{n2}(r_2) \pm \psi_{n1}(r_2)\psi_{n2}(r_1)\right]^* \frac{e^2}{r_{1,2}} \frac{1}{\sqrt{2}} \left[\psi_{n1}(r_1)\psi_{n2}(r_2) \pm \psi_{n1}(r_2)\psi_{n2}(r_1)\right] dV$$

$$\hat{V} = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r_{1,2}}$$

which yields [39]

$$E^{(1)} = \int |\psi_{n1}(r_1)|^2 \frac{e^2}{r_{1,2}} |\psi_{n2}(r_2)|^2 dV \pm \int \psi_{n1}(r_1)^* \psi_{n2}(r_2)^* \frac{e^2}{r_{1,2}} \psi_{n1}(r_2)\psi_{n2}(r_1) dV$$

Coulomb integral

exchange integral

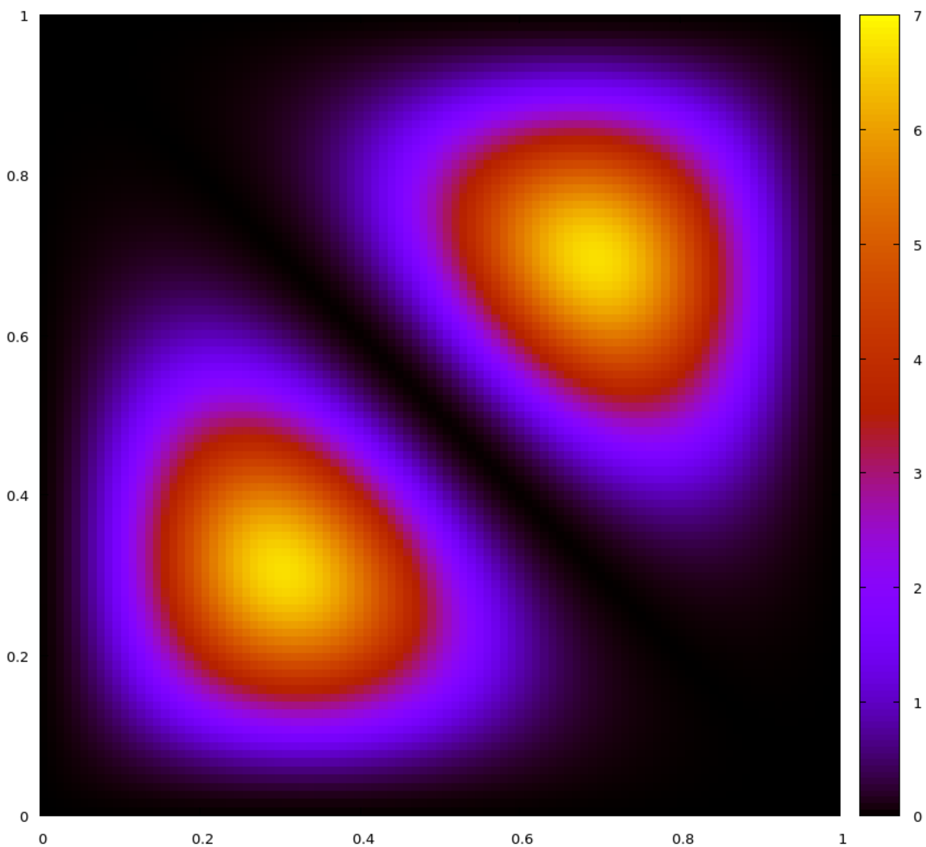
MAGNETIC MATERIALS AND HYSTERESIS

Exchange coupling

$$E^{(1)} = \int |\psi_{n1}(r_1)|^2 \frac{e^2}{r_{1,2}} |\psi_{n2}(r_2)|^2 dV \pm \int \psi_{n1}(r_1)^* \psi_{n2}(r_2)^* \frac{e^2}{r_{1,2}} \psi_{n1}(r_2)\psi_{n2}(r_1) dV$$

Coulomb integral exchange integral

Two particles in an infinite potential well – symmetric function



For the description of the image see 6 slides back

If spatial function is **symmetric** the particles tend to be closer to each other than in a classical case (due to statistical forces*) and **the electrostatic interactions increase energy of the system**

If spatial function is antisymmetric (**triplet**) the particles are repelled by statistical forces and the electrostatic interaction energy is lower than in the classical case [39, p. 301]

The exchange interactions favor parallel orientations of spins

*see the lecture of prof. T. Dietl: Physics of Exchange Interactions in Solids, Osaka/Japan, 2010.05.30 (youtube)

MAGNETIC MAT HYSTERESIS

Spin coupling

The magnetic interactions between magnetic ions in a solid depend on numerous factors (neighboring ions, temperature, external fields etc.)
In some case to describe the system one uses Hamiltonian involving simultaneous interaction between several spins [35,36]:

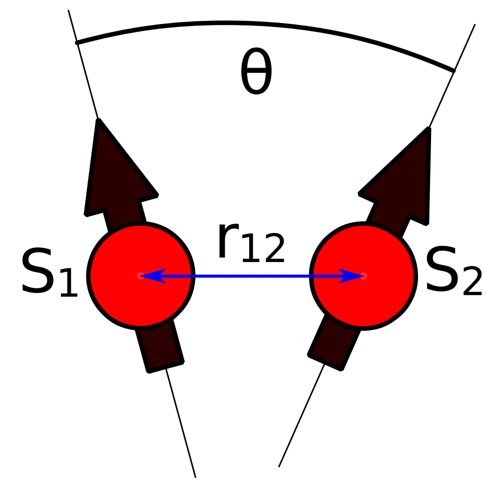
$$E_{4s} = -\sum_{ijkl} K_{ijkl}\left[(\vec{S}_i\cdot\vec{S}_j)(\vec{S}_k\cdot\vec{S}_l)+(\vec{S}_i\cdot\vec{S}_l)(\vec{S}_j\cdot\vec{S}_k)-(\vec{S}_i\cdot\vec{S}_k)(\vec{S}_j\cdot\vec{S}_l)\right]$$

the energy term involves orientations of all four spin

In some other cases it is not enough to use bilinear forms* and biquadratic forms are introduced in addition

$$E = -\sum_{ij} K_{ij}(\vec{S}_i\cdot\vec{S}_j)^2$$

In most relevant cases however it is enough to use only **two spin terms that are bilinear** [38]



$$E_{bilinear} = -\sum_{ij} K_{ij} S_1^i S_2^j = K_{xx} S_1^x S_2^x + K_{xy} S_1^x S_2^y + \ldots$$

K_{ij} is a coupling 3×3 matrix, and in matrix notation we have

$$E_{bilinear} = \vec{S}_1 [K] \vec{S}_2$$

Note the r-dependence:

$$E_{bilinear} = -\sum_{ij} K_{ij} S_1^i S_2^j = -\sum_{ij} K_{ij}(\vec{r}_{12}) S_1^i S_2^j$$

*"Form refers to a polynomial function in several variables where each term in the polynomial has the same degree. The degree of the term is the sum of the exponents." - K.C Border [37]

Spin coupling

The interaction matrix, like any 3×3 matrix [38], may be decomposed into a multiple of the identity matrix, an antisymmetric part (three different coefficients), and traceless* symmetric part:

$$K_{ij}=\begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} = J\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & D_1 & D_2 \\ -D_1 & 0 & D_3 \\ -D_2 & -D_3 & 0 \end{bmatrix} + \begin{bmatrix} A_1 & A_4 & A_5 \\ A_4 & A_2 & A_6 \\ A_5 & A_6 & A_3 \end{bmatrix}$$

$$J\vec{S}_1\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\vec{S}_2 = S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z = J\vec{S}_1\cdot\vec{S}_2$$

exchange coupling

$$E_{bilinear}=\vec{S}_1[K]\vec{S}_2$$

$$\vec{S}_1\begin{bmatrix} 0 & D_1 & D_2 \\ -D_1 & 0 & D_3 \\ -D_2 & -D_3 & 0 \end{bmatrix}\vec{S}_2 = -D_1 S_1^y S_2^x - D_2 S_1^z S_2^x + D_1 S_1^x S_2^y - D_3 S_1^z S_2^y + D_2 S_1^x S_2^z + D_3 S_1^y S_2^z$$

$$= D_1\left(S_1^x S_2^y - S_1^y S_2^x\right) - D_2\left(S_1^z S_2^x - S_1^x S_2^z\right) + D_3\left(S_1^y S_2^z - S_1^z S_2^y\right)$$

$$= \left(\hat{i}\, D_{3,} -\hat{j}\, D_{2,} \hat{k}\, D_1\right)\cdot\vec{S}_1\times\vec{S}_2 = \vec{D}\cdot\left(\vec{S}_1\times\vec{S}_2\right)$$

Dzyaloshinskii-Moriya interaction**

*trace of a matrix – a sum of diagonal elements

**note that you can encounter other spellings too: “Dzialoshinsky”, “Dzialoshinskii” ("oficial" russian transcription [Sov. Phys. JETP 5, 1259 (1957)])

Spin coupling

The interaction matrix, like any 3×3 matrix [38], may be decomposed into a multiple of the identity matrix, an antisymmetric part (three different coefficients), and traceless* symmetric part:

$$K_{ij}=\begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix}=J\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}+\begin{bmatrix} 0 & D_1 & D_2 \\ -D_1 & 0 & D_3 \\ -D_2 & -D_3 & 0 \end{bmatrix}+\begin{bmatrix} A_1 & A_4 & A_5 \\ A_4 & A_2 & A_6 \\ A_5 & A_6 & A_3 \end{bmatrix}$$

The matrix of the dipole-dipole interaction

$$E_{dipole-dipole}=\frac{-\mu_0}{4\pi|r|^3}\left[3(\hat{r}_{12}\cdot\vec{S}_1)(\hat{r}_{12}\cdot\vec{S}_2)-\vec{S}_1\cdot\vec{S}_2\right],$$

$\hat{r}_{12}$ - unit vector along the vector connecting two spins

reads

$$M_{dipole-dipole}=\frac{-\mu_0}{4\pi|r|^3}\begin{bmatrix} 3\hat{r}_x^2-1 & 3\hat{r}_x\hat{r}_y & 3\hat{r}_x\hat{r}_z \\ 3\hat{r}_x\hat{r}_y & 3\hat{r}_y^2-1 & 3\hat{r}_y\hat{r}_z \\ 3\hat{r}_x\hat{r}_z & 3\hat{r}_y\hat{r}_z & 3\hat{r}_z^2-1 \end{bmatrix}, \qquad \hat{r}_x^2+\hat{r}_y^2+\hat{r}_z^2=1$$

symmetric, traceless

Mathematica 9.0.1.0 code to get dipole-dipole matrix:

```
n =3;
wer={"x","y","z"};
r =Table[ ToExpression [StringJoin ["r",wer[[ i]]]],{i,1,n}];
S1 =Table[ ToExpression [StringJoin ["S1",wer[[ i]]]],{i,1,n}];
S2 =Table[ ToExpression [StringJoin ["S2",wer[[ i]]]],{i,1,n}];
macierz=Table[ToExpression[StringJoin["S1", wer[[i]],"*S2",wer[[j]]]],
{i,1,n},{j,1,n}];
m= Expand[ 3( r.S1)( r.S2)-S1.S2];(*write in here the spin hamiltonian (two
spin interaction), example dipole-dipole:
m= Expand[ 3( r.S1)( r.S2)-S1.S2];
*)
macierz2 =Table [Coefficient [m,macierz[[ i,j]]],{i,1,n},{j,1,n}] ;(*macierz2 is
the interaction matrix*)
TraditionalForm[macierz2]
```

*trace of a matrix – a sum of diagonal elements

Spin coupling

Anisotropic spin-spin interactions – those terms of the spin Hamiltonian that are not invariant under rotation in spin space (unaccompanied by rotation in real space) [38]

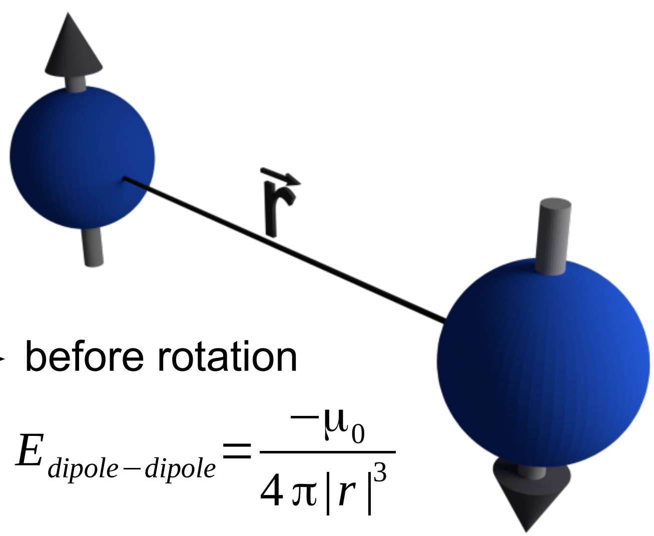
Compare two states:

- one spin points in +z direction and the other one in -z direction; both spins are on y-axis:

$$S_1^x=0,\ S_1^y=0,\ S_1^z=1;\ S_2^x=0,\ S_2^y=0,\ S_2^z=-1; \quad \hat{r}_x=0,\ \hat{r}_y=1,\ \hat{r}_z=0$$

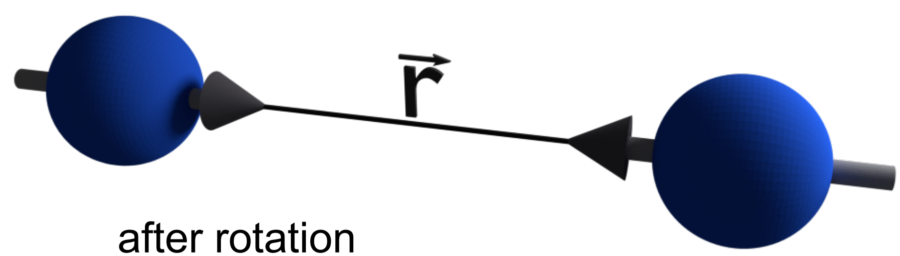
- as above but both spins are rotated by 90 Deg about x-axis

$$S_1^x=0,\ S_1^y=1,\ S_1^z=0;\ S_2^x=0,\ S_2^y=-1,\ S_2^z=0; \quad \hat{r}_x=0,\ \hat{r}_y=1,\ \hat{r}_z=0$$



before rotation

$$E_{dipole-dipole}=\frac{-\mu_0}{4\pi|r|^3}$$



after rotation

$$E_{dipole-dipole}=\frac{\mu_0}{2\pi|r|^3}$$

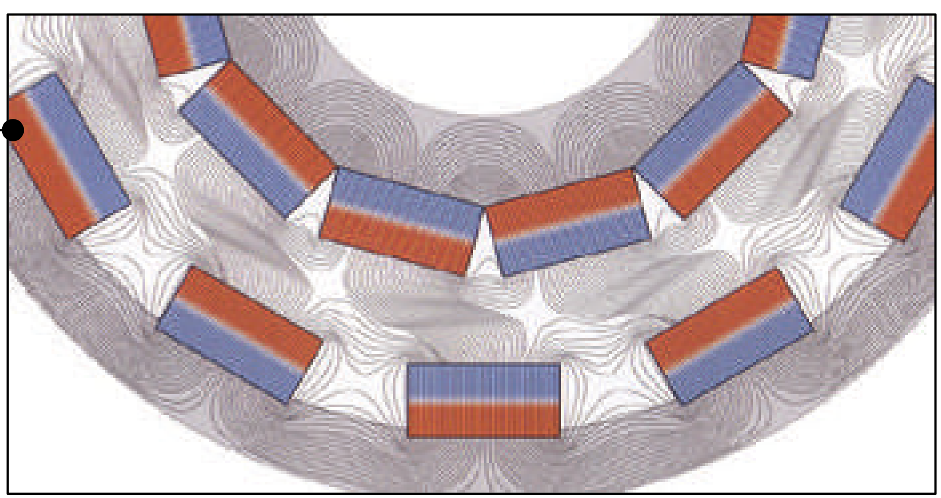
The energies obtained in both cases are different although the spins are antiparallel – dipole-dipole interaction is anisotropic

M. URBANIAK 2019
MAGNETIC MATERIALS AND HYSTERESIS

Magnetoststic couplings

- Magnetic couplings that are used in the industry for contact-less transmitting the torque in applications requiring strict separation of processed liquids and gases from the outer environment operate on the principle analogous to the one responsible for the magnetostatic interaction in thin magnetic films – *interaction between magnets*

internal and external rotors are both equipped with permanent magnets

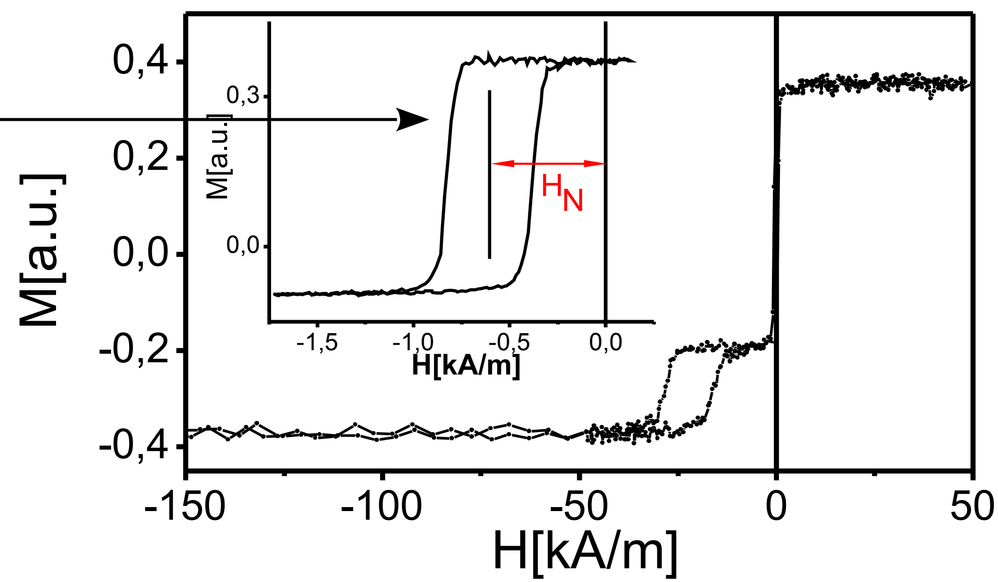


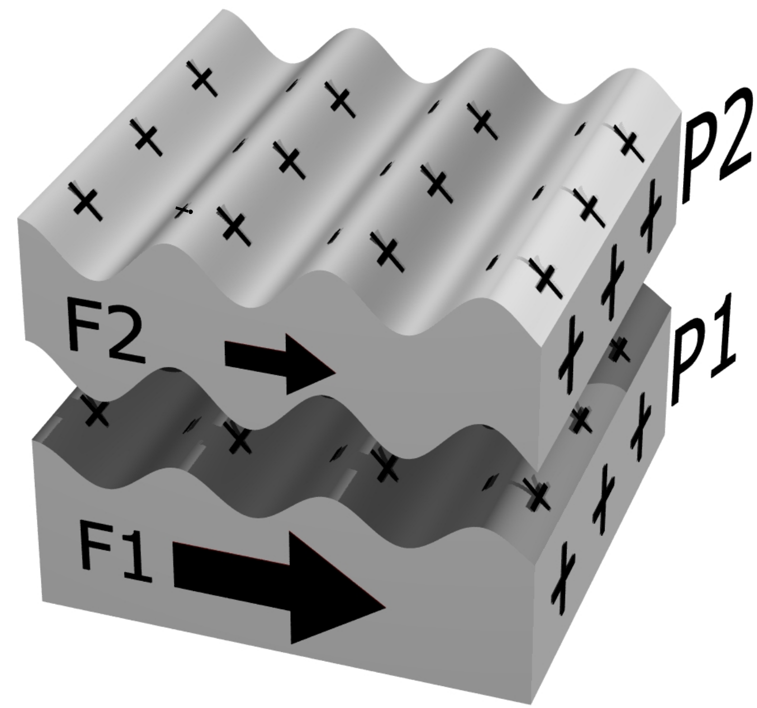
- achievable coupling torques in the range of 0.1 – 11,000 Nm*
- "If the maximum coupling torque and the maximum torsion angle are exceeded, the power transmission is interrupted" (KTR)

all images in this slide taken from: https://www.ktr.com/fileadmin/ktr/media/Tools_Downloads/kataloge/DriveTechnology.pdf, p. 224
*dst-magnetic-couplings.com/en/magnetic-couplings.html

Magnetoststic coupling – orange peel coupling

- Orange peel (OP) coupling (Néel coupling) is due to the roughness of interfaces in thin magnetic films.
- The roughness results in the appearance of surface magnetic charges.
- The OP coupling leads to the relative shift of hysterese of neighboring ferromagnetic layers:





Si(100)/100nm thermally oxidated Si/Cu(20nm)/
$Ni_{80}Fe_{20}$(10nm)/V(2.1nm)/$Ni_{80}Fe_{20}$(4nm)/$Mn_{83}Ir_{17}$(10nm)/Cu(3nm)

magnetically soft layer

exchange coupling

$$\vec{H} = -\nabla \phi_m$$

$$\phi_m(\vec{r}) = \oint_S \frac{\vec{M} \cdot \vec{ds}}{|\vec{r}|} - \int_V \frac{\nabla \cdot \vec{M}}{|\vec{r}|} d^3 r'$$

Magnetoststic coupling – orange peel coupling

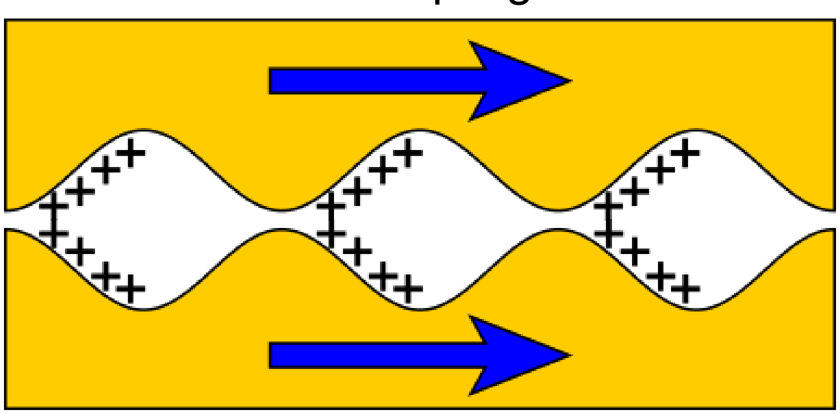
- Orange peel (OP) coupling is due to the roughnes of interfaces in thin magnetic films.
- The roughness results in the appearance of surface magnetic charges.
- The OP coupling leads to the relative shift of hystereses of neighboring ferromagnetic layers.
- If roughness profile on all interfaces is equal the shift field H_N can be shown to be given by (assuming that the hard layer is thick enough so that the influence of its second surface can be neglected):

$$H_N = \frac{\pi^2}{\sqrt{2}} \left(\frac{h^2}{\lambda t_f} \right) M_p e^{-2\pi\sqrt{2} t_s/\lambda}$$

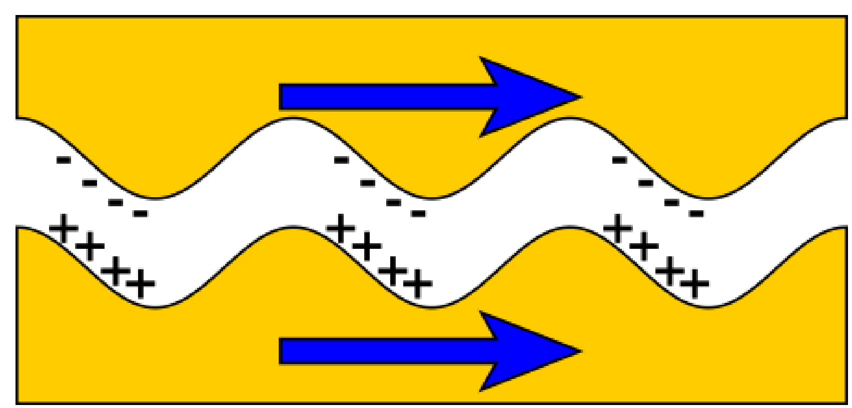
λ -wavelength of roughness modulation, t_f - thickness of „free" ferromagnetic layer, h-roughness amplitude, M_P - saturation magnetization of hard (or pinned) magnetic layer

- The coupling may be ferromagnetic or antiferromagnetic depending on a phase difference between roughnesses of neighboring interfaces (with the same direction of magnetization in neighboring layers):

AF coupling



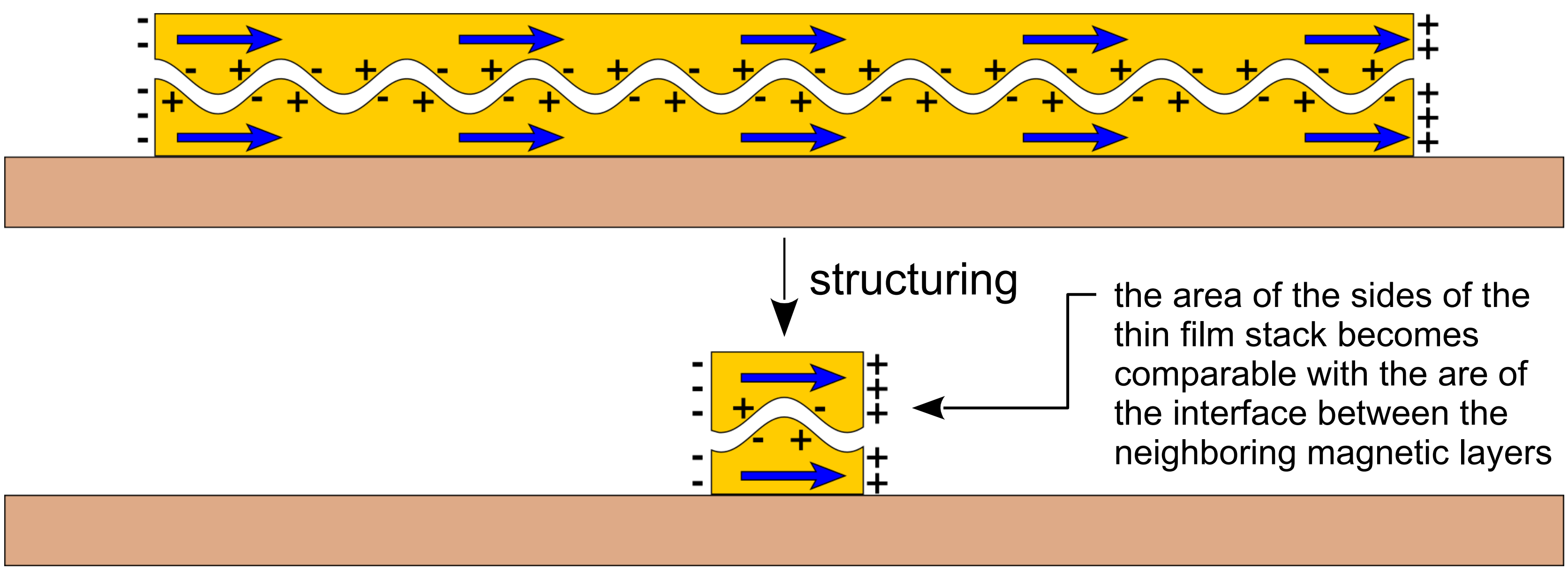
F coupling



Magnetoststic coupling – orange peel coupling

- Orange peel (OP) coupling is due to the roughnes of interfaces in thin magnetic films.
- The roughness results in the appearance of surface magnetic charges.
- The OP coupling leads to the relative shift of hystereses of neighboring ferromagnetic layers.

- Not that in extended films the influence of the magnetic fields emanating from the edges is negligible.
- If the film is structured, using for example electron lithography or deposition through a shadow mask, the edge “magnetic charges” may play a significant role in the reversal being the source of an additional coupling



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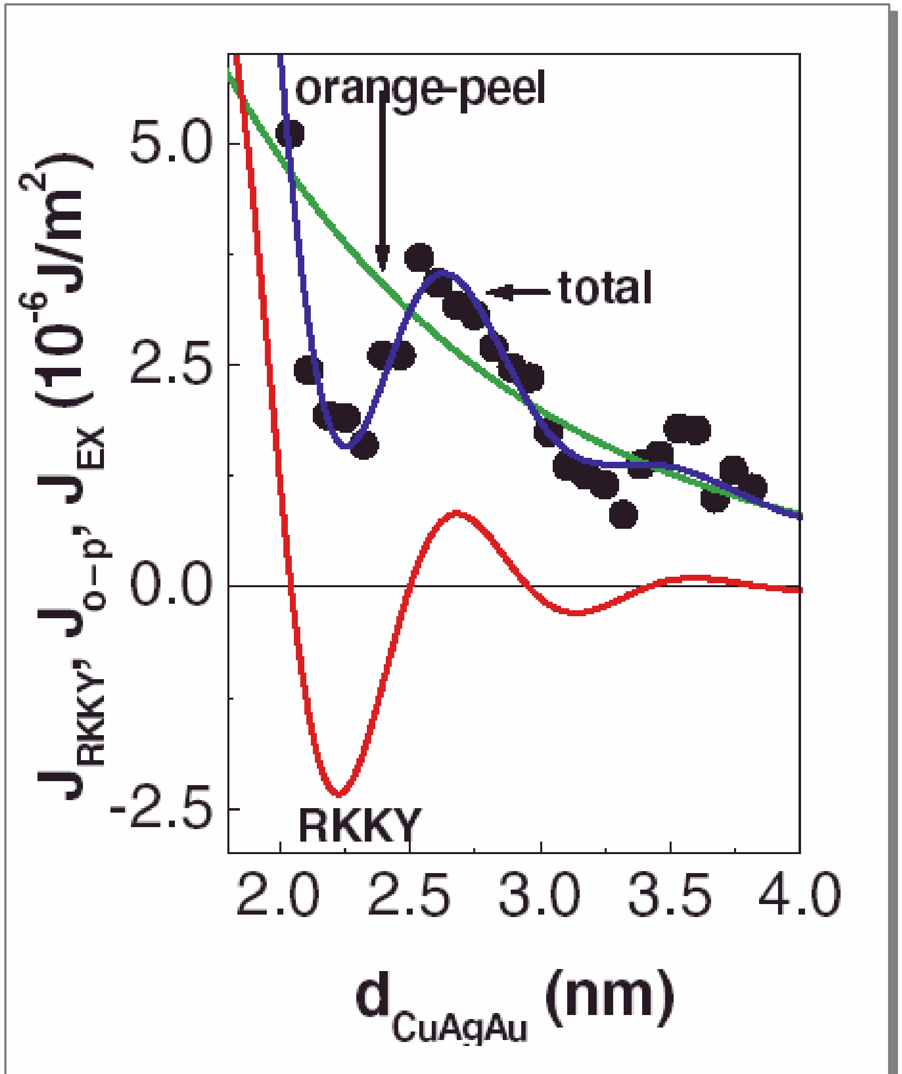
Magnetoststic coupling – orange peel coupling

- Orange peel coupling can be comparable in strength with RKKY oscillatory coupling



Py(2.5 nm)Co(2.5 nm)/CuAgAu(2,4 nm)/
Co(2.5 nm)

T. Luciński, A. Hütten, H. Brückl, T. Hempel, S. Heitmann, and G. Reiss
phys. stat. sol. (a) 196, No. 1, 97–100 (2003)

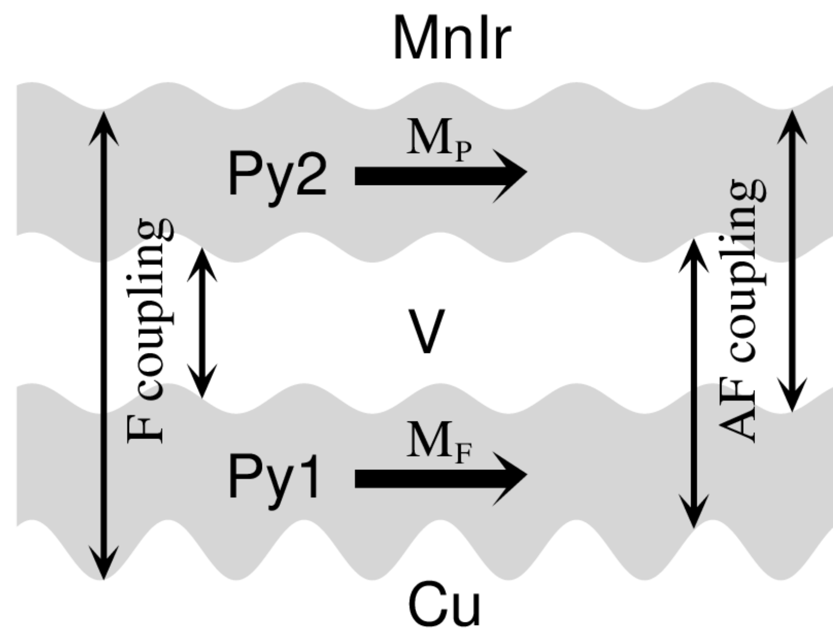
Magnetoststic coupling – orange peel coupling

- In his original paper Néel derived the coupling formula for the interaction between two semi-infinite magnetic layers
- The above description can be extended to the case of interacting thin films [16]:

- in the case shown here there are four interactions to take into account

- The interaction between the bottom surface of Py1 layer and top surface of Py2 layer leads, for example, to the following contribution to shift field:

$$H_S = \frac{\pi^2}{\sqrt{2}} \left(\frac{h_1 h_2}{\lambda t_{Py1}} \right) M_p e^{-2\pi\sqrt{2}(t_{Py1} + t_V + t_{Py2})/\lambda}$$



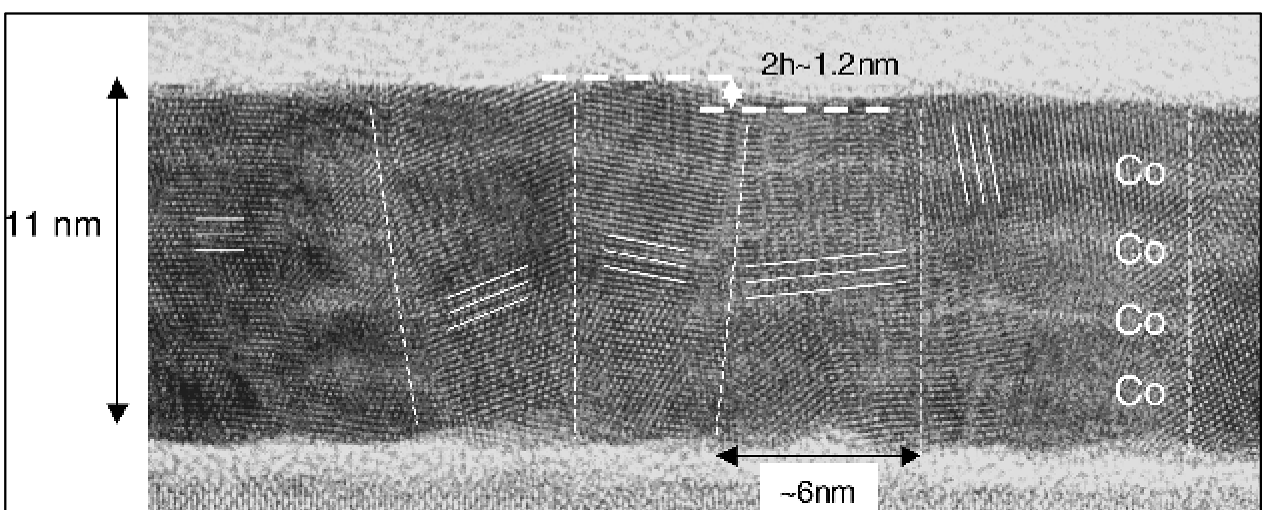
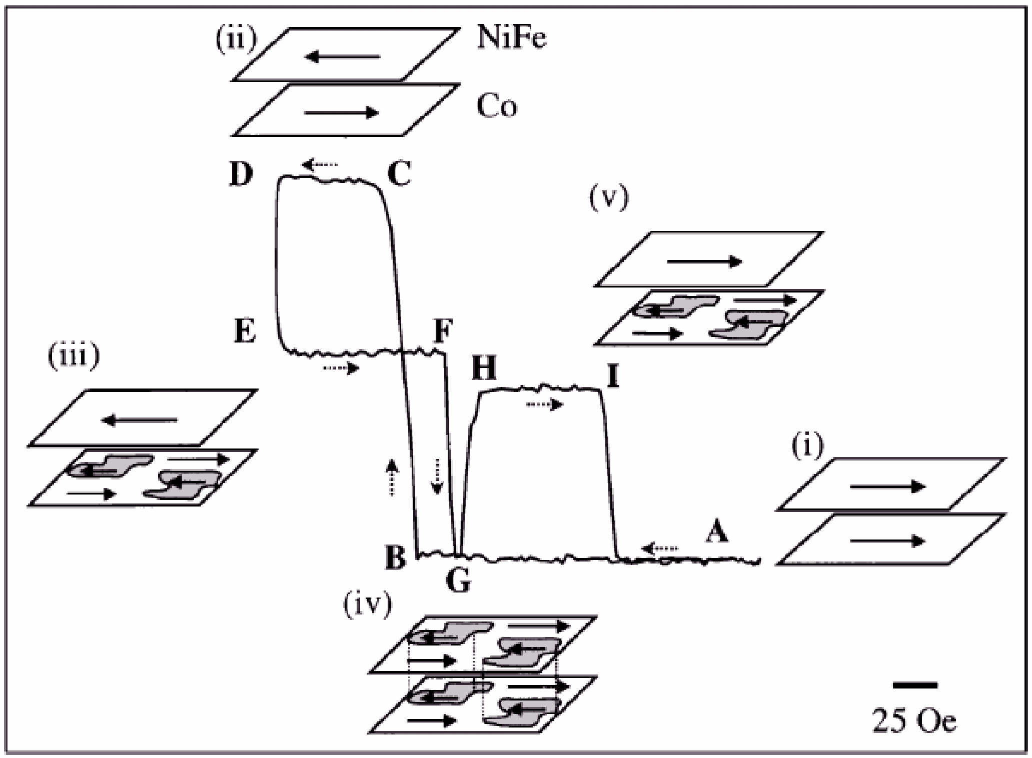


Figure 5: Cross-sectional view of a multilayer of composition $(Pt\ 1.8/Co\ 0.5)_4/Pt\ 1.8$ obtained by transmission electron microscopy. **The waviness** determined from the observation is 6 nm for **the wavelength** and 1.2 nm for the peak-to-peak amplitude.

image from: Europhys. Lett. **65**, 123 (2004), J. Moritz - F. Garcia - J. C. Toussaint - B. Dieny - J. P. Nozières

Magnetoststic coupling – domain wall coupling

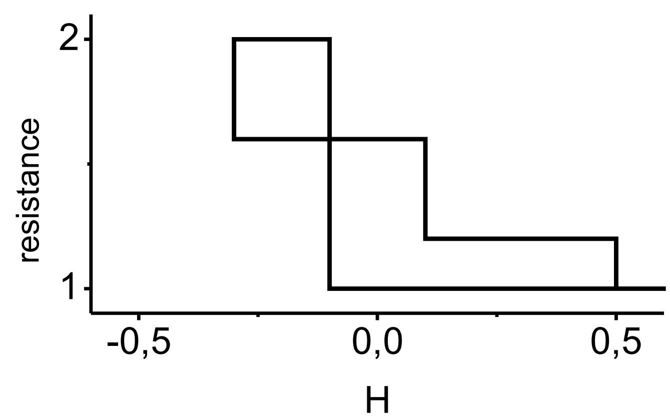
- Magnetic fields emanating from domain walls can influence magnetization reversal in neighboring layers



resistance decrease to absolute minimum- moments in neighboring layers parallel

- GaAs(100)/Co(1.8nm)/Cu(**6nm**)/ **$Ni_{80}Fe_{20}$**(6nm)
- D→E: only part of Co layer reverses
- F→G: coupling

Schematic of R(H) dependence without the coupling:



W.S. Lew et al., Phys. Rev. Lett. **90**, 217201 (2003)

RKKY-like interlayer coupling

- two Fe layers separated by a Cr wedge-shaped spacer; scanning electron microscopy with polarization analysis (SEMPA)
- measurement on a single specimen!
- up to six oscillations in coupling were observed

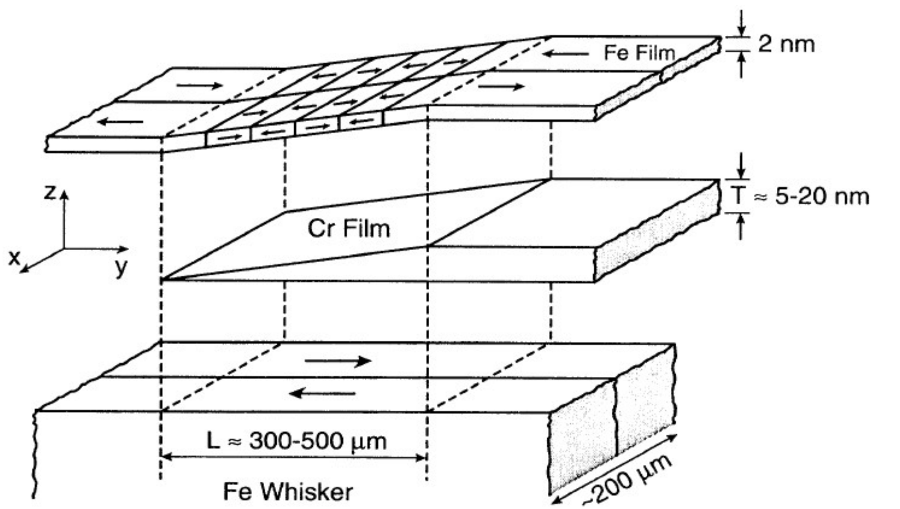


FIG. 1. A schematic exploded view of the sample structure showing the Fe(100) single-crystal whisker substrate, the evaporated Cr wedge, and the Fe overlayer. The arrows in the Fe show the direction of the magnetization in each domain. The z scale is expanded approximately 5000 times; the actual wedge angle is of order 10^{-3} deg.

Obtaining wedge-shaped films:

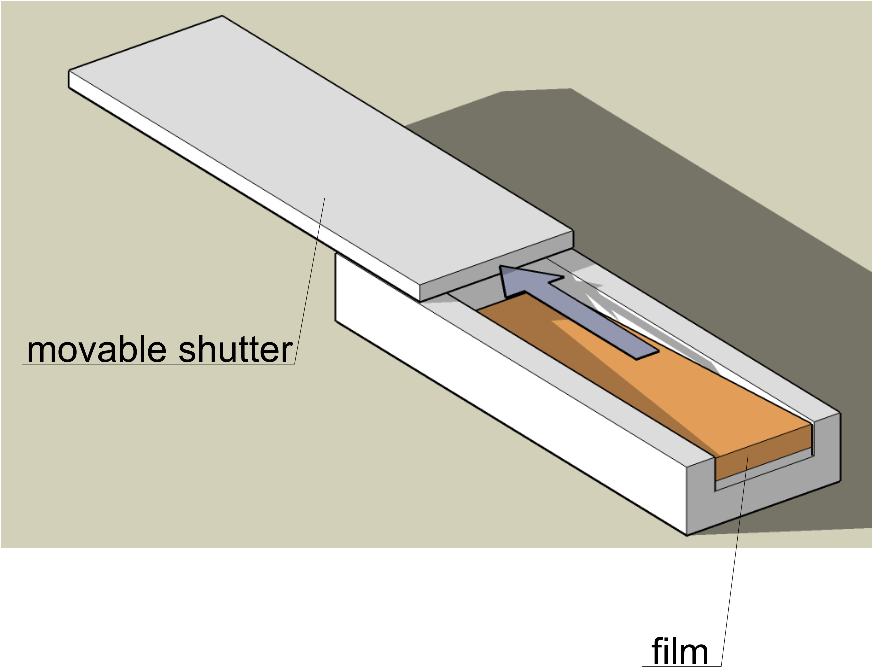


image from J. Unguris, R. J. Celotta, and D. T. Pierce Phys. Rev. Lett. **67**, 140 (1991)

RKKY-like interlayer coupling

- two Fe layers separated by a Cr wedge-shaped spacer; scanning electron microscopy with polarization analysis (SEMPA)
- measurement on a single specimen!
- up to six oscillations in coupling were observed
- different periods of coupling depending on temperature of the substrate during the film growth: samples grown at elevated temperature are of better quality and the magnetization of the upper Fe layer changes with each atomic-layer change in Cr thickness
- **“lower quality” samples display only RKKY-like coupling**

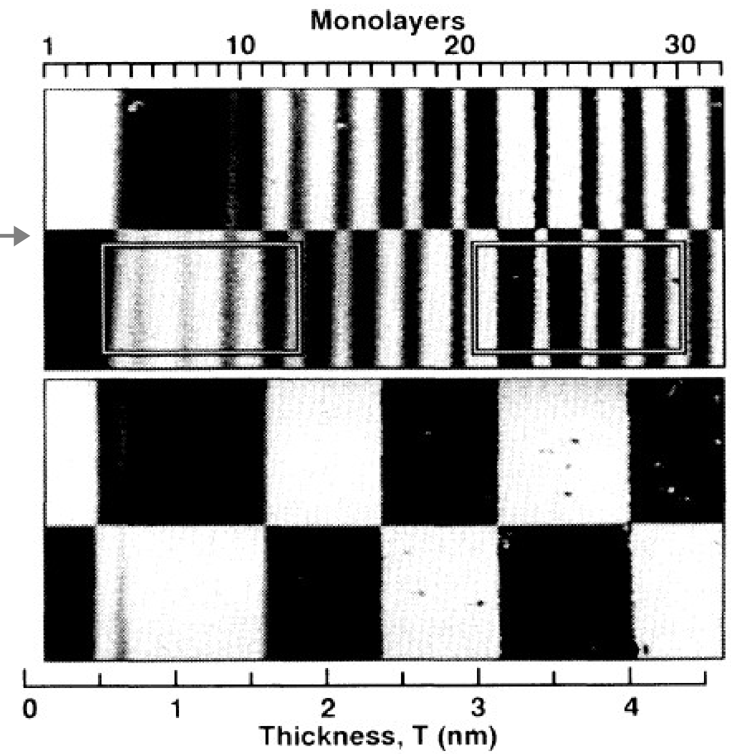


FIG. 3. The difference in the magnetic coupling of the Fe layers in the Fe/Cr/Fe sandwich for the Cr wedge grown (2.7 ML/min) on a substrate at room temperature (lower panel) and grown (7.2 ML/min) on a substrate at elevated temperature (upper panel) is clear in these SEMPA M_y images. The images in the upper and lower panels represent areas 300×280 and 350×290 μm, respectively.

grown at elevated temperatures (200-300^{o}C)

image from J. Unguris, R. J. Celotta, and D. T. Pierce Phys. Rev. Lett. **67**, 140 (1991)

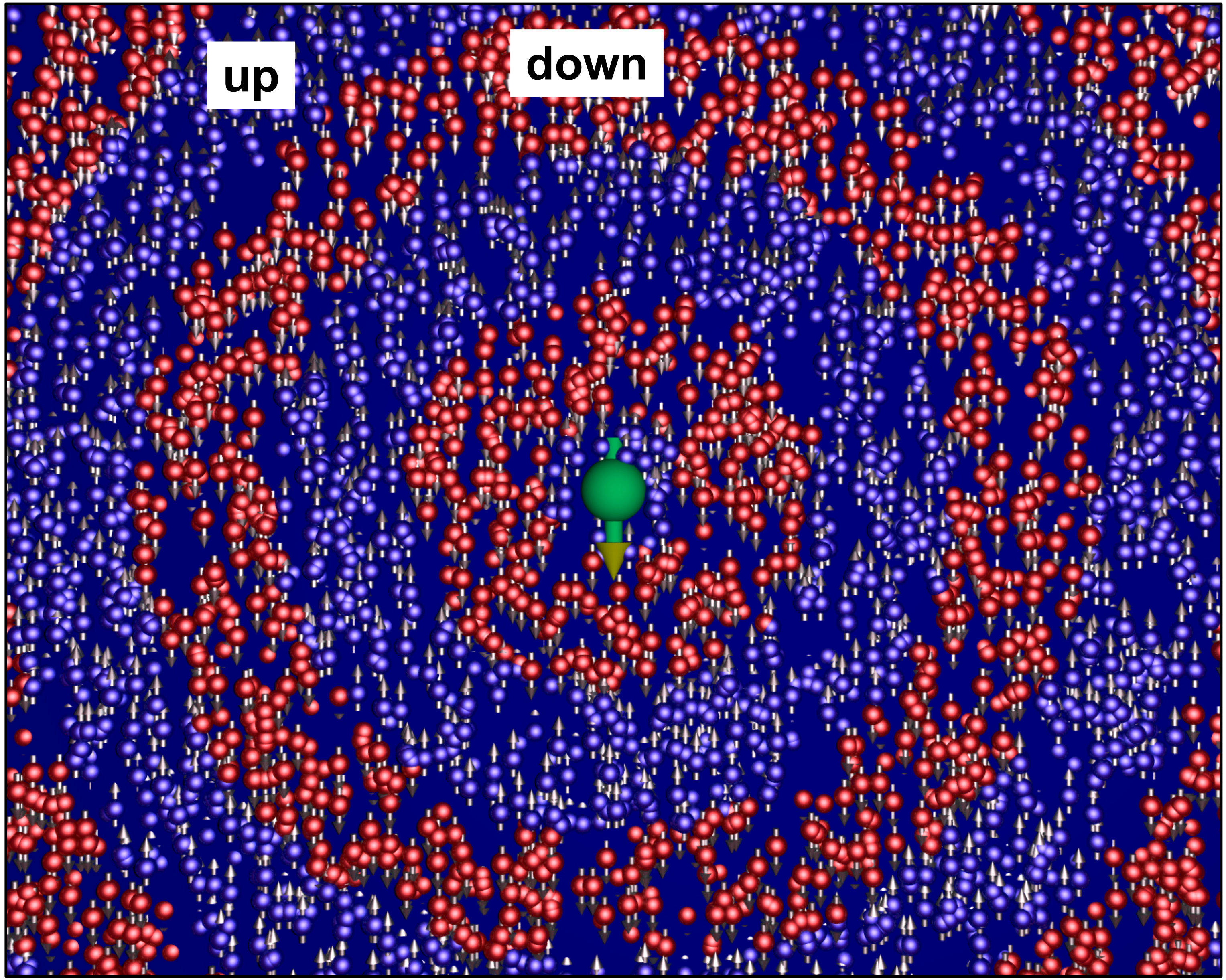
RKKY-like interlayer coupling

Magnetic impurity in a conducting medium induces spatial fluctuations of spin polarization of s-electrons about the impurity [9]

- the oscillatory term of wave number 2 k_F falls off like r^{-3} at large distances

impurity

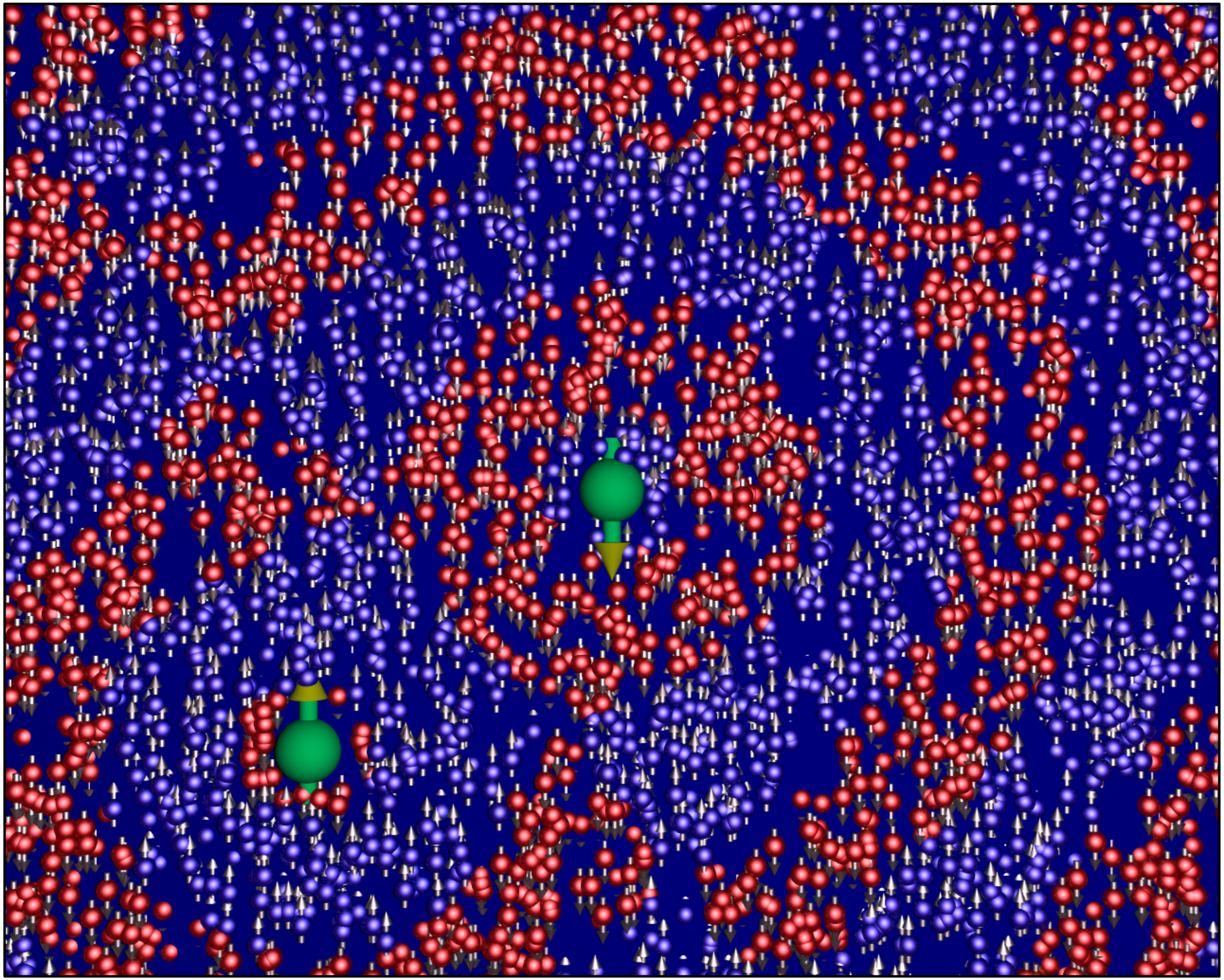
electrons



RKKY-like interlayer coupling

Magnetic impurity in a conducting medium induces spatial fluctuations of spin polarization of s-electrons about the impurity [9]

- the oscillatory term of wave number 2 k_F* falls off like r^{-3} at large distances
- the second impurity placed in the vicinity experiences interaction with the first impurity
- depending on the distance between impurities the interactions may be **ferromagnetic** or **antiferromagnetic**



*Fermi wave vector

RKKY-like interlayer coupling

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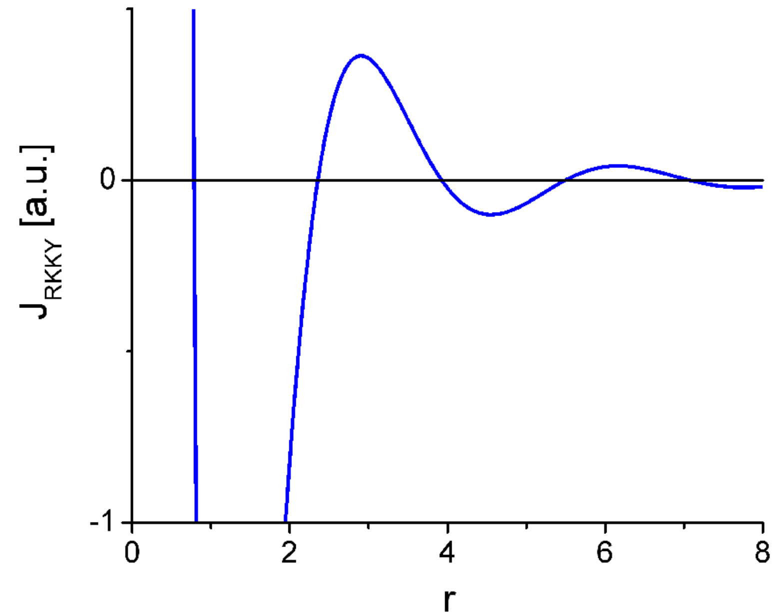
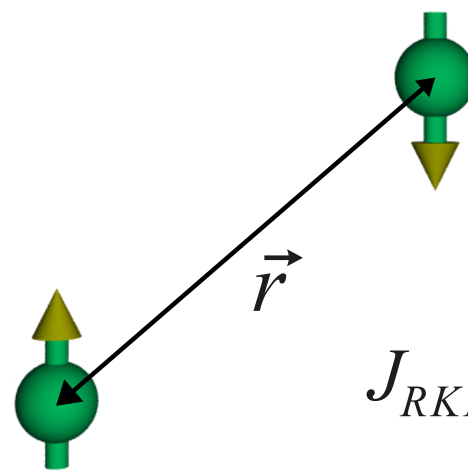




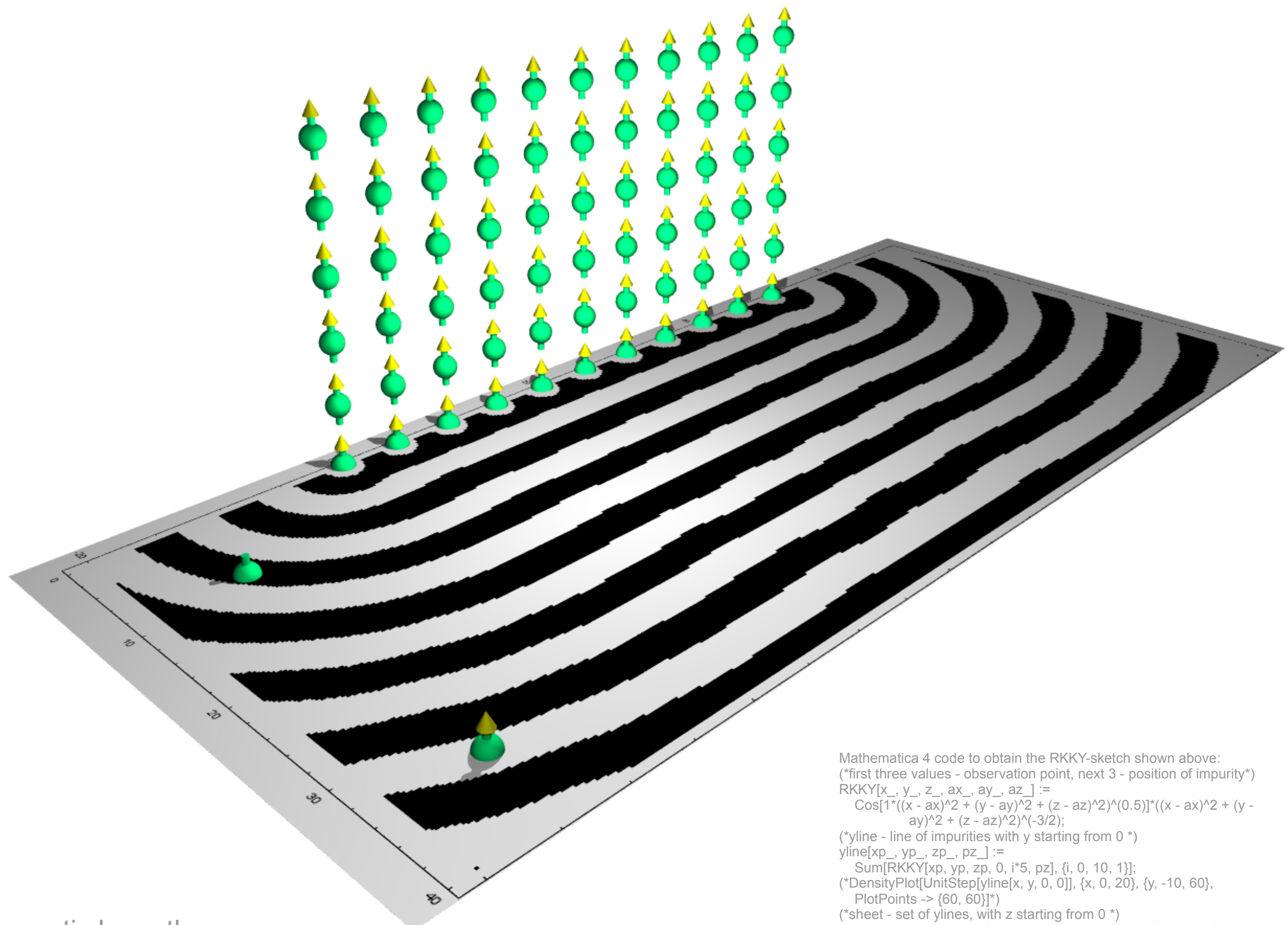
$$J_{RKKY} \propto \frac{1}{r^3} \cos\left(2 k_F r\right)$$

RKKY-like interlayer coupling

A plane composed of exchange coupled impurities creates spatial oscillations of spin polarization in the direction perpendicular to its surface

- if the moments are strongly coupled ferromagnetically they form a ferromagnetic layer
- a similar, parallel, layer or multilayer placed a certain distance away experiences ferromagnetic or antiferromagnetic coupling depending on a distance from the first layer

schematic drawing of a RKKY spin polarization due to single atom thick (11×11atoms) layer of impurities*




```
Mathematica 4 code to obtain the RKKY-sketch shown above:
(*first three values - observation point, next 3 - position of impurity*)
RKKY[x_, y_, z_, ax_, ay_, az_] :=
   Cos[1*((x - ax)^2 + (y - ay)^2 + (z - az)^2)^(0.5)]*((x - ax)^2 + (y -
         ay)^2 + (z - az)^2)^(-3/2);
(*yline - line of impurities with y starting from 0 *)
yline[xp_, yp_, zp_, pz_] :=
   Sum[RKKY[xp, yp, zp, 0, i*5, pz], {i, 0, 10, 1}];
(*DensityPlot[UnitStep[yline[x, y, 0, 0]], {x, 0, 20}, {y, -10, 60},
   PlotPoints -> {60, 60}]*)
(*sheet - set of ylines, with z starting from 0 *)
sheet[xq_, yq_, zq_]  = Sum [ yline[xq, yq, zq, i*5], {i, 0, 10, 1}];
DensityPlot[UnitStep[sheet[x, y, 25]], {x, 0, 40}, {y, -20, 70},
  PlotPoints -> {200, 200*   9/4  }, AspectRatio -> 9/4, Mesh -> False,
  ImageSize -> 600]
```

in case of quasi-infinite/real ferromagnetic layer the lines delimiting areas of opposite spin polarization would not be curved except at the ends

*the drawing shows the sign of the coupling (black and gray correspond to positive and negative spin polarization)

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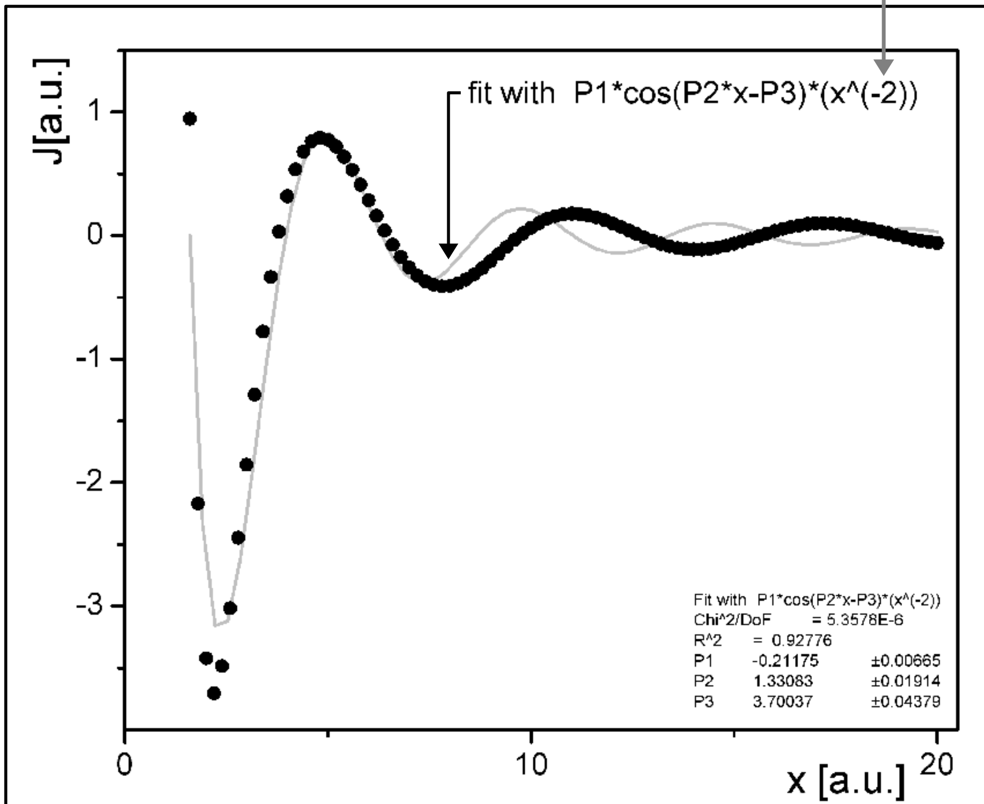
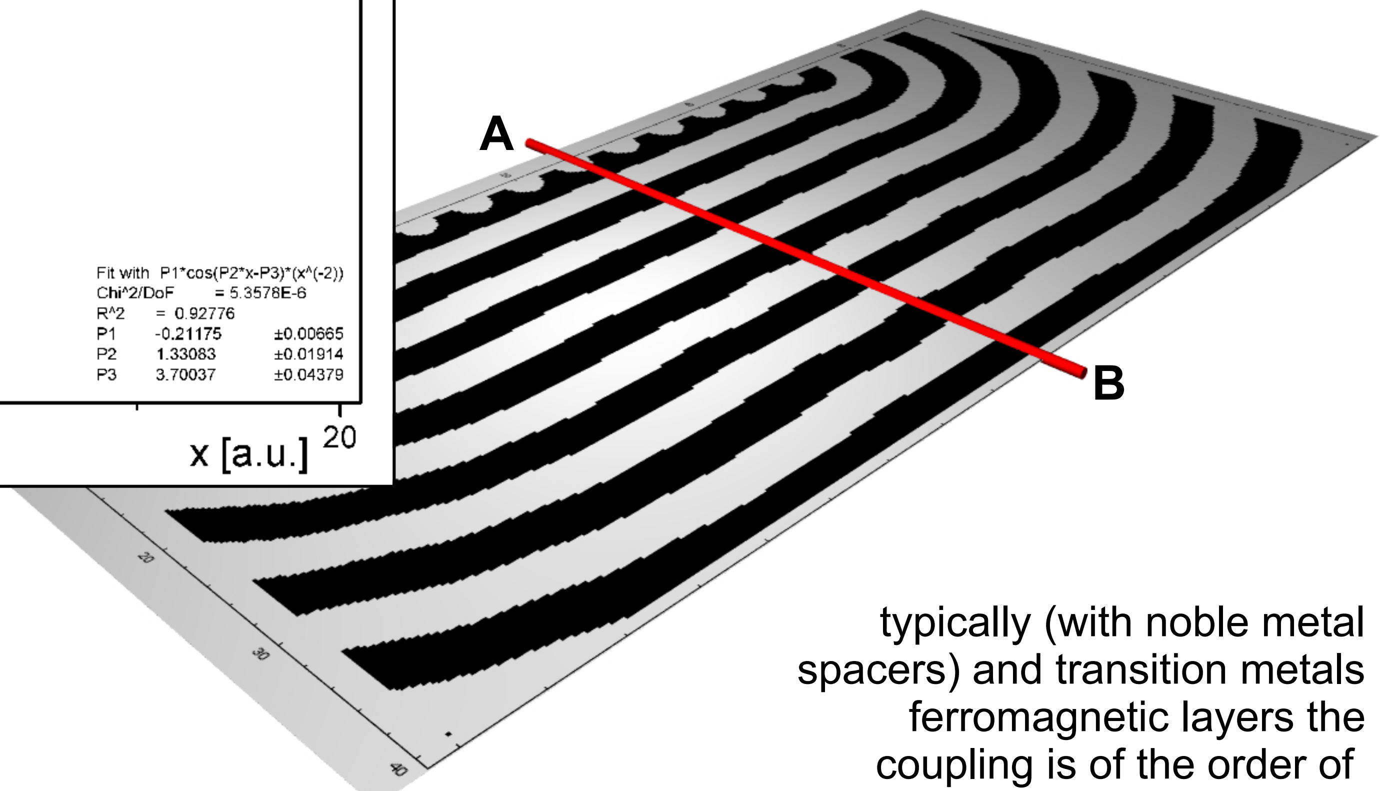
RKKY-like interlayer coupling

Theoretical considerations show that the coupling between **two ferromagnetic layers** is inversely proportional to the square of the spacer thickness [30]

$$J_{RKKY} \propto \frac{1}{r^2}$$



the coupling along AB line



typically (with noble metal spacers) and transition metals ferromagnetic layers the coupling is of the order of 1×10^{-6} Jm^{-2} in the first antiferromagnetic maximum

*the drawing shows the sign of the coupling (black and gray correspond to positive and negative spin polarization)

RKKY-like coupling and giant magnetoresistance

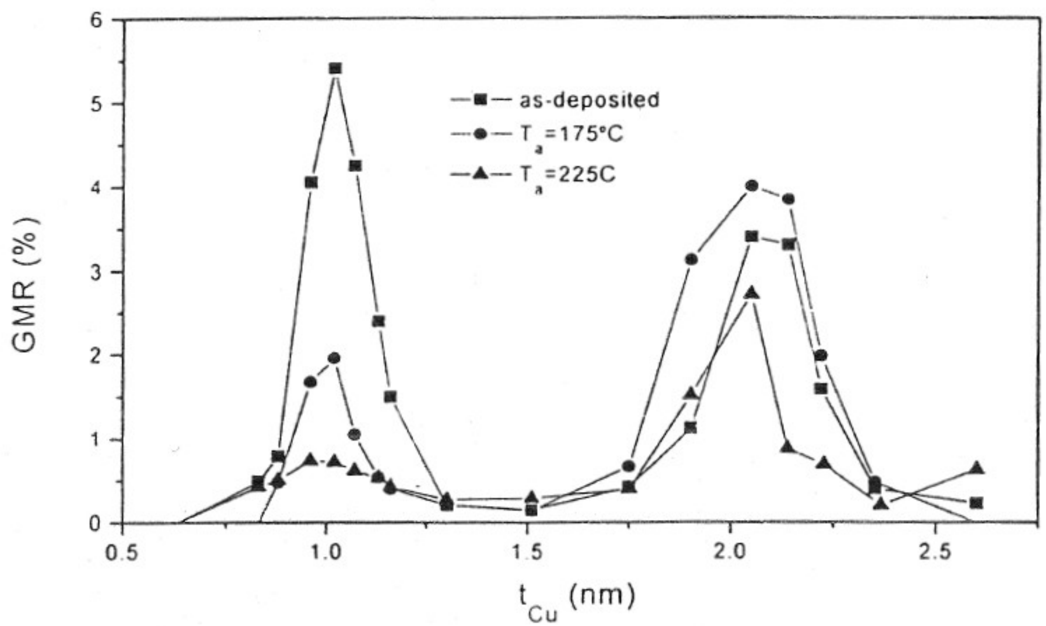


Fig. 1. GMR as a function of the Cu sublayer thickness for the as deposited and annealed samples.

- $Si(100)/Cu(20nm)[Ni_{83}Fe_{17}(2nm)/Cu(t_{Cu})]_{100}$
- GMR reflects the oscillatory character of the RKKY-like coupling between permalloy layers
- in MLs with identical magnetic layers (the same switching fields) GMR can be observed only for spacer thicknesses corresponding to antiferromagnetic coupling; otherwise the magnetic field does not change relative orientation of magnetic moments of neighboring layers

image from: F. Stobiecki, T. Luciński, R. Gontarz, M. Urbaniak, Materials Science Forum 287, 513 (1998)

RKKY-like coupling and giant magnetoresistance

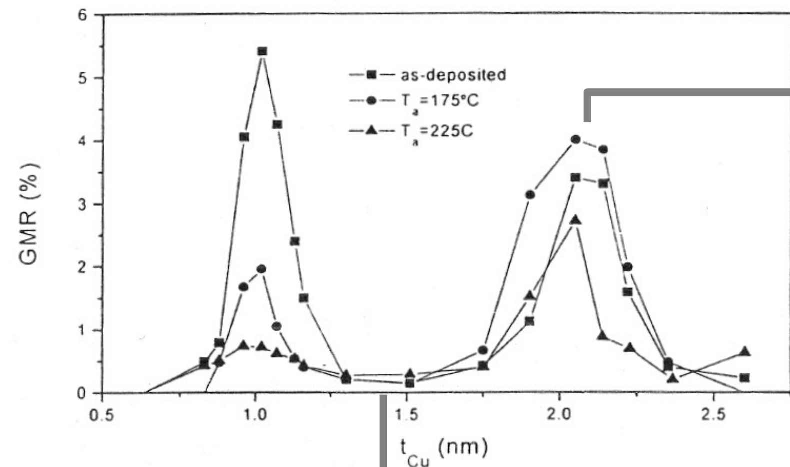
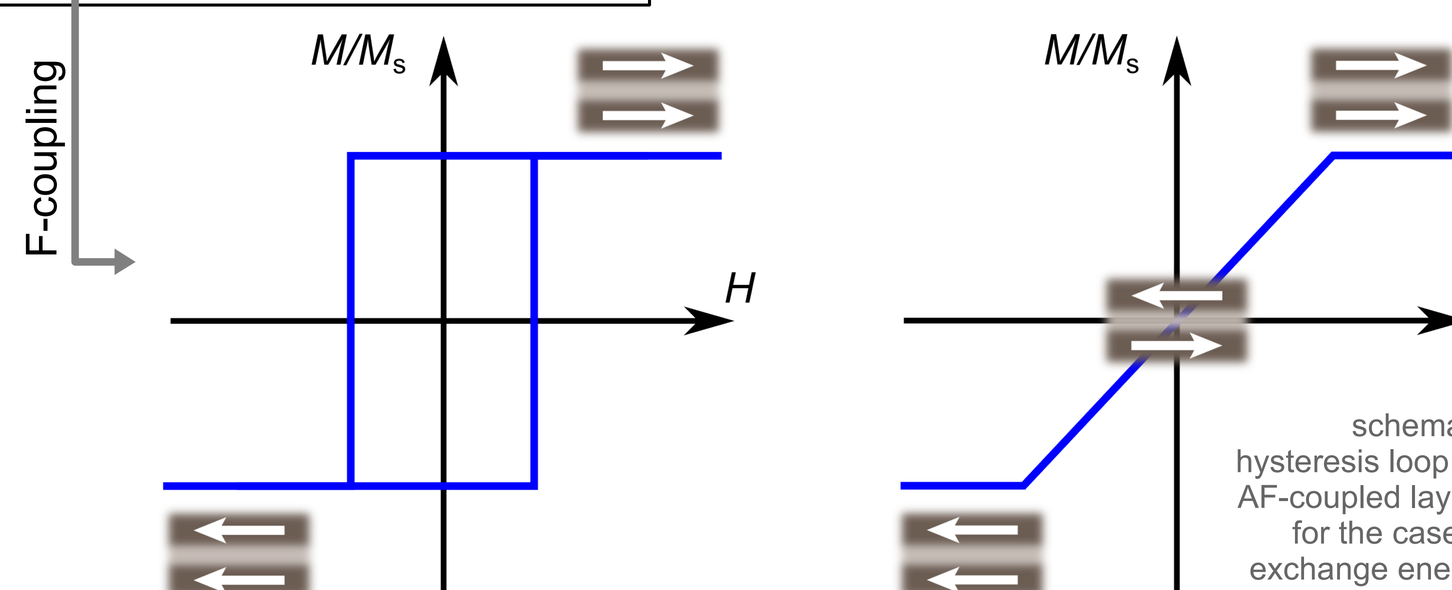


Fig. 1. GMR as a function of the Cu sublayer thickness for the as deposited and annealed samples.



schematic hysteresis loop for AF-coupled layers for the case of exchange energy much exceeding magnetic anisotropy

image from: F. Stobiecki, T. Luciński, R. Gontarz, M. Urbaniak, Materials Science Forum 287, 513 (1998)

Dzyaloshinskii-Moriya interaction (**DMI**) – antisymmetric exchange

- The bilinear terms of the coupling: $E_{bilinear} = -\sum_{ij} K_{ij} S_1^i S_2^j = K_{xx} S_1^x S_2^x + K_{xy} S_1^x S_2^y + \ldots$

$$J \vec{S}_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \vec{S}_2 = J \vec{S}_1 \cdot \vec{S}_2$$

exchange coupling

$$\vec{S}_1 \begin{bmatrix} 0 & D_1 & D_2 \\ -D_1 & 0 & D_3 \\ -D_2 & -D_3 & 0 \end{bmatrix} \vec{S}_2 = \vec{D} \cdot (\vec{S}_1 \times \vec{S}_2)$$

Dzyaloshinskii-Moriya interaction

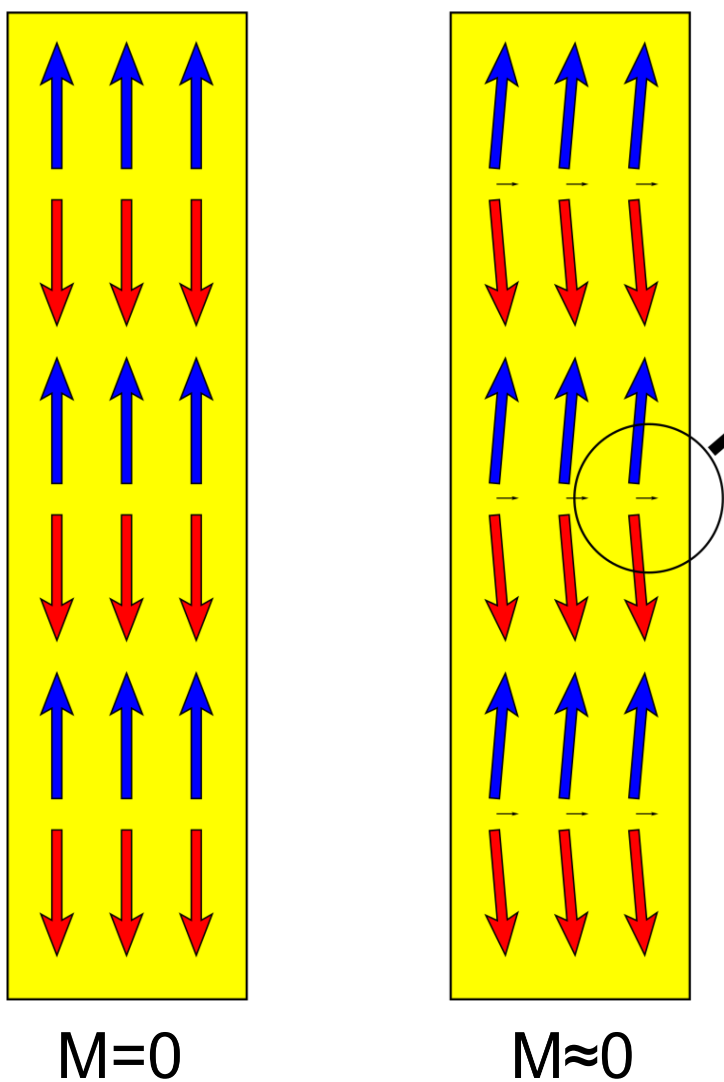
$$\vec{S}_1 \left[-\frac{\mu_0}{4\pi |r|^3} \begin{bmatrix} 3\hat{r}_x^2 - 1 & 3\hat{r}_x \hat{r}_y & 3\hat{r}_x \hat{r}_z \\ 3\hat{r}_x \hat{r}_y & 3\hat{r}_y^2 - 1 & 3\hat{r}_y \hat{r}_z \\ 3\hat{r}_x \hat{r}_z & 3\hat{r}_y \hat{r}_z & 3\hat{r}_z^2 - 1 \end{bmatrix} \right] \vec{S}_2$$

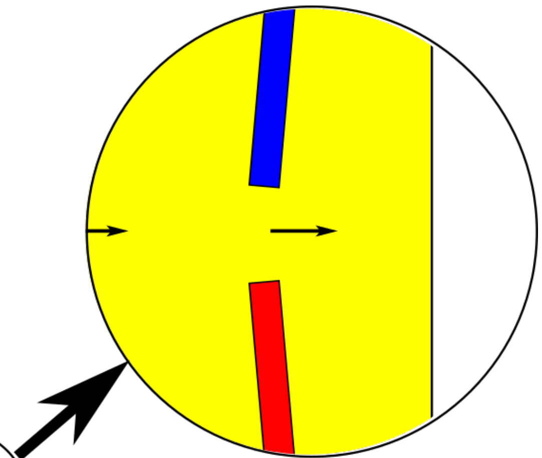
dipole-dipole interaction

Dzyaloshinskii-Moriya interaction

Weak ferromagnetism:

- the magnetization of a sample is by a factor 10^{-2} to 10^{-5} lower than the magnetization of constituent magnetic lattices





canting of magnetic moments in sublattices of an antiferromagnet creates a tiny resultant magnetic moment in each cell

$FeBO_3$

the interaction between Fe atoms/ spins is mediated by oxygen atoms

when “the symmetry allows coincidence of magnetic and resonant forbidden scattering” “ the sign of the Dzyaloshinskii–Moriya vector could be measured with resonant X-ray diffraction by observing interference between the resonant and magnetic scattering amplitudes.”

this type of coupling was introduced when investigating “weak ferromagnets” (example α-Fe_2O_3) by I. E. Dzyaloshinskii [Sov. Phys. JETP **5**, 1259(1957)]

im

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Dzyaloshinskii-Moriya interaction

NATURE PHYSICS DOI: 10.1038/NPHYS2859 LETTERS

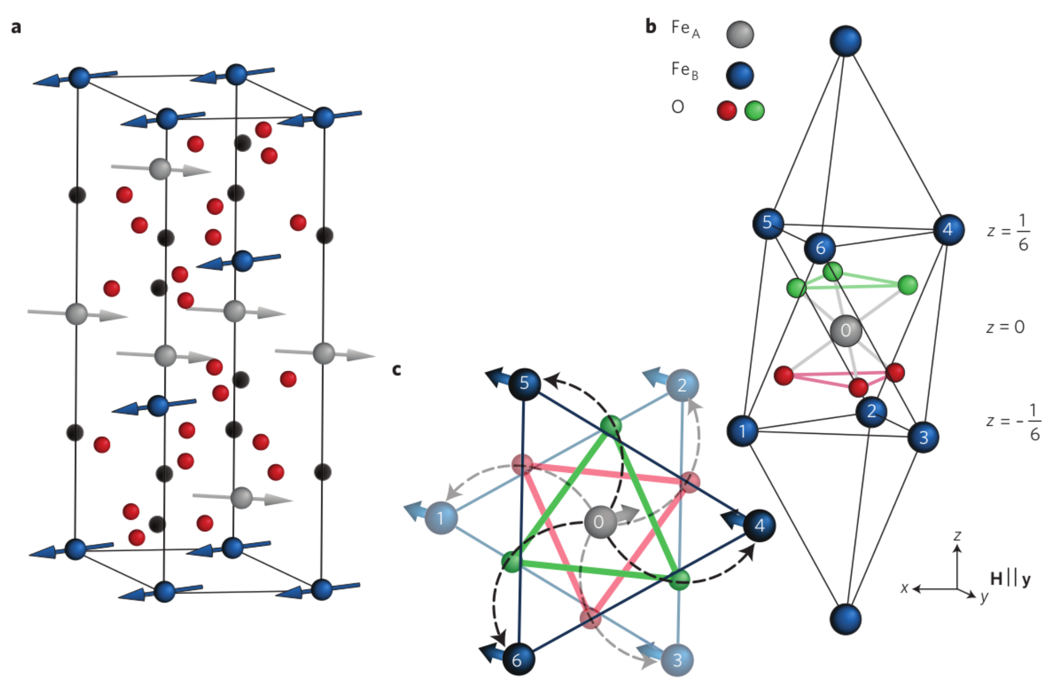

Figure 1 | Atomic and magnetic order in $FeBO_3$. **a**, A magnetic (hexagonal) unit cell, showing oxygen atoms (red), boron atoms (black), and two symmetry-related magnetic iron sublattices (blue and grey) with moments tilted between the two. **b**, The local environment of one of the grey (A-site) Fe atoms, showing neighbouring B-site Fe atoms (blue). The upper and lower oxygen triangles are coloured green and red, and boron atoms are removed for clarity. **c**, The same structure viewed from the top, highlighting the twisted superexchange paths from the A-site Fe atom to the upper Fe layer (dark blue) and the lower layer (pale blue) via the oxygen triangles.

image from V. E. Dmitrienko et al., Nature Physics **10**, 202 (2014)

- $FeBO_3$
- the interaction between Fe atoms/ spins is mediated by oxygen atoms
- when “the symmetry allows coincidence of magnetic and resonant forbidden scattering” “ the sign of the Dzyaloshinskii–Moriya vector could be measured with resonant X-ray diffraction by observing interference between the resonant and magnetic scattering amplitudes.”
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$$E = \vec{D} \cdot (\vec{S}_1 \times \vec{S}_2)$$

Dzyaloshinskii-Moriya interaction

The calculated Dzyaloshinskii–Moriya vector linking iron atoms 0 and 1 (Fig. 1), for example, is D_{01} = (−0.25, 0,−0.24) meV. [V.E. Dmitrienko, *et al.*]

$$E = \vec{D} \cdot \left(\vec{S}_1 \times \vec{S}_2 \right)$$

Then the direction of the DM-vector an be determined according to the following rules* [102 and references therein]:

Consider two spins located at R_1 and R_2 . The middle is labeled as $\tilde{R} = (R_1+R_2)/2$.

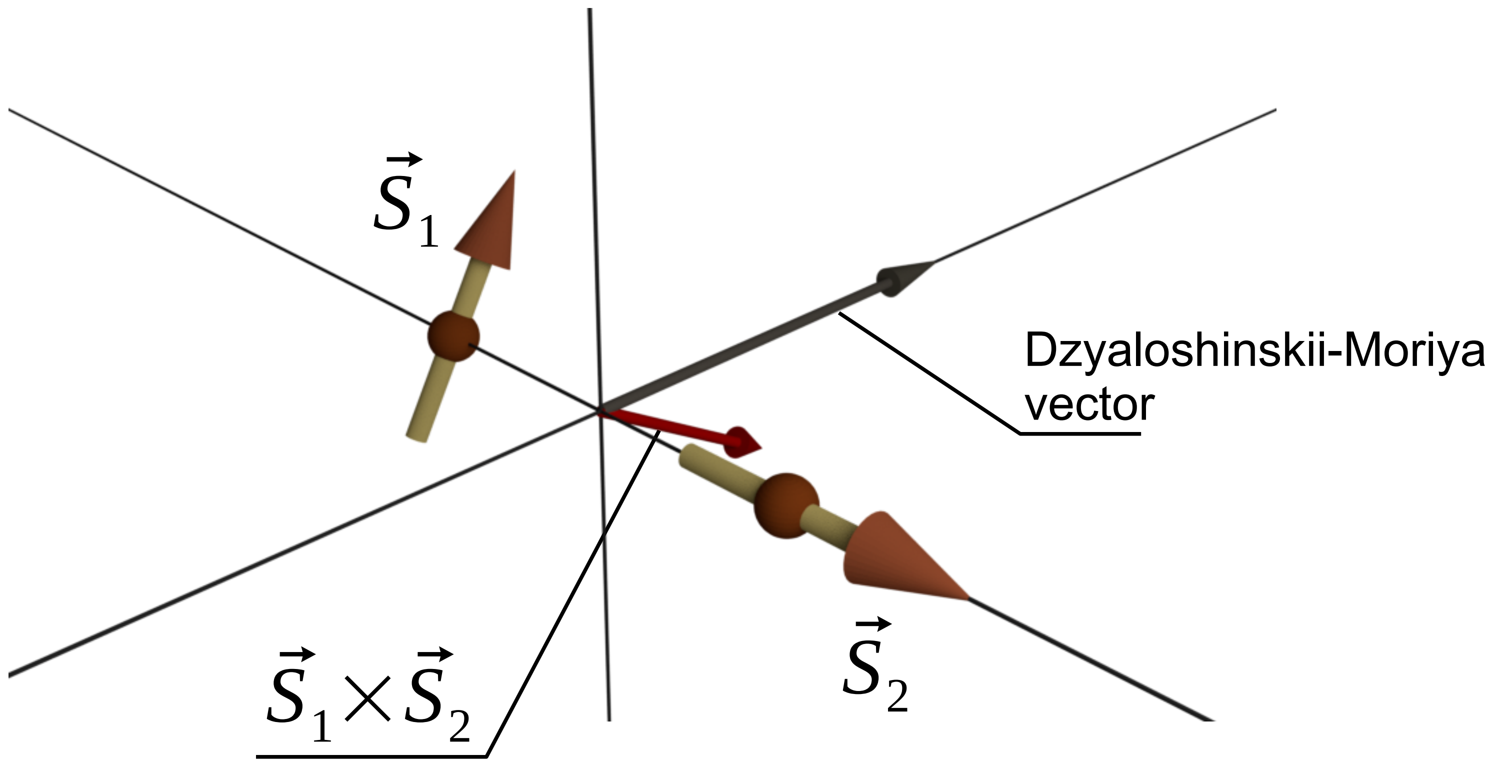
- If a center of inversion is located at $\tilde{R}$: D = 0.
- If a mirror plane perpendicular to R1−R2 includes $\tilde{R}$ then $D \perp (R_1 - R_2)$.
- If a mirror plane includes R_1 and R_2 then D⊥ mirror plane.
- If a two-fold rotation axis perpendicular to $R_1 - R_2$ includes $\tilde{R}$ then D⊥rotation axis.
- If a n-fold rotation axis (n ≥ 2) includes R_1 and R_2 then $D \parallel (R_1 - R_2)$.

[102]: B. Zimmermann, dissertaton 2010, Institut für Festkörperforschung (IFF) Forschungszentrum Jülich

- Note that Dzyaloshinskii-Moriya interaction is “chiral” in that sense that it favors one chirality of spin pair in favor of the other:

$$E_1 = \vec{D}\cdot(\vec{S}_1 \times \vec{S}_2) \ \ \textbf{\textit{not equal}} \ \ \vec{D}\cdot\left(\vec{S}_1 \times (-\vec{S}_2)\right) = E_2$$

i.e. the two configurations with equal angle between the interacting spins have different energies (this is due to the configuration of the surrounding atoms)



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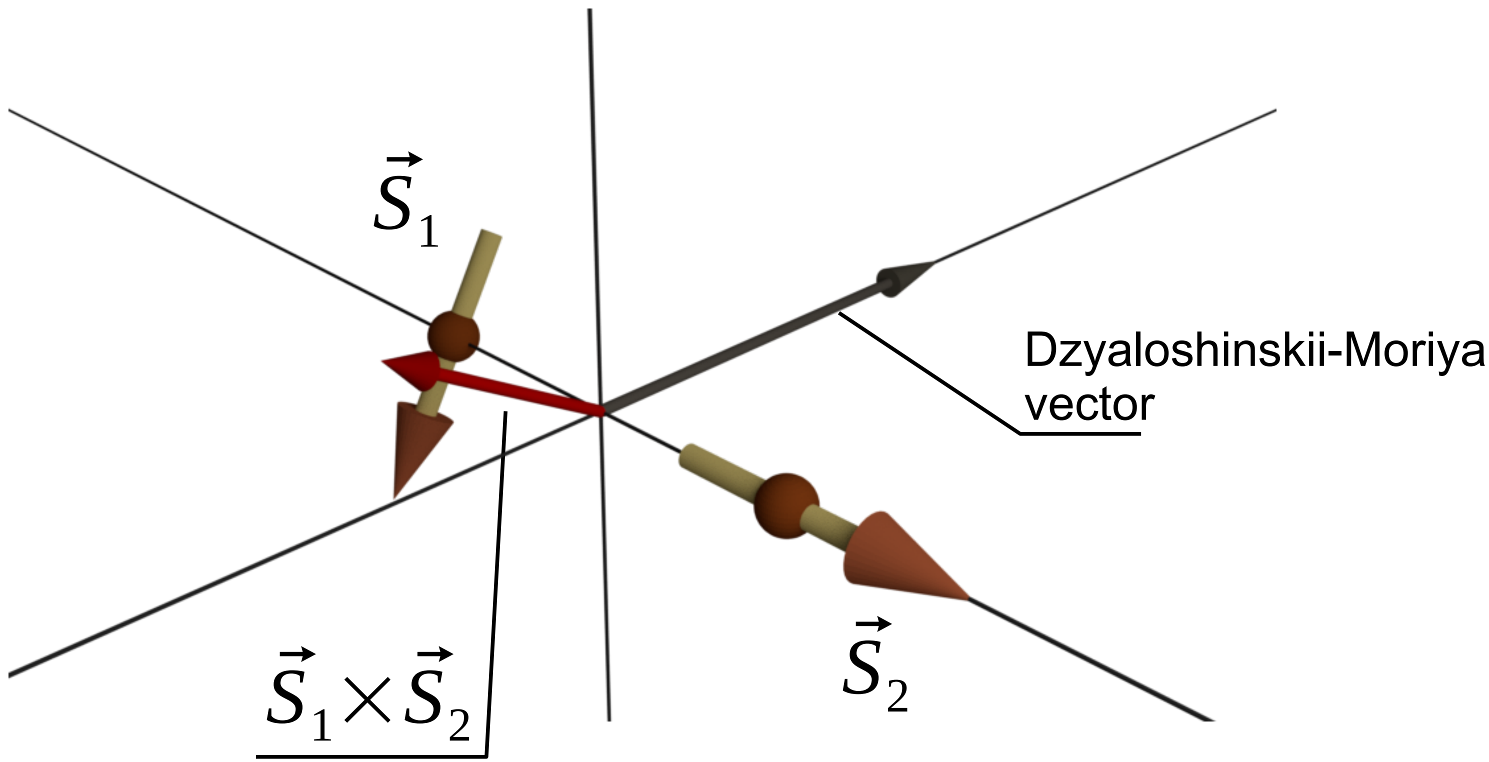
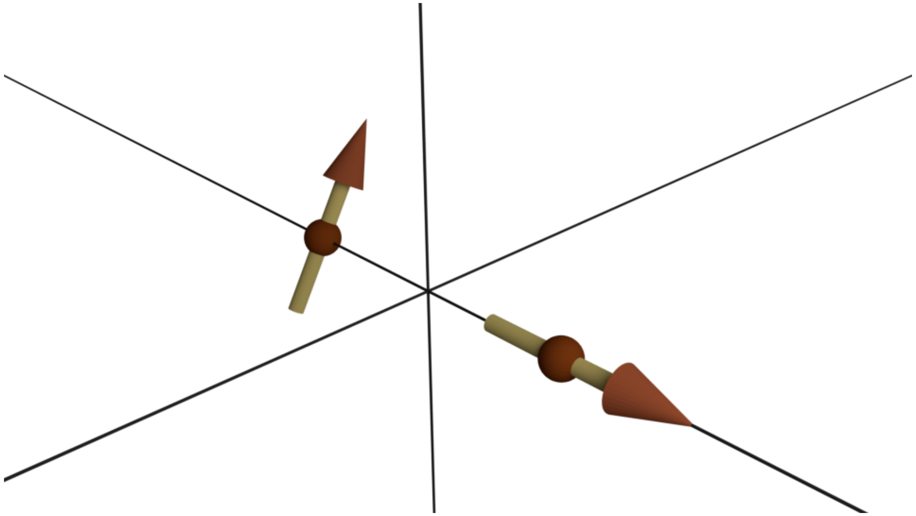


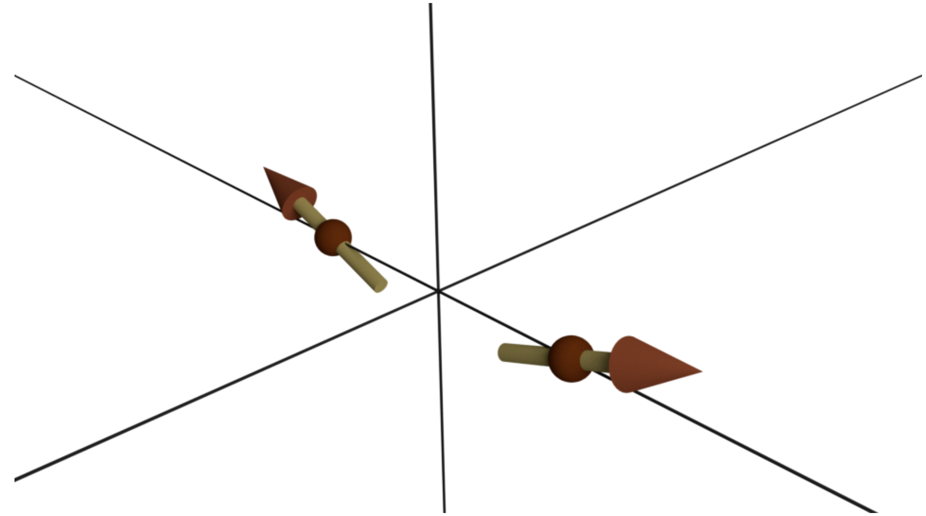
- Different sign of a dot product of DM vector with a cross product of interacting spins – depending on the direction of DM vector the clockwise or counterclockwise orientation is favored; this is not the case for anisotropic exchange interaction

Dzyaloshinskii-Moriya interaction

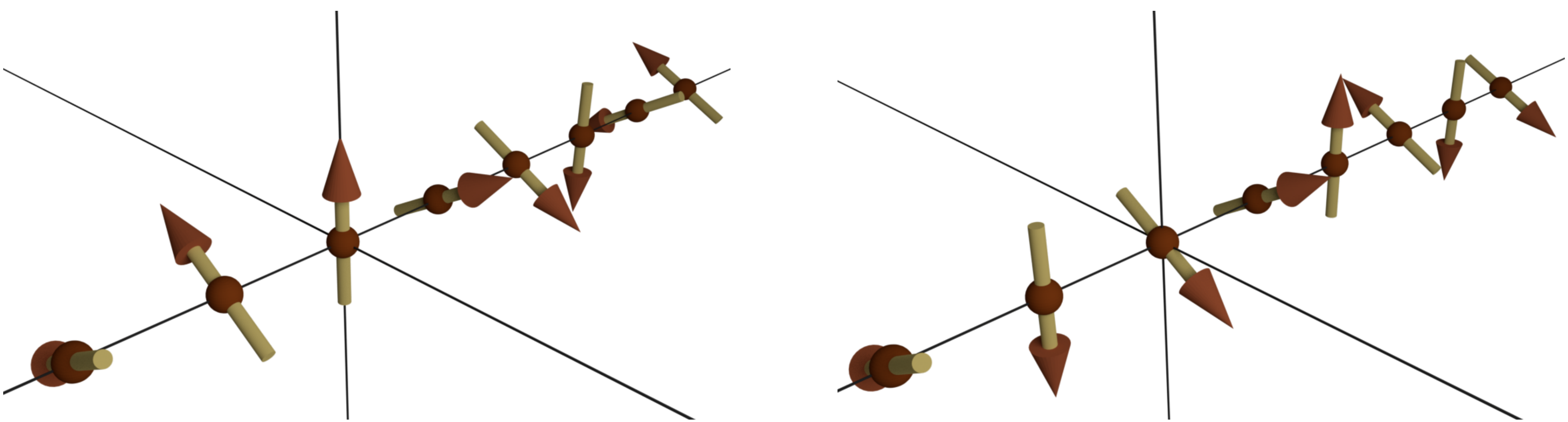
DMI alone favors perpendicular orientation of interacting magnetic moments



DMI coupled with exchange coupling favors canting of spins



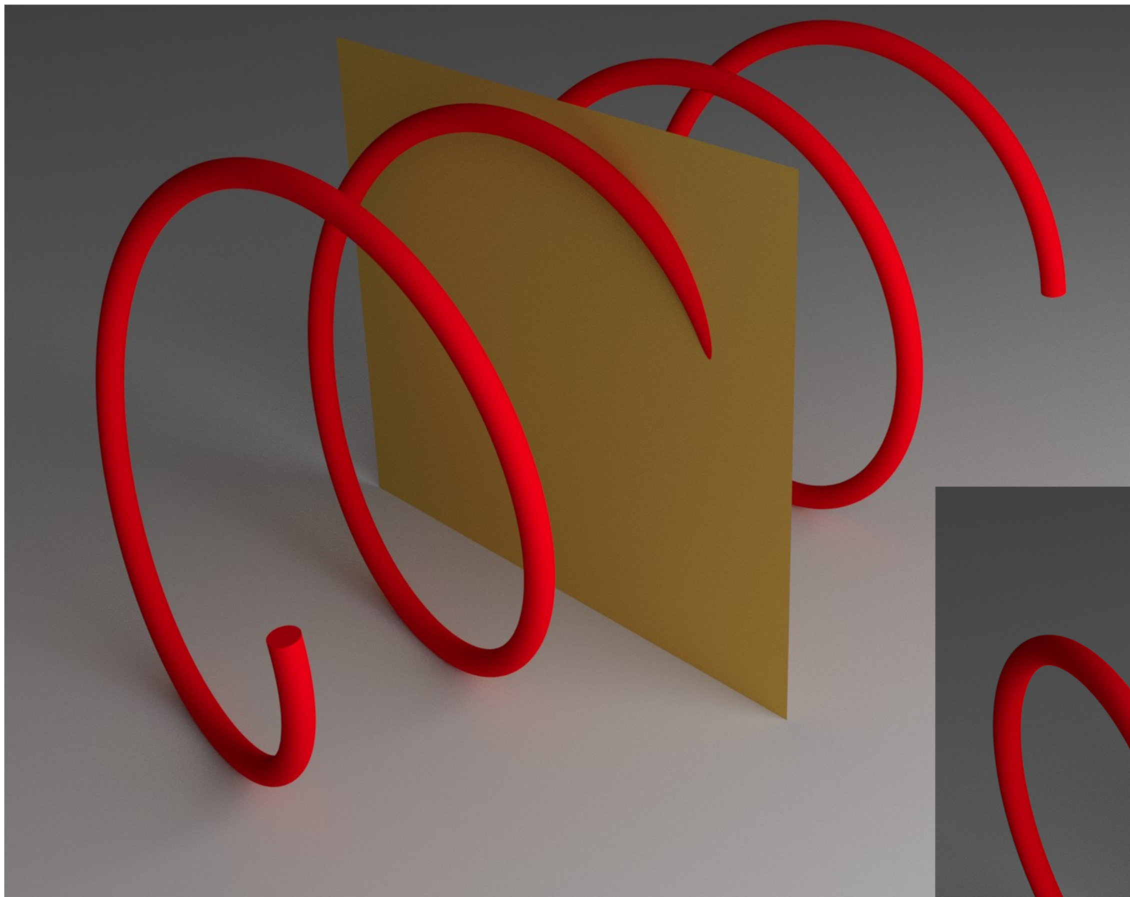
DMI coupled with exchange coupling and periodicity of the lattice can lead to a spiral states with various chirality* [101]



*S. Blügel, P. Grünberg,"Complex Magnetism" in Lecture Notes of the 45 th IFF Spring School, Forschungszentrum Jülich, 2014

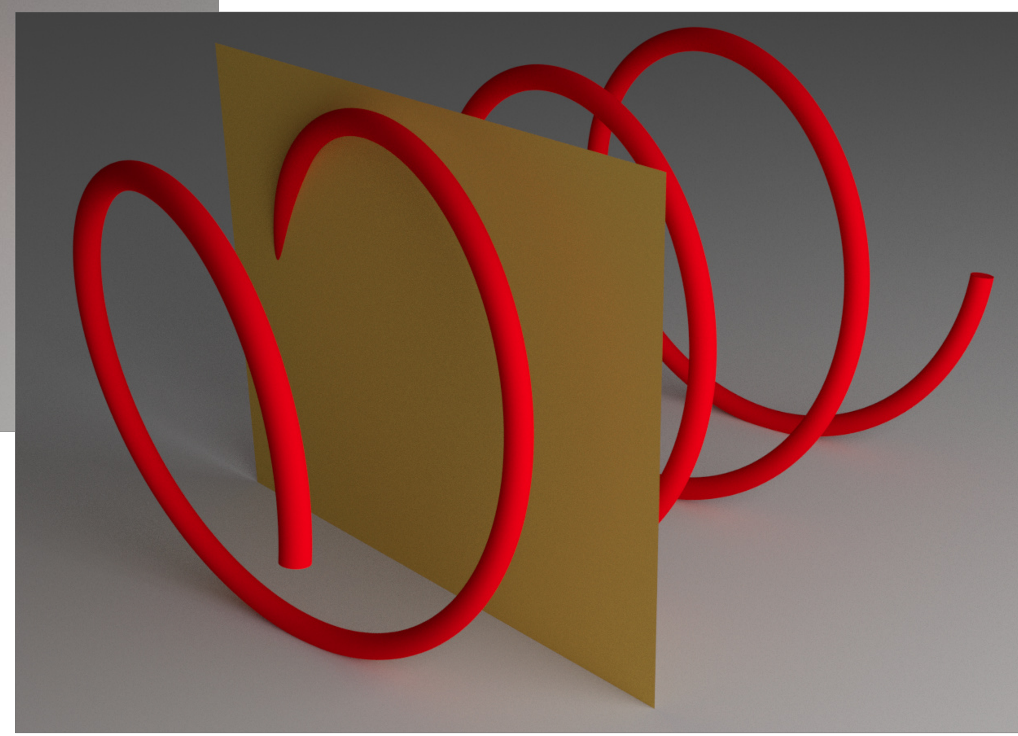
Chirality

“A right-handed helix is one that turns clockwise as you move along the length of the helix” * [103]



Right-handed helix, P or Δ

Left-handed helix, M or Λ



[103]: J. P. Riehl, Mirror-Image Asymmetry: An Introduction to the Origin and Consequences of Chirality, John Wiley & Sons, Inc. 2010

Chiral magnetic structure – an example

- $Ba_3NbFe_3Si_2O_{14}$
- this magnetic structure is characterized by **two kinds** of magnetic chiralities:

  - triangular chirality

  - helical chirality

image source: V. Simonet, M. Loire, and R. Ballou, Eur. Phys. J. Special Topics **213**, 5–36 (2012)

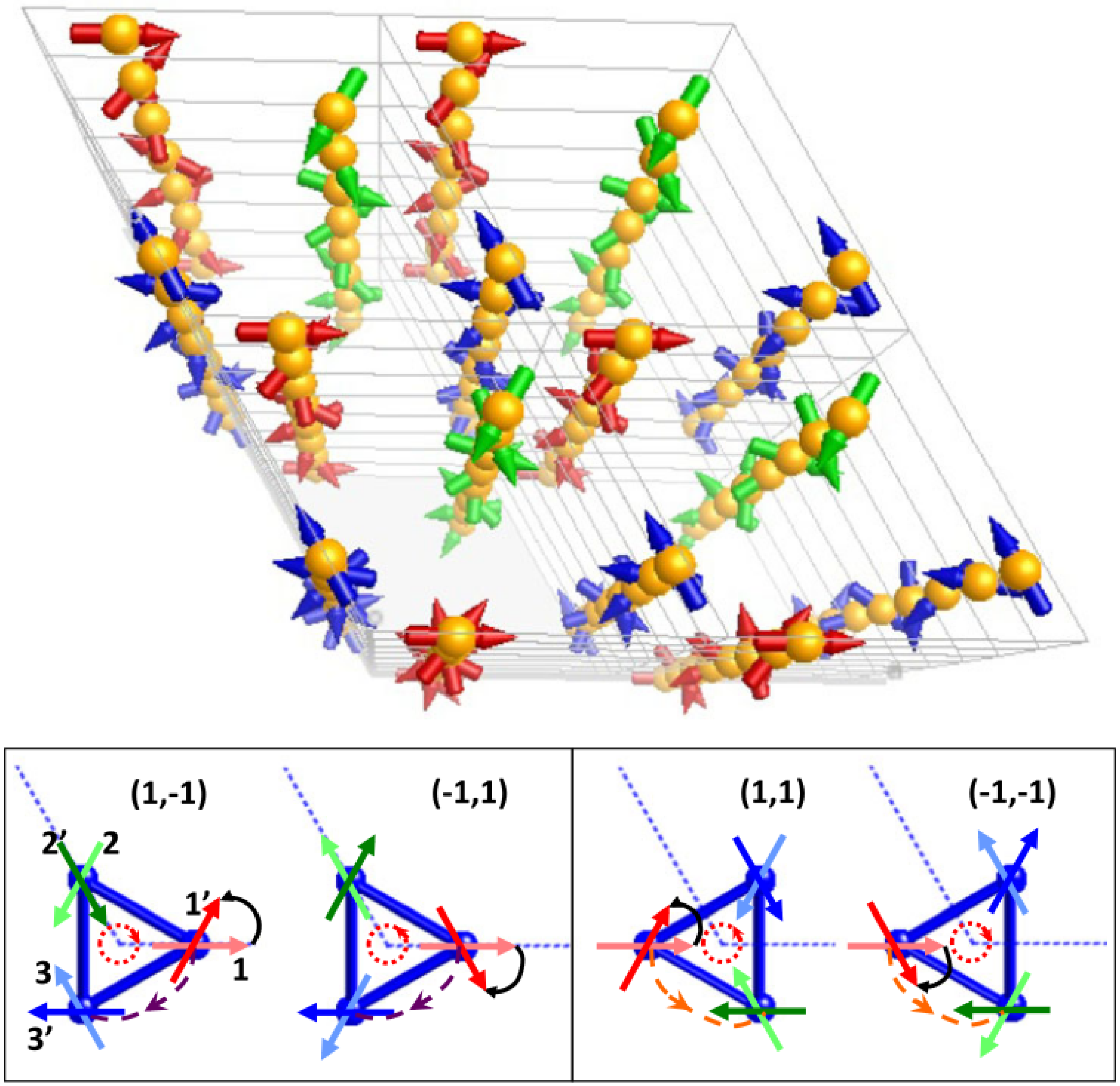


Fig. 6. Top: magnetic structure of $Ba_3NbFe_3Si_2O_{14}$ with different colors for the three Bravais lattices. Below: representation of the magnetic structures associated with the 4 possible chiral ground states (helical chirality=±1, triangular chirality=±1). The light colored moments lie in one layer and the darker colored ones in the next layer along the **c** axis, a black curved arrow defines the helical chirality. The red arrowed circle materializes the triangular chirality. The structural chirality is related to the strongest diagonal exchange between the two layers, which is shown as a purple/orange dashed arrow path for negative/positive structural chirality.

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