Transport properties of topological insulators

Andrea Droghetti
School of Physics and CRANN, Trinity College Dublin, IRELAND

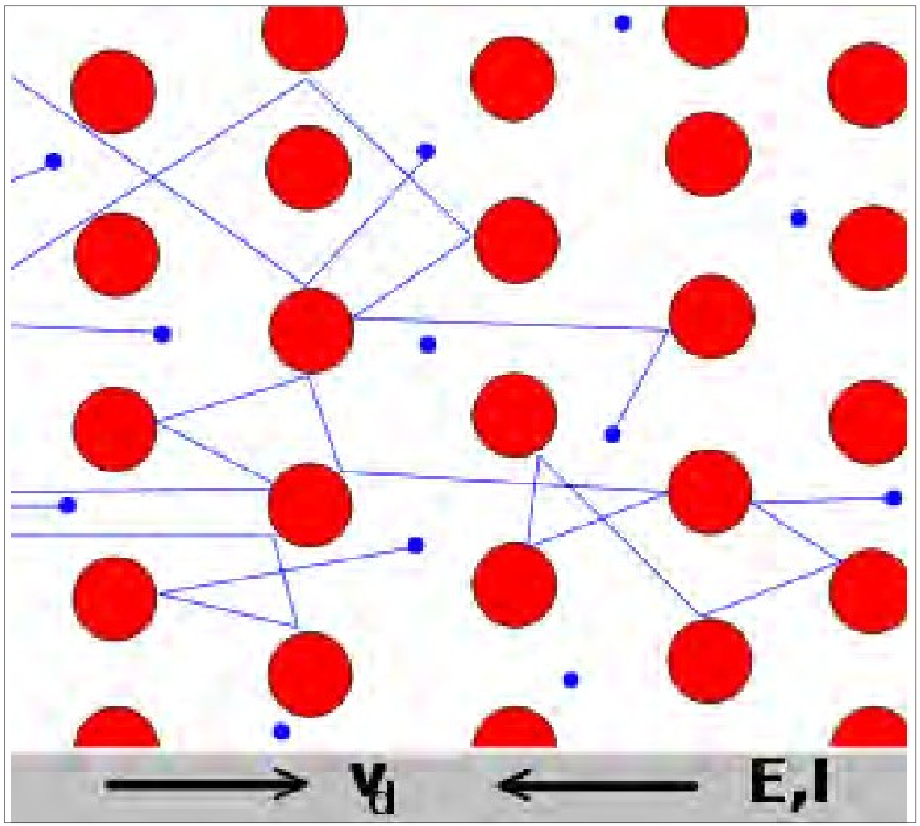
- Basic course on electronic transport
- Topological insulators (Kane-Mele model/Bi_2Se_3)
- Kondo impurity in a topological insulator

- Basic course on electronic transport
- Topological insulators (Kane-Mele model/Bi_2Se_3)
- Kondo impurity in a topological insulator

Classical transport: Drude model and Ohm's law

CRANN

Length of the sample >> electron mean free path



- Electrons are viewed as particles in a pinball
- Resistance results from (back) scattering
- Conductivity and resistivity (characteristic of the metal)

$$\sigma = \frac{1}{\rho} = \frac{\mathbf{J}}{\mathbf{E}} = \frac{en\mathbf{v_d}}{\mathbf{E}}$$

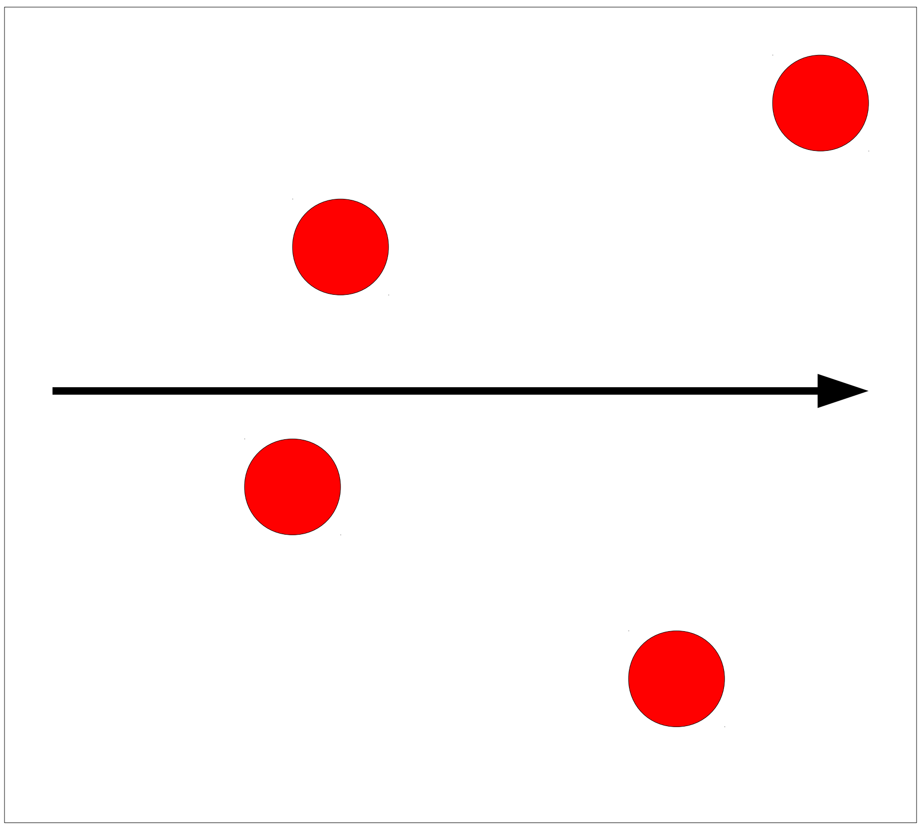
- Conductance

$$G = \sigma \frac{\text{transverse area}}{\text{length}}$$

Quantum transport: ballistic regime

CRANN

Length of the sample < electron mean free path



- Electrons are viewed as waves
- Solve Schrodinger equation and find the eigenmodes
- Calculate transmission probability of the eigenmodes
- “Conductance is transmission”

$$G = \frac{2e^2}{h} \sum_{n=1}^{N} T_n$$

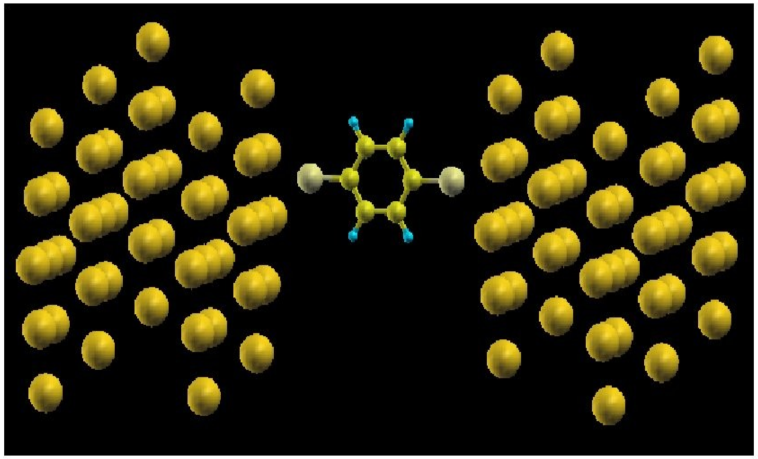
Landauer formula

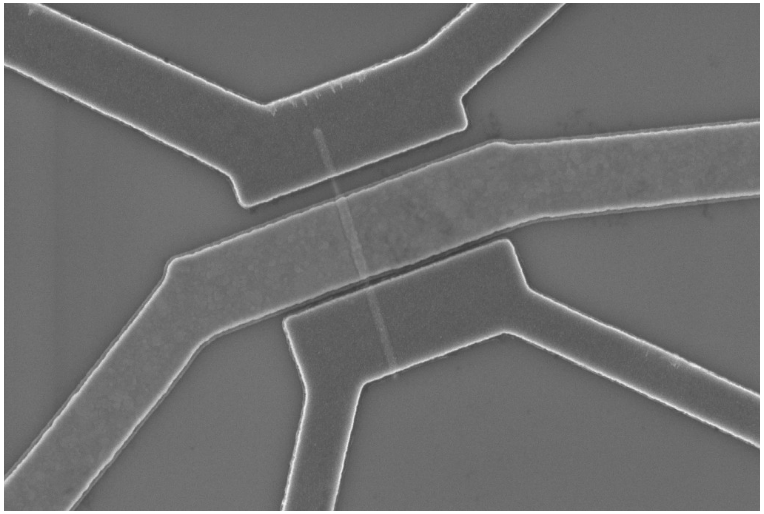
- Resistance only comes from the contacts

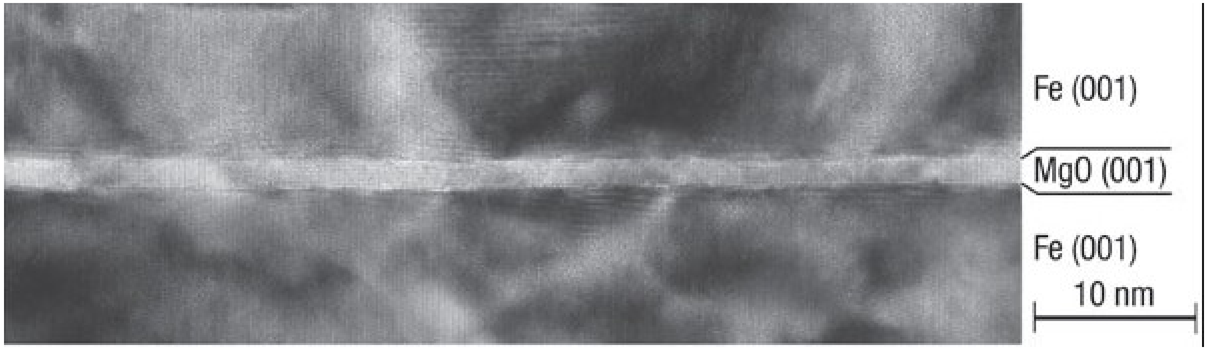
S. Datta, **Electronic Transport in Mesoscopic Systems**, Cambridge University Press (1995)

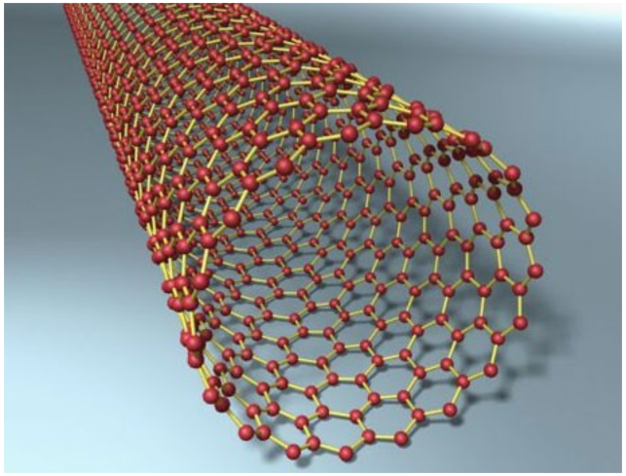
Quantum transport: ballistic regime

Examples of ballistic conductors

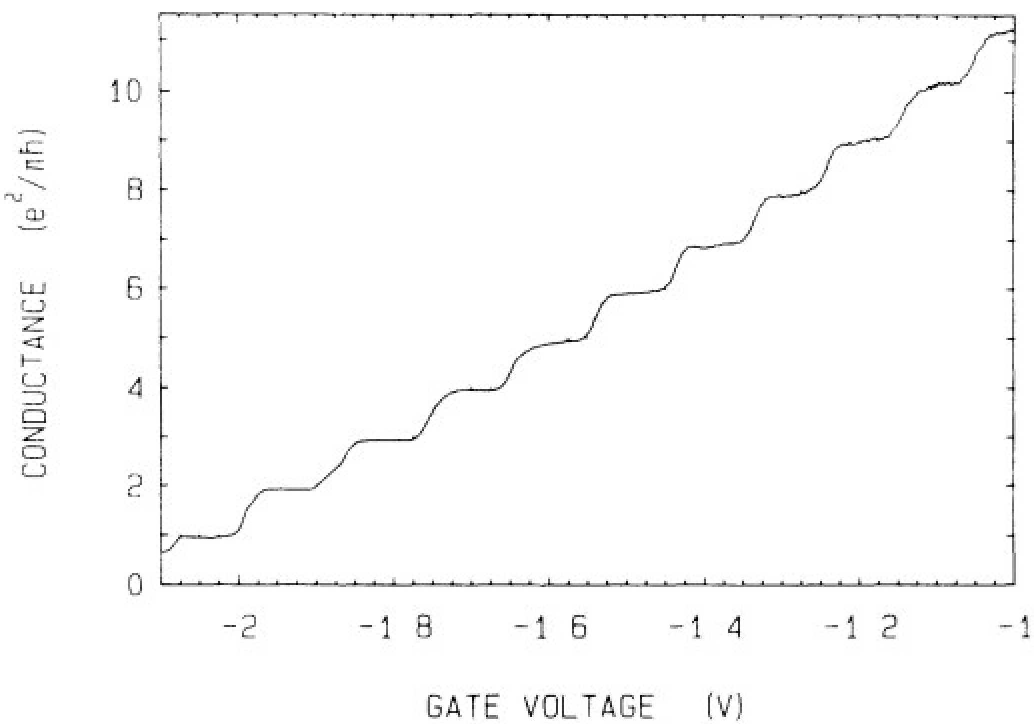








Quantum transport: ballistic regime



B.J. Van Wees, Phys. Rev. Lett. **60**, 848 (1988)

$$G = \frac{2e^2}{h} \sum_{n=1}^{N} T_n$$

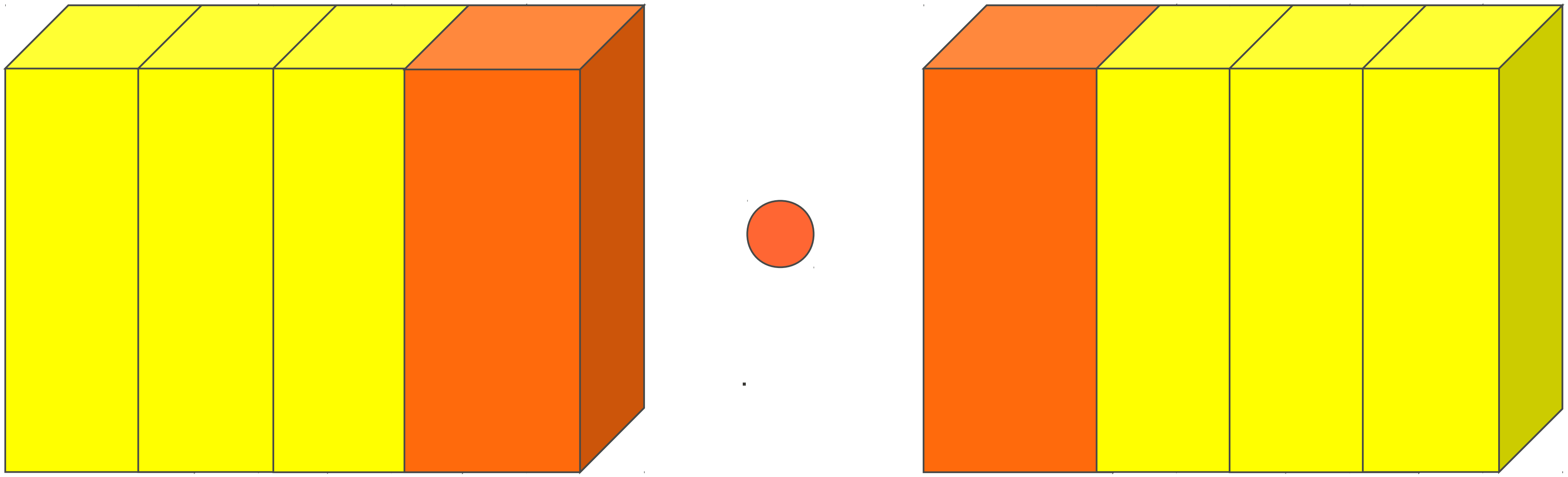
Quantum transport: ballistic regime

“Conductance is transmission”

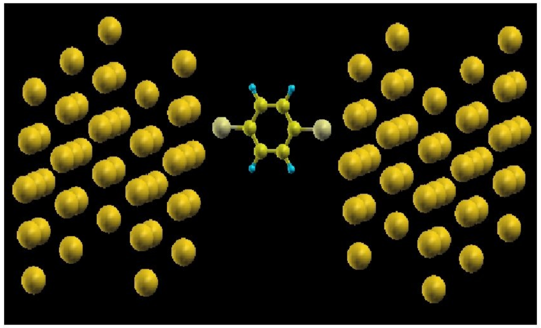
$$G = \frac{2e^2}{h} \sum_{n=1}^{N} T_n$$

How can we calculate the transmission for “real” systems?

Quantum transport

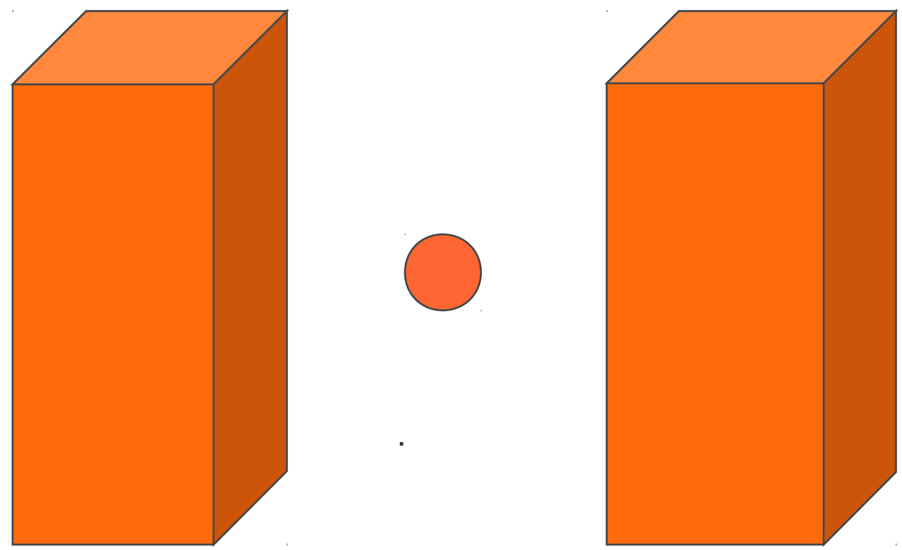


$$H_L + H_{LM} + H_M + H_{MR} + H_R$$



Quantum transport

$\Sigma_L +$

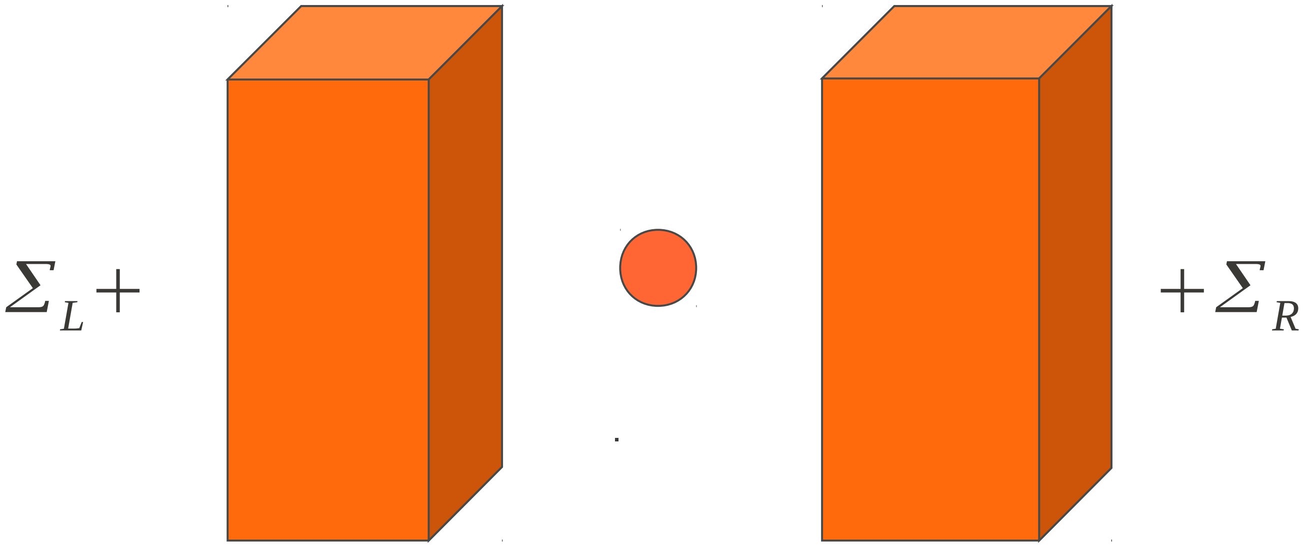


$+\Sigma_R$

$$H_M + \Sigma_R + \Sigma_L$$

A.R. Rocha et al., Phys. Rev. B **73**, 085414 (2006)
I. Rungger and S. Sanvito, Phys. Rev. B **78**, 035407 (2008)

Quantum transport



$$G(E) = [E - H_M - \Sigma_R(E) - \Sigma_L(E)]^{-1}$$

Quantum transport

$$G(E) = [E - H_M - \Sigma_R(E) - \Sigma_L(E)]^{-1}$$

$$\Gamma_{L(R)}(E) = i[\Sigma_{L(R)}(E) - \Sigma^{\dagger}_{L(R)}(E)]$$

$$\boxed{T(E) = \mathrm{Tr}[\Gamma_L(E) G(E)^{\dagger} \Gamma_R(E) G(E)]}$$

The Theoretical Tool: *Smeagol*

CRANN

- DFT based quantum transport
- Scales to large systems (N>10,000 atoms)
- Many functionals (LDA/GGA, LDA+U, LDA+SIC...)
- Spin-polarized, non-collinear, spin-orbit
- Constrained DFT
- Current induced forces
- Spin-torque
- Andreev reflection
- Molecular dynamics under finite bias (under testing)
- Interfaced with Siesta and with FHI-AIMS (under development)
- GW based transport (under development)

Smeagol

Non-equilibrium Electronic Transport

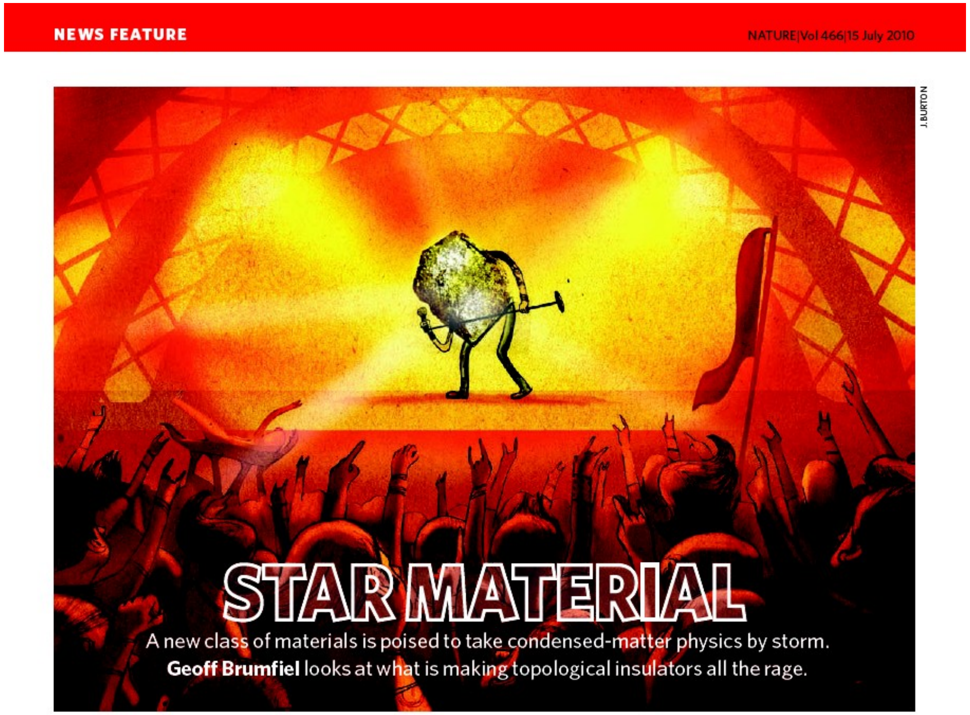
www.smeagol.tcd.ie

Initial development by A.R. Rocha and S. Sanvito (Dublin)
in collaboration with C. Lambert (Lancaster)
Actual full-time maintainer I. Rungger (Dublin)

- Scratch course on electronic transport
- Topological insulators (Kane-Mele model/Bi_2Se_3)
- Kondo impurity in a topological insulator

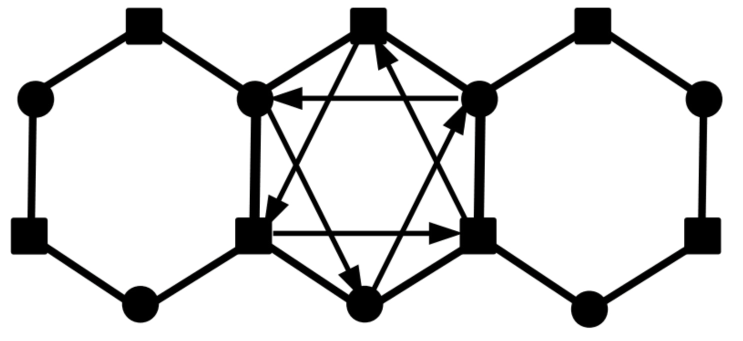
Application: Topological Insulators

CRANN



Application: Topological Insulators

$$H_{Haldane} = t \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \Delta \sum_i \xi_i c_i^{\dagger} c_i + t_2 \sum_{\langle\langle i,j \rangle\rangle} e^{i\nu_{ij}\phi} c_i^{\dagger} c_j$$



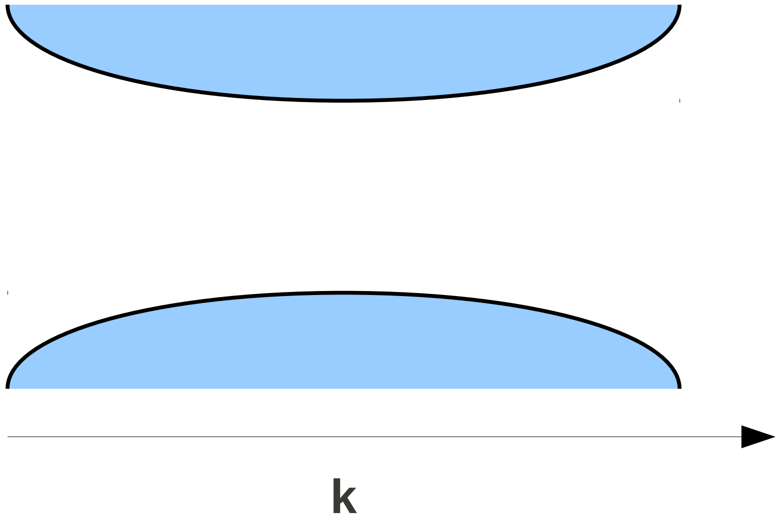
F.D.M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988)

Application: Topological Insulators

$$H_{Haldane} = t\sum_{\langle ij\rangle} c_i^\dagger c_j + \Delta\sum_i \xi_i c_i^\dagger c_i + t_2 \sum_{\langle\langle i,j\rangle\rangle} e^{i\nu_{ij}\phi} c_i^\dagger c_j$$

Kane-Mele model

$$H = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} = \begin{pmatrix} H_{Haldane} & 0 \\ 0 & H_{Haldane} \end{pmatrix}$$



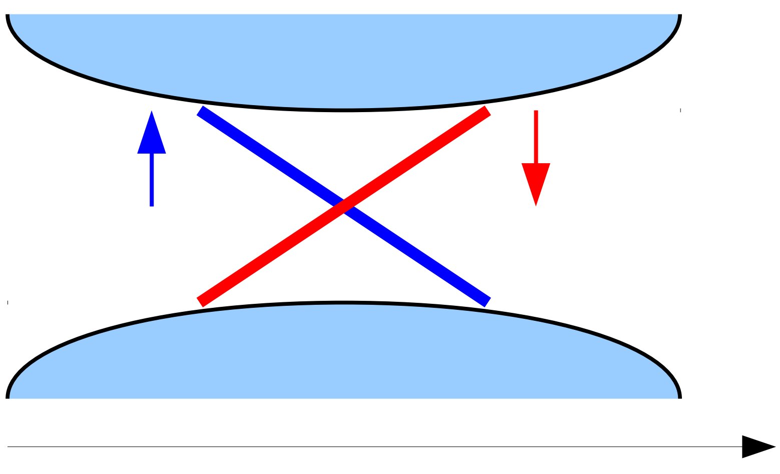
C.L. Kane and E.J .Mele, Phys. Rev. Lett., **95**, 146802 (2005)

Application: Topological Insulators

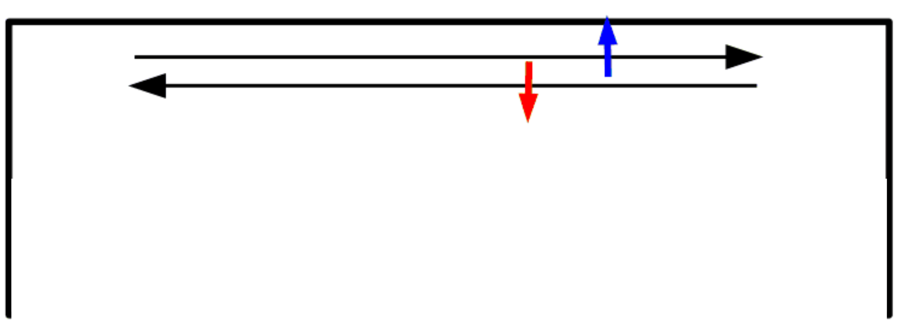
$$H_{Haldane} = t\sum_{\langle ij\rangle} c_i^\dagger c_j + \Delta\sum_i \xi_i c_i^\dagger c_i + t_2 \sum_{\langle\langle i,j\rangle\rangle} e^{i\nu_{ij}\phi} c_i^\dagger c_j$$

Kane-Mele model

$$H = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} = \begin{pmatrix} H_{Haldane} & 0 \\ 0 & H_{Haldane} \end{pmatrix}$$



k



C.L. Kane and E.J. Mele, Phys. Rev. Lett., **95**, 146802 (2005)

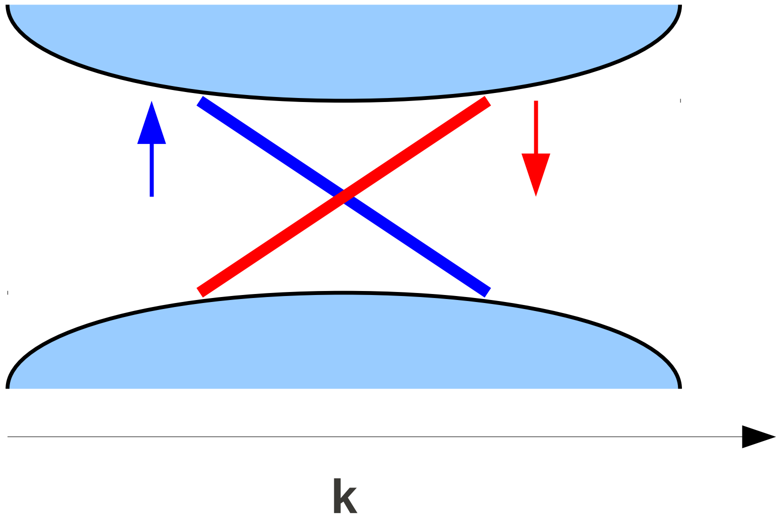
Application: Topological Insulators

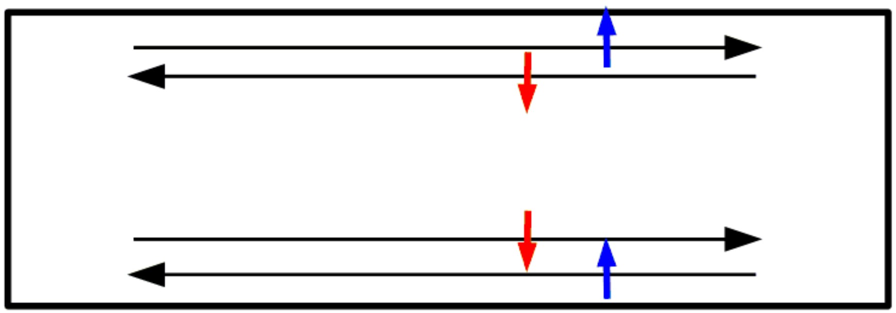
CRANN

$$H_{Haldane} = t\sum_{\langle ij\rangle} c_i^\dagger c_j + \Delta \sum_i \xi_i c_i^\dagger c_i + t_2 \sum_{\langle\langle i,j\rangle\rangle} e^{i\nu_{ij}\phi} c_i^\dagger c_j$$

Kane-Mele model

$$H = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} = \begin{pmatrix} H_{Haldane} & 0 \\ 0 & H_{Haldane} \end{pmatrix}$$

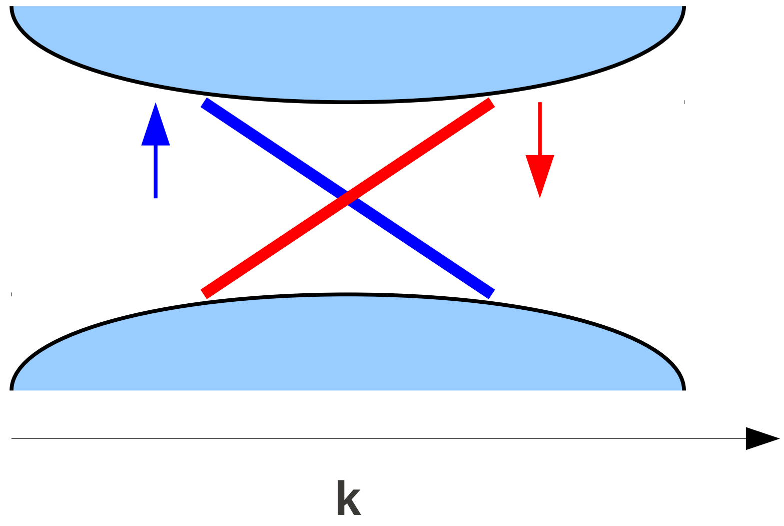


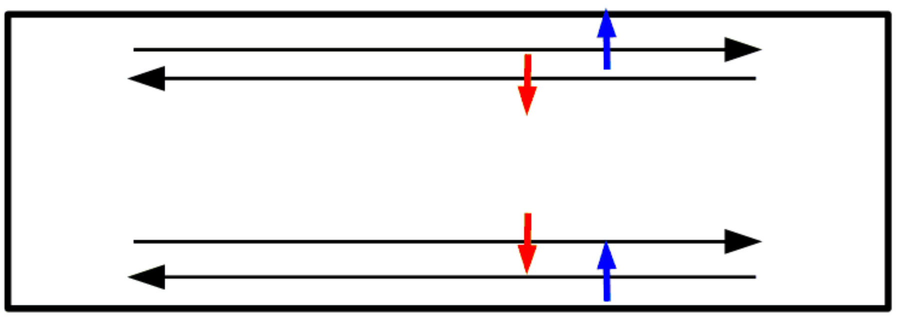


C.L. Kane and E.J. Mele, Phys. Rev. Lett., **95**, 146802 (2005)

Application: Topological Insulators

CRANN

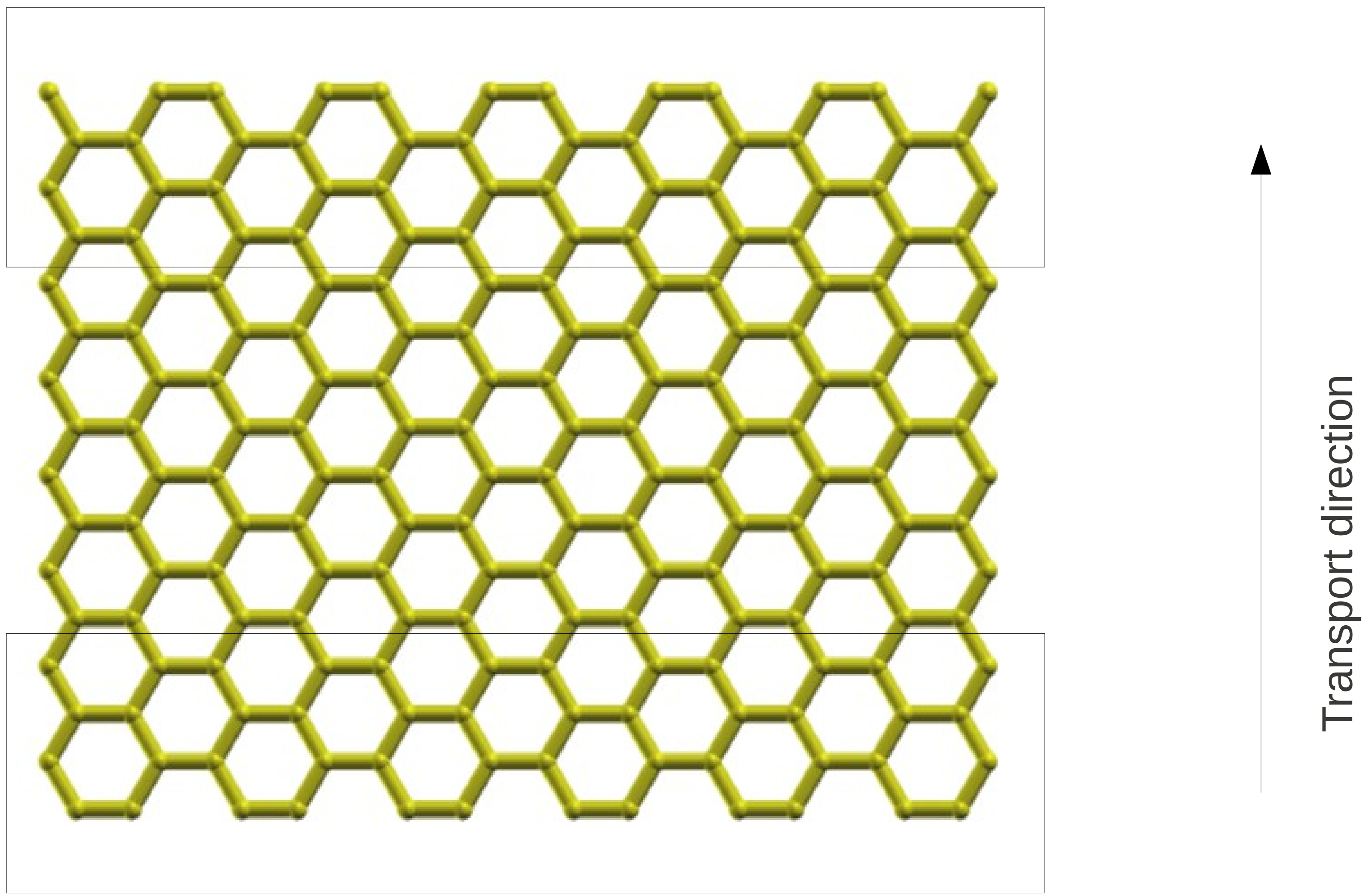




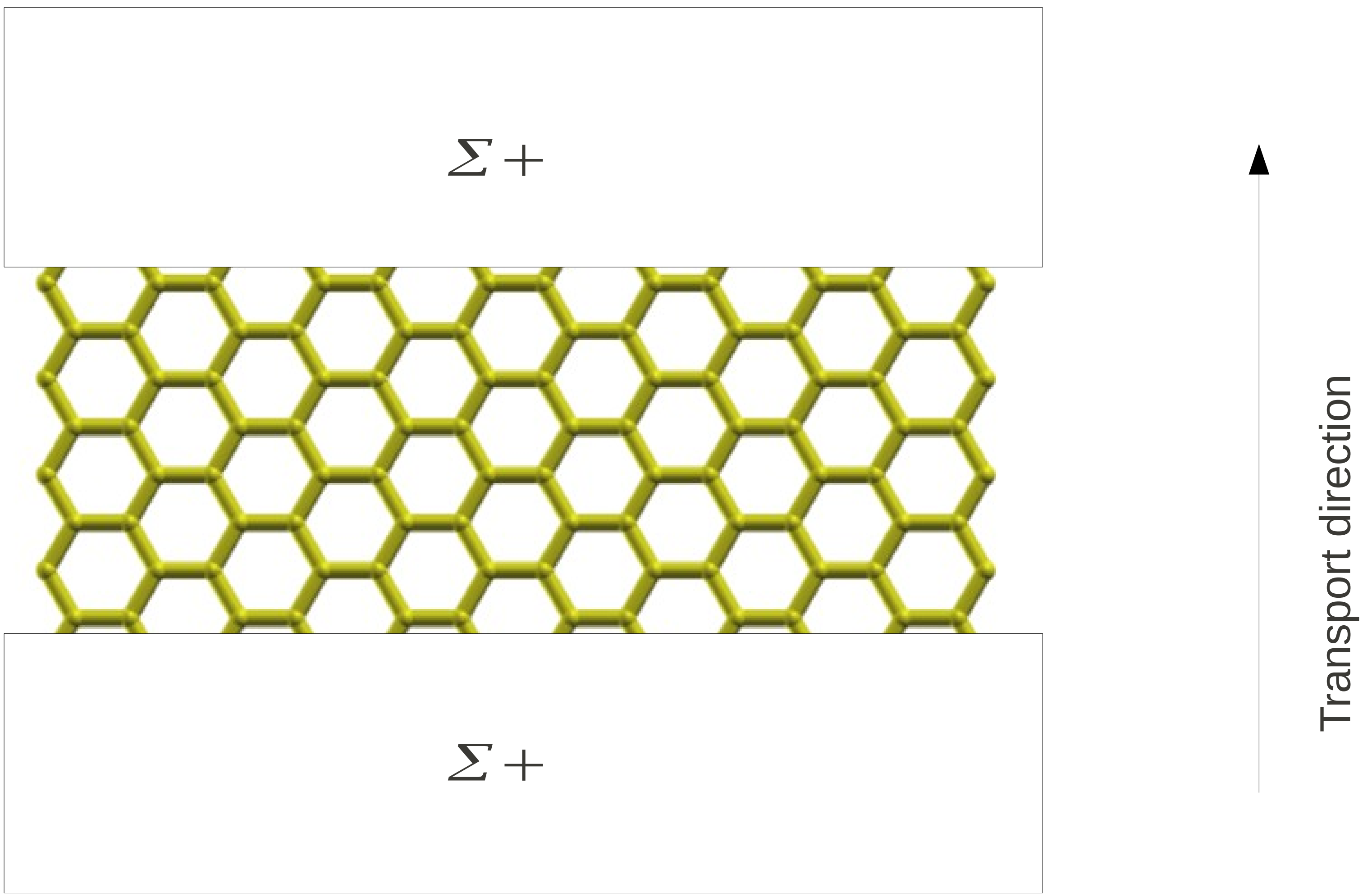
Edge states are protected by time reversal symmetry

- Kramers degeneracy protects band crossing
- Elastic backscattering is forbidden
- Conservation of S_z not essential

Application: Topological Insulators

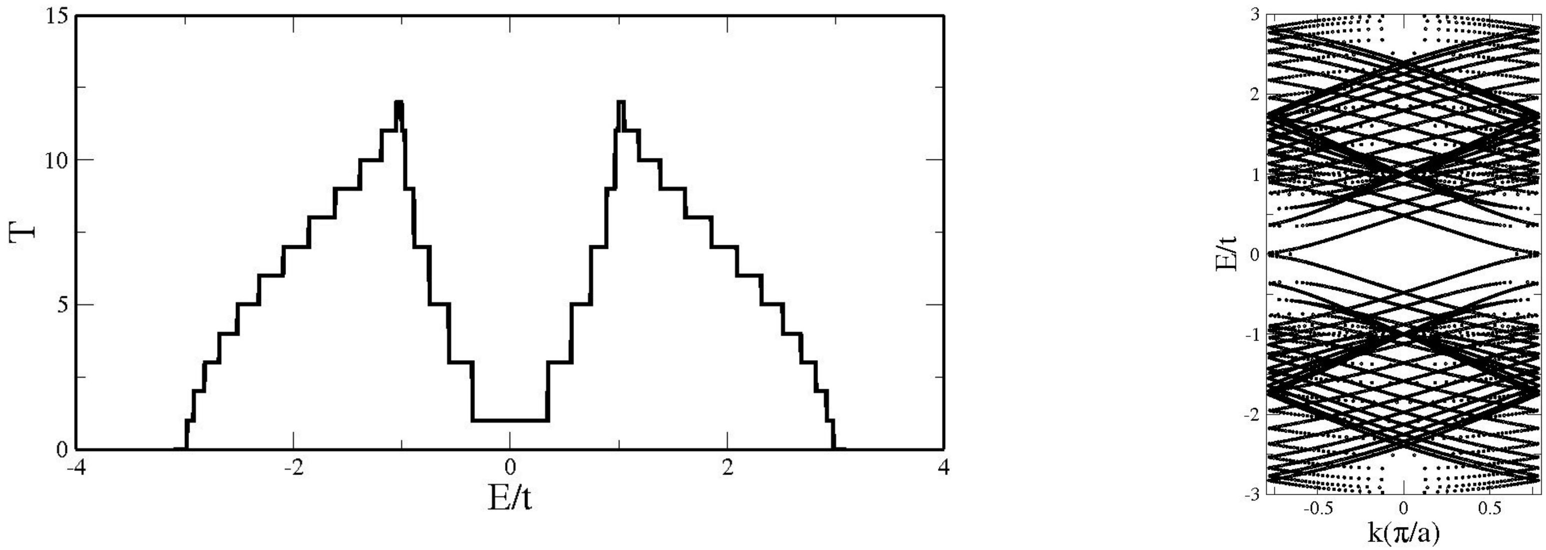


Application: Topological Insulators

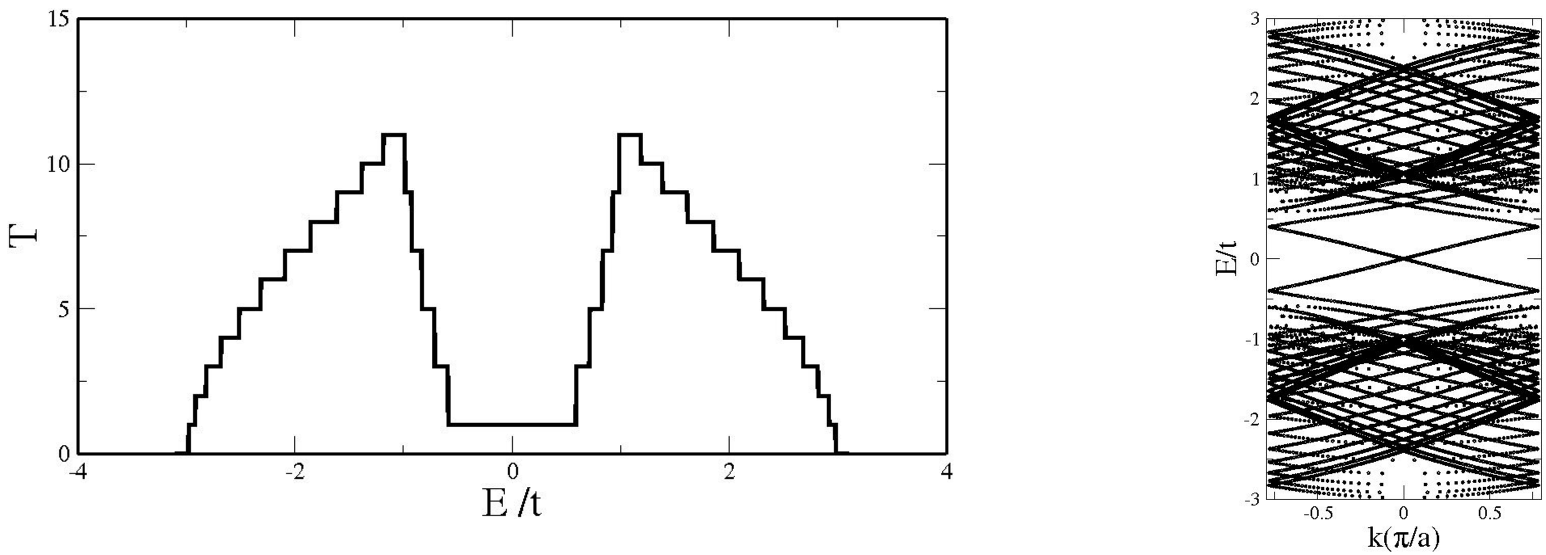


Application: Topological Insulators

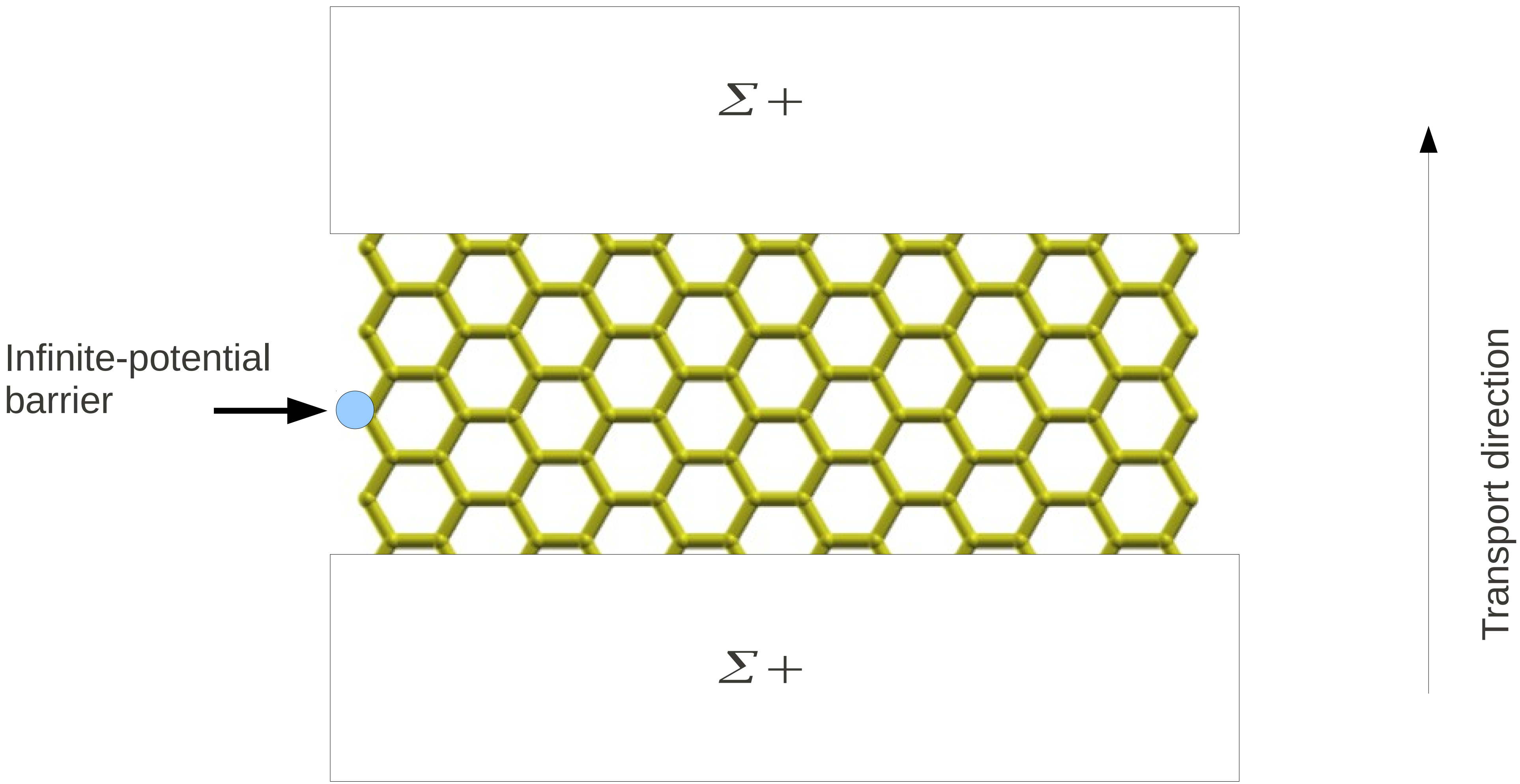
Graphene nanoribbon



Kane-Mele nanoribbon

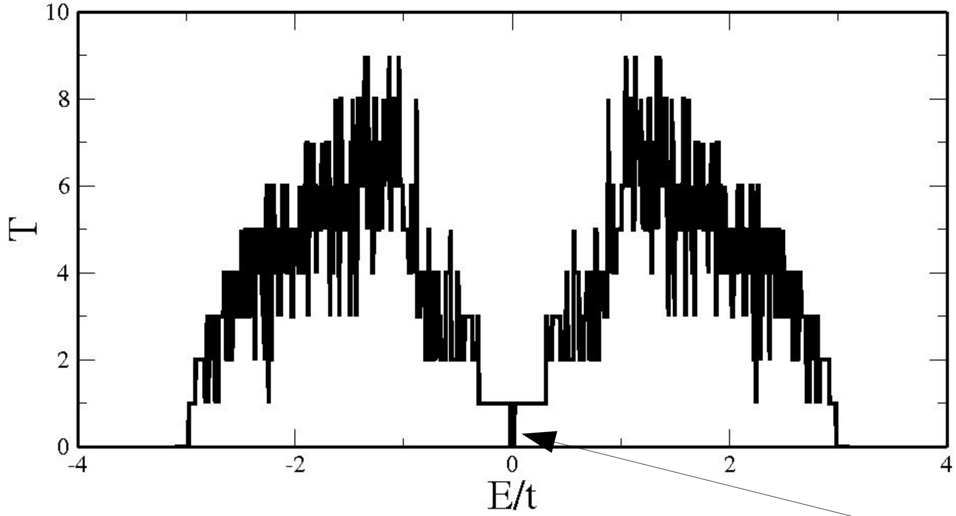


Application: Topological Insulators



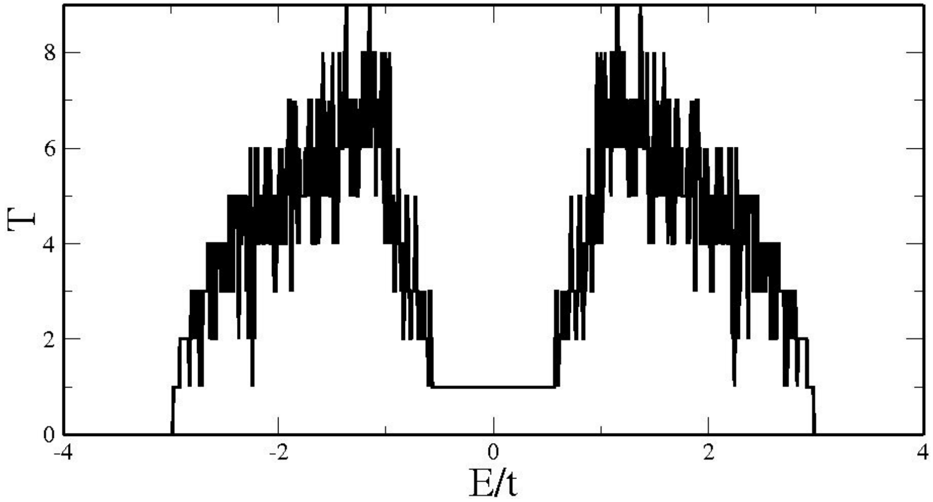
Application: Topological Insulators

Graphene nanoribbon



Transmission drops to zero

Kane-Mele nanoribbon



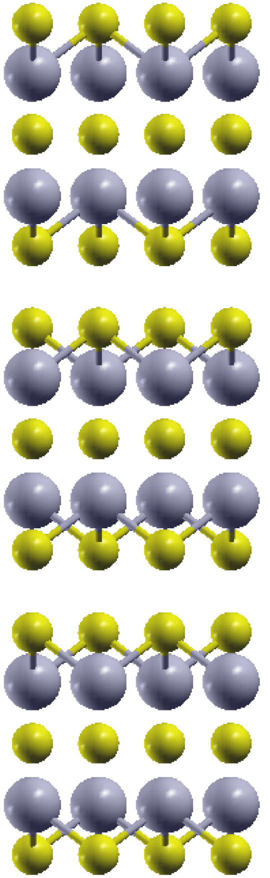
Edge states are protected by time reversal symmetry

- Kramers degeneracy protects band crossing
- Elastic backscattering is forbidden

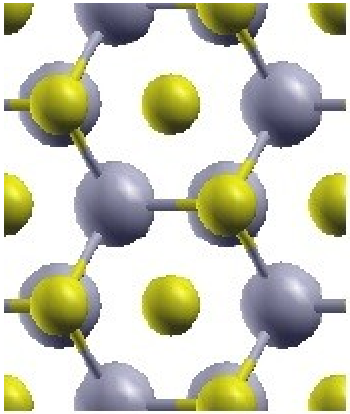
Application: Topological Insulators

Bi_2Se_3

Side view

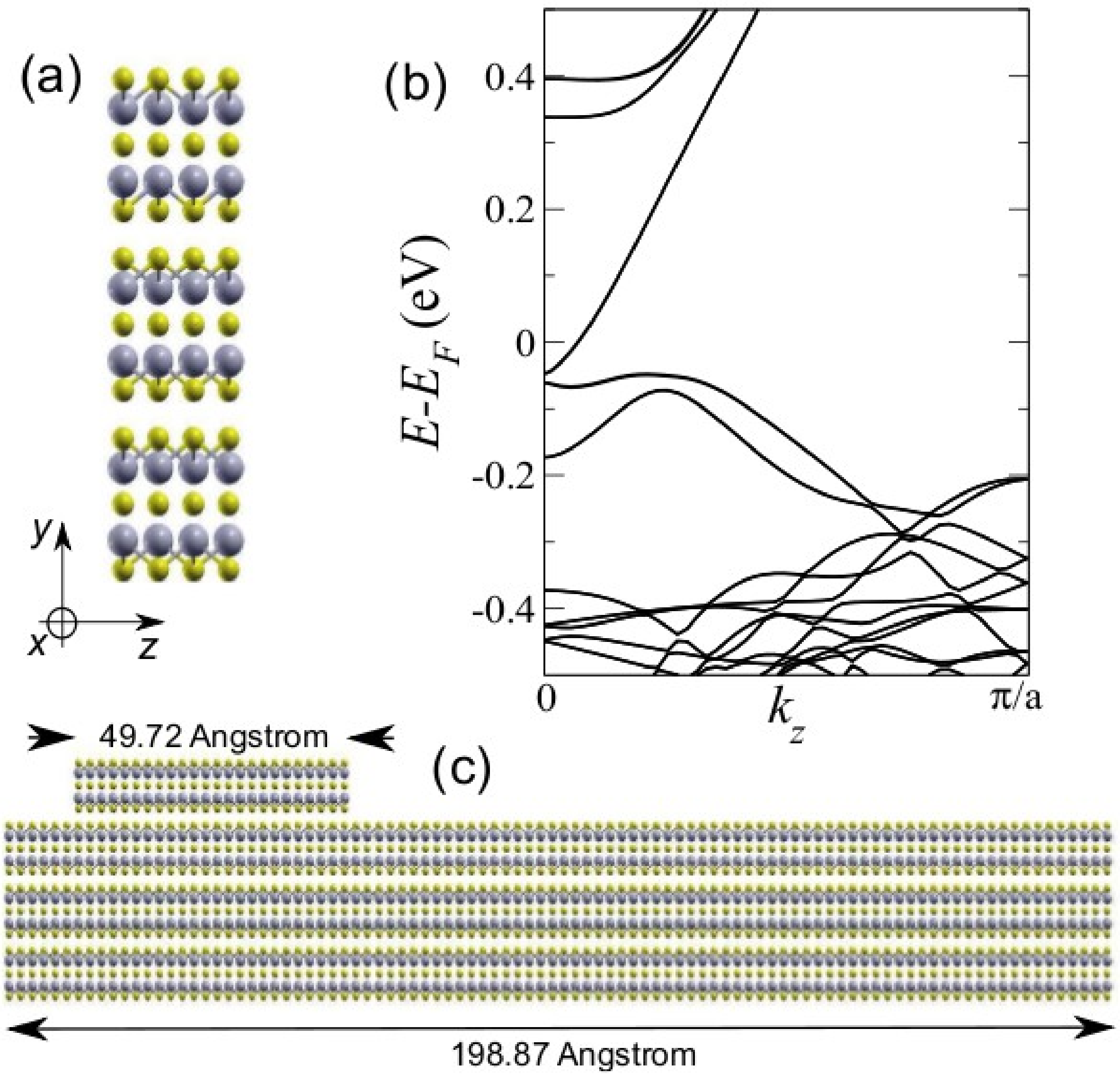


Top view



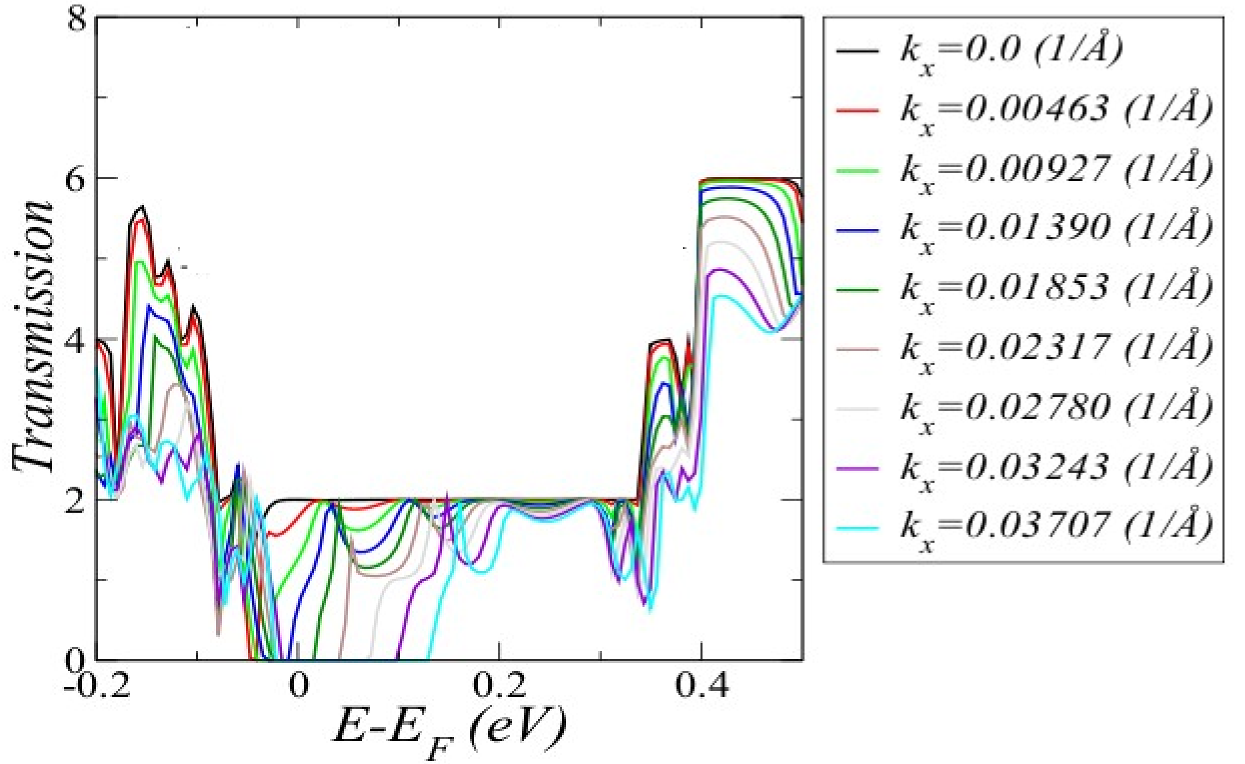
H. Zhang et al., Nat. Phys. **5**, 438 (2009)
Y. Xia et al., Nat. Phys. **5**, 398 (2009)

Application: Topological Insulators



Application: Topological Insulators

For Bi_2Se_3



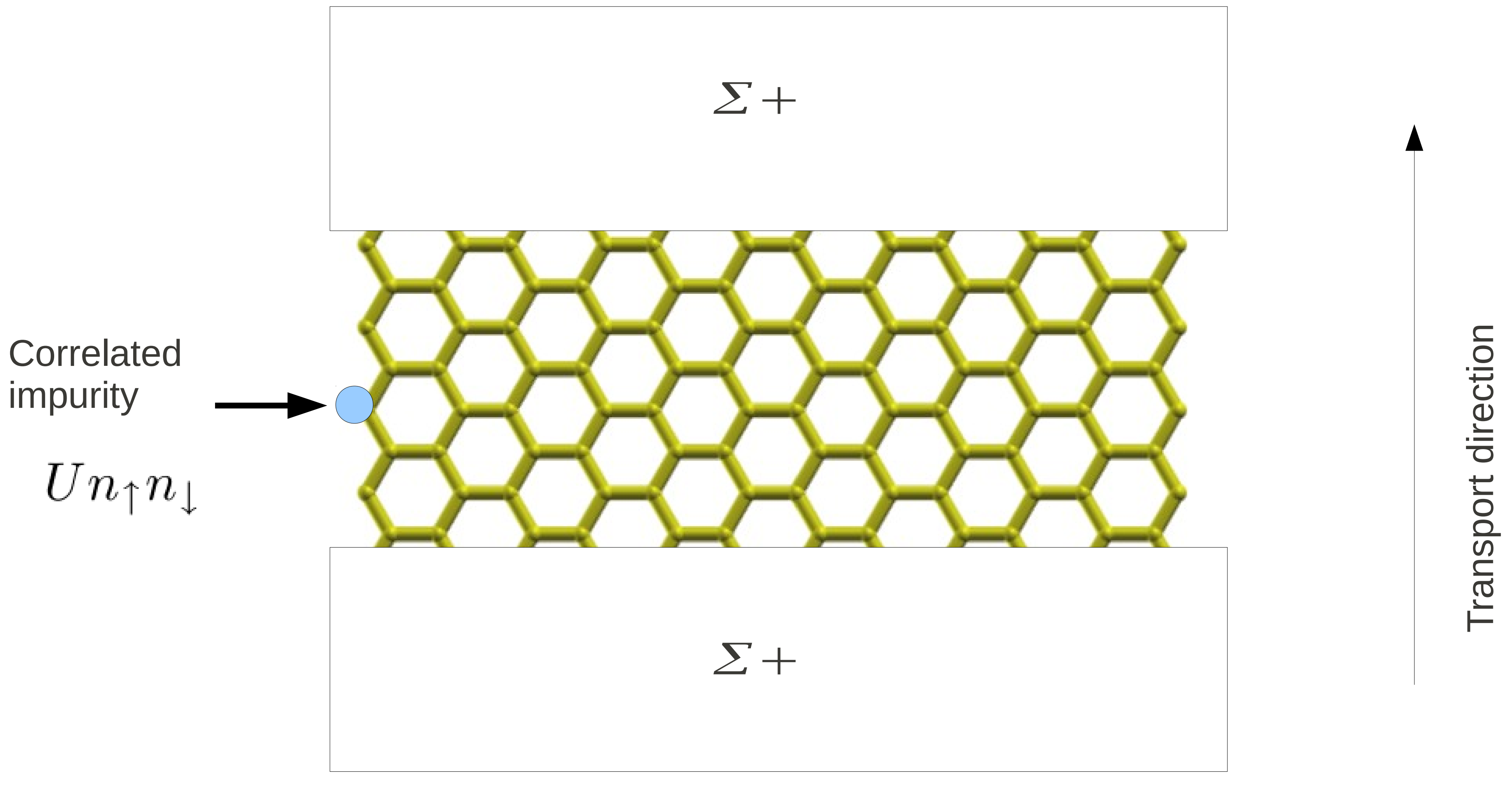
A. Narayan, I. Rungger, A. Droghetti and S. Sanvito, in preparation

- Basic course on electronic transport

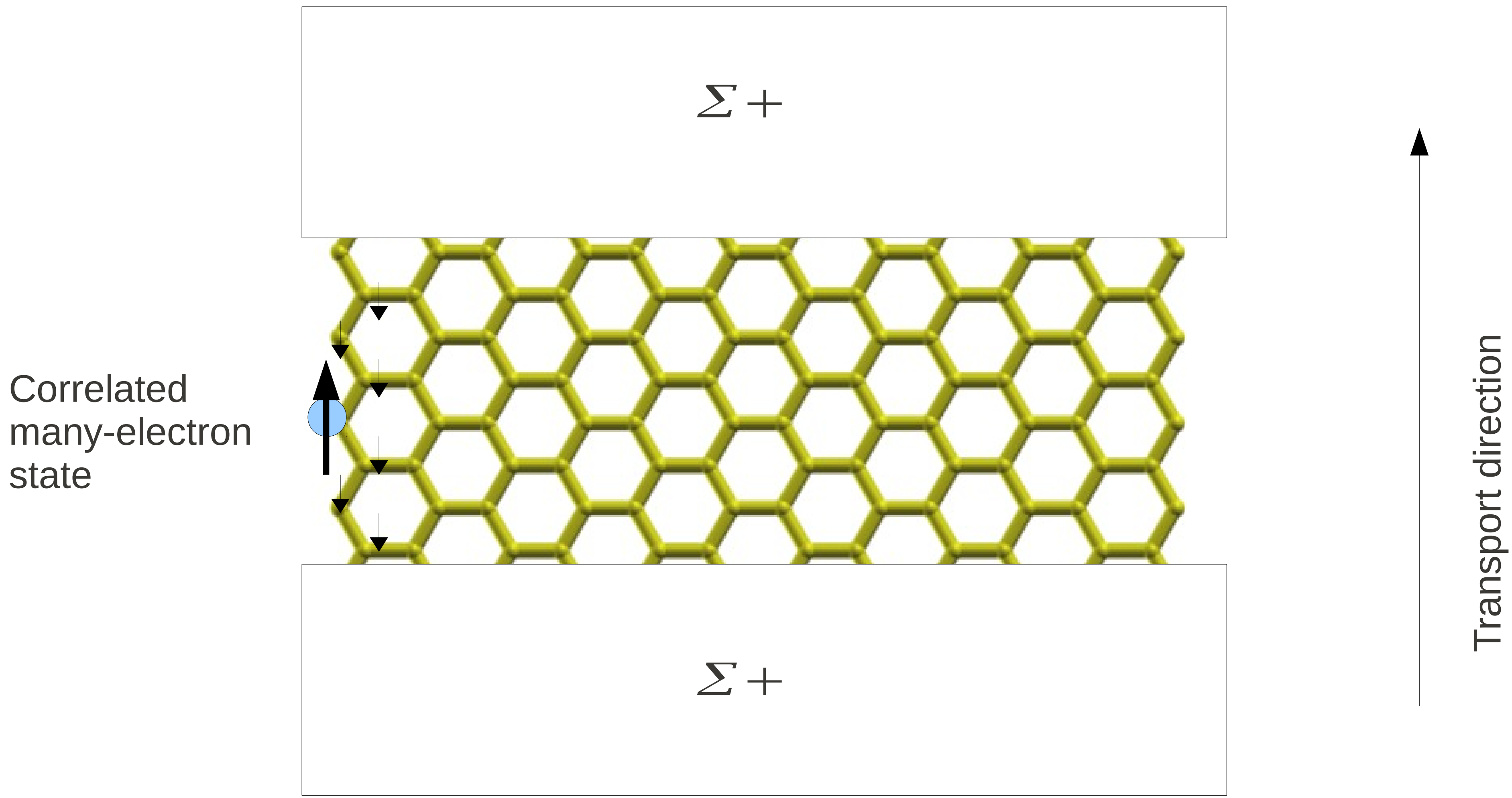
- Topological insulators (Kane-Mele model/Bi_2Se_3)

- Kondo impurity in a topological insulator

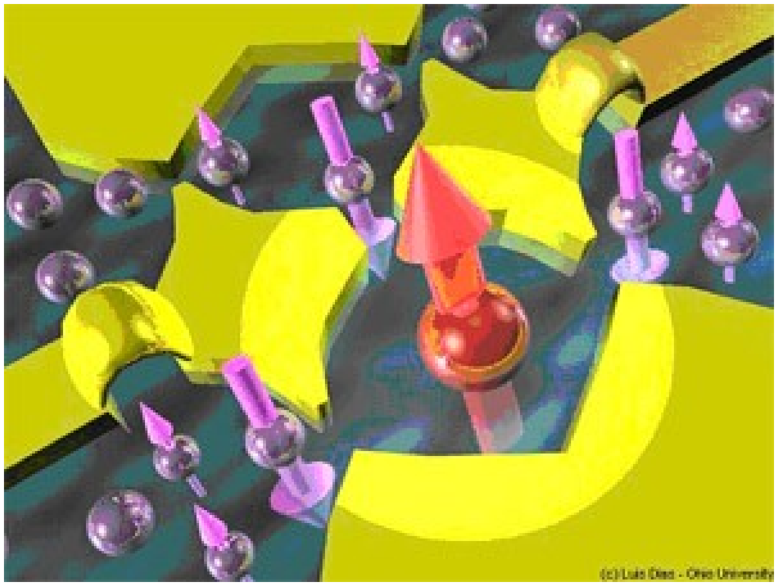
Application: Topological Insulators



Kondo effect

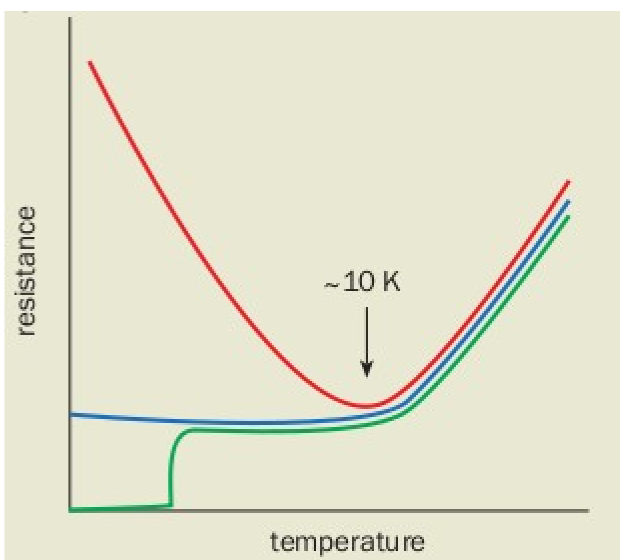


Kondo effect

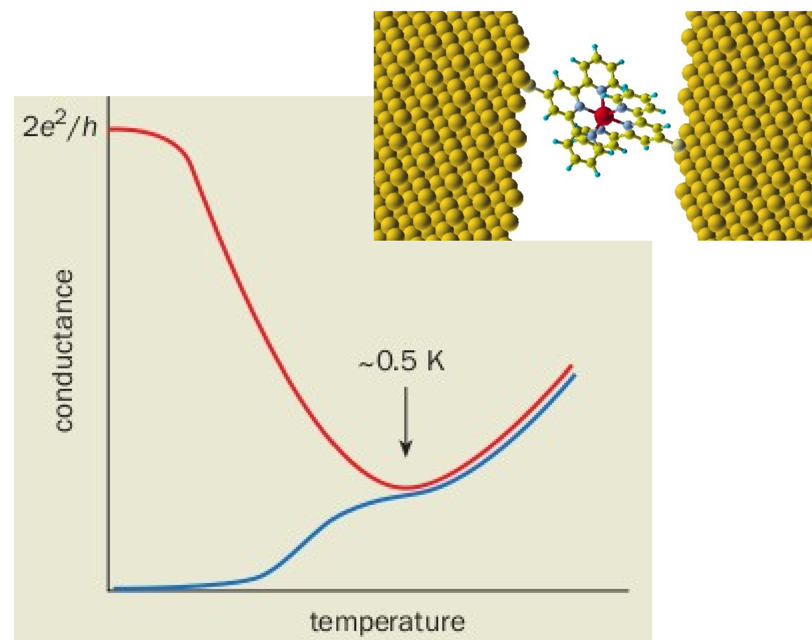


L. Kouwenhoven and L.Glazman,
Revival of Kondo effect, Physics World, January 2001

A.C. Hewson
The Kondo Problem to Heavy Fermion,
Cambridge University Press 1993



In metals



In single molecules devices

$$\begin{pmatrix} G_0^{ii} & G_0^{id} \\ G_0^{di} & G_0^{dd} \end{pmatrix}$$

$$\begin{pmatrix} G^{ii} & G^{id} \\ G^{di} & G^{dd} \end{pmatrix} = \begin{pmatrix} G_0^{ii} & G_0^{id} \\ G_0^{di} & G_0^{dd} \end{pmatrix} + \begin{pmatrix} G_0^{ii} & G_0^{id} \\ G_0^{di} & G_0^{dd} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \Sigma^{dd} \end{pmatrix} \begin{pmatrix} G^{ii} & G^{id} \\ G^{di} & G^{dd} \end{pmatrix}$$

Dyson Equation

The algorithm

CRANN

$$G_o^{dd}(i\omega_n) \rightarrow$$

Continuous-time quantum Monte Carlo

E.Gull, A.J. Millis, A.I. Lichtenstein, A.N. Rubtsov, M. Troyer, P. Werner, Rev. Mod. Phys. **83**, 349 (2011)

$$\omega_n = \frac{(2n+1)\pi}{\beta}$$

$$\downarrow$$

$$\Sigma^{dd}(i\omega_n)$$

$$G^{dd}(i\omega_n)$$

$$\downarrow$$

Analytic continuation

$$i\omega_n \rightarrow \omega - i\eta$$

$$\Sigma^{dd}(\omega)$$

Pade approximation

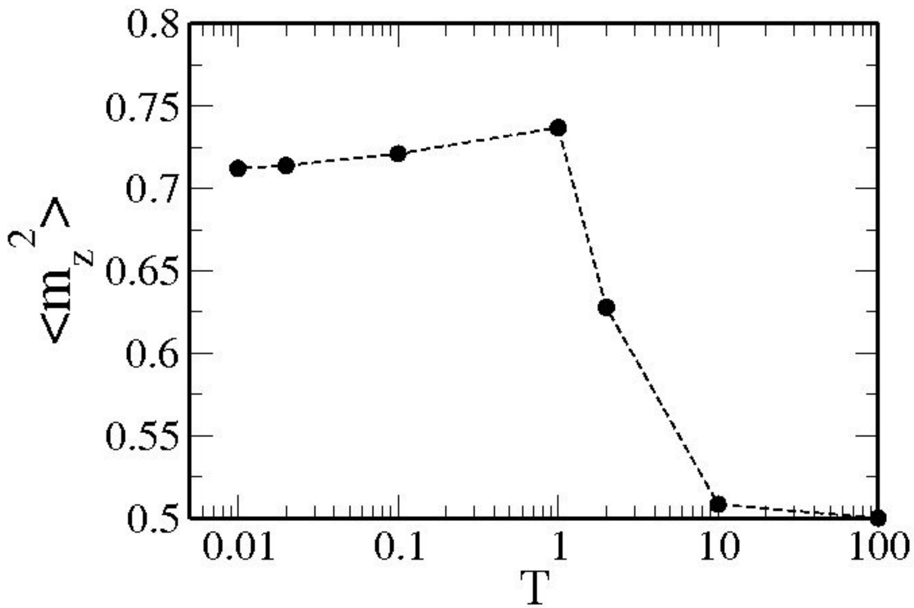
H.J. Vidberg & J.W. Serene, J. Low Temp. Phys. **29**, 179 (1977)

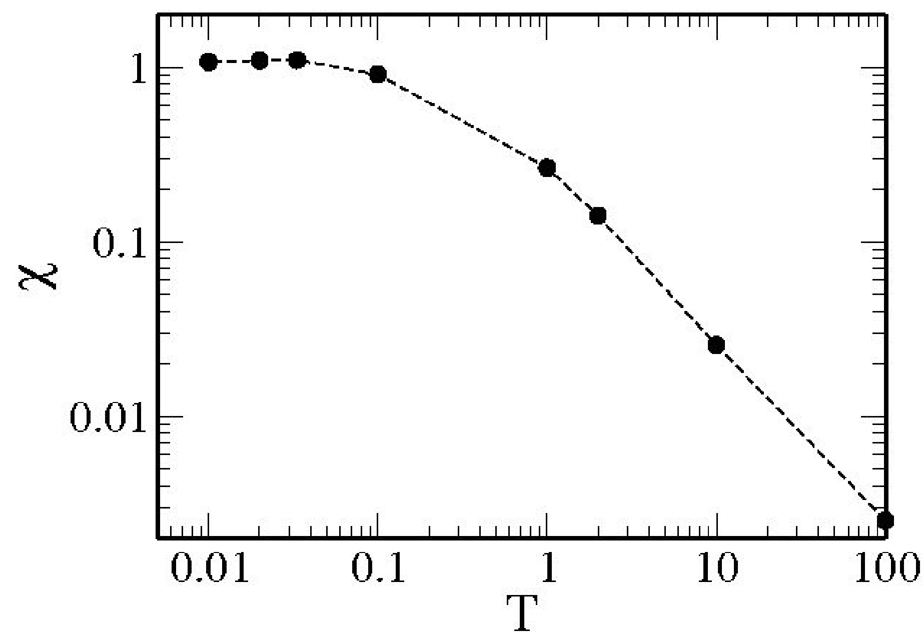
Maximum entropy method

M. Jarrell & J.E. Gubernatis, Phys. Reports **269**, 133 (1996)

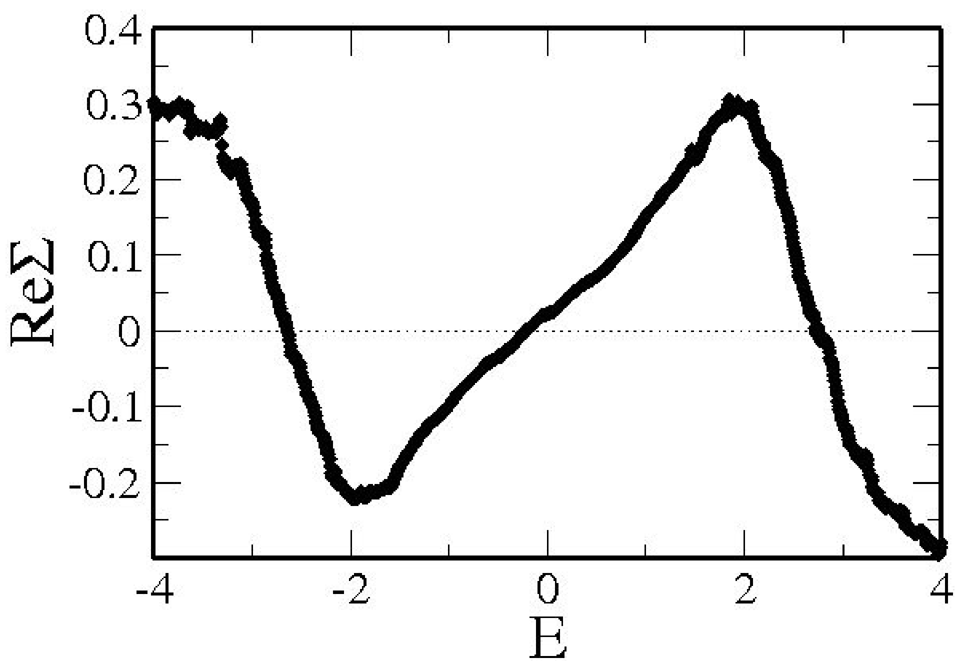
Stochastic optimization

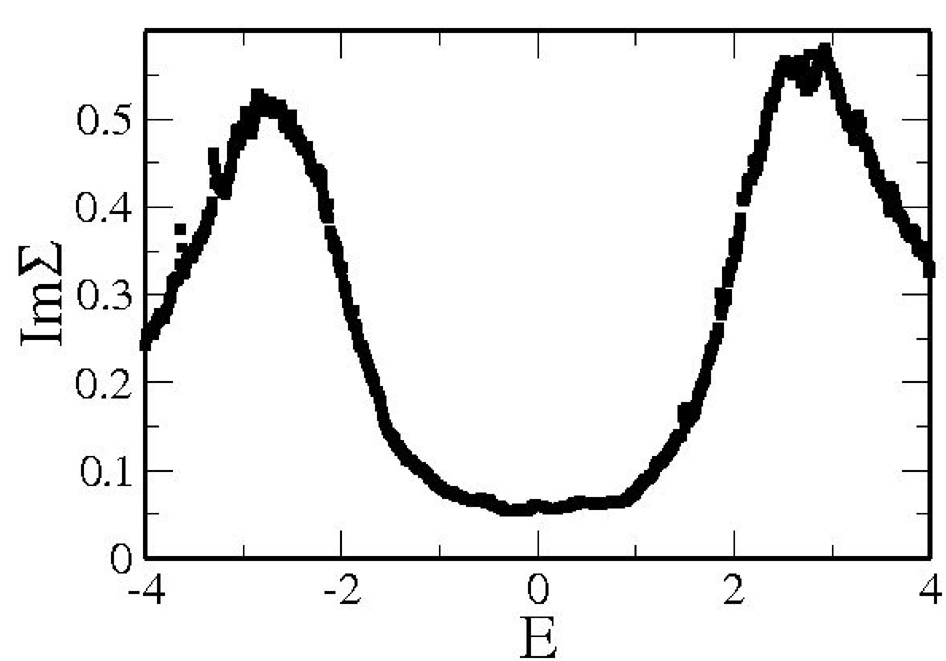
A.S. Mishchenko, Phys. Rev. B **269**, 62 (2000)


0.8
0.75
0.7
0.65
0.6
0.55
0.5
$<m_z^2>$
0.01
0.1
1
10
100
T


1
0.1
0.01
χ
0.01
0.1
1
10
100
T

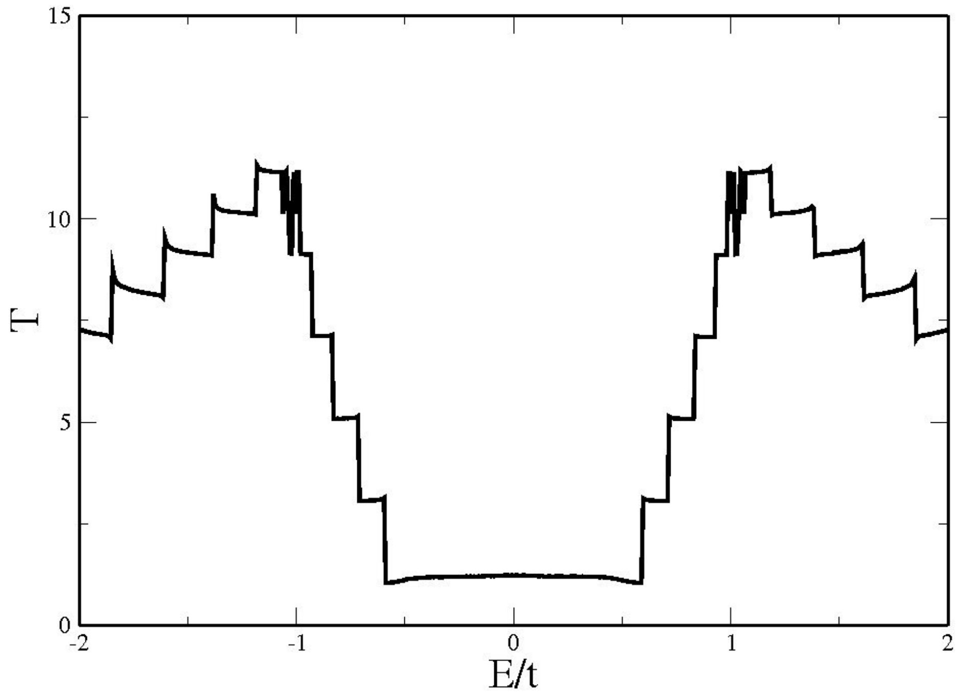
CRANN





$$\begin{pmatrix} G^{ii} & G^{id} \\ G^{di} & G^{dd} \end{pmatrix} = \begin{pmatrix} G_0^{ii} & G_0^{id} \\ G_0^{di} & G_0^{dd} \end{pmatrix} + \begin{pmatrix} G_0^{ii} & G_0^{id} \\ G_0^{di} & G_0^{dd} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \Sigma^{dd} \end{pmatrix} \begin{pmatrix} G^{ii} & G^{id} \\ G^{di} & G^{dd} \end{pmatrix}$$

$$T(E) = \mathrm{Tr}[\Gamma_L(E) G(E)^\dagger \Gamma_R(E) G(E)]$$



Transmission

A. Droghetti, I. Rungger, S. Sanvito, in preparation

Conclusions

CRANN

• “Conductance is transmission”.

• Numerical demonstration that back-scattering is forbidden in topological insulators in accordance with low-energy models.

• Kondo screening “protects” the edge state from back-scattering even in presence of magnetic impurities.

• The presented scheme, which allows to study zero-bias transport properties of Kondo systems, can be easily implemented in a DFT+transport code.

Ivan Rungger (Smeagol code maintainer)

Awadhesh Narayan (DFT calculations for Bi_2Se_3)

Stefano Sanvito (the boss)

CRANN

go raibh maith agat

("a thousand good things would be on you")