Effective model of antiferromagnetic MnTe and anisotropic magnetoresistance

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solid state physics

materials science

anisotropic magnetoresistance (AMR) iron, permalloy, (Ga,Mn)As

antiferromagnets

## MnTe: an antiferromagnet







Kriegner et al. '17 doi: 10.1103/PhysRevB.96.214418

#### MnTe: a semiconductor



# The goal:

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

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





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



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## AMR: the new twist

# AMR: the new twist antiferromagnets!



**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.

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

300

350

Temperature (K)

400

#### 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)



$$H = \frac{\hbar^2}{2m_0} \begin{bmatrix} ak_x^2 + bk_y^2 + ck_z^2 + dk_yk_z & (a-b)k_xk_y + dk_xk_z \\ (a-b)k_xk_y + dk_xk_z & bk_x^2 + ak_y^2 + ck_z^2 - dk_yk_z \end{bmatrix}$$

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



#### competing maxima at the VB top: the idea



$$H = \left(\begin{array}{cc} E_X & 0\\ 0 & E_Z \end{array}\right)$$

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





 $(\angle 1)$ Born approximat  $(1 - \cos \theta_{vv'})$ , how to of scattering that for each the Bloch states from Eq. the president of the product of the has the scattering particulatoring use<sup>31</sup>  $\theta_{vv'}$ , the angle subtended by the teles  $V_{n'}(\mathbf{k}')$  to take into account  $\mathbf{r}_{nk}$  which  $\mathbf{r}_{mk}$  here  $\mathbf{k}_{n}$  is the second representation of the second repre the fermi en the full impurity potential **k** in case the combined effect of <sup>h</sup> the SOI n and  $\mathbf{R}^{2}$ on distorts the Fermi surfaces as suggested by the der to estimate conscience win acts ig. 1(a). tional Mn act as acceptors where here in a static ito no beyond subtended by the static ito and the static ito angle subtended by the static i cipate in the ferromagnetic, (b) dan dor, (Cd, Who Rate in of the Control of the ging the magnetic and nonmaled etoc k Bin was provided to the south of the souther the sou magnetization discattening Ferfalsbourges chersing bereater and sketch in Figthe Bloch states From Eq. (2), the set of  $M^{C}$  Substitutional Mn act as acceptors and their magnetic part  $\lambda \mathbf{k}' \mathbf{h}'$ ments participate in the for romagnetic control for the participate in the formation of the second o ering matrix elements between awledging states agenetic and reputagenetic provision onian (2).5 In the six-sband Wottakon of Eq. (2), the DUT 415 and Motaginer ?? magneticupation and the state magneticupation energy level/matrix element. Briefly speaking, the k=0 en- $M_{nn'} = \langle z_{\mathbf{k}'n'} | \alpha \langle z_{\mathbf{k}'n'} | \alpha \langle z_{\mathbf{k}'n'} \rangle$ based(4)on ergy levels are first fixed from Ref. 5 and the matrix elements are then adjusted to obtain the band diagram; as a result there are 10 (18) adjustable parameters in  $5\sqrt{T_{H}}e_{M}$ , S, where we = 0 angle subtended by the where k = 0 energy lifer, the scattering matrix elements between two eigenstates core constant, alence band to obtain Luttinger parameters, and for the key parameters are the matrix elements. Here, they were nd thally to respect the contract the contract of the the second for the contract of the contr the a penervale provints de the Brilbying gone. The ened Coulonio, at the the the brilbying gone. The energy of the coulon of th ty bully of this method. Figures 3-3 show the band structed acceptors and we of the and GaAs obtained with our kin model on and in a to Substitutional Mnife



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



# how to deal with exchange - a toy model wavefunctions



# how to deal with exchange - a toy model wavefunctions



# $H = H_b + H_{so} + H_{ex}$ 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.)



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





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



### 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

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# 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)



### anisotropic bands (due to exchange+SO)



#### conductivity: Boltzmann approach



### conductivity: Boltzmann approach



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

$$\tau = \hbar/2\Gamma \qquad \qquad M^C = V(|\mathbf{k} - \mathbf{k}'|)\mathbb{I}, \quad V(q) = -\frac{e^2}{\varepsilon} \frac{1}{q^2 + q_{TF}^2}$$
  
transport relax. time 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





# Crystalline Hamiltonian

• Lowest order expansion

#### What is the basis?

 $p_x$ ,  $p_y$  orbitals

### AMR: crystalline and non-crystalline components

