SIGNATURES OF SPIN-ORBIT DRIVEN ELECTRONIC TRANSPORT IN TRANSITION- METAL-OXIDE INTERFACES

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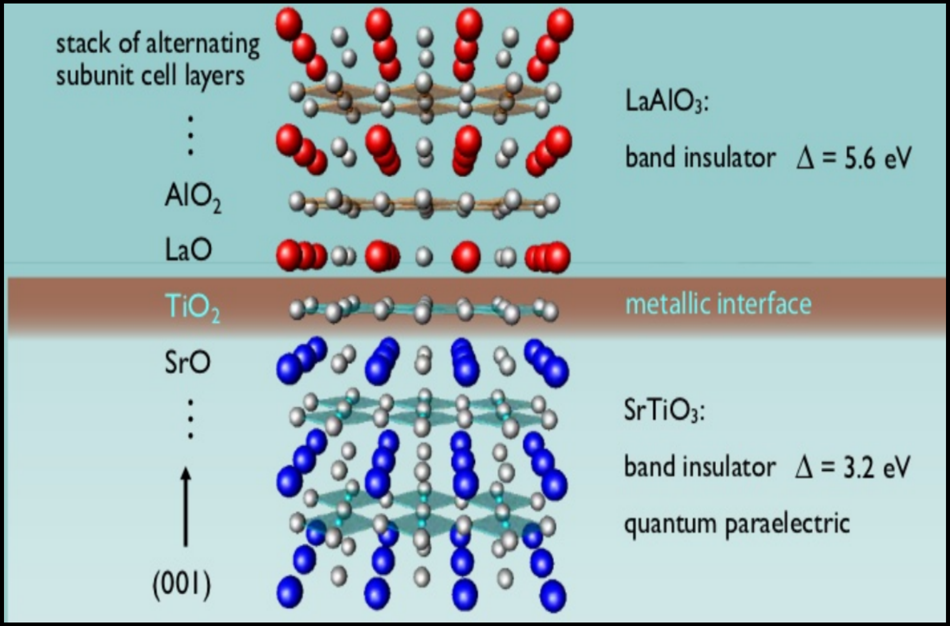
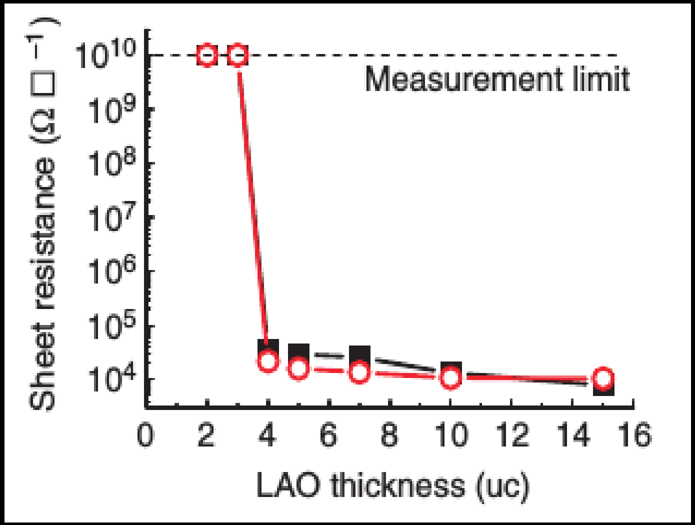
Bad Honnef, 19-22 September 2016

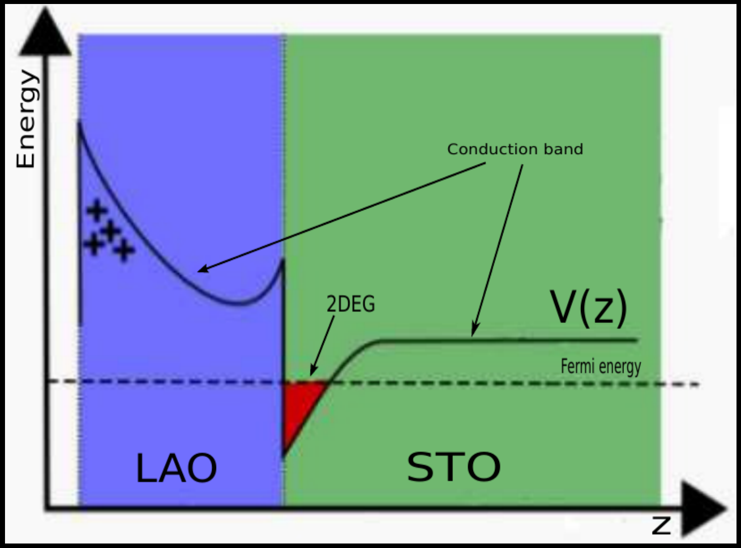
LAO/STO heterostructure:

conducting interface between two insulators

conducting *interface beyond*
critical thickness of 3 unit cells
Ohtomo & Hwang Nature 427 (2004)



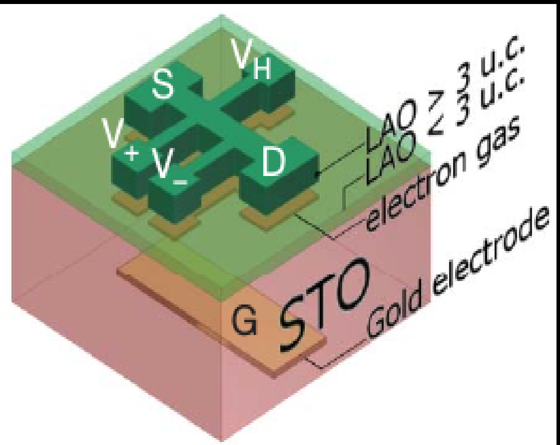




Surface reconstruction → quantum-well confinement
z-extension of the conducting region ~ 2 – 10 nm
(lattice constant = 0.4 nm)

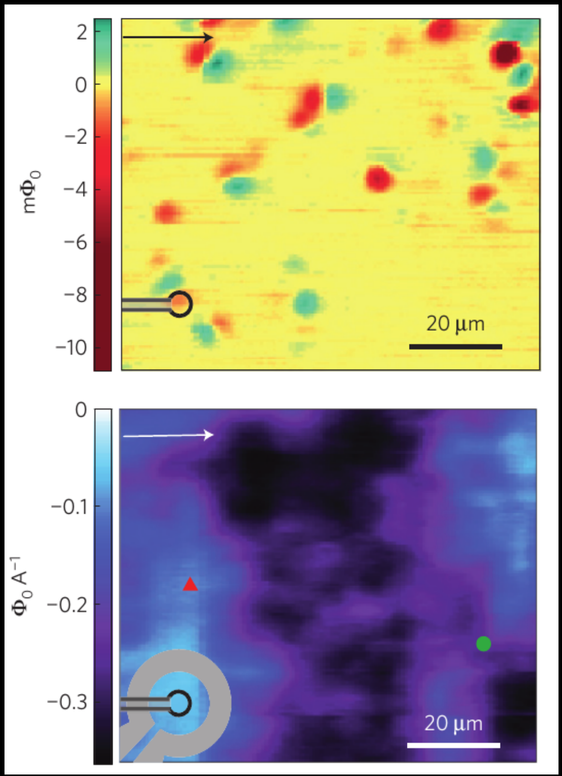
Electric-field control of the Ground State

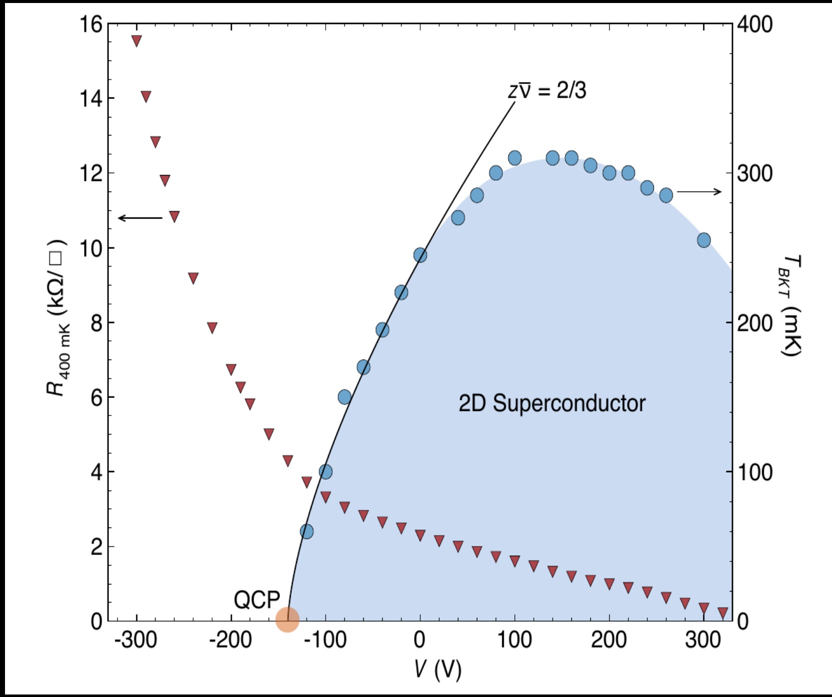
Caviglia *et al.*, Nature 456, 624-627 (2008)

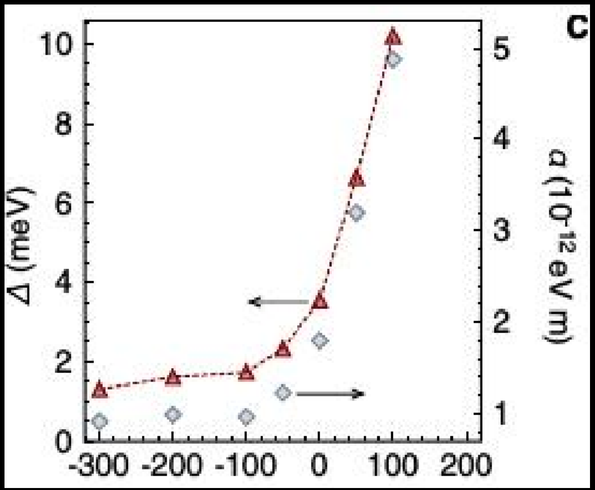


Bulk – insulating substrate with high dielectric constant ($10^3 - 10^4$ at low-*T*) allows large modulation of the carrier density at the interface via an applied gate - voltage

- Symmetry of the SC order parameter?
- Superconductivity vs. Spin-Orbit coupling (Top. SC?)



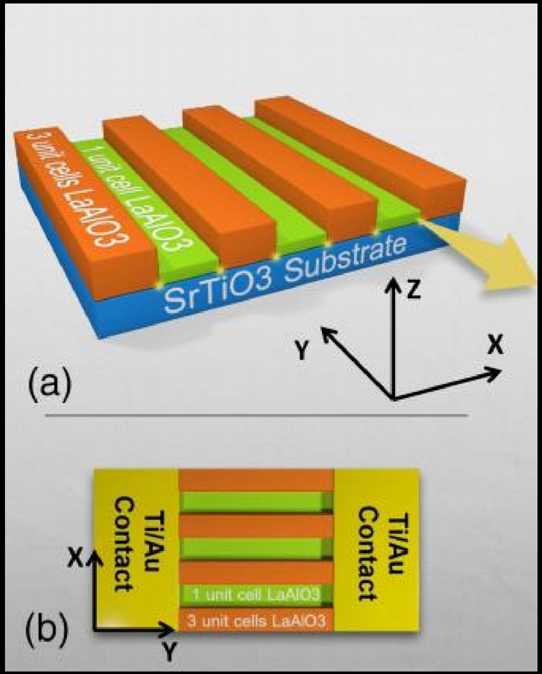




Caviglia *et al.*, PRL 104, 126803 (2010)

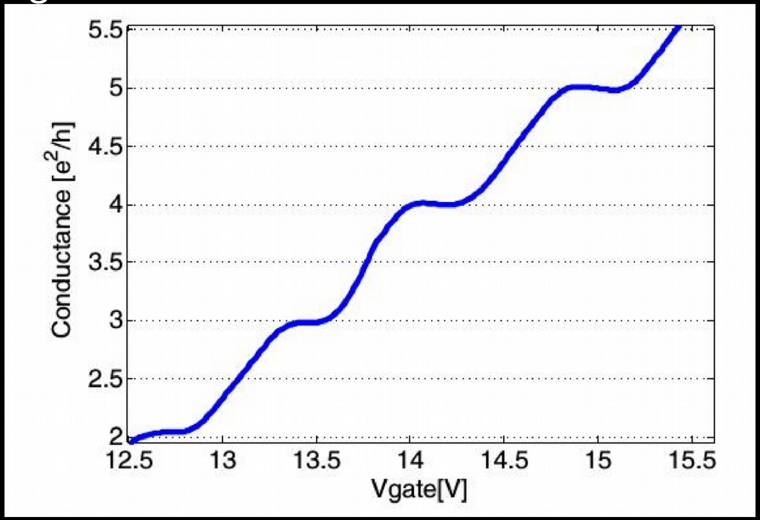
- Coexistence of magnetism and superconductivity? Bert *et al.*, Nat. Phys. (2011) Bert *et al.*, PRB (2012)
- Interactions between localized moments and conducting electrons (e.g. Kondo)? Joshua et al. PNAS (2013), Ruhman et al. PRB (2014)

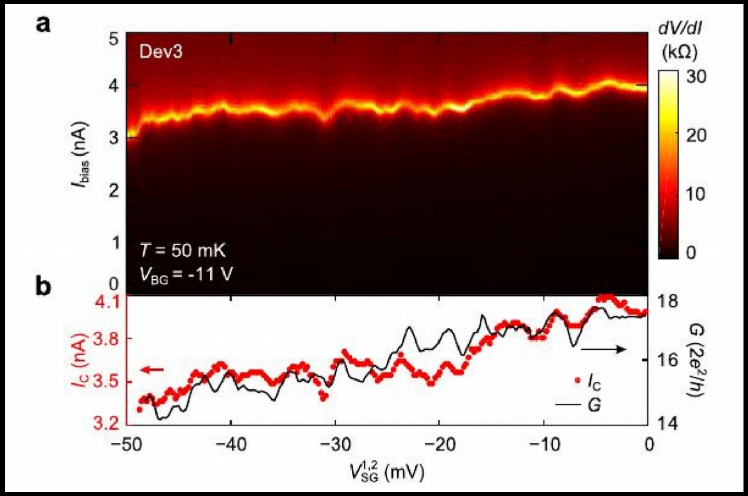
Nanostructures



1D Quantum Wire with quantized conductance

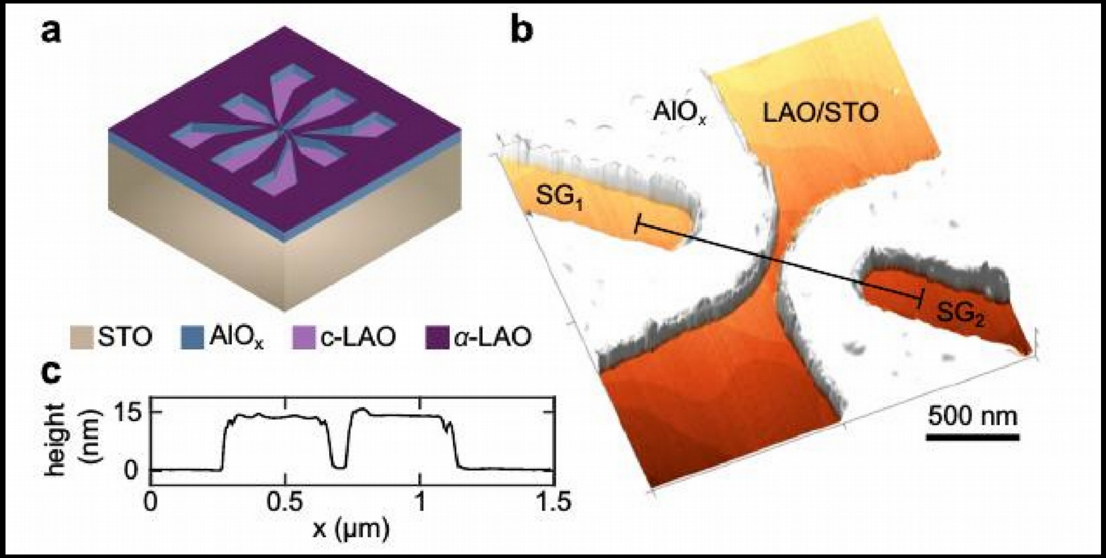
Ron and Dagan, PRL **112**, 136801 (2014)





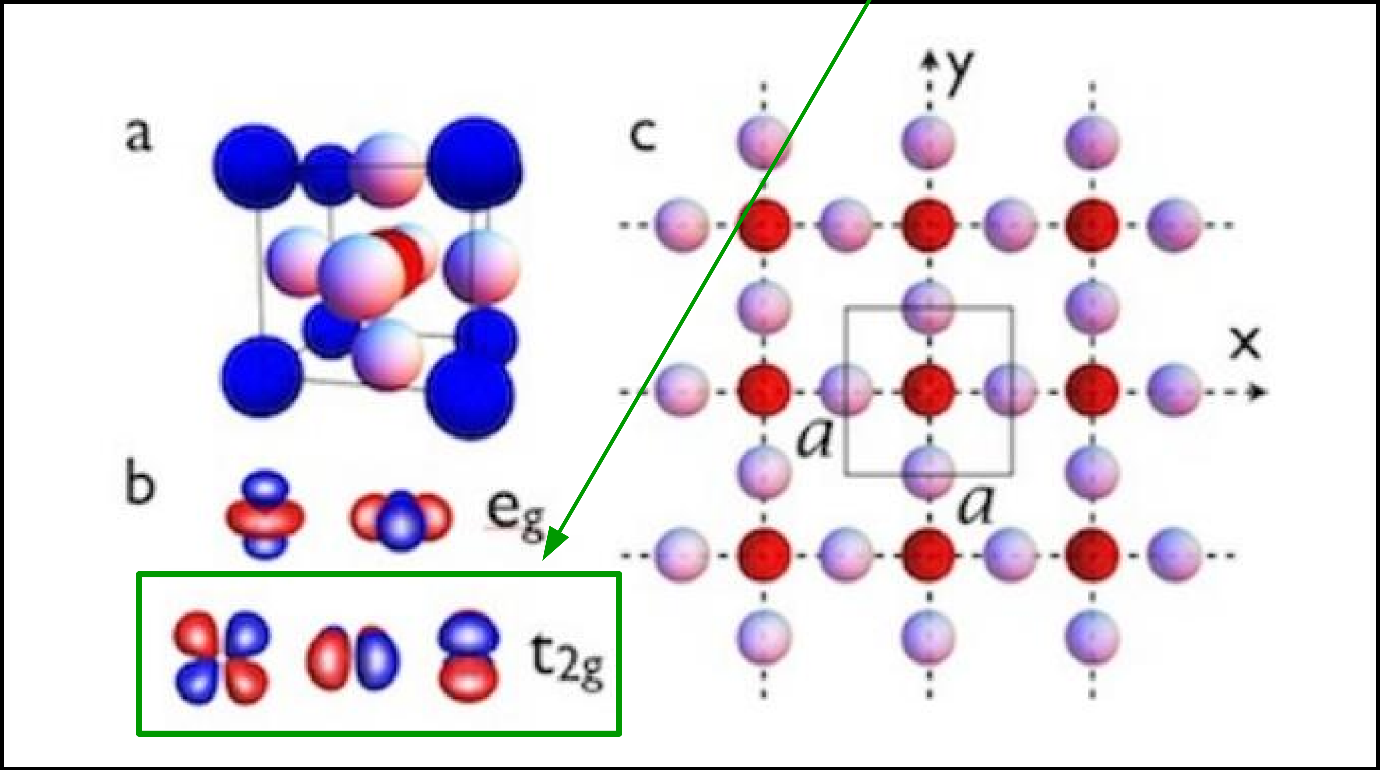
Side-gate tunable Josephson Junctions

A. Monteiro, D. Groenendijk, N. Manca, E. Mulazimoglu, S. Goswami, L. Vandersypen, A. Caviglia, **arXiv:1609.03304**



Electronic structure of the interface

Conduction bands derived from (d_{xy}, d_{xz}, d_{yz}) **Ti-orbitals**



Khalsa, Lee and MacDonald, PRB **88**, 041302(R) (2013)

"Sharp confinement" : Hamiltonian and band structure

Kinetic Hamiltonian

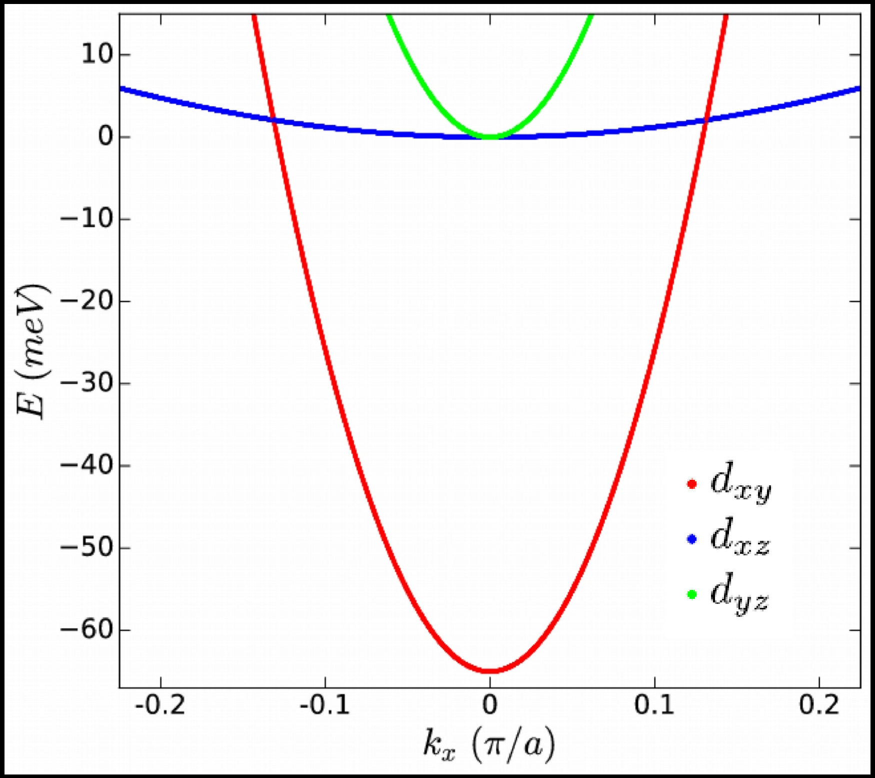
$$H_\mathrm{K} = \begin{pmatrix} \epsilon_{xy}(k) - \Delta_\mathrm{E} & 0 & 0 \\ 0 & \epsilon_{xz}(k) & \delta(k) \\ 0 & \delta(k) & \epsilon_{yz}(k) \end{pmatrix} \otimes \hat{\sigma}_0$$

$$\epsilon_{xy}(k) = 2t_l(2 - \cos k_x - \cos k_y)$$

$$\epsilon_{xz}(k) = 2t_l(1 - \cos k_x) + 2t_h(1 - \cos k_y)$$

$$\epsilon_{yz}(k) = 2t_h(1 - \cos k_x) + 2t_l(1 - \cos k_y)$$

$$\delta(k) = 2t_d \sin k_x \sin k_y$$



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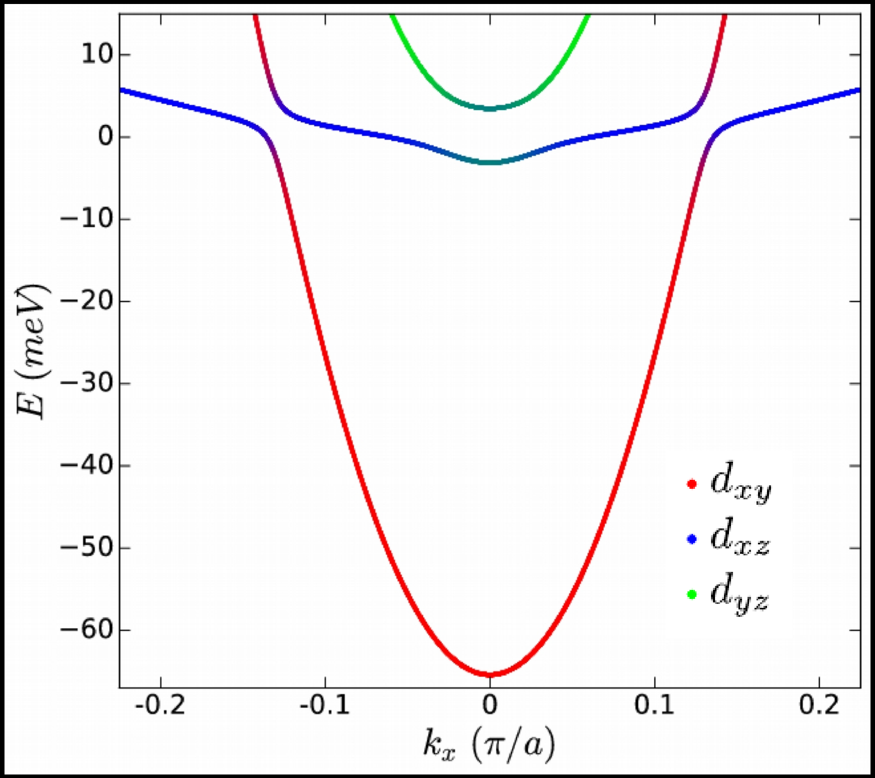
Atomic spin-orbit

$$H_\mathrm{SO} = \frac{\Delta_\mathrm{SO}}{2} \begin{pmatrix} 0 & i\hat{\sigma}_x & -i\hat{\sigma}_y \\ -i\hat{\sigma}_x & 0 & i\hat{\sigma}_z \\ i\hat{\sigma}_y & -i\hat{\sigma}_z & 0 \end{pmatrix}$$



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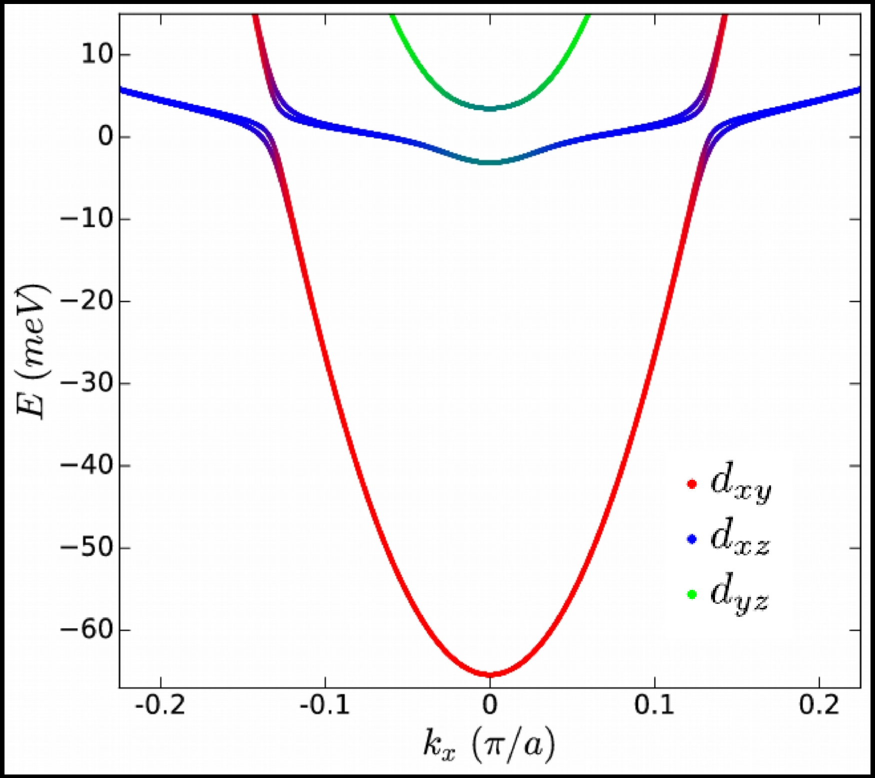
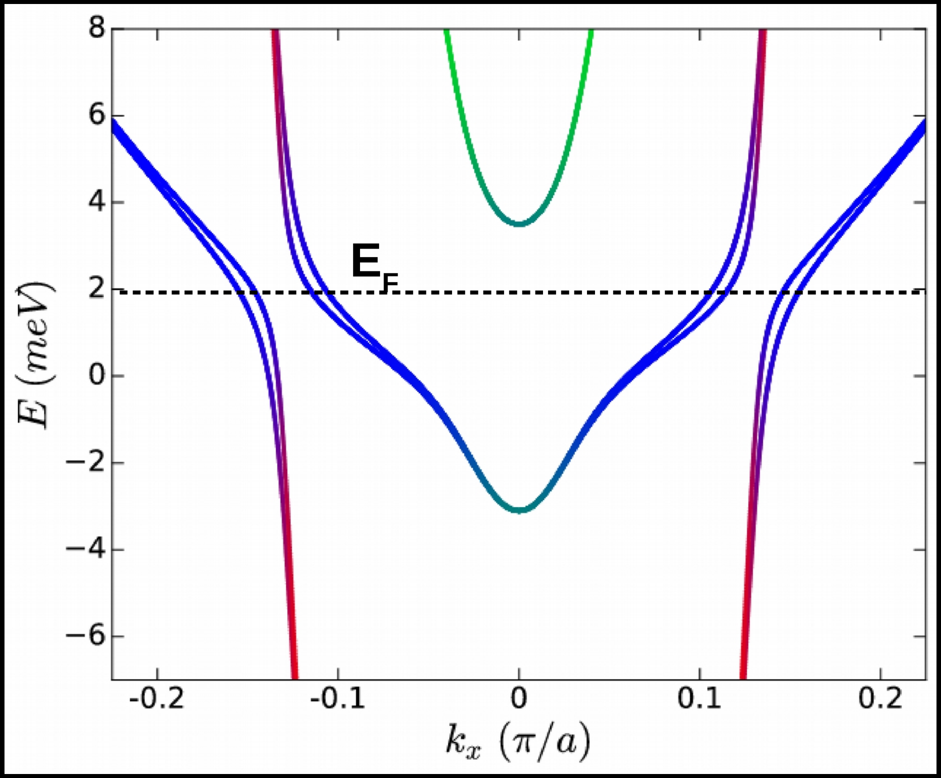
Inversion symmetry breaking

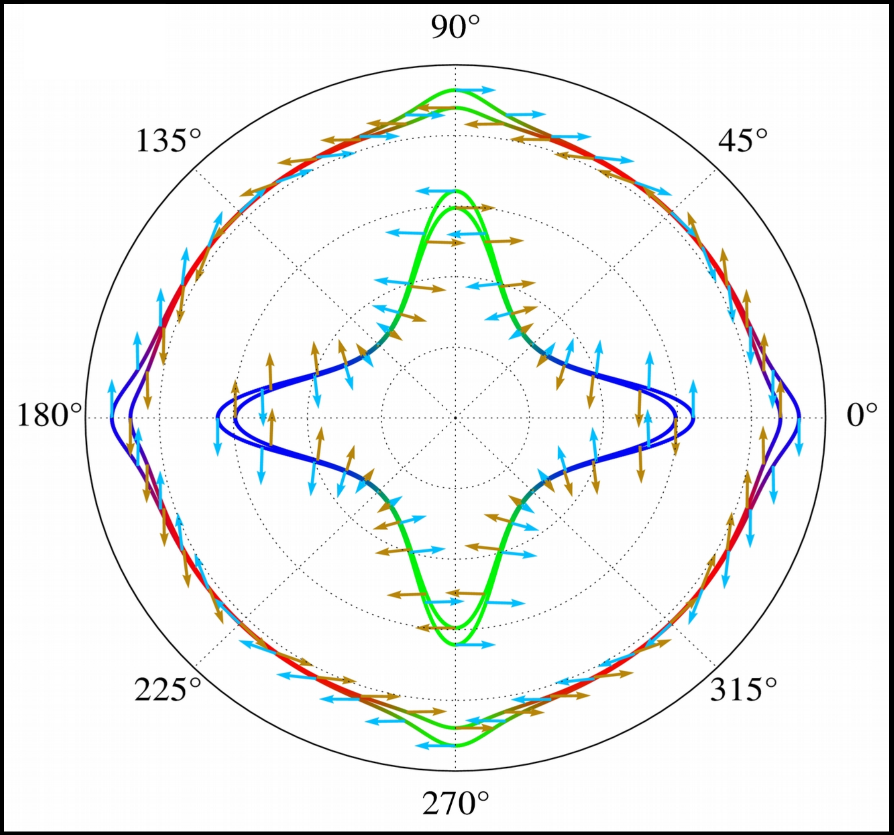
$$H_{\mathrm{Z}} = \Delta_{\mathrm{Z}} \begin{pmatrix} 0 & i \sin k_y & i \sin k_x \\ -i \sin k_y & 0 & 0 \\ -i \sin k_x & 0 & 0 \end{pmatrix} \otimes \hat{\sigma}_0$$

Khalsa, Lee and MacDonald, PRB 2013



Spin-orbit interaction gives band-mixing





- Electronic states with mixed orbital character at certain directions in the BZ
- In presence of scattering by disorder, transitions between different bands are allowed for any kind of potential (no need for "special" impurities)

- Spin-splitting not simply linear in *k* (unlike conventional Rashba-systems)
- maximally enhanced near the band (avoided) crossings

Boltzmann transport equation
for scattering by impurities

$f_{\mathbf{k},\nu} = f_0 + g_{\mathbf{k},\nu}$ $g_{\mathbf{k},\nu} = \mathbf{\Lambda}_{\mathbf{k},\nu} \cdot \mathbf{E}$ $\mathbf{\Lambda}_{\mathbf{k},\nu}$ **Vector mean-free-path**

$$-e(\mathbf{v}_{\mathbf{k},\nu} \cdot \mathbf{E})\partial f_0/\partial \epsilon_{\mathbf{k},\nu} - (e/\hbar)(\mathbf{v}_{\mathbf{k},\nu} \times \mathbf{B}) \cdot \nabla_{\mathbf{k}} g_{\mathbf{k},\nu} =$$

Field-driven evolution

$$\sum_{\mathbf{k}',\nu'} Q_{\mathbf{k}\nu,\mathbf{k}'\nu'}(g_{\mathbf{k},\nu} - g_{\mathbf{k}',\nu'})$$

$$Q_{\mathbf{k}\nu,\mathbf{k}'\nu'} \sim e^{-\xi^2|\mathbf{k}-\mathbf{k}'|^2/2} |\langle u_{\mathbf{k},\nu}|u_{\mathbf{k}',\nu}\rangle|^2$$

momentum-dependent scattering amplitude due to extended impurities

depends on the spin- and orbital-polarization of the states

$$\mathbf{\Lambda} = (\Lambda^x, \Lambda^y)$$

We solve the matrix equations

$$\Lambda^{x,y} = \mathcal{M} v^{x,y}$$

$$\Lambda^{x,y} = \begin{pmatrix} \Lambda^{x,y}_{i_1 n} \\ \Lambda^{x,y}_{i_2 n} \\ \cdot \\ \cdot \\ \cdot \\ \Lambda^{x,y}_{i_k m} \end{pmatrix}$$

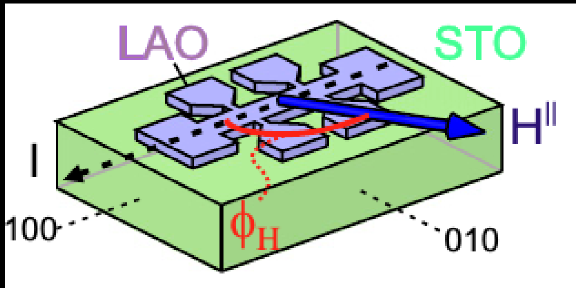
The two indices count respectively the number of discretized points on a single Fermi surface (i) and the number of bands (n)

$$\mathcal{M}_{in,jm} = -\frac{d\,l_{in}}{|\mathbf{v}_{in}|}\, q_{in,jm}$$

Scattering OUT

$$\mathcal{M}_{in,in} = \sum_{j,m} \frac{d\,l_{in}}{|\mathbf{v}_{in}|}\, q_{in,jm}$$

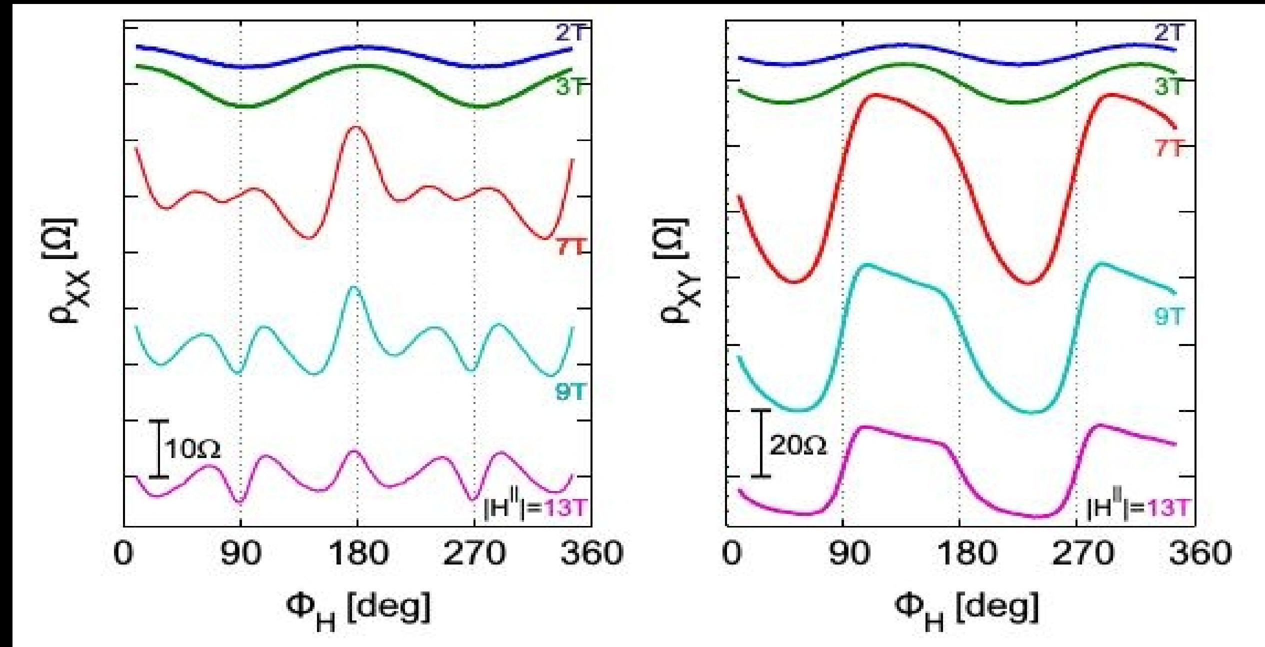
Scattering IN



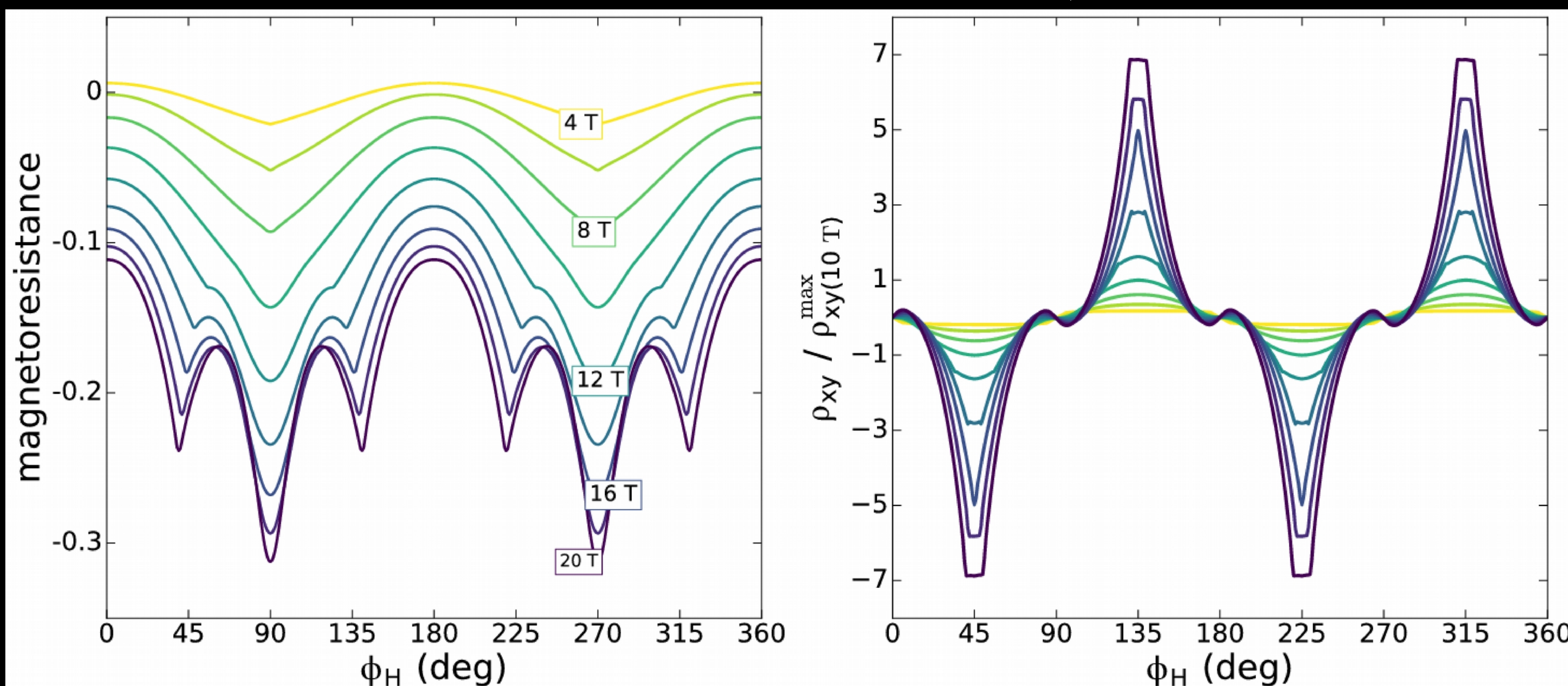
Joshua et al. PNAS **110**, 9633 (2013)

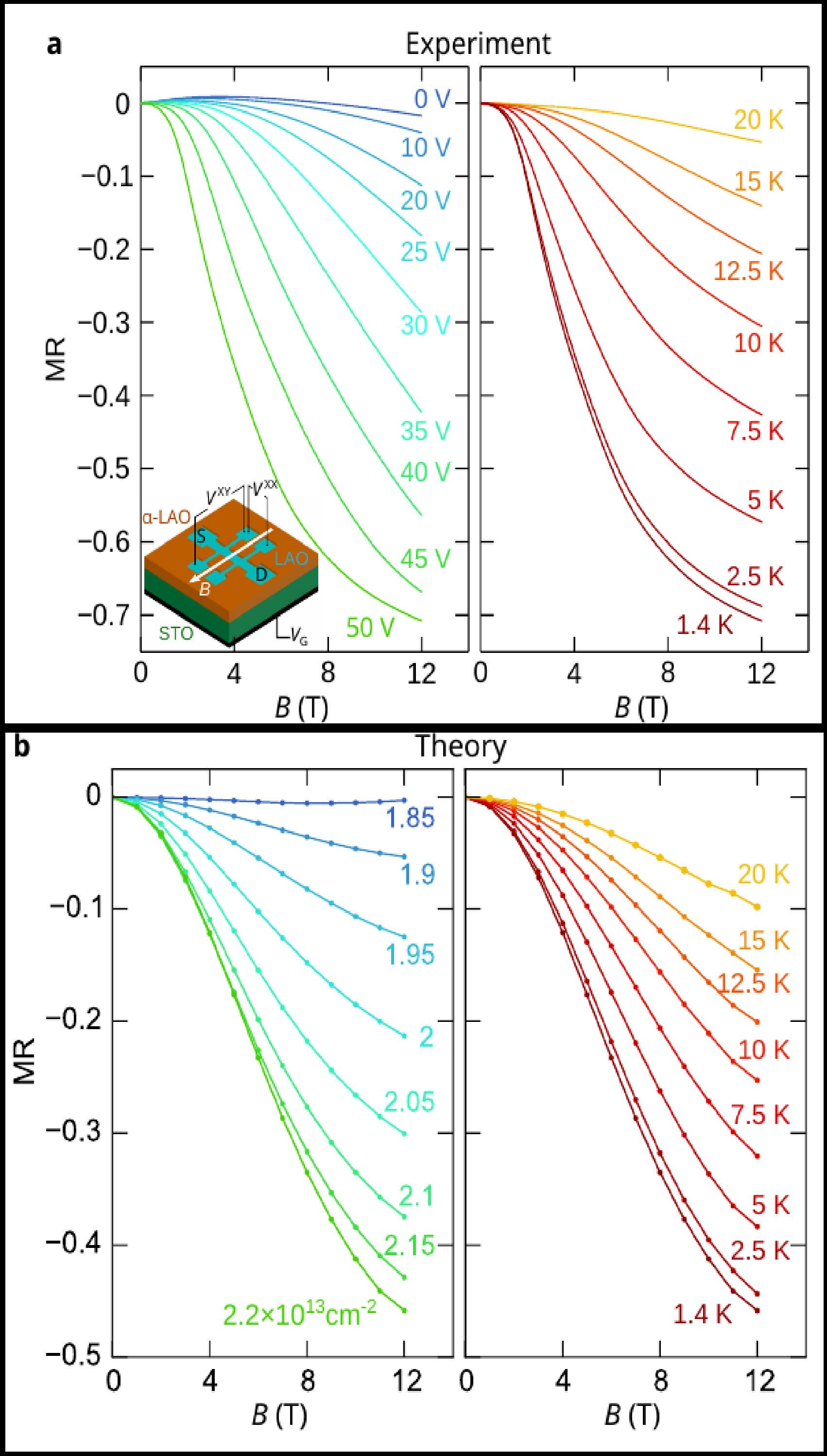
EXPERIMENTS show…

- very anisotropic negative MR
- large "Hall" resistivity with square-wave-like modulation



THEORY N. Bovenzi and M. Diez, **arXiv:1609.00663**





M. Diez, A. Monteiro, G. Mattoni, E. Cobanera,T. Hyart, E. Mulazimoglu, N. Bovenzi, C. Beenakker, A. Caviglia, PRL **115**, 016803 (2015)

Curves at fixed (low) temperature as a function of the gate-voltage (density)

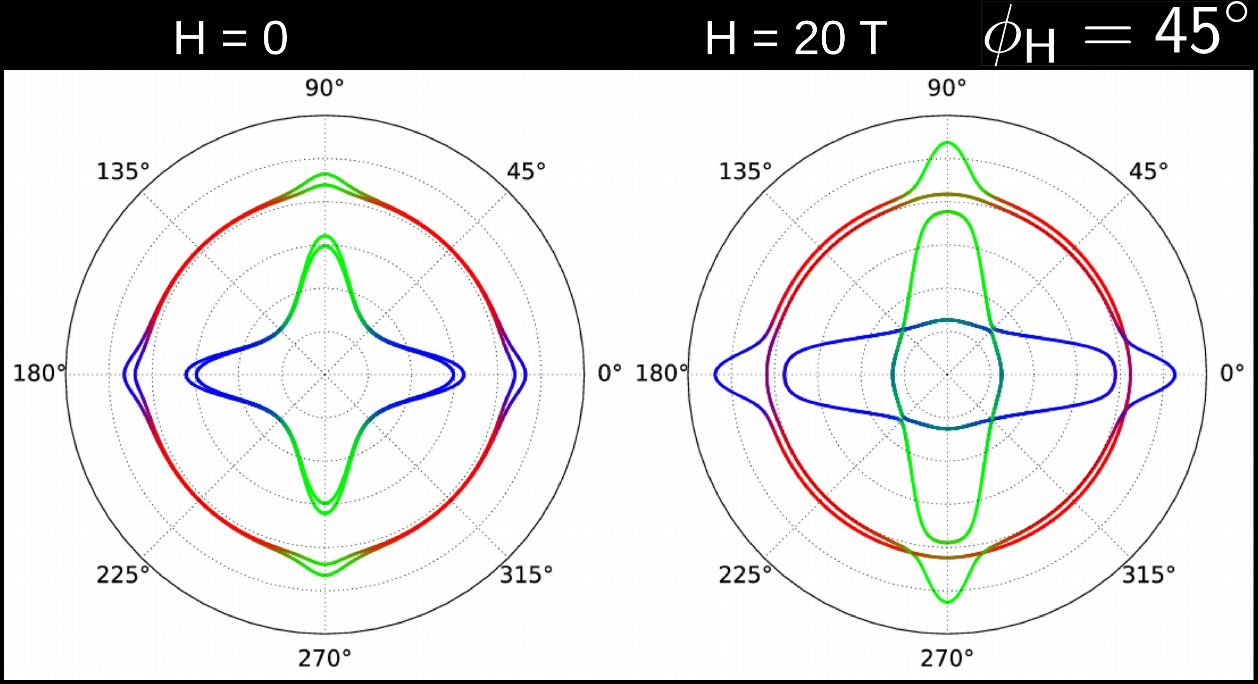
And

Curves at fixed (high) voltage as a function of temperature look similar

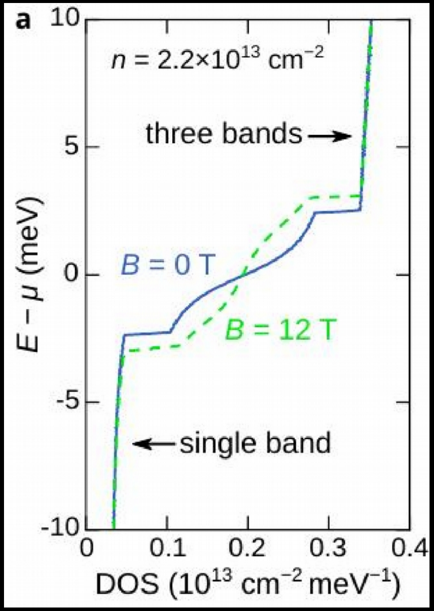
CLASSICAL EFFECTS:

- Suppression of *inter-band* scattering produces negative MR

- *Intra-band* scattering is anisotropically enhanced when the the magnetic field balances the spin-orbit field at points of maximal SO-hybridization (***effective Lorentz force***)



- Voltage/temperature symmetry of the curves naturally comes from downwards-renormalization of the chemical potential at finite *T*

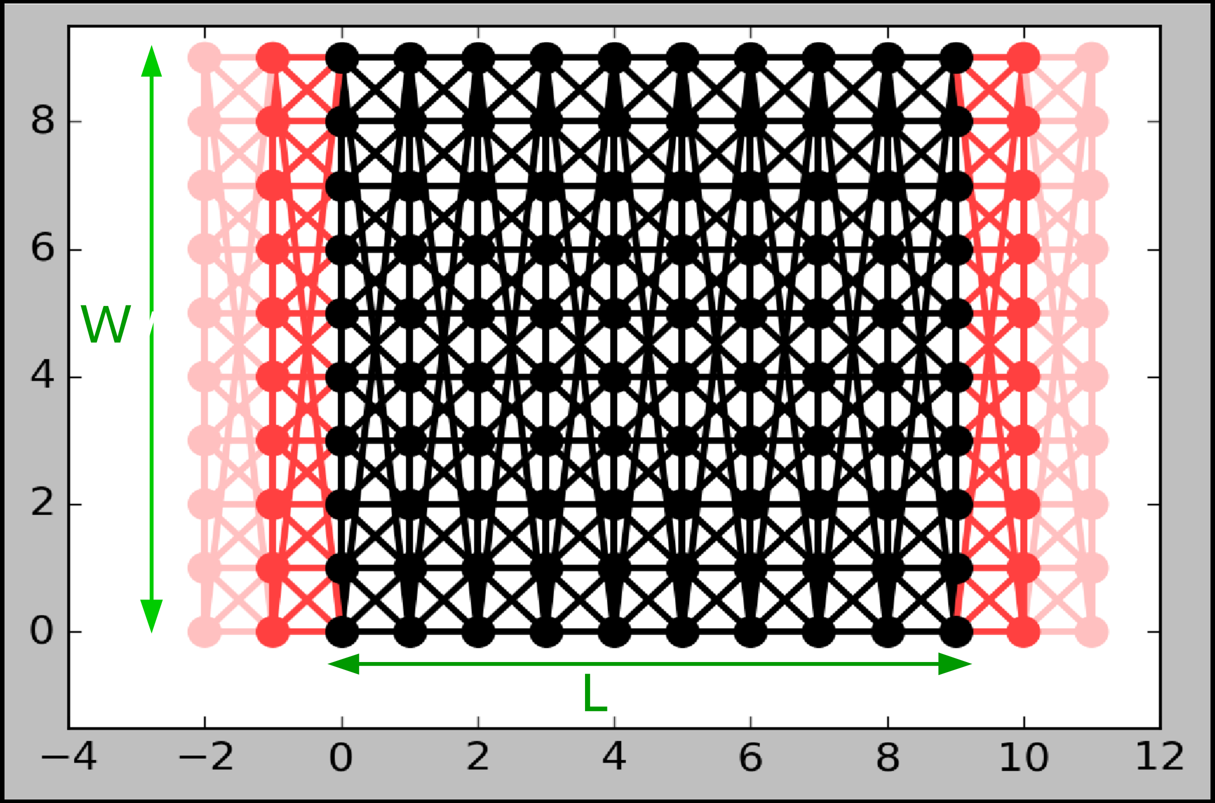


Current understanding and challenges…

- Spin-orbit coupling affects the band structure in a way that is not perturbatively treatable
- Orbital-mixing effects need to be properly modeled
- Implications for (diffusive) nanostructures (Thoulesse energy *vs.* spin-orbit energy)?
- What if the low-disorder approximation is not reliable?

Next future: Quantum Transport simulations

Kwant toolbox C. W. Groth, M. Wimmer, A. R. Akhmerov and X. Waintal, NJP **16**, 063065 (2014)



$$\Psi_{out} = S\Psi_{in}$$

Scattering matrix

✔ Arbitrary disorder strength (not perturbative)

✗ No interactions

Landauer formula

$$G = \frac{e^2}{h} Tr(tt^\dagger)$$