Effective model of antiferromagnetic MnTe and anisotropic magnetoresistance

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KCL

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UR

solid state physics

materials science

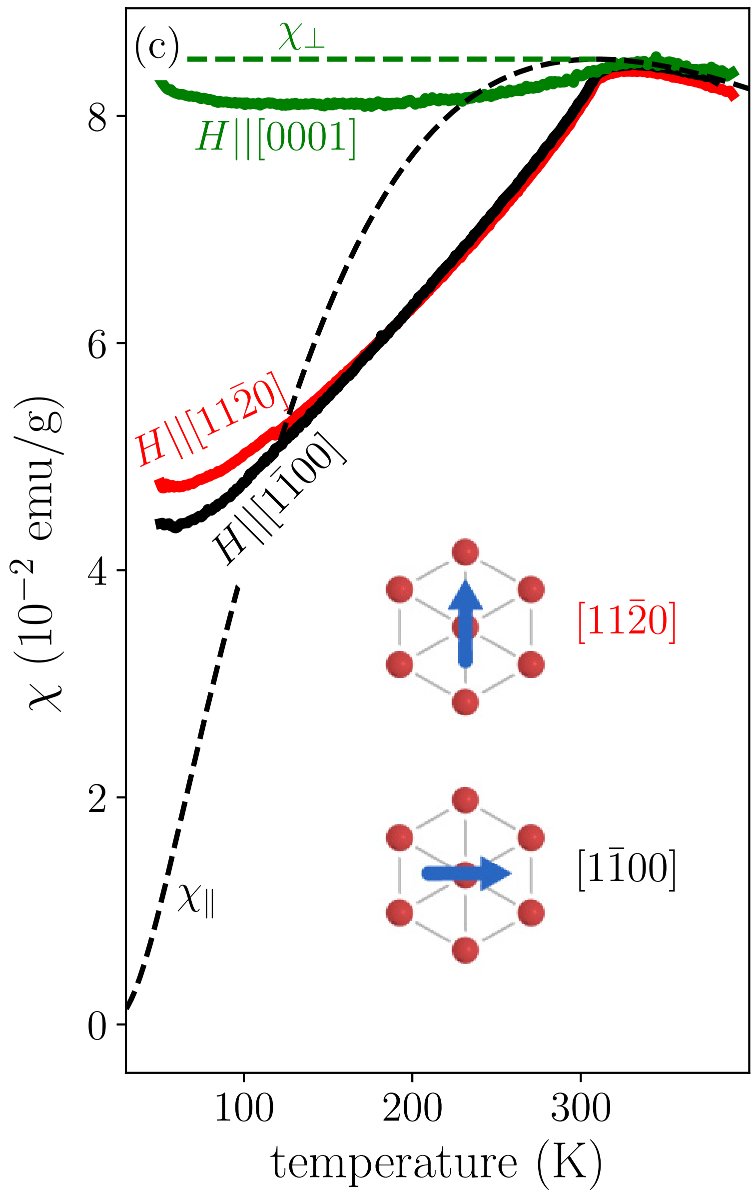
anisotropic magnetoresistance (AMR)

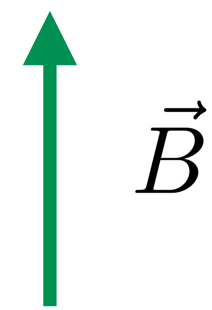
iron, permalloy, (Ga,Mn)As

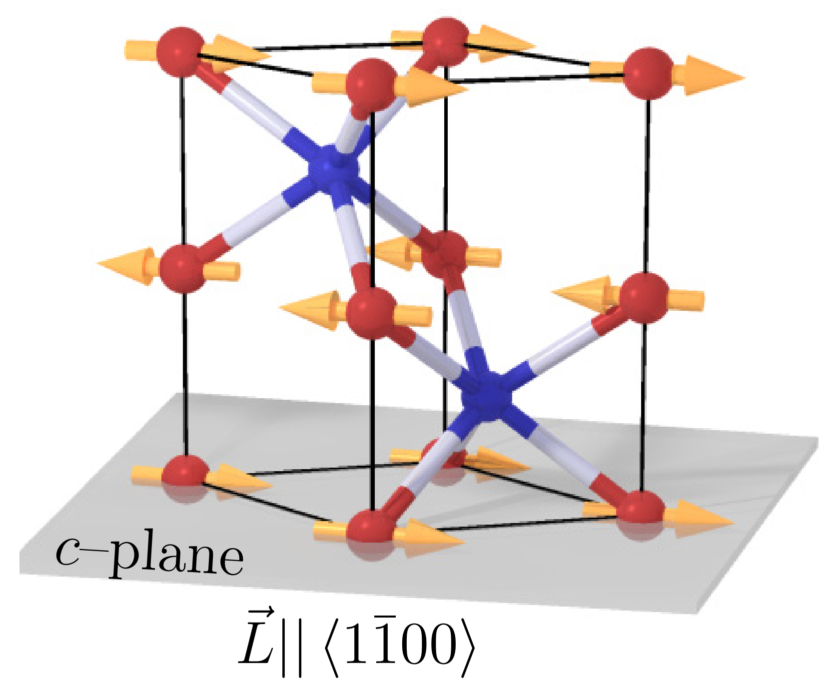
antiferromagnets

MnTe: an antiferromagnet

Magnetometry





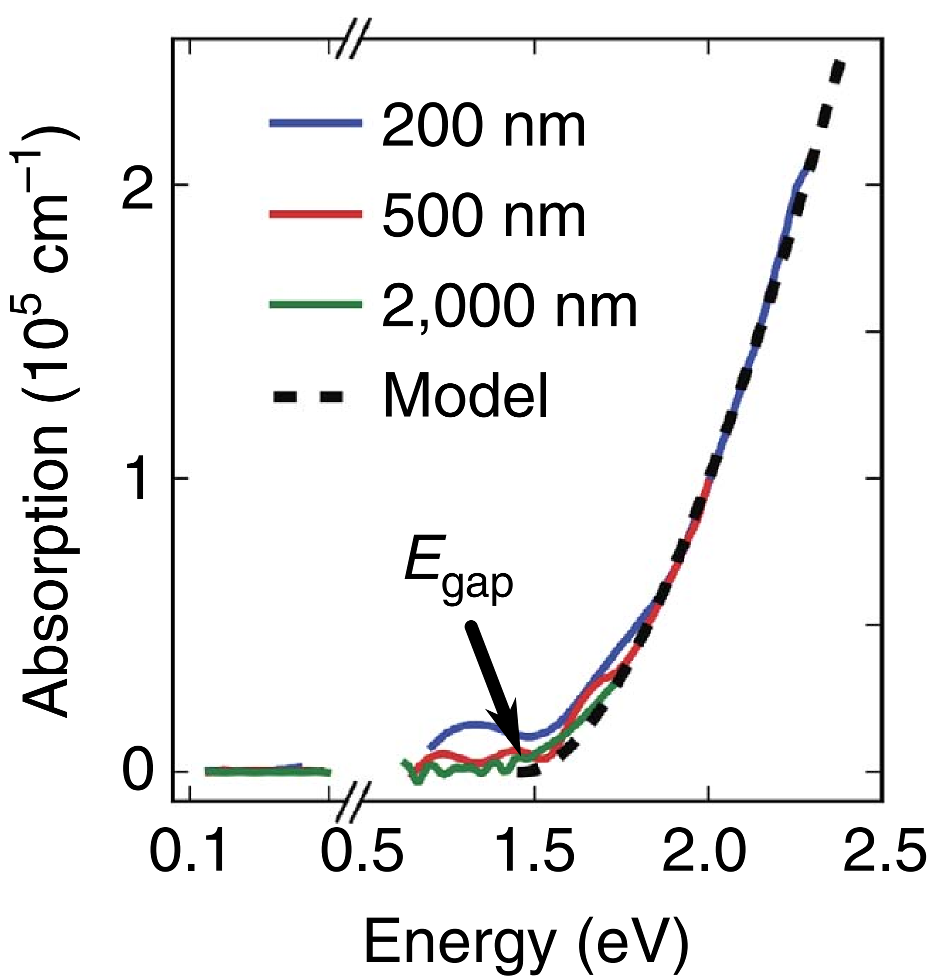


Kriegner et al. '17

doi: 10.1103/PhysRevB.96.214418

MnTe: a semiconductor

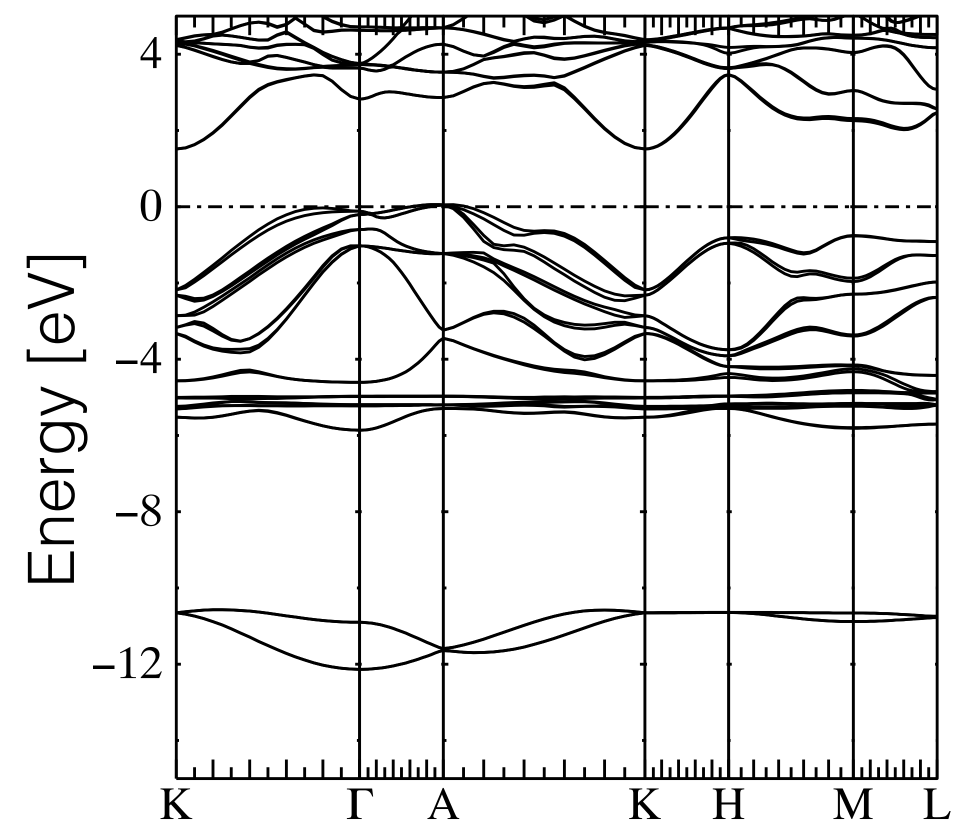
absorption on thin layers



Kriegner et al. '16

doi: 10.1038/ncomms11623

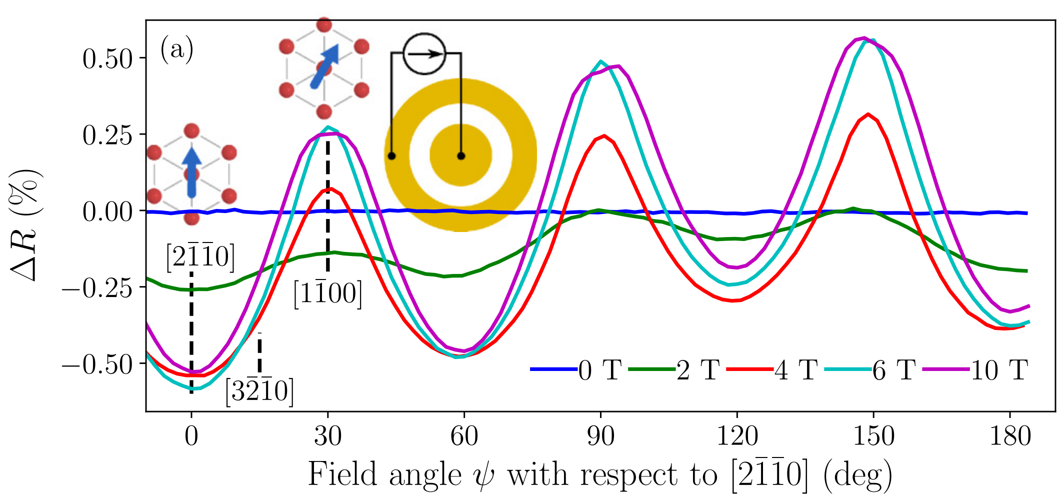
QSGW



The goal:

- construct an effective model
- analyse magnetic anisotropies
- AMR modelling

- non-crystalline components (Hall)
- crystalline components (Corbino)



Kriegner et al. '17

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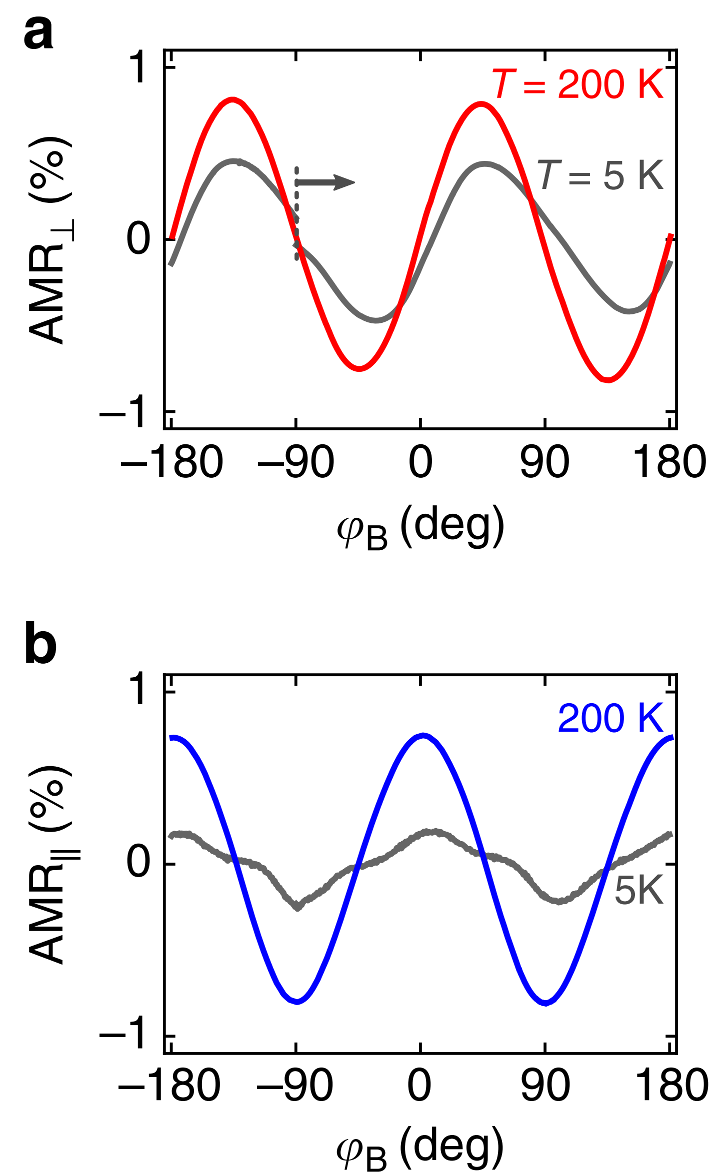
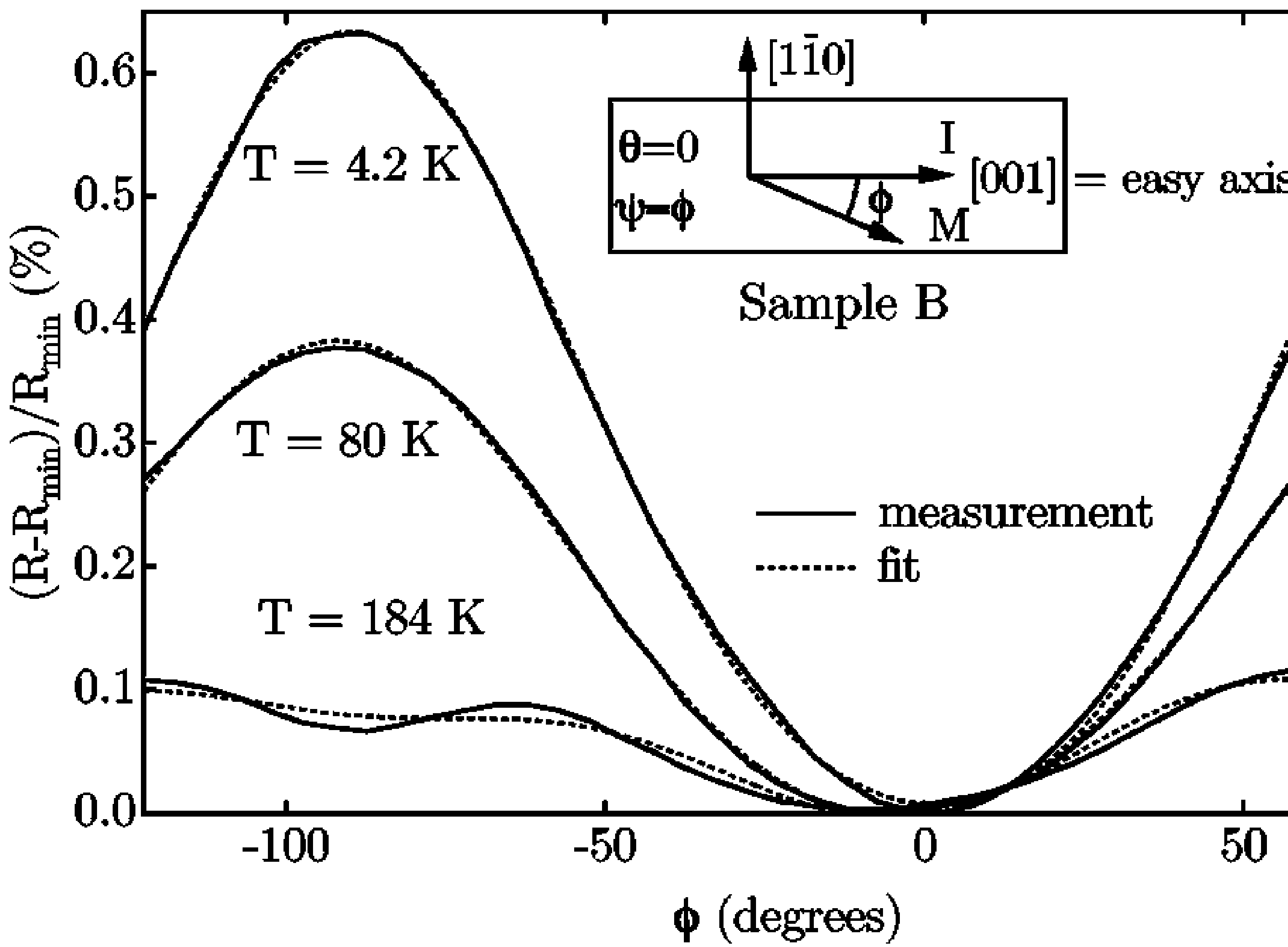


Kriegner et al. '16

doi: 10.1038/ncomms11623

AMR: an “old” phenomenon



- discovered in mid 19th century
- more recently: epitaxial films (here, Fe)

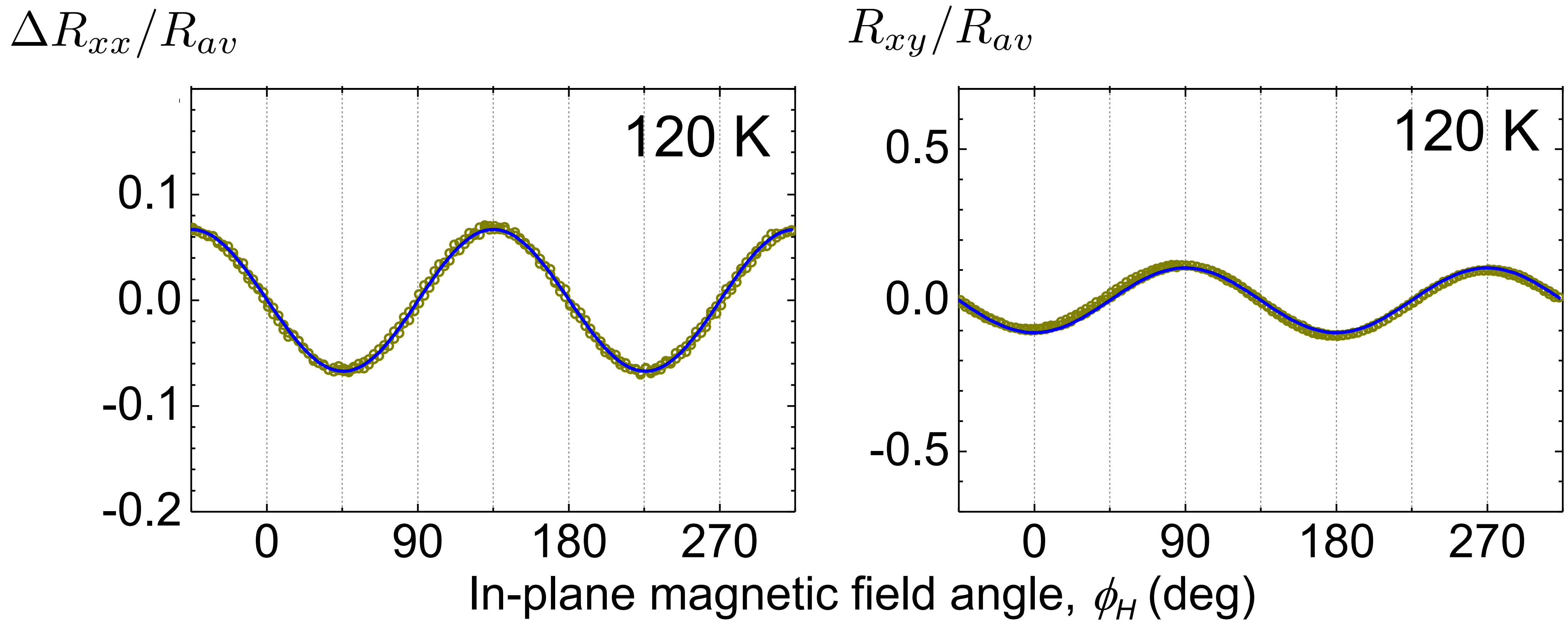
van Gorkom et al. ’01

doi: 10.1103/PhysRevB.63.134432

AMR: an “old” phenomenon - still explored

(Ga,Mn)As - ferromagnetic semiconductor, here ~10% Mn

longitudinal: $R_{\|}$ transversal: $R_{\perp}$

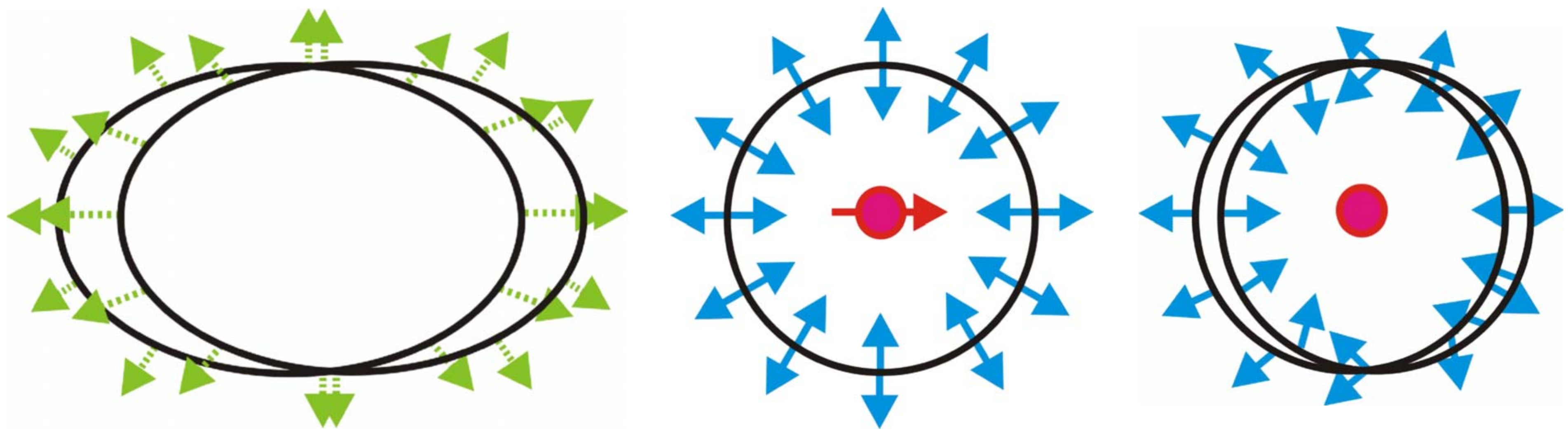


$\phi = \phi_H + \theta,\ \theta = 45^\circ$

Miyakozawa et al. ’16
10.1063/1.4944328

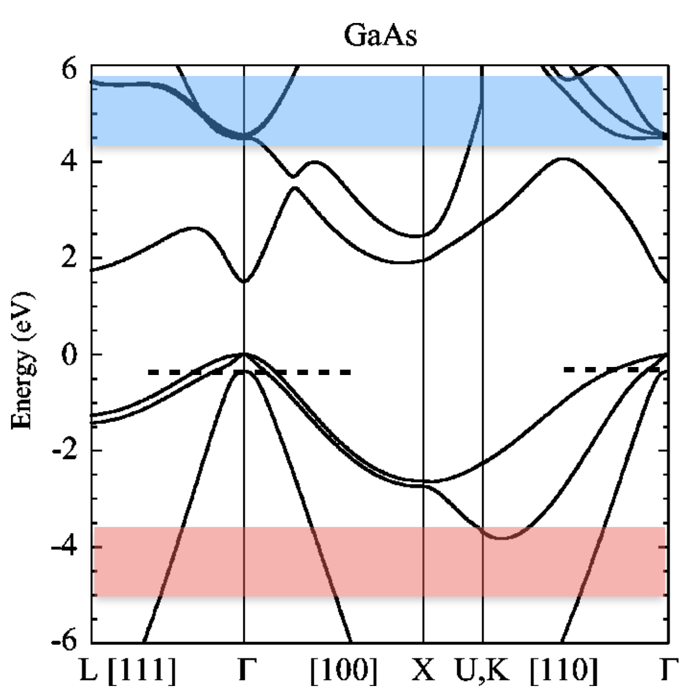
$$\Delta\rho_{xx}/\rho_0 = C_I \cos 2\phi \qquad \rho_{xy}/\rho_0 = C_I \sin 2\phi$$

AMR: the idea of analysis

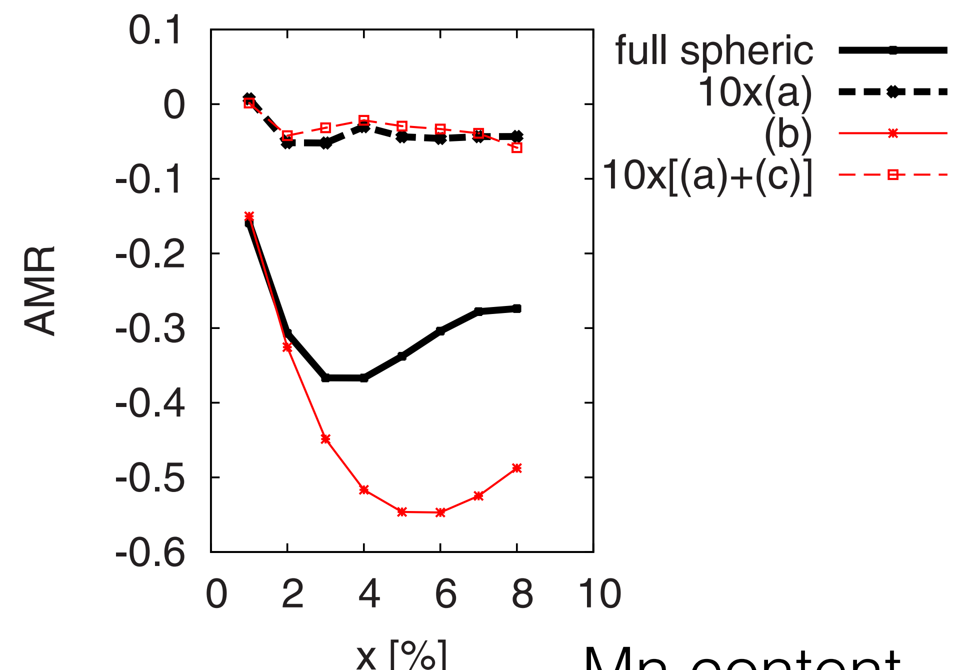


(a) (b) (c)

example: ferromagnetic (Ga,Mn)As



- Mn dopants: both magnetic and non-mag. char.
- VB: p-states of As
- Mn 3d states split the VB top



… Mn content

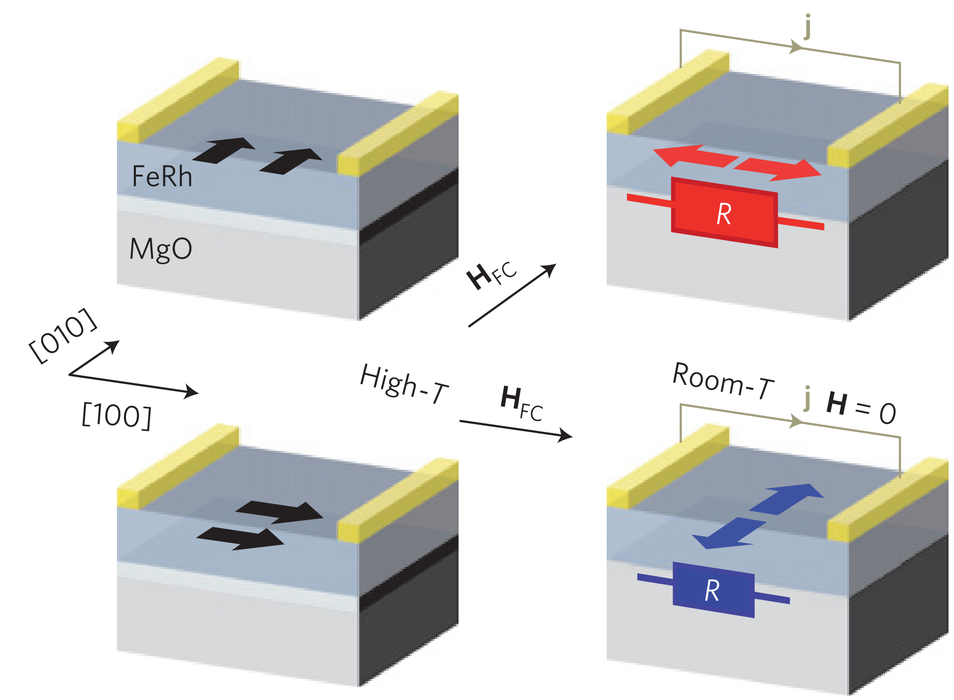
$$H = H_{KL} + (J_{pd}/\mu_B)\vec{M}\cdot\vec{s}$$

the humble myself et al. '09

doi: 10.1103/PhysRevB.80.165204

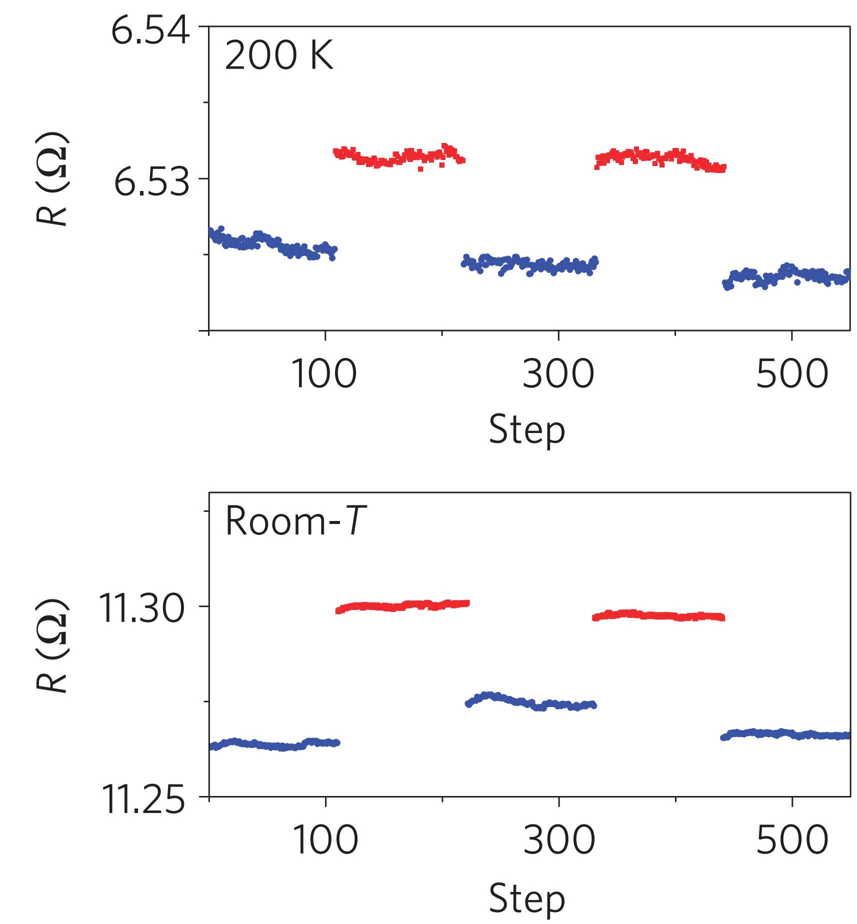
AMR: the new twist

AMR: the new twist antiferromagnets!



- AFM at low T, FM at higher T
- cool-down in magnetic field
- 'memory', read-out via AMR

Marti et al. '14
10.1038/nmat3861



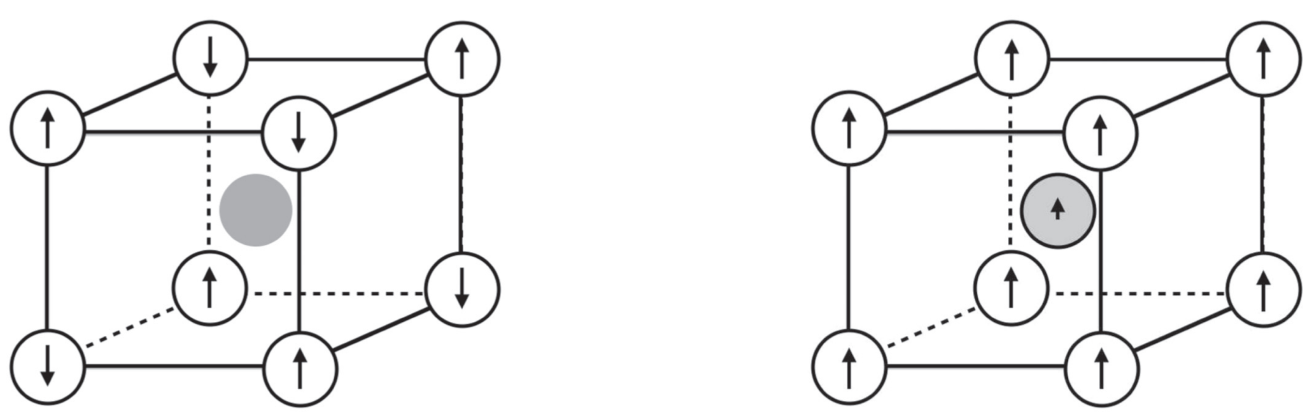
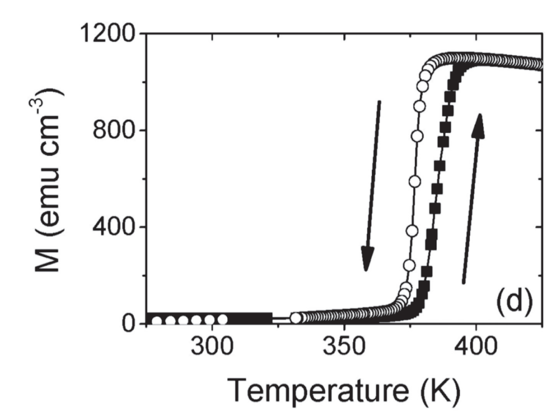


Figure 5. Structure of bulk FeRh. In the AF phase (left), the Rh atom (grey) has no magnetic moment while the Fe magnetic moments are ordered as indicated. Except for a different lattice constant (see text), the crystal structure remains unchanged in the FM phase (right); magnetic moment of the Rh atoms is then non-zero and parallel with that of Fe atoms.

FeRh



Saidl et al. '15
10.1088/1367-2630/18/8/083017

MnTe in hexagonal NiAs structure

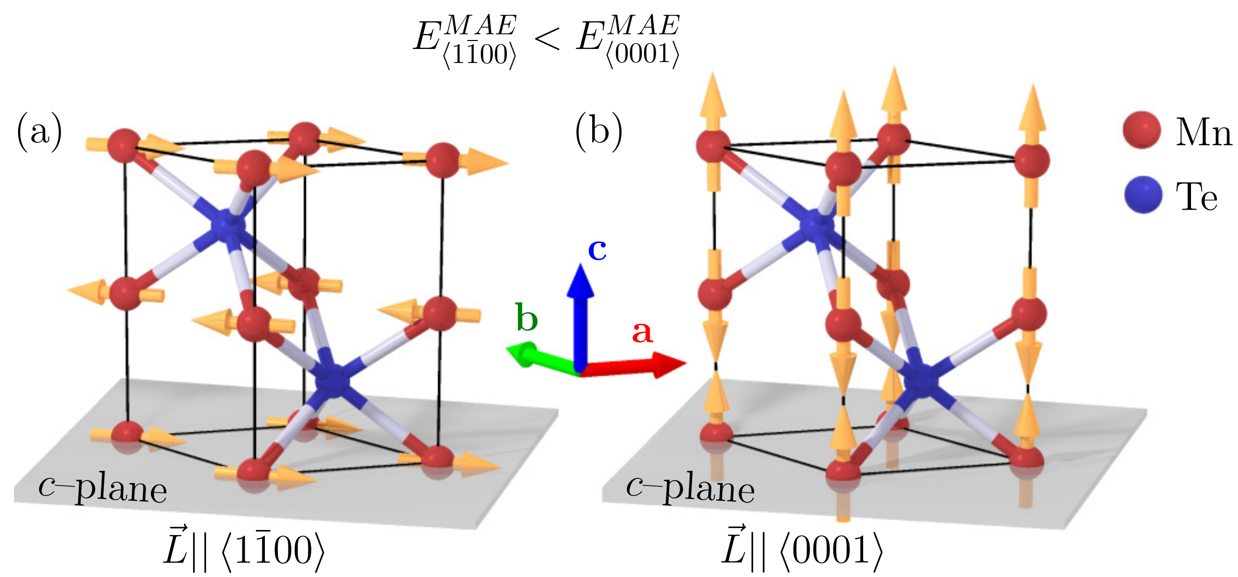
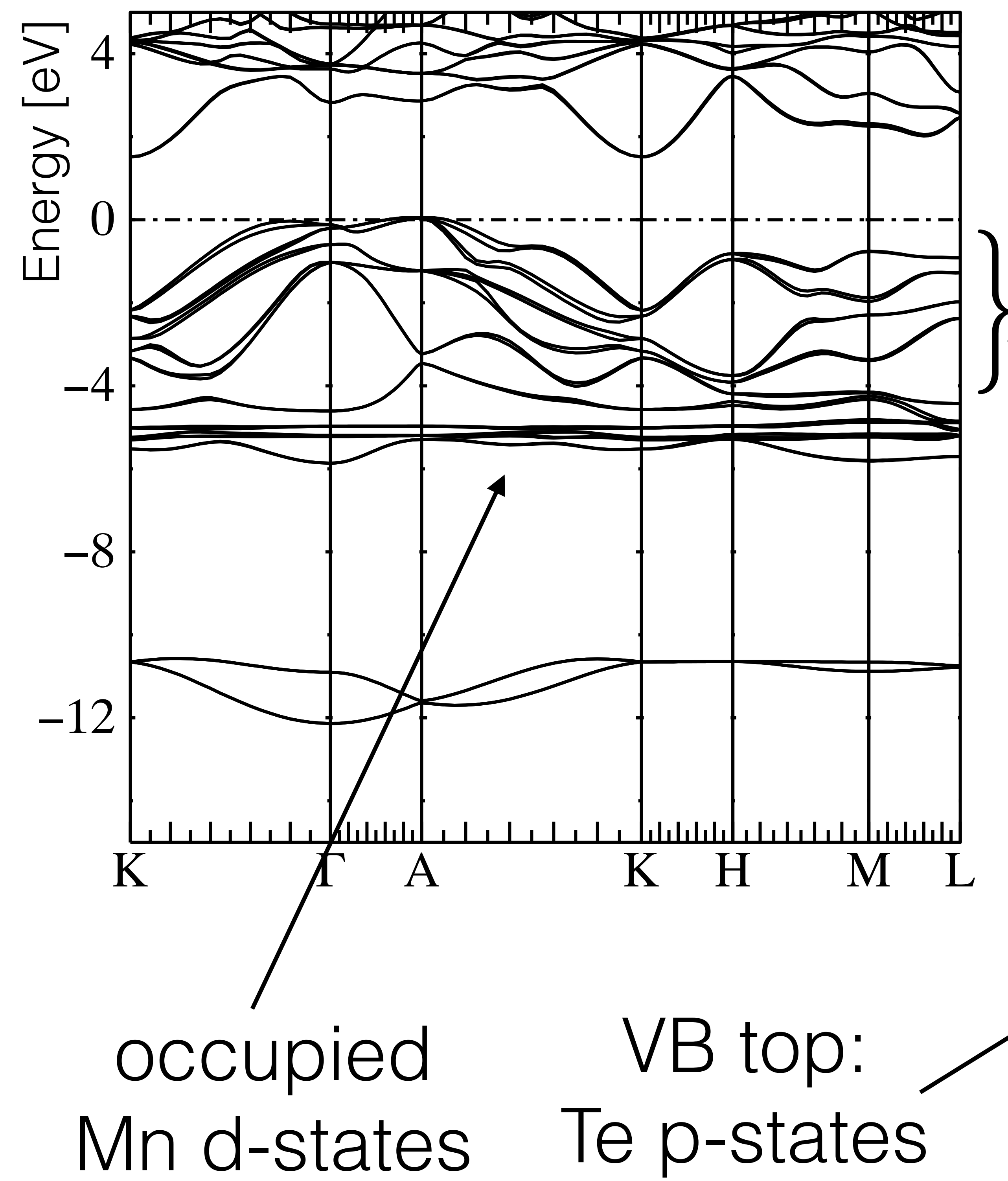
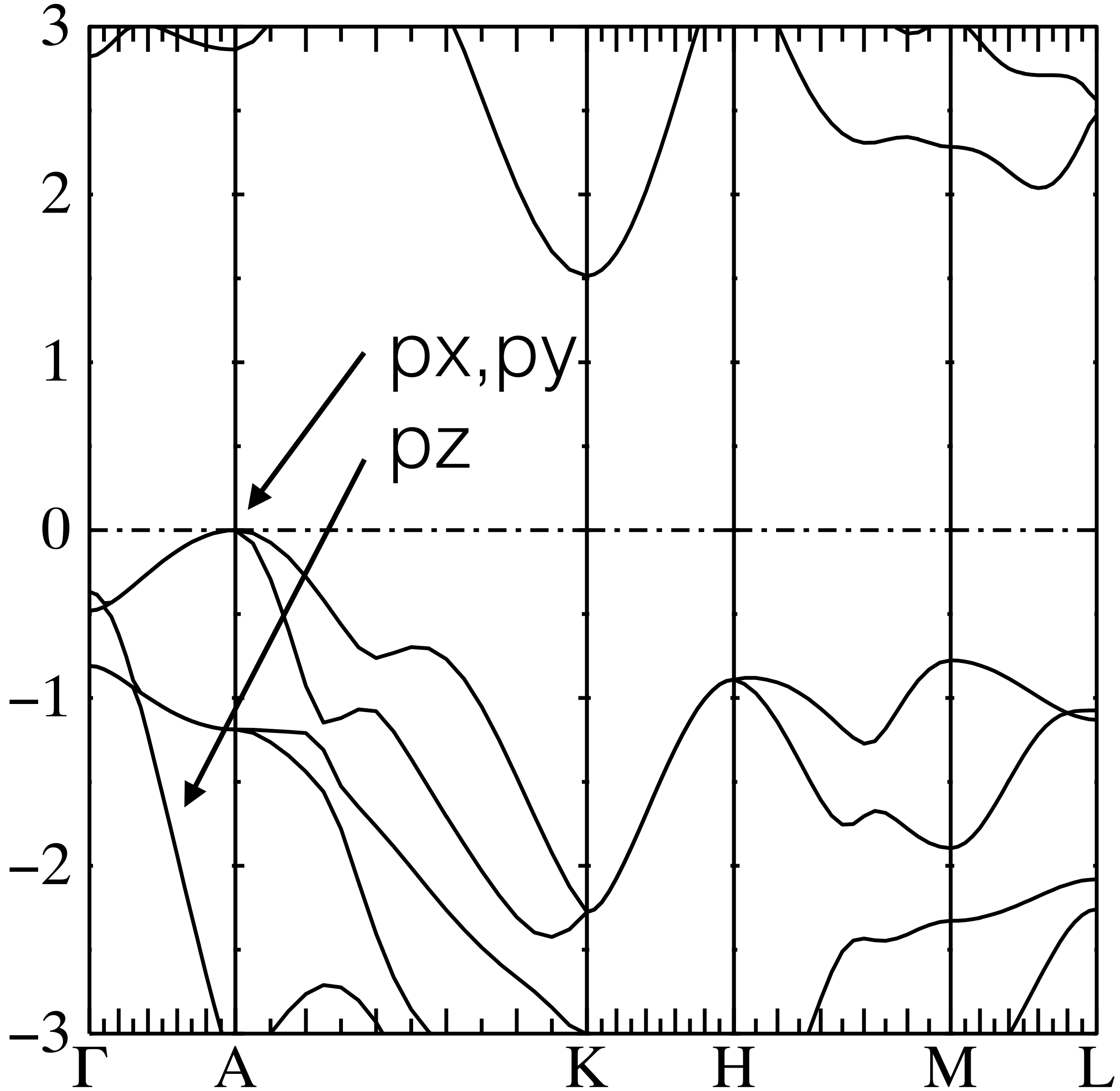


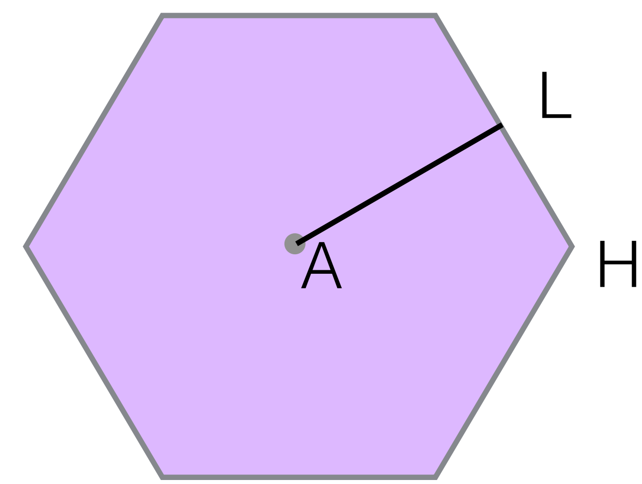
FIG. 1. Sketch of the atomic and possible magnetic structures of antiferromagnetic hexagonal MnTe. (a) In-plane/c plane (ground state) and (b) out-of-plane/c-axis (hard axis) orientation of the magnetic moments of Mn with the Néel vector $\vec{L}$ along $\langle 1\bar{1}00\rangle$ and $\langle 0001\rangle$ are shown. The hexagonal basal plane, i.e., the c plane is indicated by a gray plane, while red, green, and blue arrows show the directions of the unit cell axes.

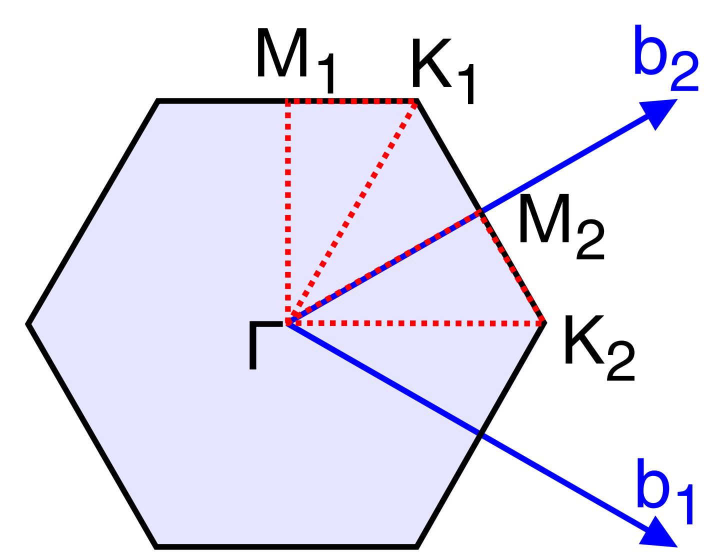


detail of the VB (no SO)



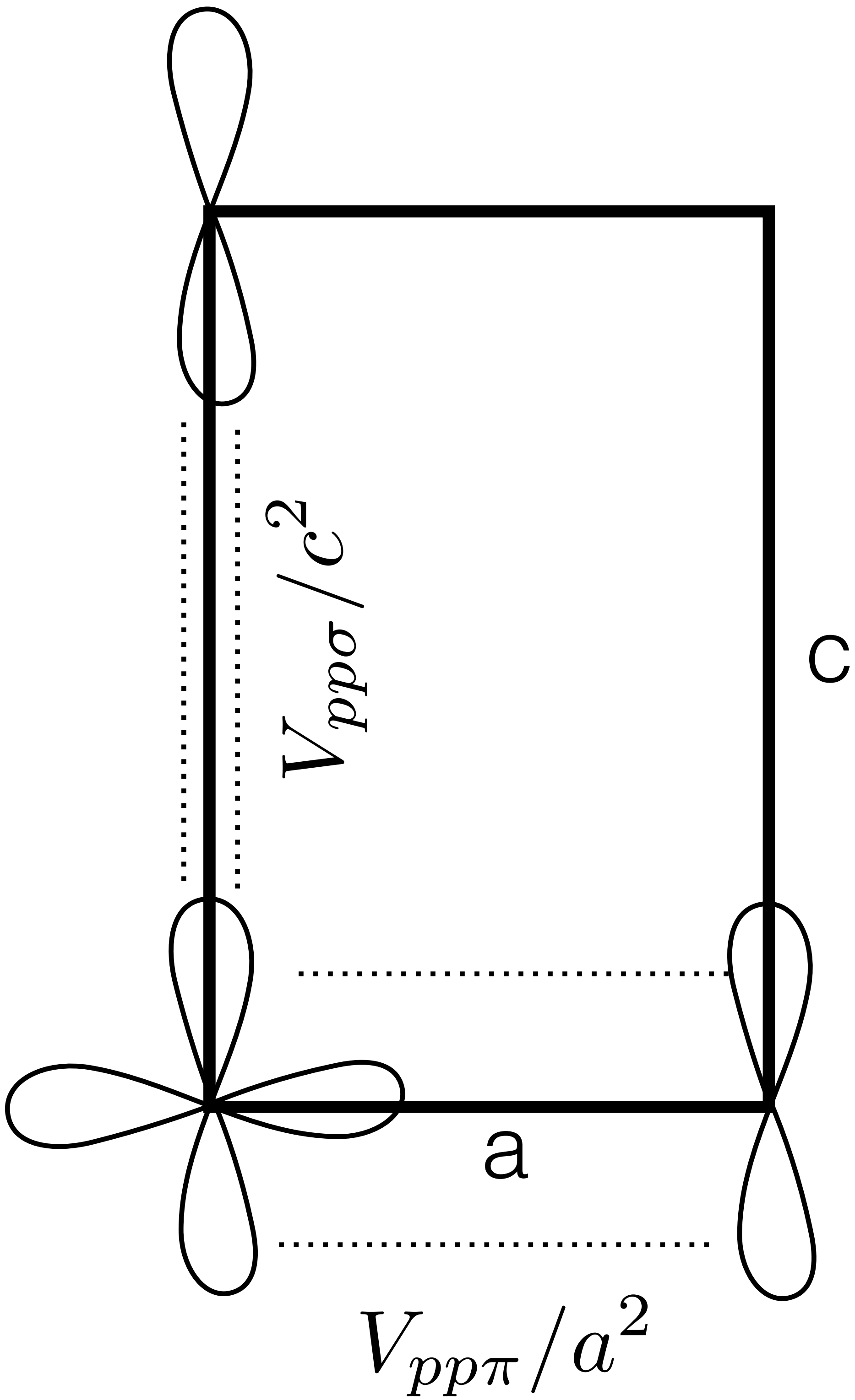
- warping in kx,ky plane neglected
- d=0 for simplicity (warping away from kz=0)





$$H=\frac{\hbar^2}{2m_0}\left[\begin{array}{cc} ak_x^2+bk_y^2+ck_z^2+dk_yk_z & (a-b)\,k_xk_y+dk_xk_z \\ (a-b)\,k_xk_y+dk_xk_z & bk_x^2+ak_y^2+ck_z^2-dk_yk_z \end{array}\right]$$

competing maxima at the VB top: the idea

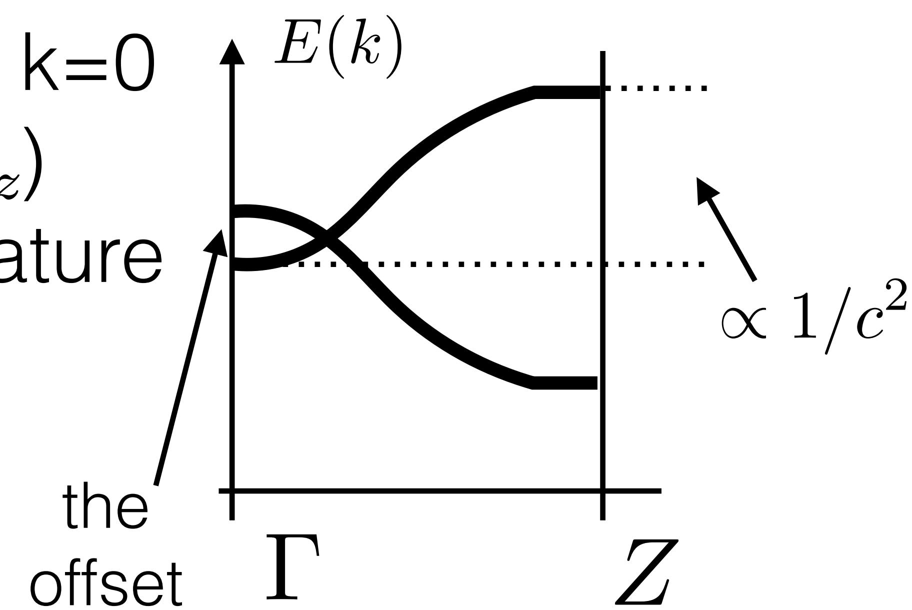


$$H = \begin{pmatrix} E_X & 0 \\ 0 & E_Z \end{pmatrix}$$

$$E_X = \frac{2V_{pp\pi}}{a^2}\cos ak_x + \frac{2V_{pp\sigma}}{c^2}\cos ck_z$$

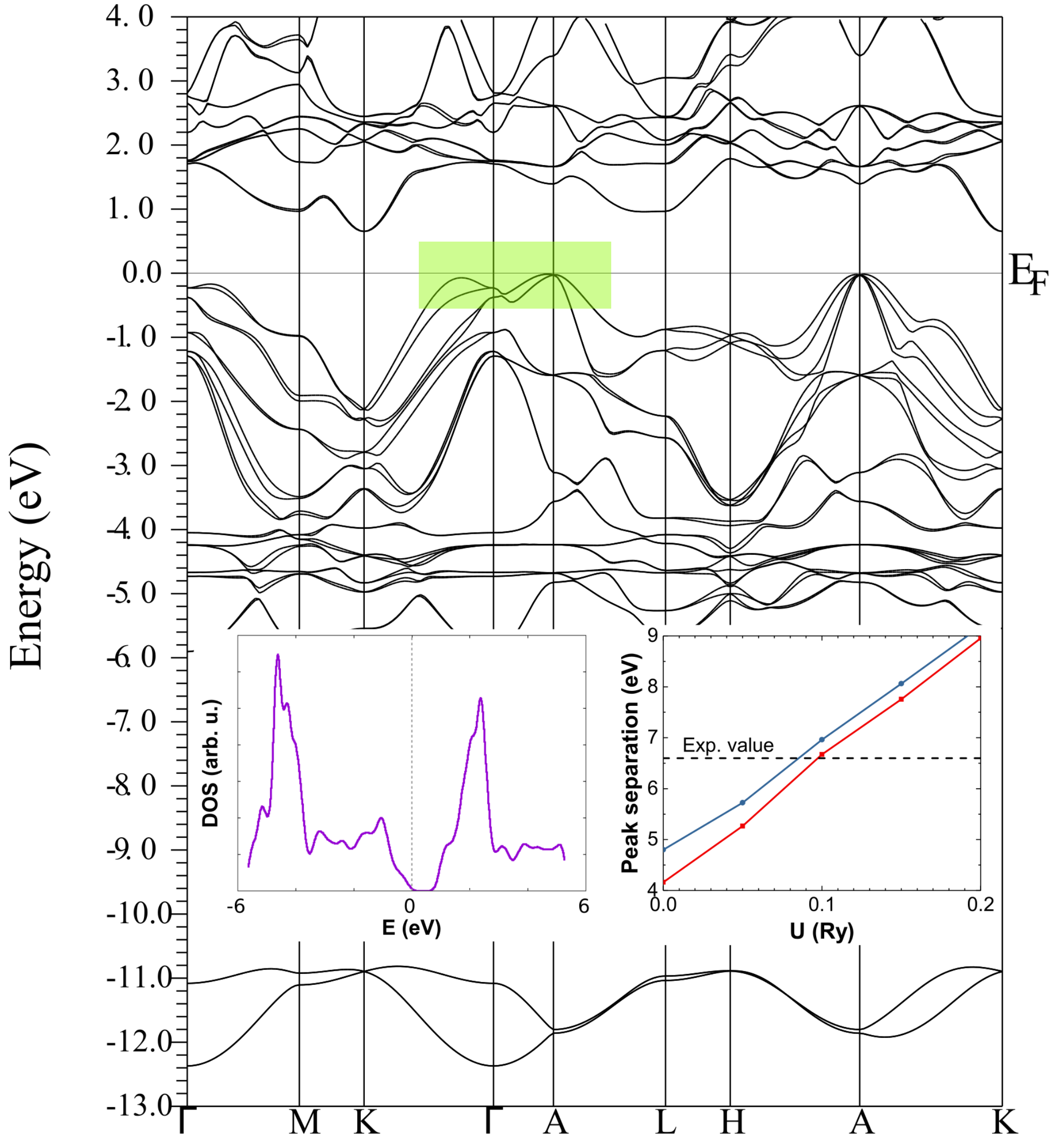
$$E_Z = \frac{2V_{pp\sigma}}{a^2}\cos ak_x + \frac{2V_{pp\pi}}{c^2}\cos ck_z + \Delta_z$$

- degenerate at k=0 for a=c (negl. Δ_z)
- opposite curvature for $V_{pp\sigma}V_{pp\pi} < 0$

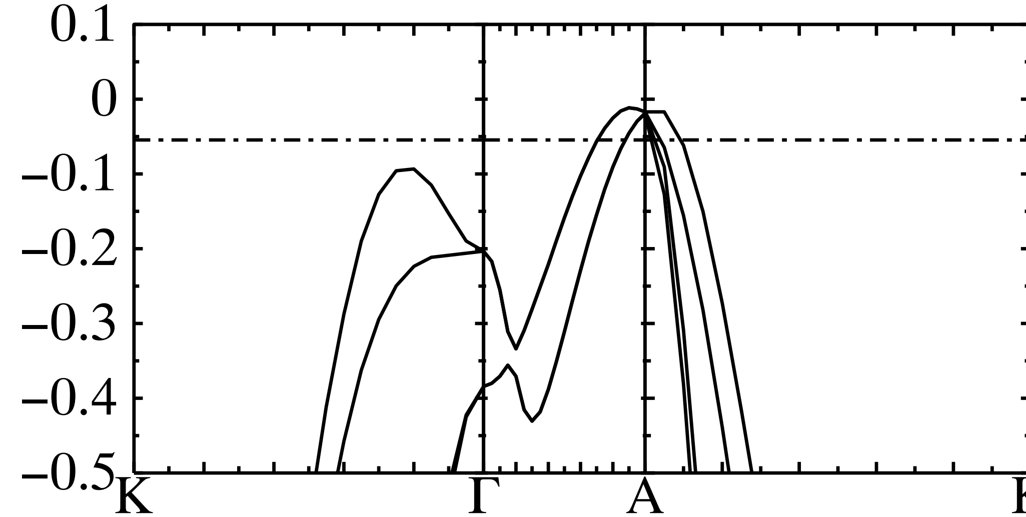


competing maxima at the VB top: *ab initio*

DFT+U



GW



type	a/c	position of max.
Ref. [1]	0.409/0.643	
bulk	0.414/0.671	around A
SrF_2 LT	0.4135/0.6655	around A
SrF_2 RT	0.4148/0.672	around A
InP RT	0.417/0.669	VBM1≈VBM2
InP LT	0.417/0.660	Γ-K line

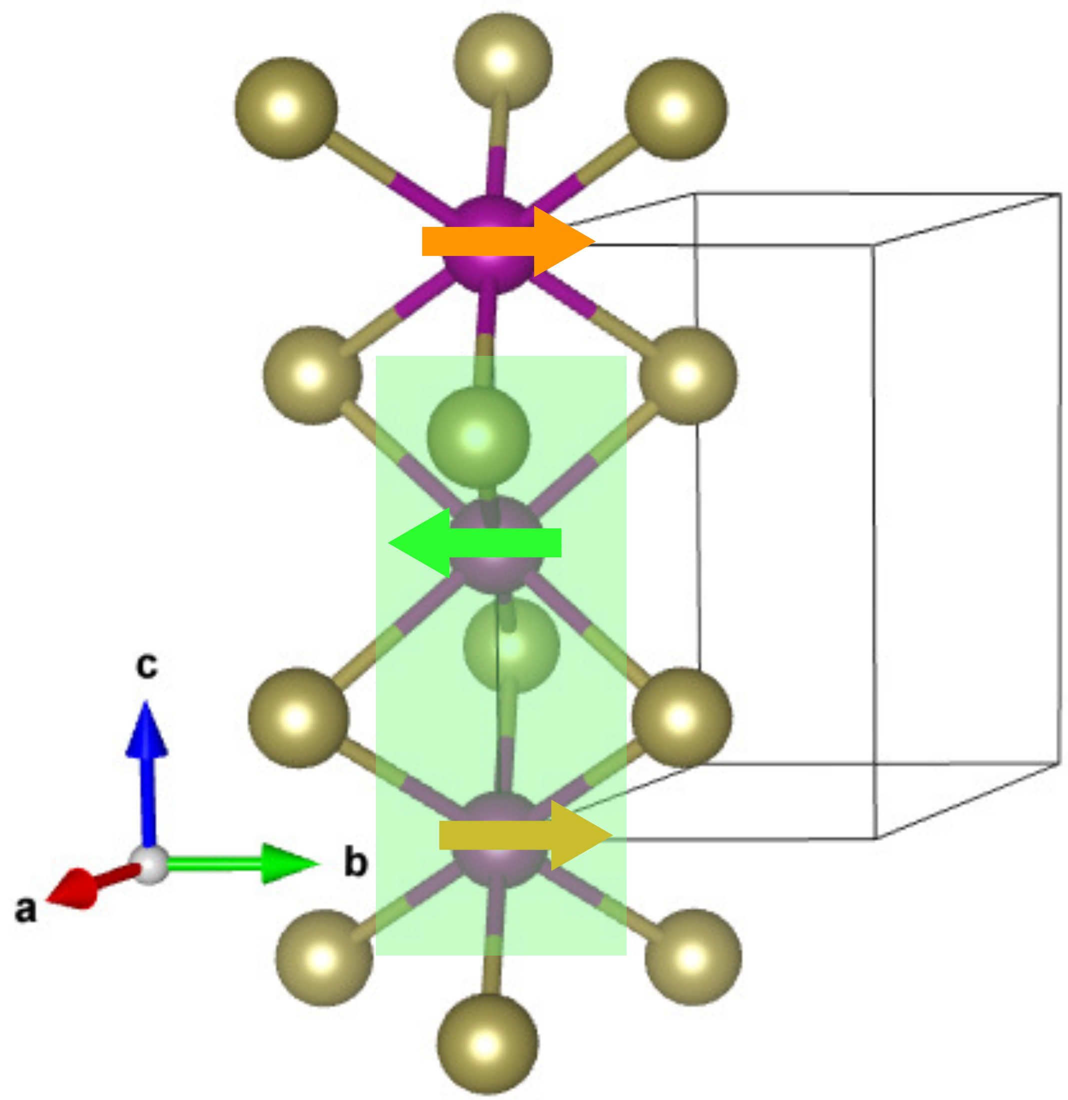
how to deal with exchange

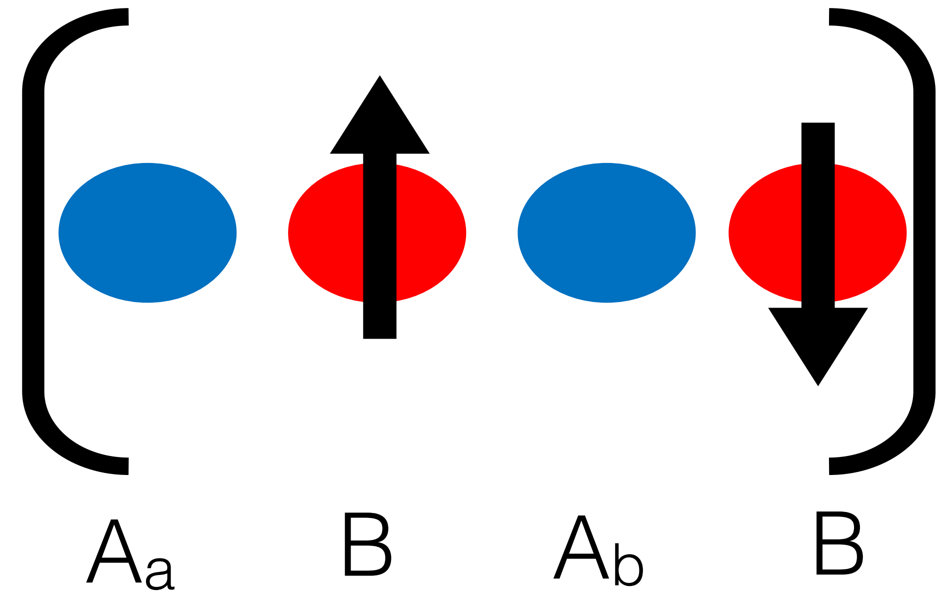
ferromagnetic semiconductor

$$H = H_{KL} + (J_{pd}/\mu_B)\vec{M} \cdot \vec{s}$$

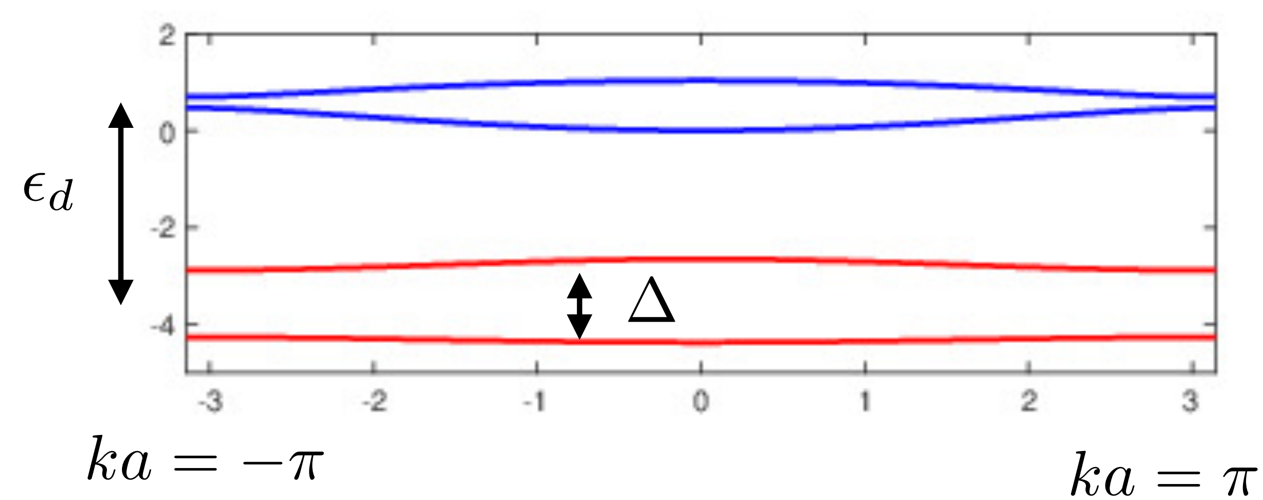
but in an antiferromagnet???

how to deal with exchange - a toy model

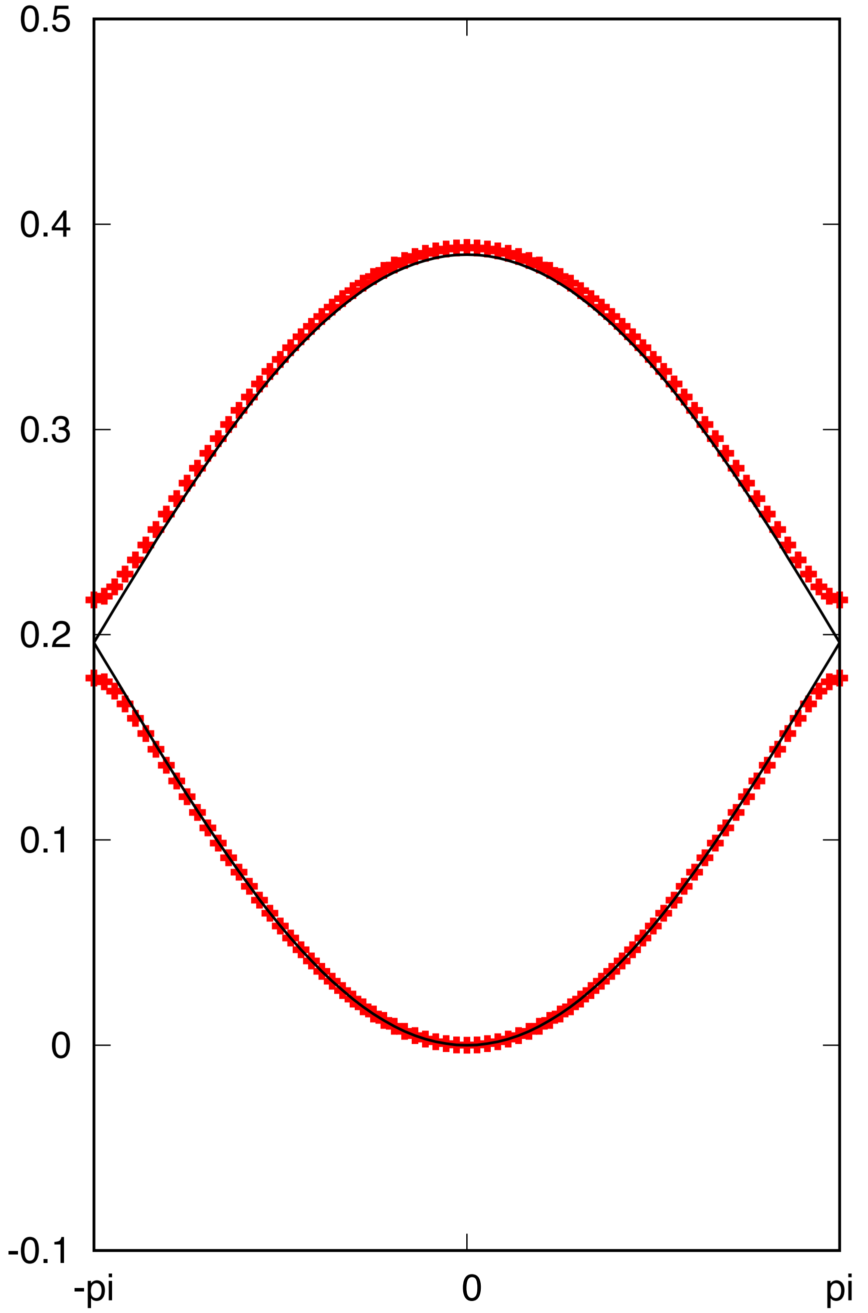




$$H = \begin{pmatrix} 0 & t & 0 & te^{-ika} \\ t & \epsilon_d + \Delta & t & 0 \\ 0 & t & 0 & t \\ te^{ika} & 0 & t & \epsilon_d - \Delta \end{pmatrix}$$

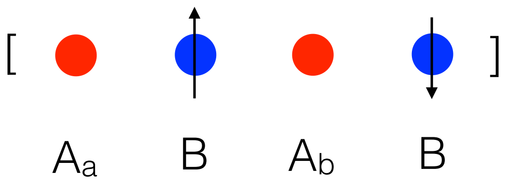


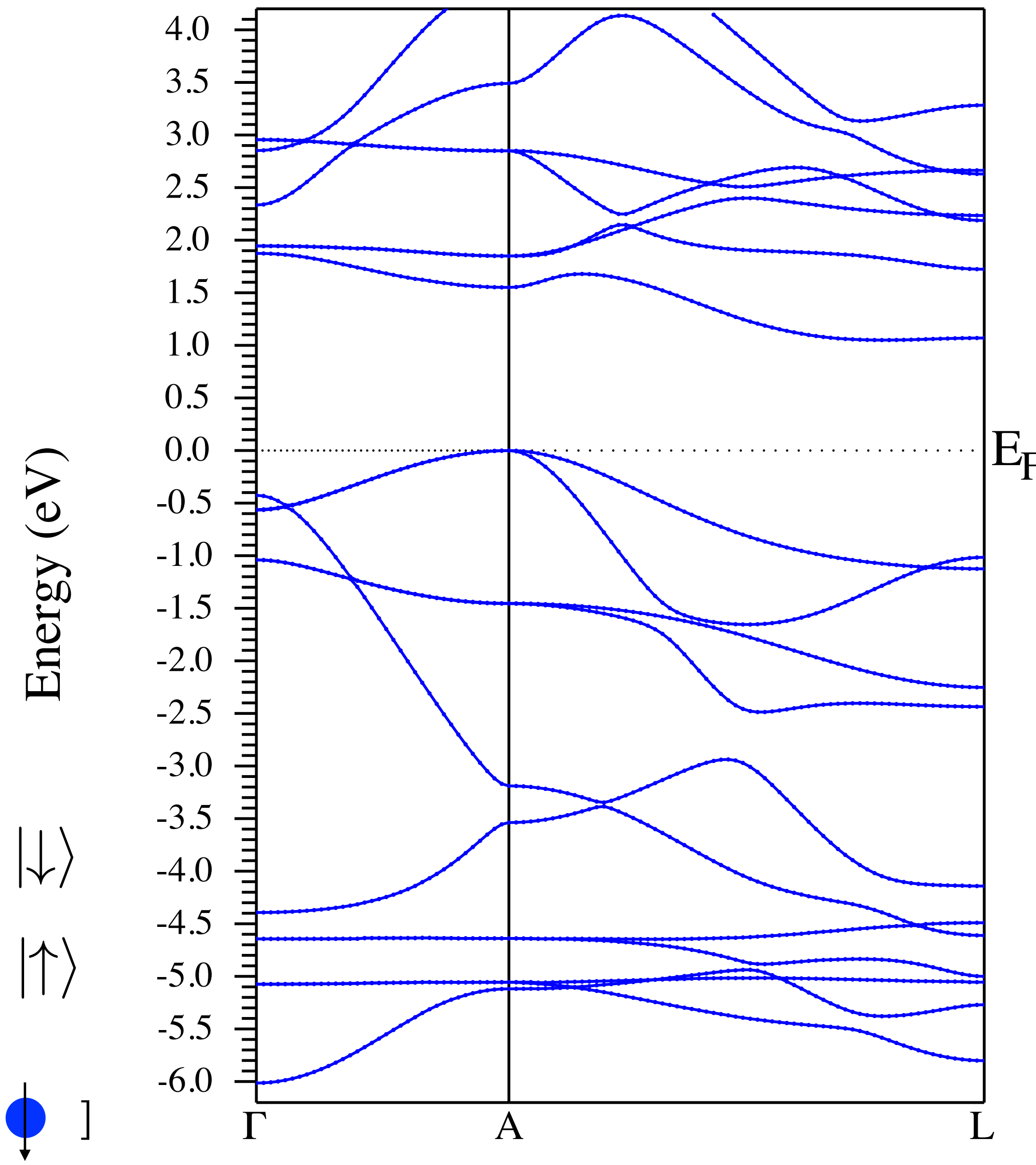
how to deal with exchange - a toy model wavefunctions



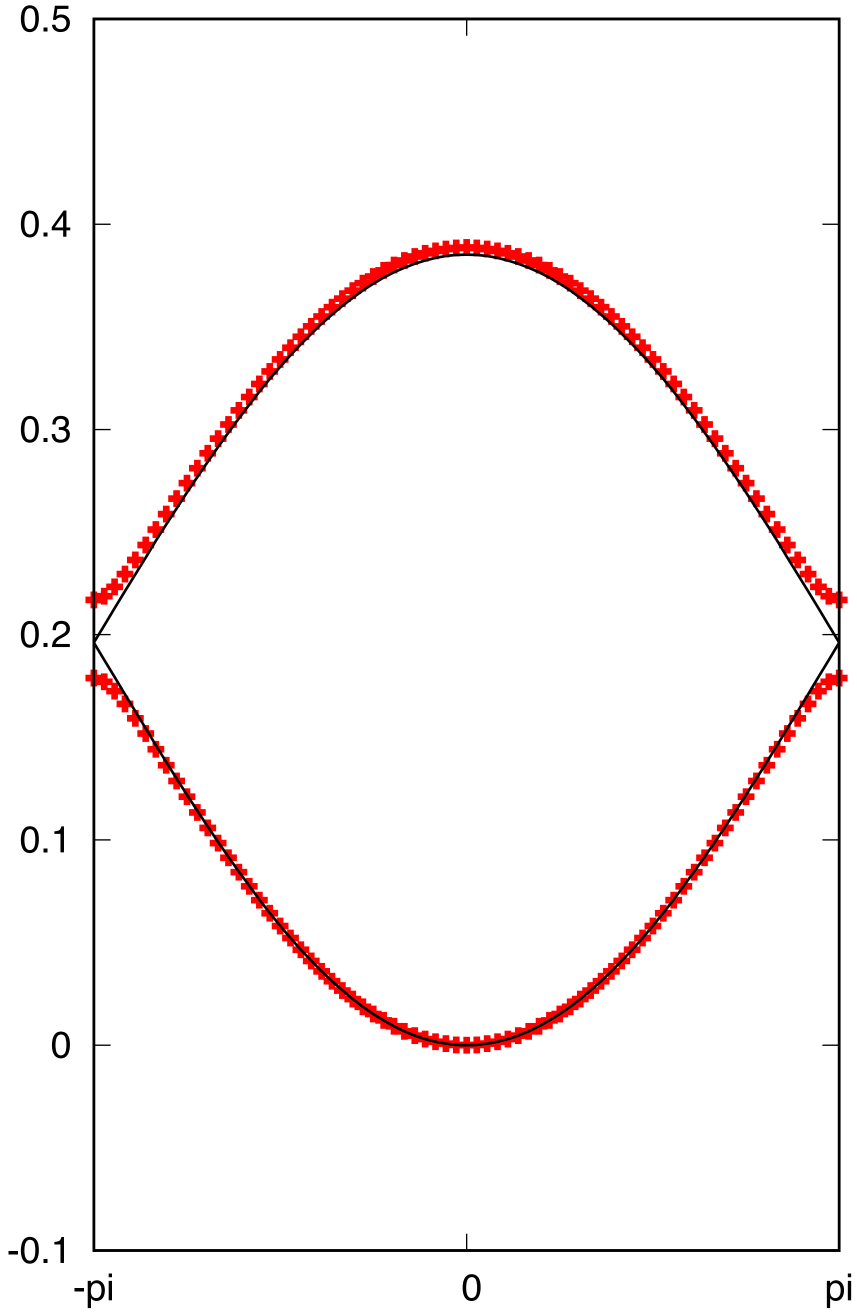
$$(|a\rangle - |b\rangle) \otimes |\downarrow\rangle$$

$$(|a\rangle + |b\rangle) \otimes |\uparrow\rangle$$



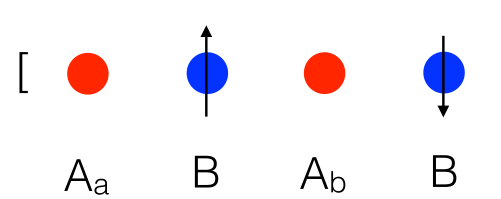


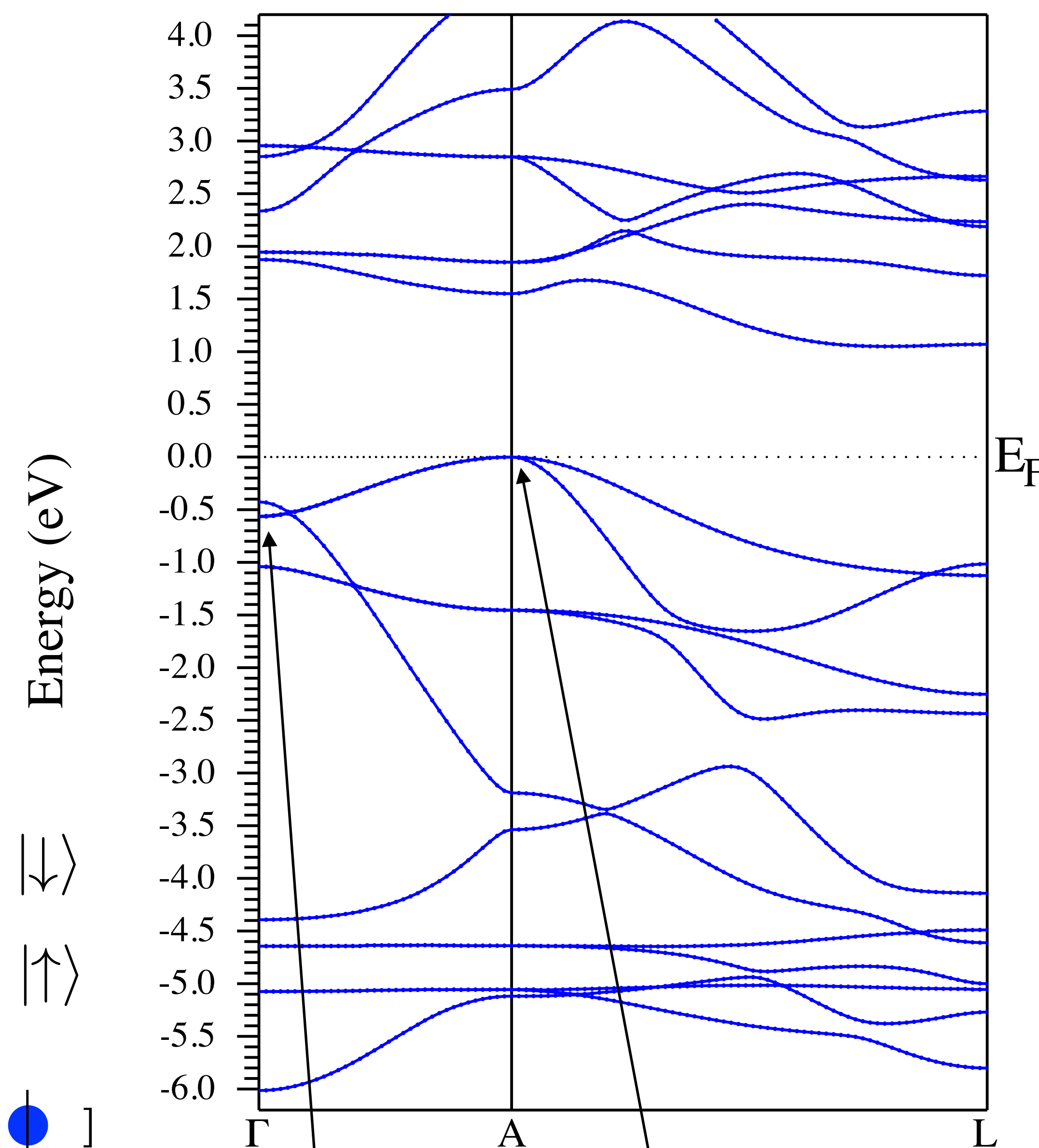
how to deal with exchange - a toy model
wavefunctions

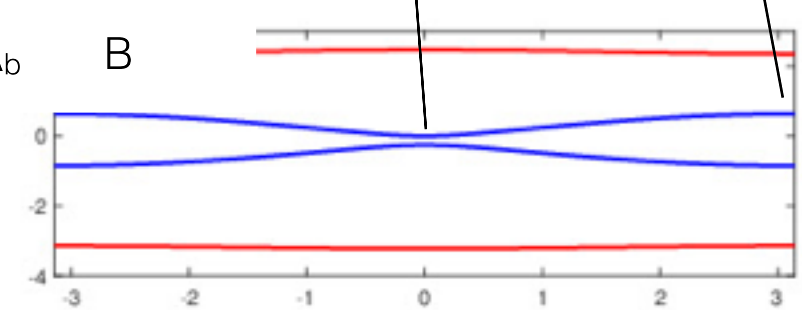


$$(|a\rangle - |b\rangle) \otimes |\downarrow\rangle$$

$$(|a\rangle + |b\rangle) \otimes |\uparrow\rangle$$







$$\Delta > \epsilon_d$$

$$H = H_b + H_{so} + H_{ex}$$

changed to

$$H = H_{be} + H_{so}$$

& matrix els. of H_{so} recalculated

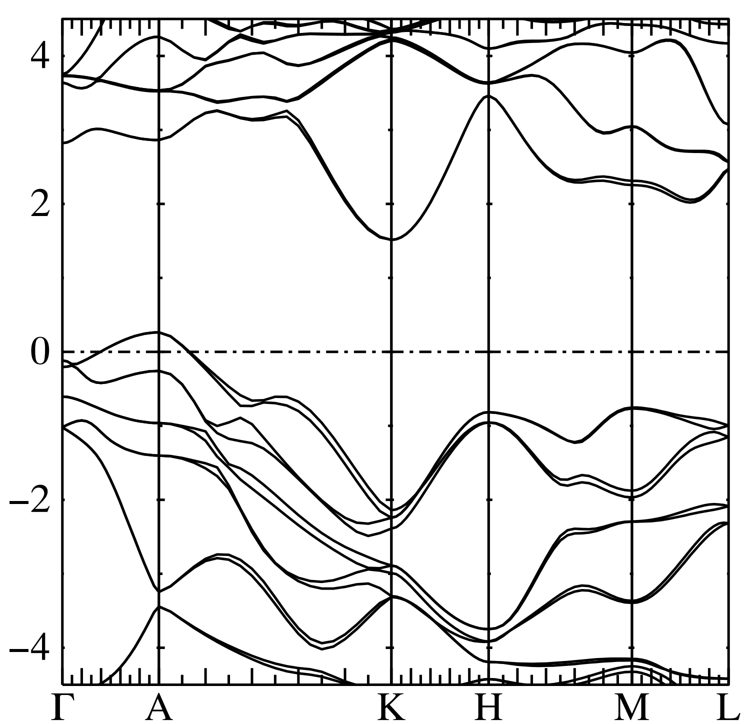
$$H = H_b + H_{so} + H_{ex}$$

changed to

$$H = H_{be} + H_{so}$$

detail of the VB - effect of spin-orbit (SO) int.
(zero order eff.)

$\vec{m}_{1,2} \parallel \hat{z}$

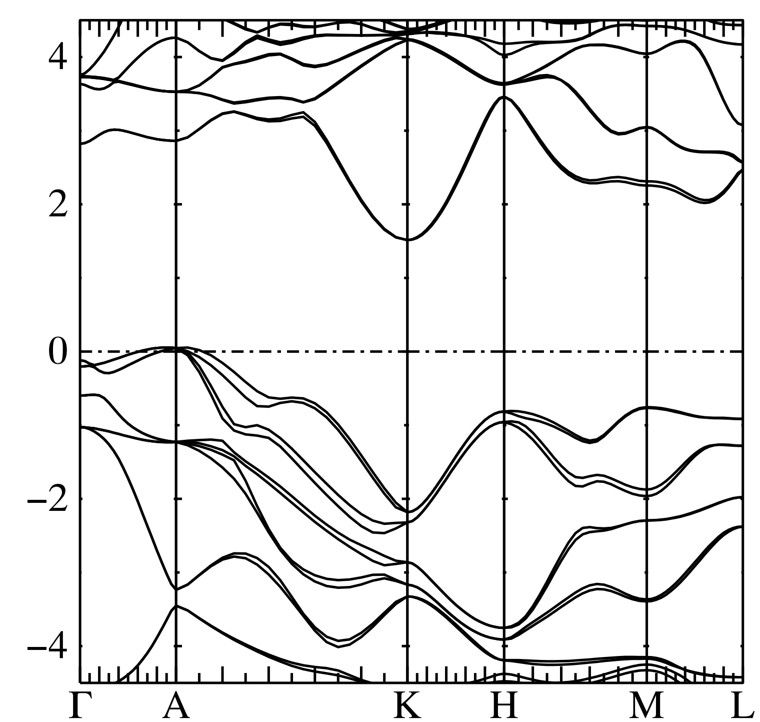


$$H_{so} = \lambda \vec{S} \cdot \vec{L}$$

$$H_{so} = \begin{pmatrix} 0 & i\lambda \\ -i\lambda & 0 \end{pmatrix}$$

$$H_{so} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\vec{m}_{1,2} \parallel \hat{x}$



detail of the VB - effect of spin-orbit (SO) int. (zero order eff.)

$$\vec{m}_{1,2} \parallel \hat{z}$$

$$H_{be} = \begin{pmatrix} ak_x^2 & 0 & 0 \\ 0 & bk_x^2 & 0 \\ 0 & 0 & \epsilon_z \end{pmatrix}$$

$$\vec{m}_{1,2} \parallel \hat{x}$$

$$H_{so} = \begin{pmatrix} 0 & i\lambda & 0 \\ -i\lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$H_{so} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i\lambda \\ 0 & -i\lambda & 0 \end{pmatrix}$$

$$\pm\lambda, \epsilon_z$$

$$0, \lambda^2/\epsilon_z, \epsilon_z - \lambda^2/\epsilon_z$$

~ 1 eV

~ 1 meV

$$H_{so} = \Delta_z S_z L_z + \Delta_{xy}(S_x L_x + S_y L_y)$$

$$2\Delta_z$$

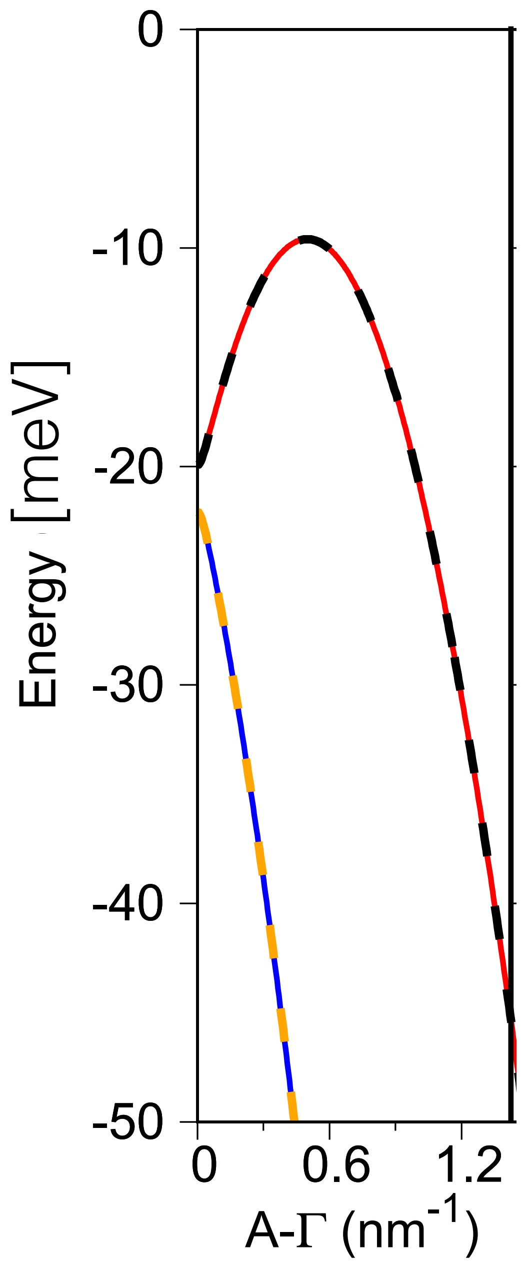
$$\Delta_{xy}^2/\epsilon_z$$

$$\Delta_z \approx 0.27 \text{ eV}$$

$$\Delta_{xy} \approx 0.06 \text{ eV}$$

detail of the VB - effect of spin-orbit (SO) int.
(next order eff.?)

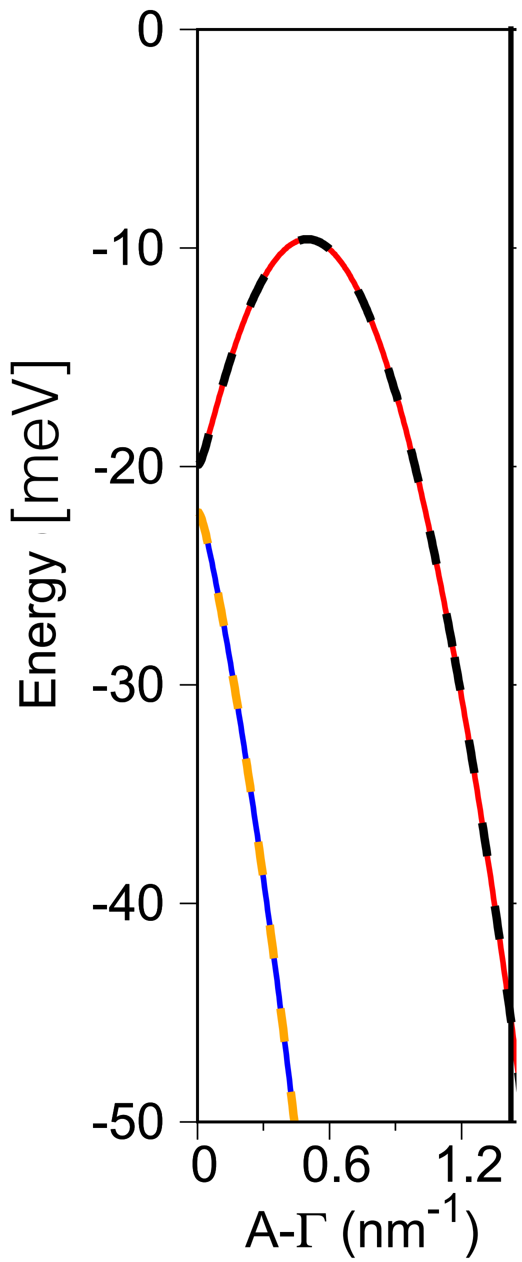
splitting along
$A-\Gamma$ line



similar to Rashba?

detail of the VB - effect of spin-orbit (SO) int. (first order eff.)

splitting along $A - \Gamma$ line



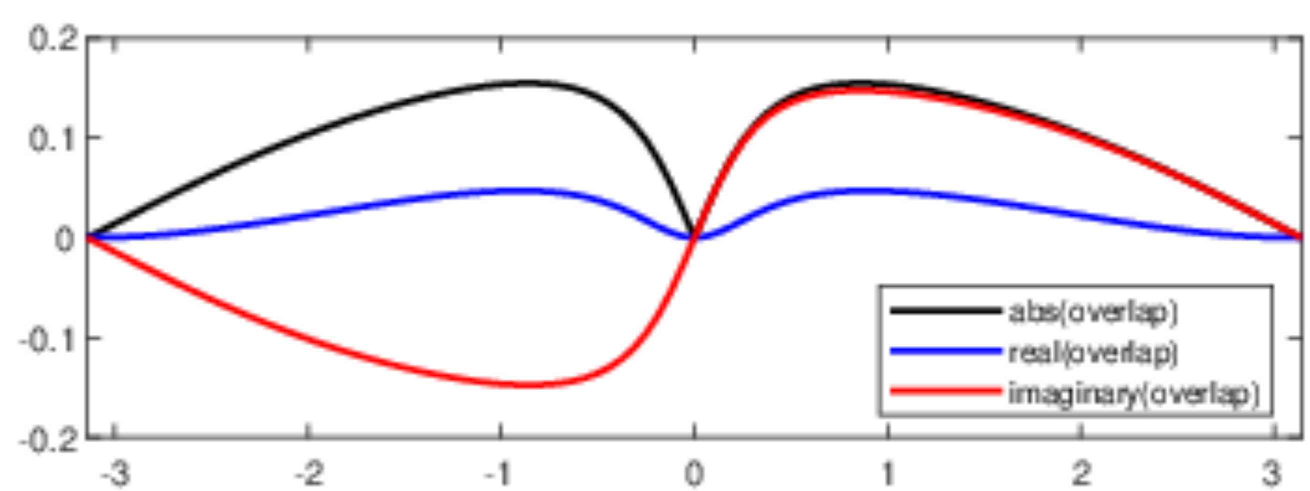
block structure

$(|a\rangle + |b\rangle) \otimes |\uparrow\rangle \qquad (|a\rangle - |b\rangle) \otimes |\downarrow\rangle$

$$\begin{pmatrix} ak_x^2 + bk_y^2 + ck_z^2 & x & & \\ x & ak_y^2 + bk_x^2 + ck_z^2 & & \\ & & ak_x^2 + bk_y^2 + ck_z^2 & x \\ & & x & ak_y^2 + bk_x^2 + ck_z^2 \end{pmatrix}$$

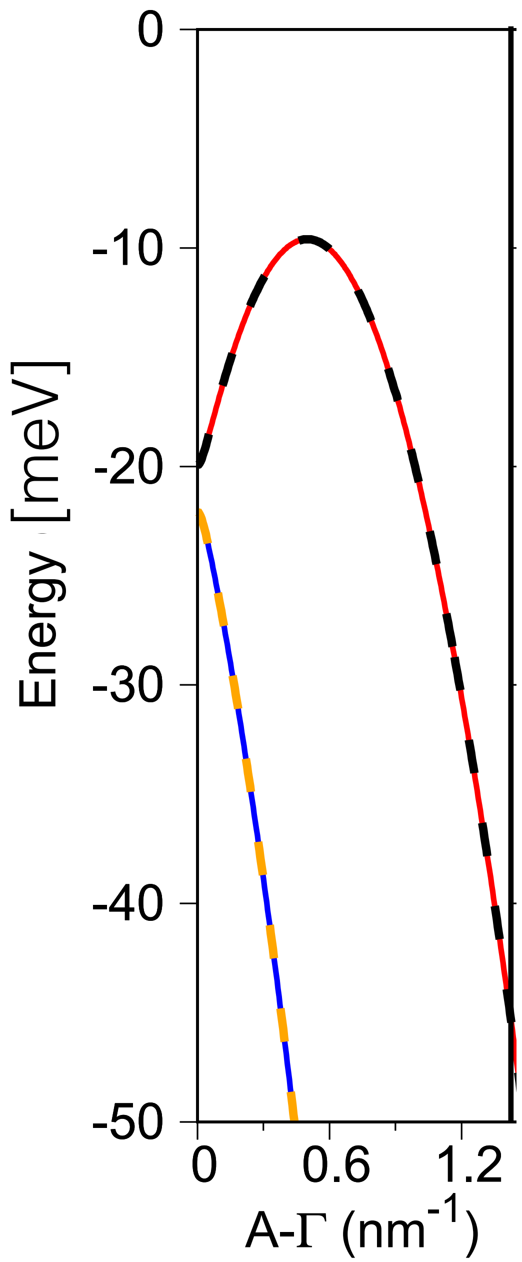
$$\begin{pmatrix} & x & & it\Delta_z \\ x & & -it\Delta_z & \\ & it\Delta_z & & x \\ -it\Delta_z & & x & \end{pmatrix}$$

overlaps in the toy model



detail of the VB - effect of spin-orbit (SO) int. (first order eff.)

splitting along $A-\Gamma$ line



state 1

$$(|a\rangle + |b\rangle) \otimes |\uparrow\rangle$$

state 2

$$(|a\rangle - |b\rangle) \otimes |\downarrow\rangle$$

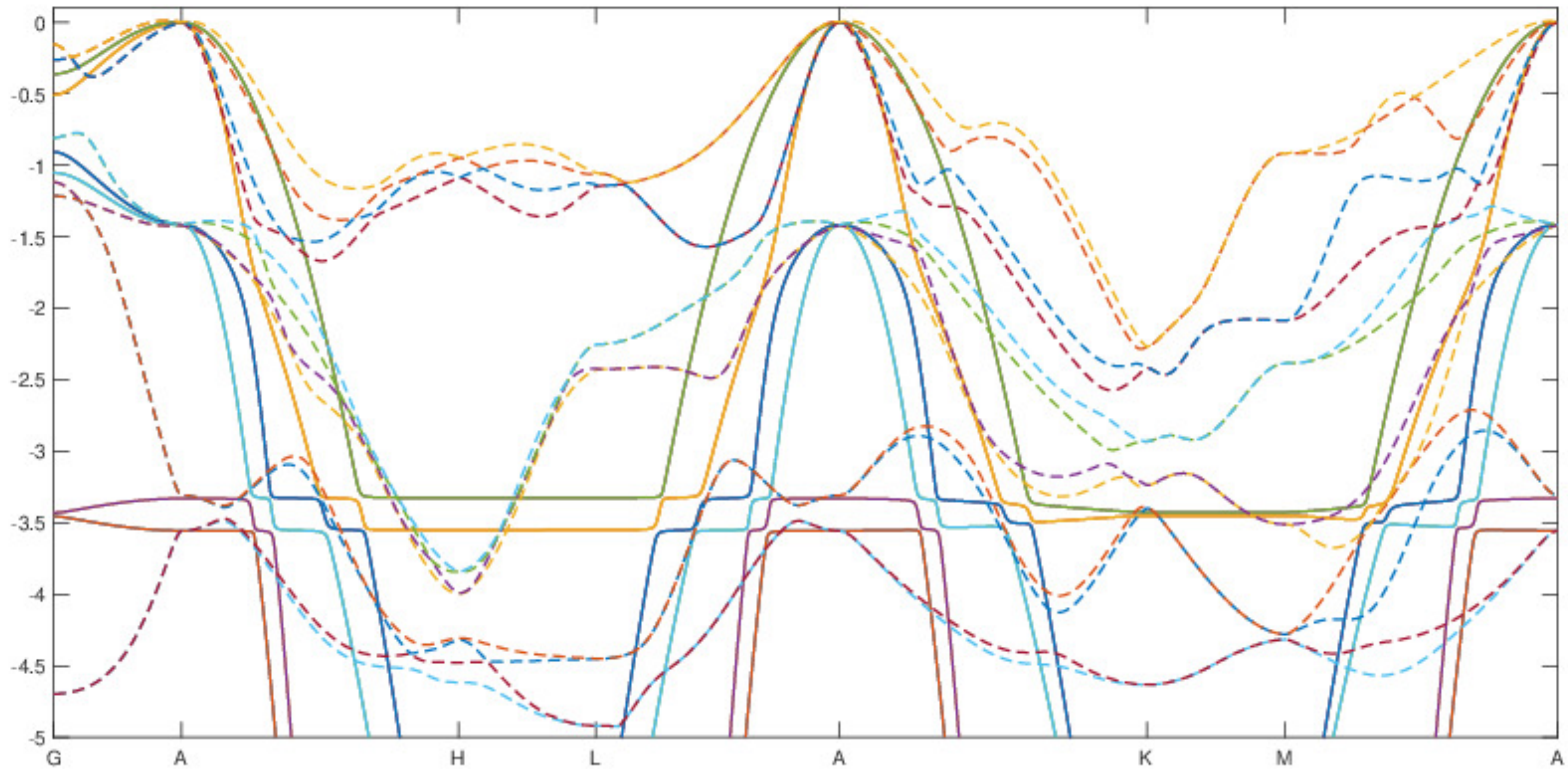
$$H_{be} = \begin{pmatrix} ak_x^2 + bk_y^2 + ck_z^2 & x & 0 & & & \\ x & bk_x^2 + ak_x^2 + ck_z^2 & 0 & & & \\ 0 & 0 & \epsilon_z & & & \\ & & & ak_x^2 + bk_y^2 + ck_z^2 & x & 0 \\ & & & x & bk_x^2 + ak_x^2 + ck_z^2 & 0 \\ & & & 0 & 0 & \epsilon_z \end{pmatrix}$$

$$\vec{m}_{1,2} \parallel \hat{x}$$

$$H_{so} = \begin{pmatrix} & & & 0 & it\Delta_z & t\Delta_{xy} \\ & & -i\Delta_{xy} & -it\Delta_z & 0 & 0 \\ & i\Delta_{xy} & & -t\Delta_{xy} & 0 & 0 \\ 0 & it\Delta_z & -t\Delta_{xy} & & & \\ -it\Delta_z & 0 & 0 & & & i\Delta_{xy} \\ t\Delta_{xy} & 0 & 0 & & -i\Delta_{xy} & \end{pmatrix}$$

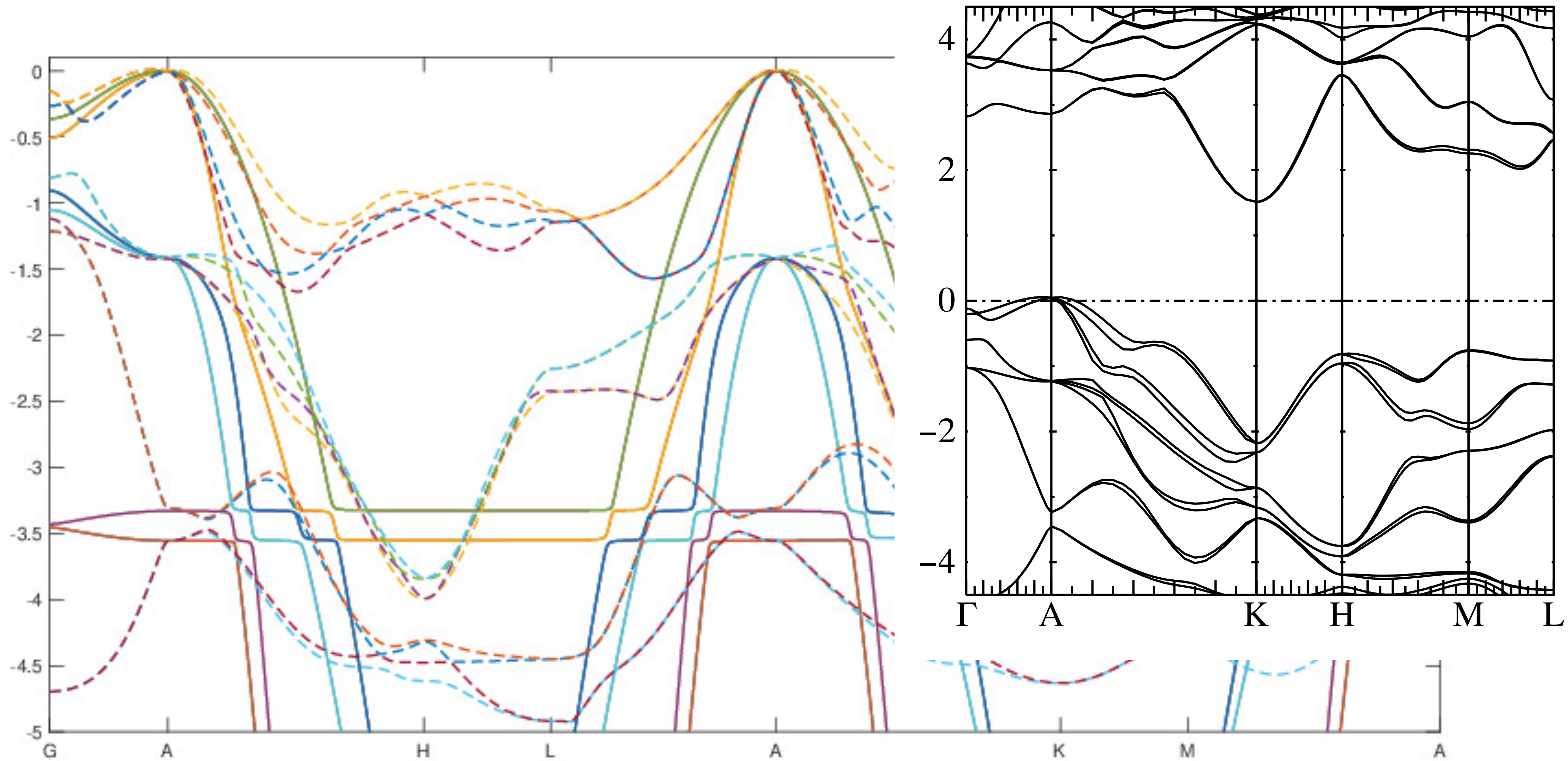
$$t = \langle 1|2\rangle \propto k_z$$

More realistic toy model: 12 bands



- based on toy model (4 atoms)
- downfolded to two Te atoms
- 3 orbitals (x,y,z)
- 2 spins, incl. SO

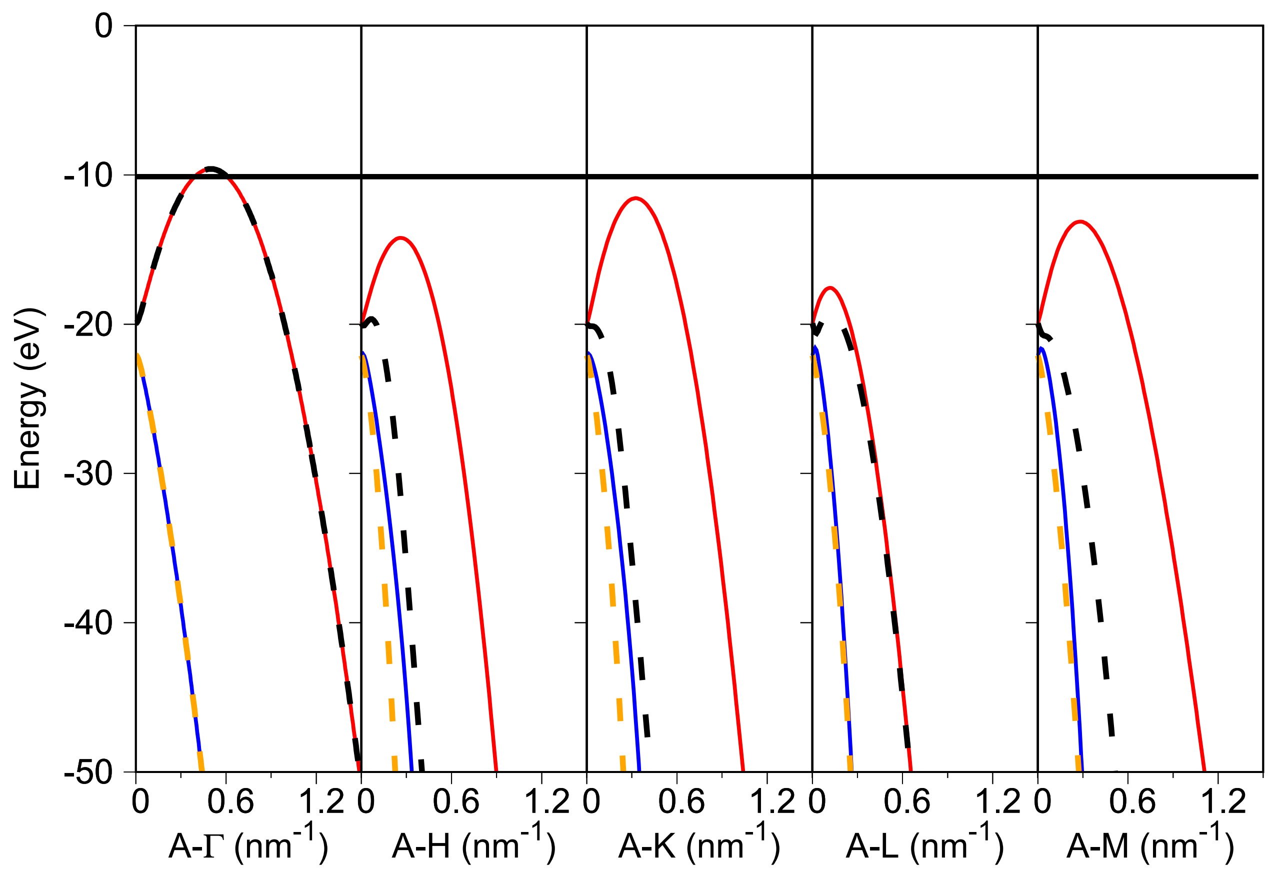
More realistic toy model: 12 bands

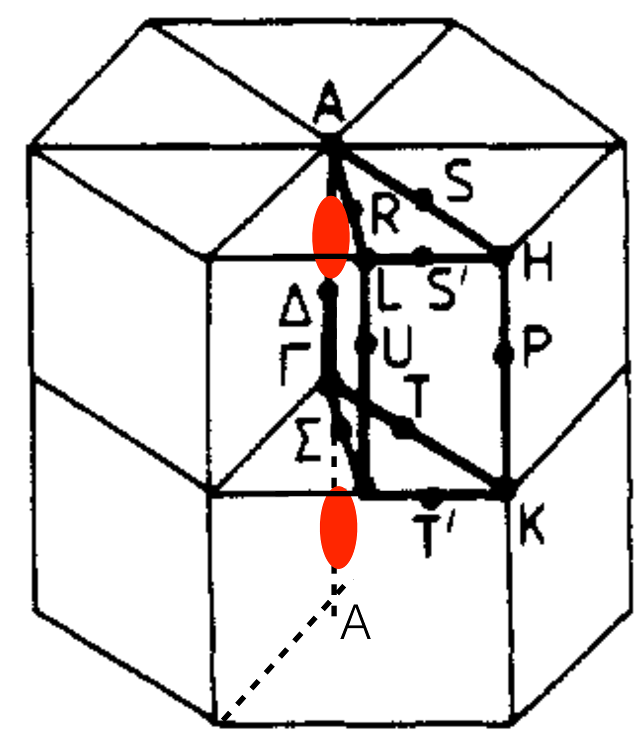


- based on toy model (4 atoms)
- downfolded to two Te atoms
- 3 orbitals (x,y,z)
- 2 spins, incl. SO

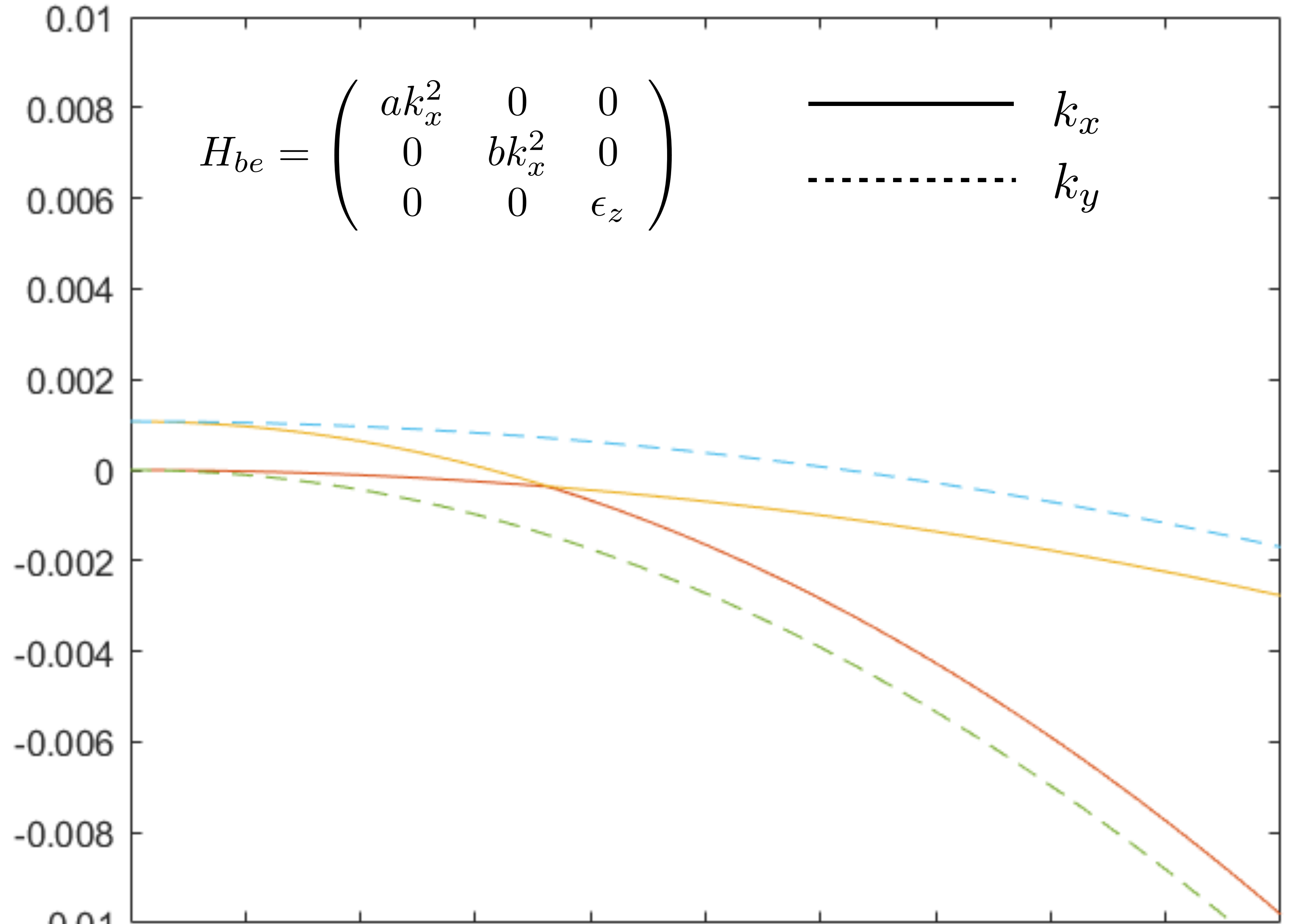
detail of the VB - effect of spin-orbit (SO) int. (first order eff.)

$$H_{be} = \frac{\hbar^2}{2m_0}\begin{pmatrix} ak_x^2 + bk_y^2 + ck_z^2 & (a-b)k_xk_y \\ (a-b)k_xk_y & ak_y^2 + bk_x^2 + ck_z^2 \end{pmatrix}$$





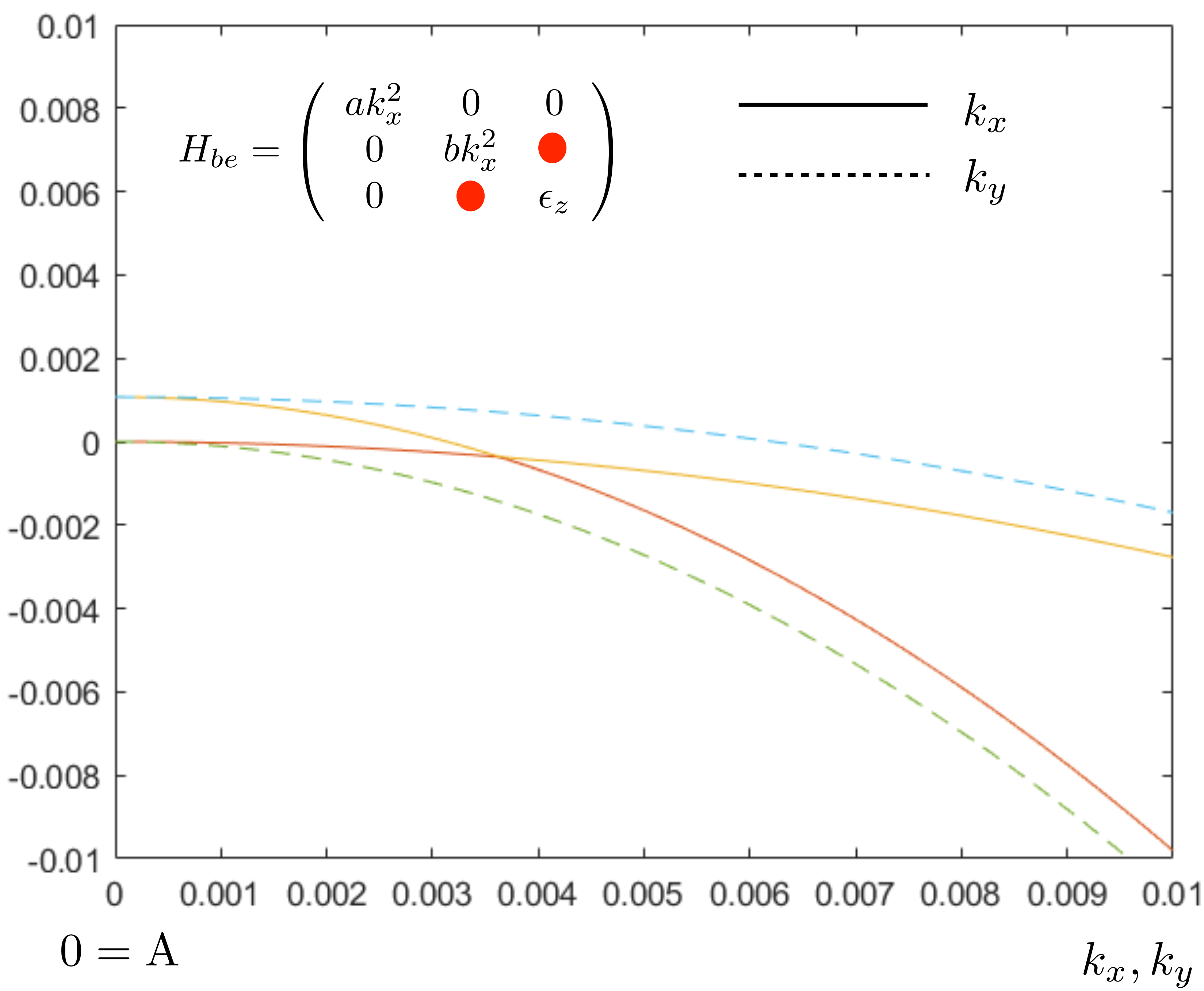
anisotropic bands (due to exchange+SO)

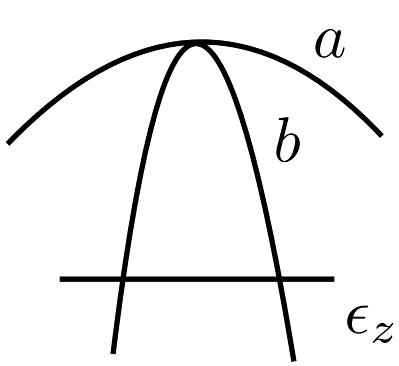


$0 = \mathrm{A}$

k_x, k_y

anisotropic bands (due to exchange+SO)

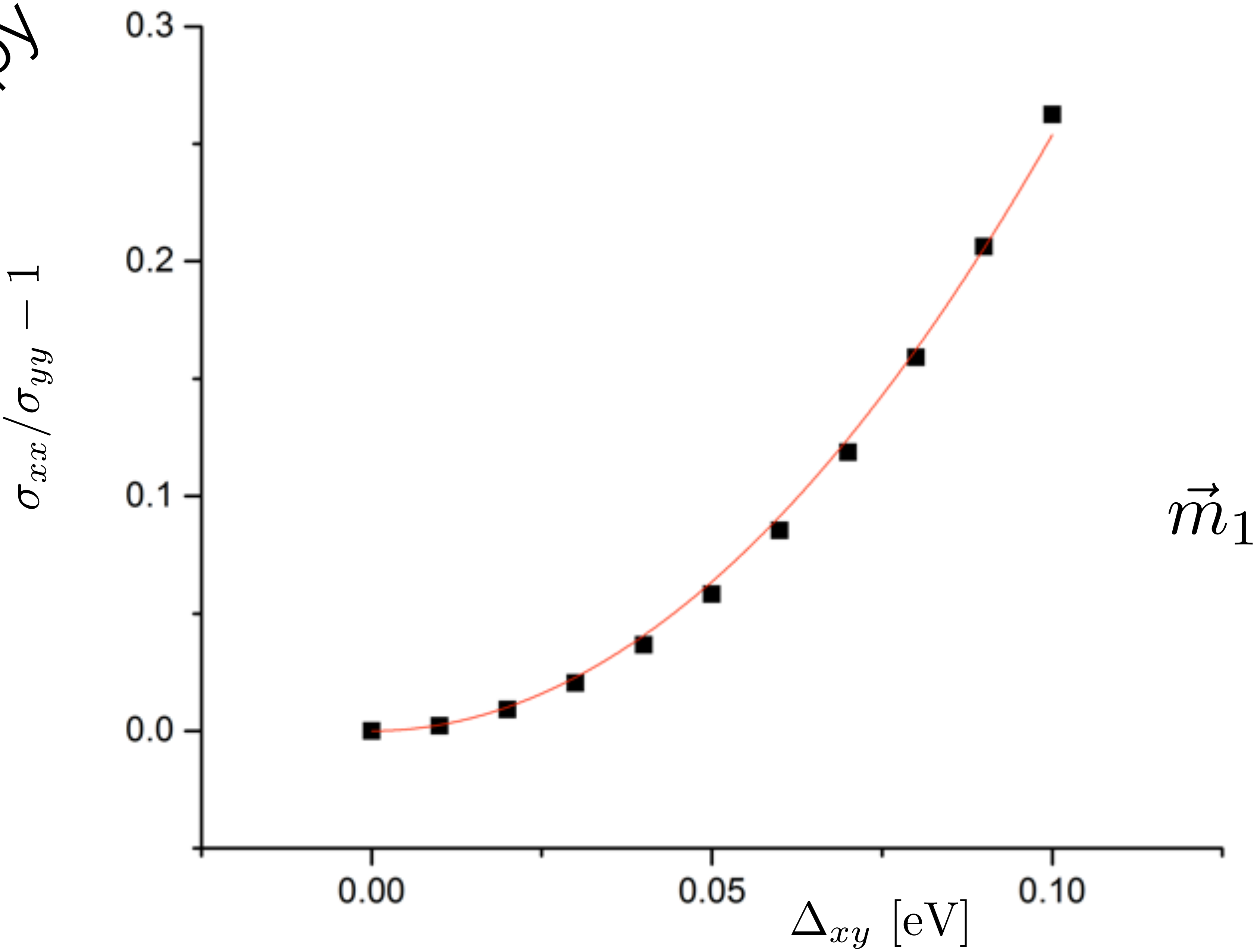




conductivity: Boltzmann approach

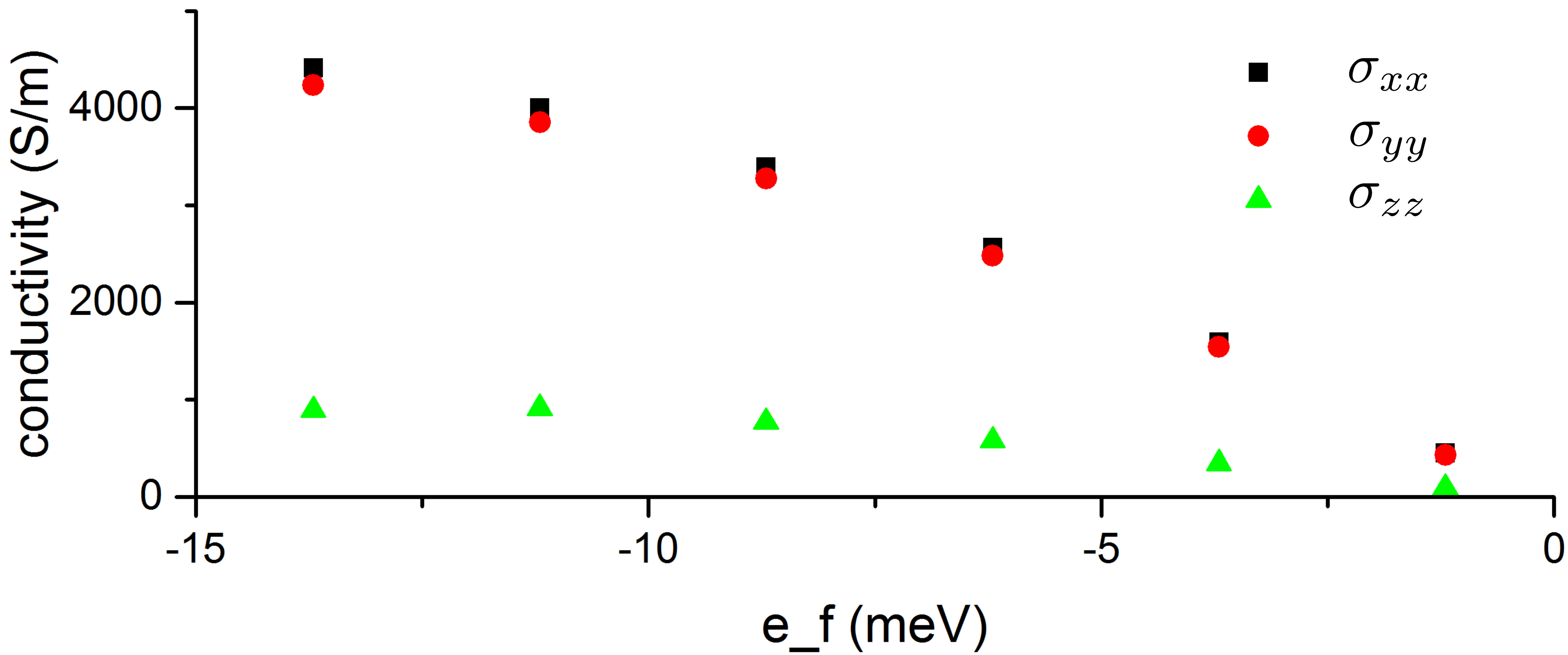
$$\sigma_{xx} = e^2\tau \int \frac{d^3k}{(8\pi^2)} v_x^2 \delta(E_k - E_F)$$

anisotropy



$$\vec{m}_{1,2} \parallel \hat{x}$$

conductivity: Boltzmann approach



$$\Gamma_{n,\mathbf{k}} = \frac{2\pi}{\hbar} N_{\mathrm{Mn}} \times \sum_{n'} \int \frac{d^3k'}{(2\pi)^3} |M_{nn'}^{\mathbf{k}\mathbf{k}'}|^2 \delta[E_n(\mathbf{k}) - E_{n'}(\mathbf{k}')] \times (1 - \cos\ \theta_{vv'}),$$

$$\tau = \hbar / 2\Gamma$$

transport relax. time

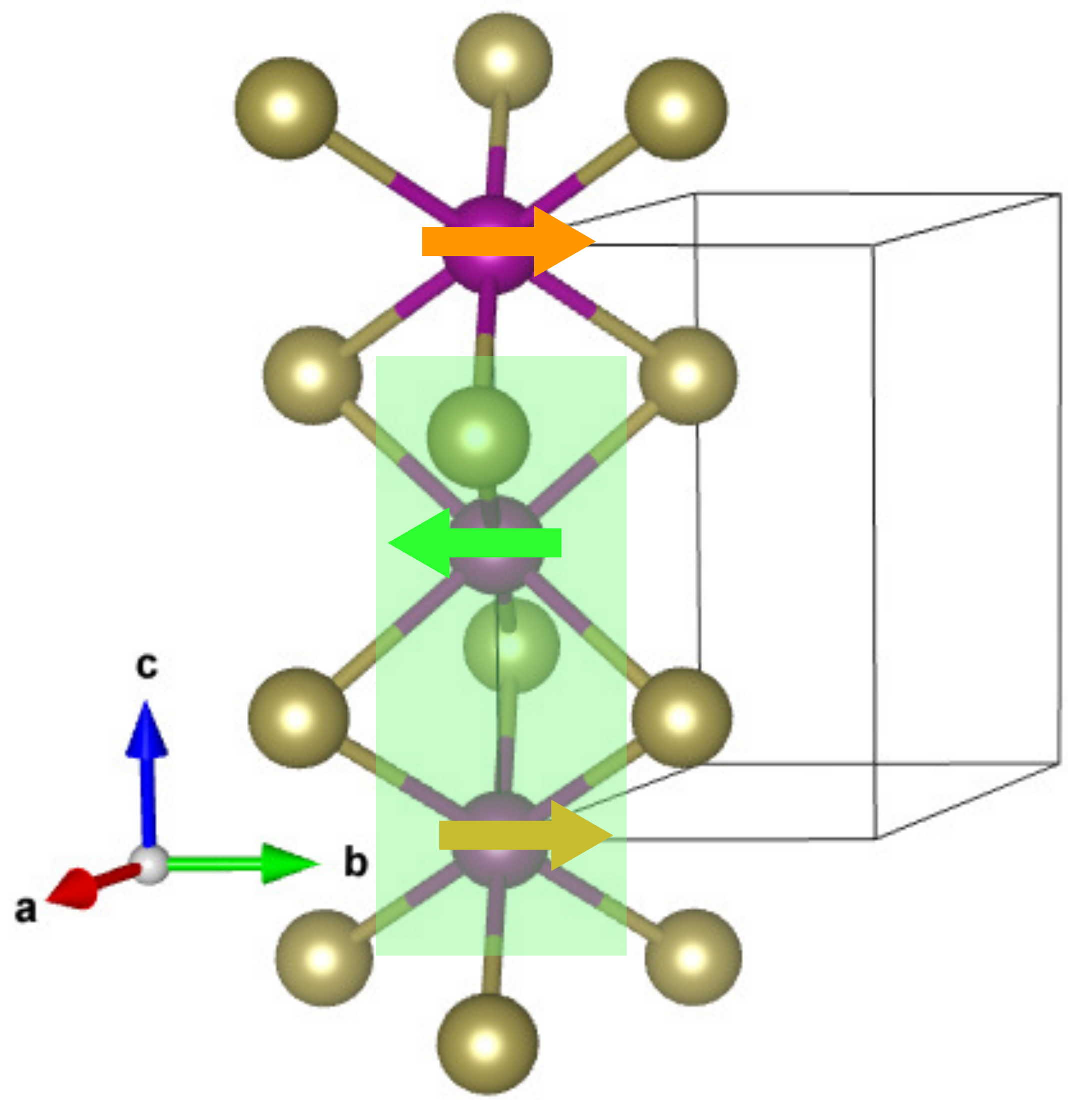
$$M^C = V(|\mathbf{k} - \mathbf{k}'|)\mathbb{1}, \quad V(q) = -\frac{e^2}{\varepsilon} \frac{1}{q^2 + q_{TF}^2}$$

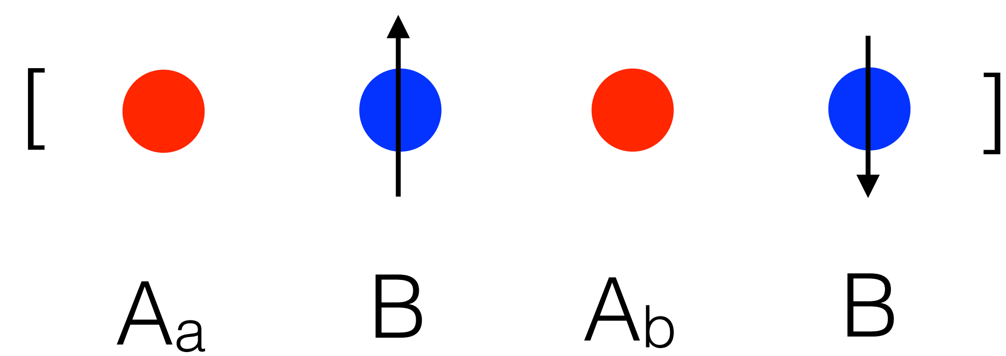
Thomas-Fermi screening

Conclusions

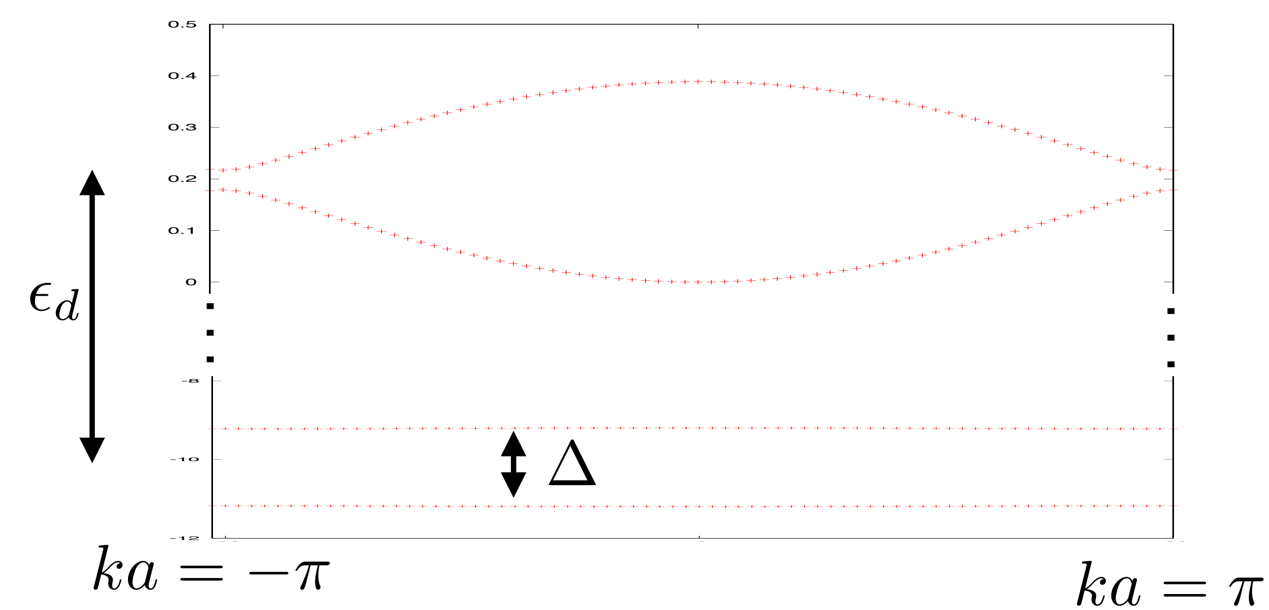
- competing VB maxima - to be resolved by advanced ab initio
- effective model components: band, SO, exchange (band+exchange go together)
- complicated structure in the vicinity of A-point
- conductivity can easily be evaluated, scattering treated e.g. by Fermi golden rule
- some symmetry-breaking terms still to be identified

how to deal with exchange - a toy model



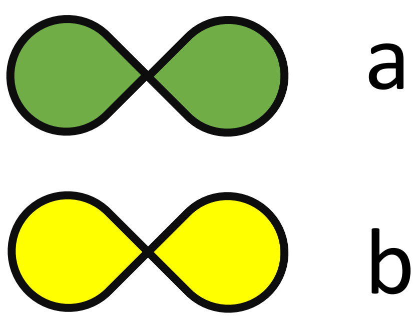


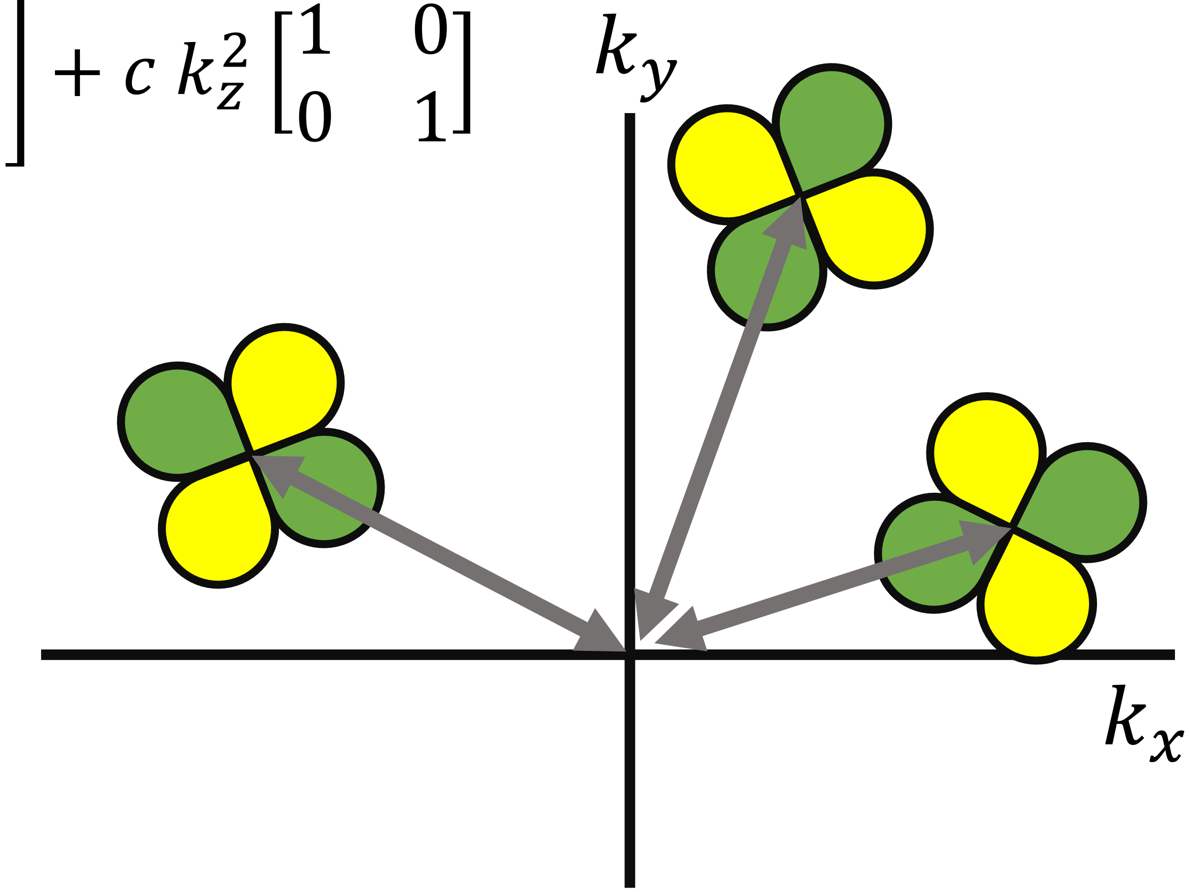
$$H = \begin{pmatrix} 0 & t & 0 & te^{-ika} \\ t & \epsilon_d + \Delta & t & 0 \\ 0 & t & 0 & t \\ te^{ika} & 0 & t & \epsilon_d - \Delta \end{pmatrix}$$



Crystalline Hamiltonian

- Lowest order expansion
- $H = \begin{bmatrix} a\,k_x^2 + b\,k_y^2 & (a-b)k_xk_y \\ (a-b)k_xk_y & b\,k_x^2 + a\,k_y^2 \end{bmatrix} + c\,k_z^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$





What is the basis?

p_x, p_y orbitals

AMR: crystalline and non-crystalline components

$$\Delta\rho_L/\rho_{av} = C_I \cos 2\phi + C_{I,C}\cos(2\phi+4\theta) + C_C\cos(4\phi+4\theta) + C_U\cos(2\phi+2\theta)$$

$$\Delta\rho_T/\rho_{av} = C_I \sin 2\phi - C_{I,C}\sin(2\phi+4\theta)$$

de Ranieri et al., NJP '08