Computational electronics from atomic principles

- basics of electronic transport

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- Introduction: need for quantum transport from atomic first principles, mini course of quantum transport theory, NEGF-DFT method.
- Spin-orbit: helical spin states in topological insulator Bi_2Se_3.
- Disorder: non-equilibrium vertex correction theory. Roughness scattering.
- Other issues, large systems;
- Summary

Today's field effect transistor:

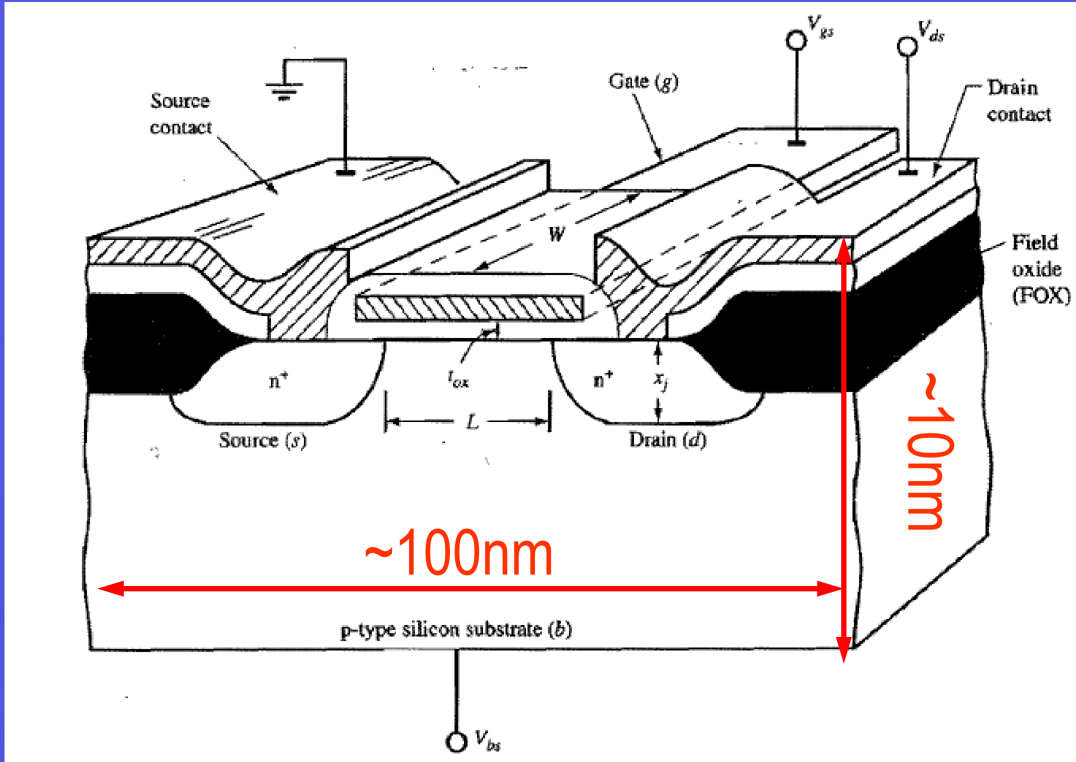


Figure 3.1. Three-dimensional view of basic MOSFET device structure. (After Arora, 1993.)

Picture from Taur and Ning, Fundamentals of Modern VLSI Devices

2011: L=22nm

2013 (?): L=14nm

To model, needs ~10,000 to 70,000 Si atoms in the channel region.

DFT: ~1000 atoms.

One of the many problems of technology: discrete materials

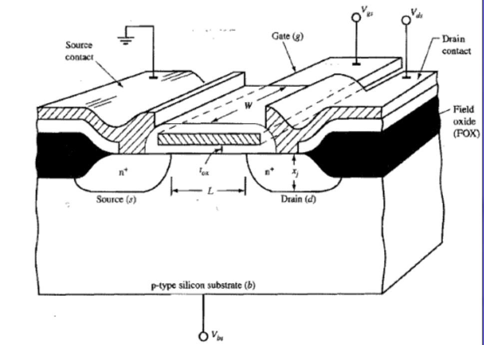


Figure 3.1. Three-dimensional view of basic MOSFET device structure. (After Arora, 1993.)

Picture from Taur and Ning, Fundamentals of Modern VLSI Devices

Huge device to device variability:

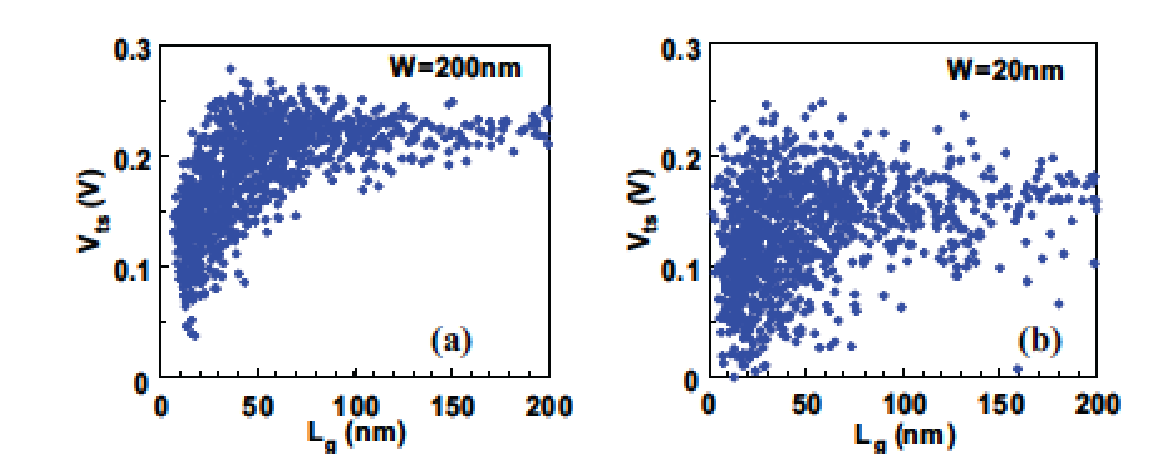


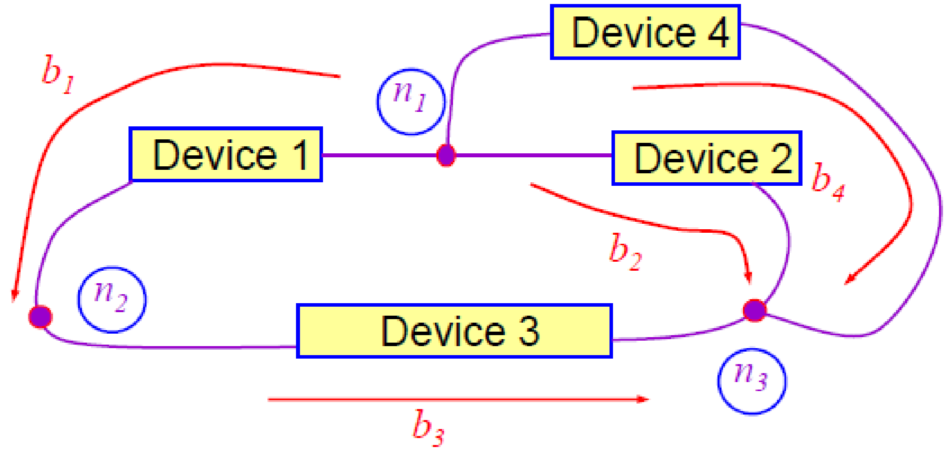
Fig. 1 Experimental saturation threshold voltage, V_{ts}, of NMOS transistors with L_g down to 20nm for (a) width=200nm and (b) width=20nm at V_d=1.0V.

F.L. Yang et al., in *VLSI Technol. Tech. Symp. Dig., pp. 208, June 2007.*

If every transistor behaves differently, difficult to design circuit.

Today's Circuit simulation:

What is a circuit?

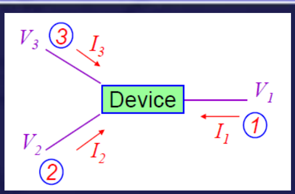


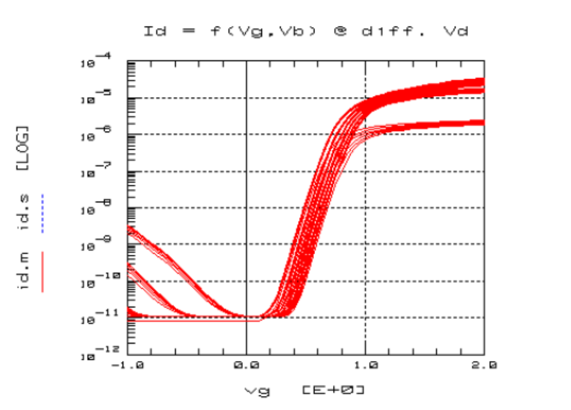
- it represents different devices interconnecting each other
- forming nodes (n_1, n_2, n_3) and branches (b_1, b_2, b_3, b_4)
- for given node voltages, each device calculates its contribution to the branch currents

How do we know device parameters?

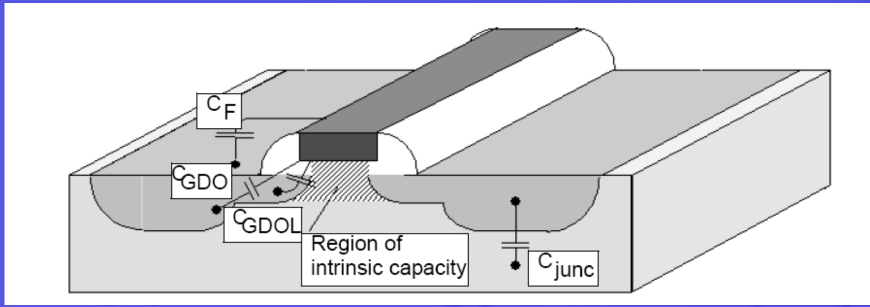
Munsun Chan (HKUST)

Device parameters: measured in foundry

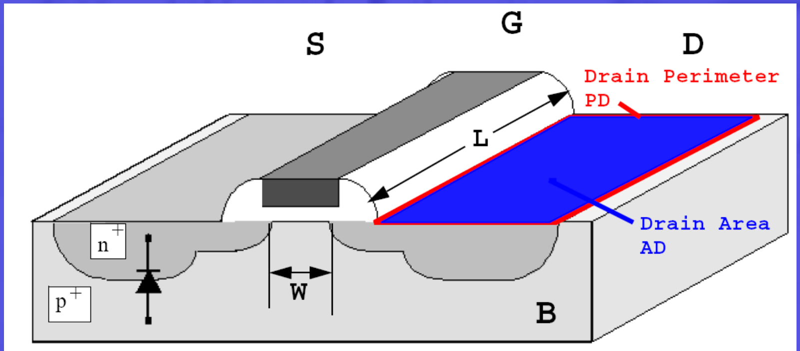




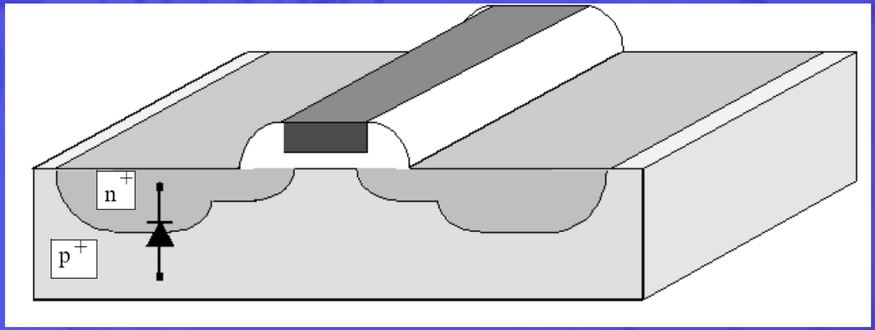
transconductances



capacitance



Geometry scaling



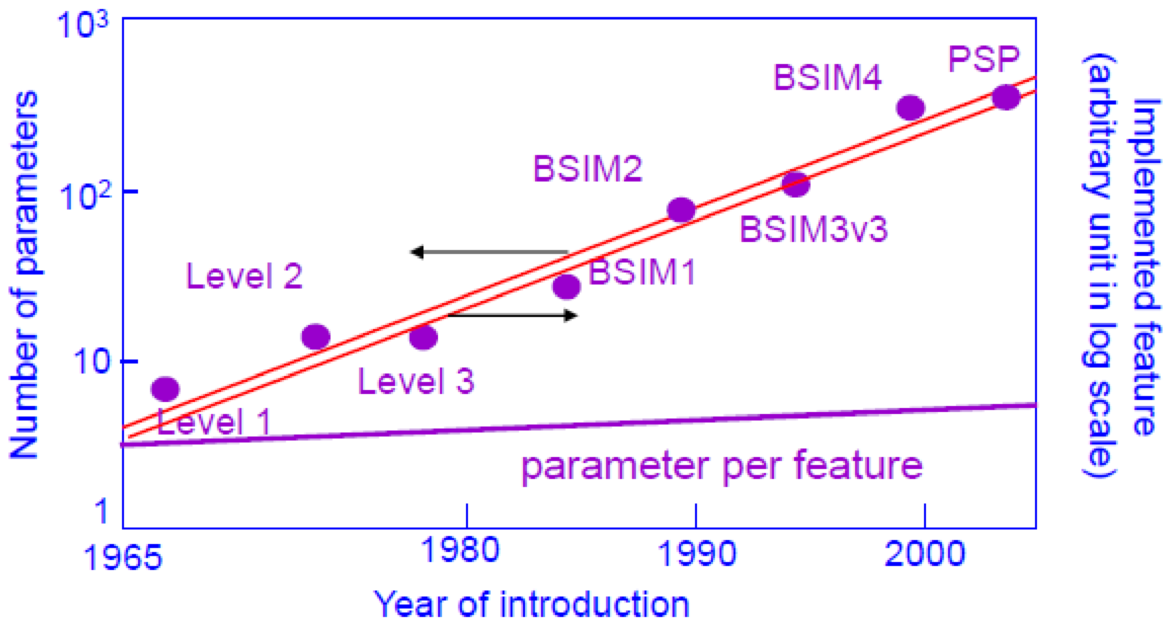
diodes

Several hundred parameters are needed.

Today: the Moore's law of fitting parameters

Number of parameter double every 18 months

Also reflects the complexity in modern technology

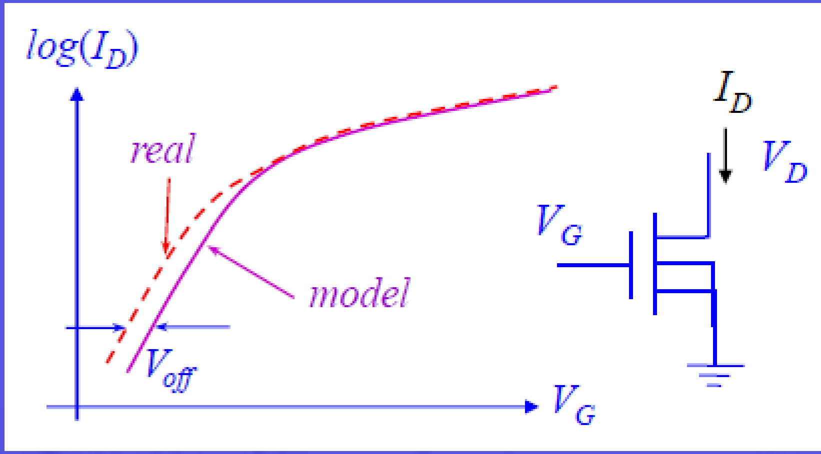


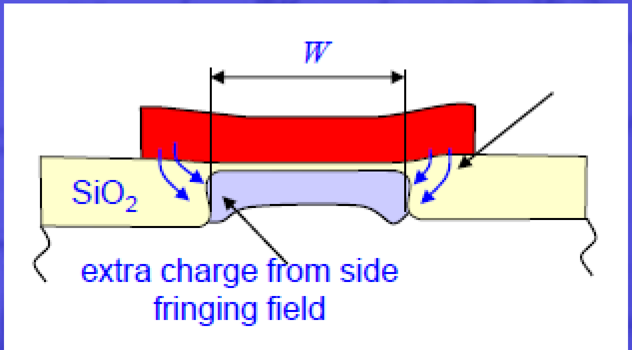
Strong correlation with technology

Munsun Chan (HKUST)

Why there are so many fitting parameters ?

Munsun Chan (HKUST)



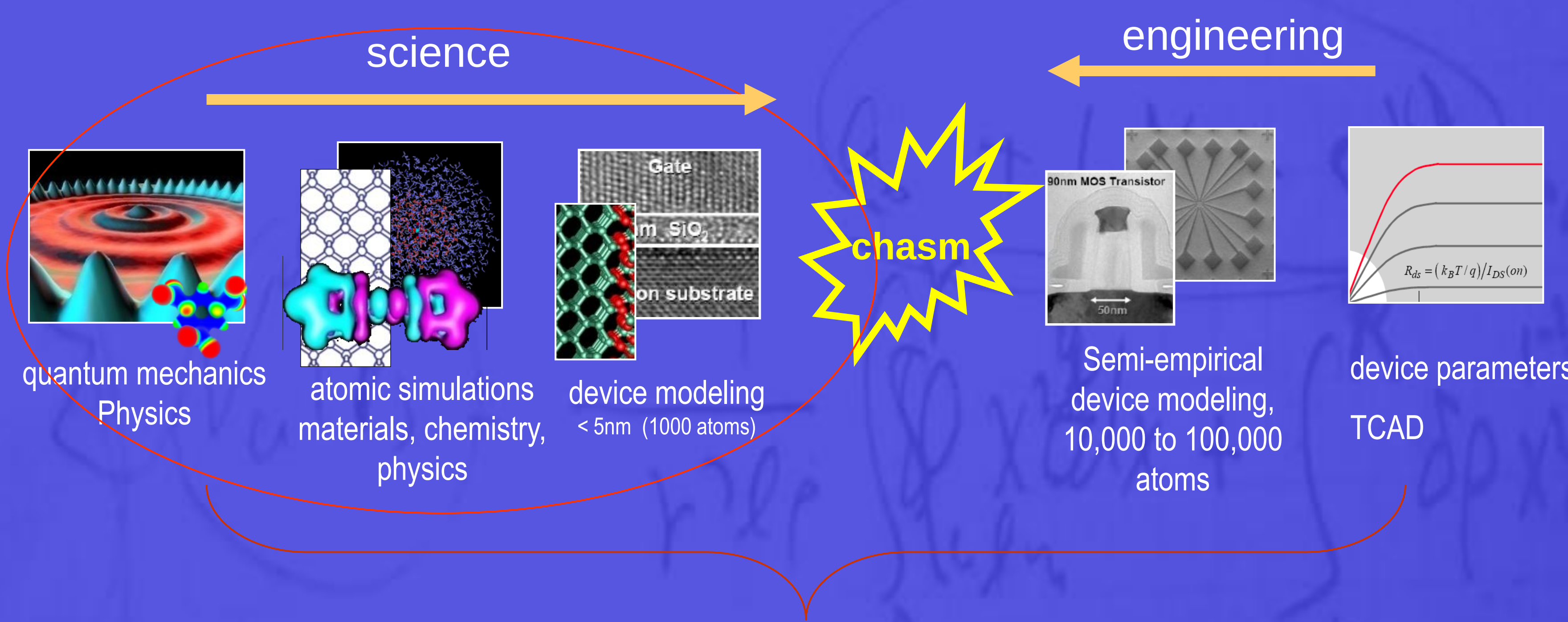


Model can be beautiful, real device can be ugly.

Parameters are added to take into account the fringing field.

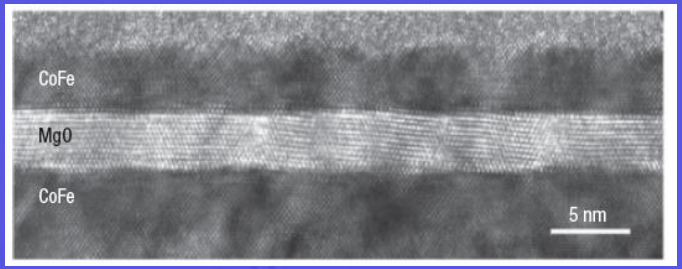
More and more parameters are added to account for changes of device.

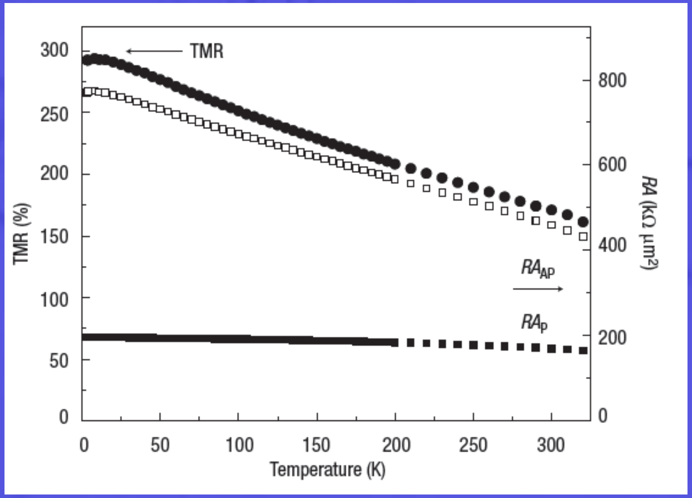
Can we calculate the device parameters?



Quantitative prediction of quantum transport from atomic first principles without any parameter

Computational nanoelectronics: quantum transport





S. Parkin et al. Nature Materials, 3, 862 (2004).

- Quantum tunneling;
- Coherence, decoherence;
- Interference;
- Spintronics;
- Photovoltaics;
- Topological insulators;
- Quantum materials;
- …

Computational nanoelectronics must include:

- discrete materials – atomic first principles;
- quantum transport in discrete materials;
- non-equilibrium quantum transport conditions;
- reasonably accurate results: band gap, conductance …
- hundreds and up to 100,000 atoms, *parameter-free modeling;*
- reasonably wide scope of materials and device structures;
- reasonably fast computation…

Mini course of quantum transport theory:

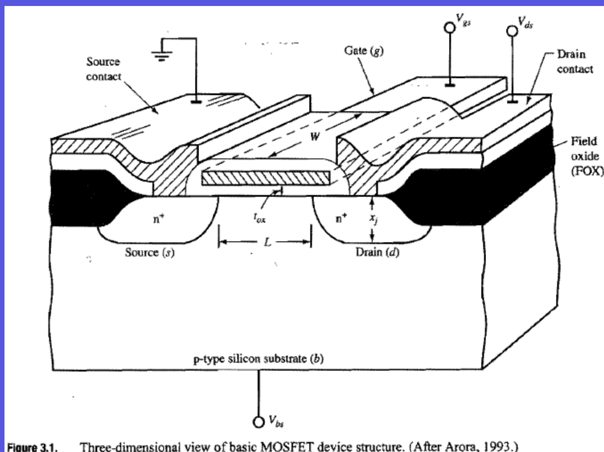
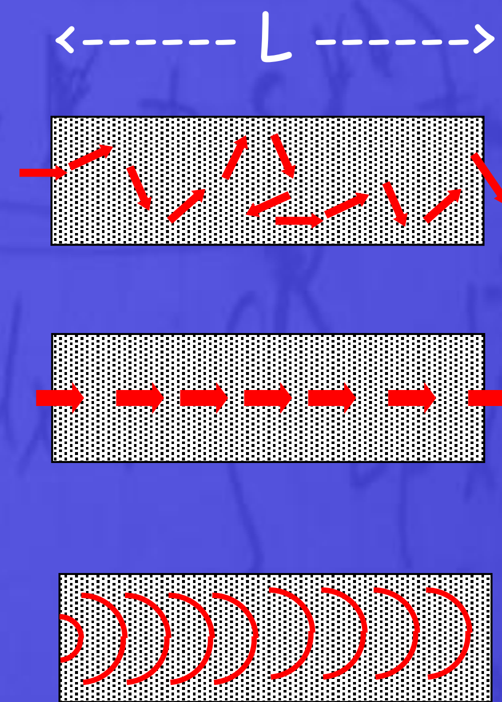


Figure 3.1. Three-dimensional view of basic MOSFET device structure. (After Arora, 1993.)

Picture from Taur and Ning, Fundamentals of Modern VLSI Devices

	Channel Length, L
	1 mm
Top	0.1 mm
	10 μm
1975	1 μ m
2000	0.1 μm
	10 nm
2016	1 nm
Bottom	0.1 nm

Macroscopic dimensions

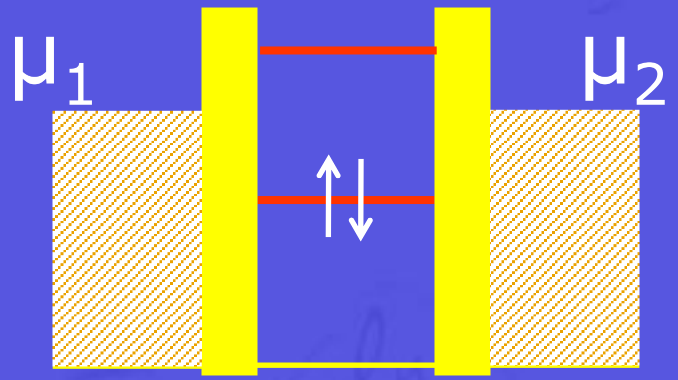


Atomic dimensions

Physics has changed from classical to quantum.

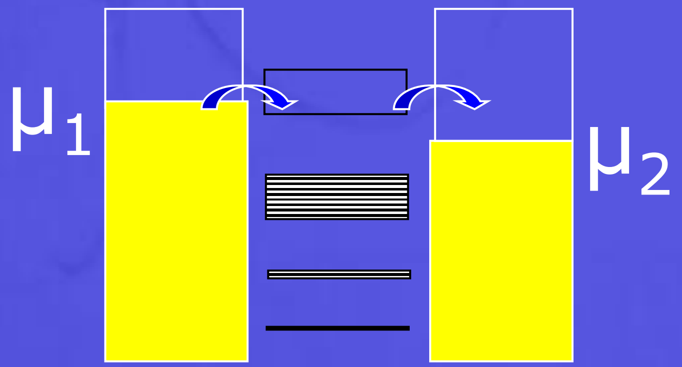
S. Datta, Nanotechnology, 15, S433 (2004)

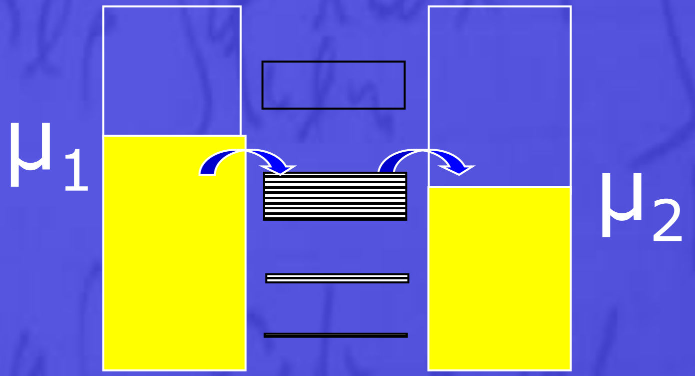
Why current flows ?



No net current flows when $\mu_1 = \mu_2$

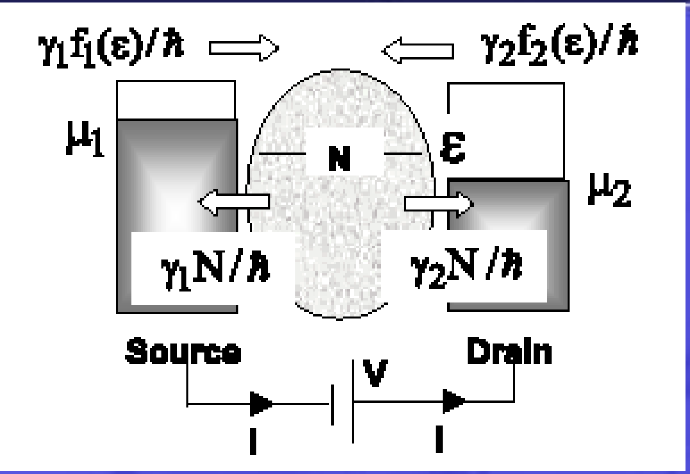
Current flows in the following situations: competition of left and right reservoirs.





Derivation of a current formula: (single level)

Left electrode wants to see f_1 electrons in the channel; right electrode wants see f_2 electrons there. In the end, the number of electrons in the channel is some number N, which is in between f_1 and f_2.



Therefore, current in left and right electrodes will be proportional to (f_i – N)

$$I_1 = (-e)\frac{\gamma_1}{\hbar}(f_1 - N)$$

$$I_2 = (-e)\frac{\gamma_2}{\hbar}(f_2 - N)$$

In steady state, flow-in = flow-out,

hence: $I_1 + I_2 = 0$

We then obtain: $$N = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

S. Datta, Nanotechnology, 15, S433 (2004)

Plug N into the current formula: $I_1 = (-e)\frac{\gamma_1}{\hbar}(f_1 - N)$

We arrive at:

$$I = I_1 = -I_2 = \frac{e}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}[f_1(\varepsilon) - f_2(\varepsilon)]$$

There is no current flow if $f_1 = f_2$. This happens if the energy level ε is below or above the electrochemical potentials of the two electrodes. Only when $\varepsilon \sim \mu_i$ do we get any current. This is correct physics.

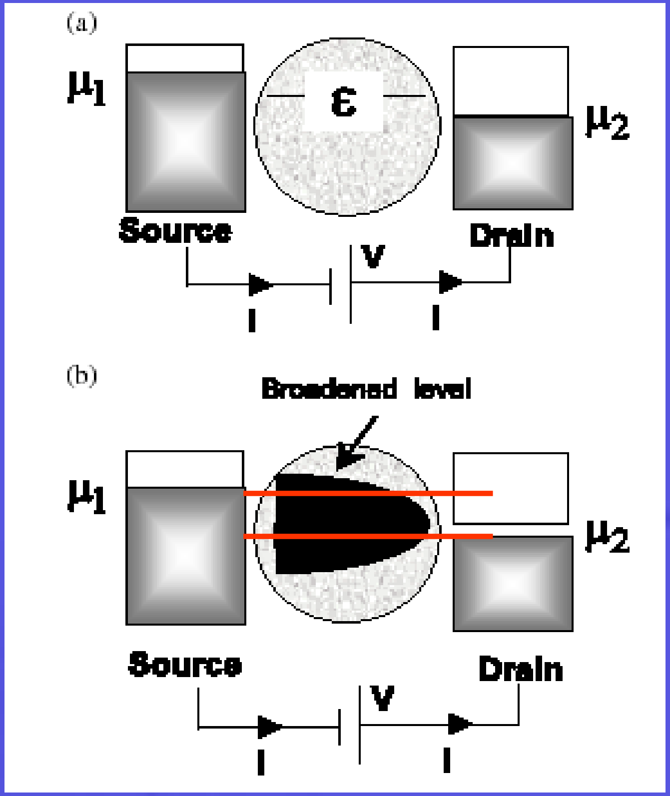
Consider the case of low temperature, so that $f_1(\varepsilon) \approx 1,\ f_2(\varepsilon) \approx 0$. Then, assuming symmetric coupling: $\gamma_1 = \gamma_2$,

We obtain: $$I = \frac{e}{2\hbar}\gamma_1$$

---WRONG in comparison to experiment

S. Datta, Nanotechnology, 15, S433 (2004)

Why wrong ? Because we assumed the level to have zero width - not true if there are electrodes



S. Datta, Nanotechnology, 15, S433 (2004)

$$I = \frac{e}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}[f_1(\varepsilon) - f_2(\varepsilon)]$$

WRONG

$$I = \frac{e}{\hbar}\int_{-\infty}^{+\infty} dE\, DOS(E)\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}[f_1(E) - f_2(E)]$$

CORRECT

- DOS enters formula due to broadening of level

DOS for a single broadened level:

$$DOS(E) = \frac{1}{2\pi}\frac{\gamma}{(E-\varepsilon)^2 + (\gamma/2)^2}$$

$$\gamma = \gamma_1 + \gamma_2$$

Formula for electric current:

Define a transmission coefficient:

$$T(E) \equiv 2\pi\ DOS(E)\ \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}$$

Therefore:

$$I = \frac{e}{h} \int_{-\infty}^{+\infty} dE\ T(E) [\, f_1(E) - f_2(E)]$$

CORRECT

- Landauer formula for charge current

Although we "derived" the Landauer formula for a device with one level, the formula is generally true.

To compute current, just find the transmission coefficient.

Low bias conductance:

At very low temperature: $f_1(E) - f_2(E) = 1 \quad if \;\; \mu_1 > E > \mu_2$

Otherwise this factor is zero. Therefore the current is reduced to:

$$I = \frac{e}{\hbar}\int_{\mu_2}^{\mu_1} dE\, T(E) \approx \frac{e(\mu_1 - \mu_2)}{h} T(\mu) = \frac{e^2}{h} T(\mu) V_D$$

$$G = \frac{e^2}{h} T(\mu)$$

- Landauer formula for conductance

Conductance quanta:

For a perfectly transmitting level, T=1.

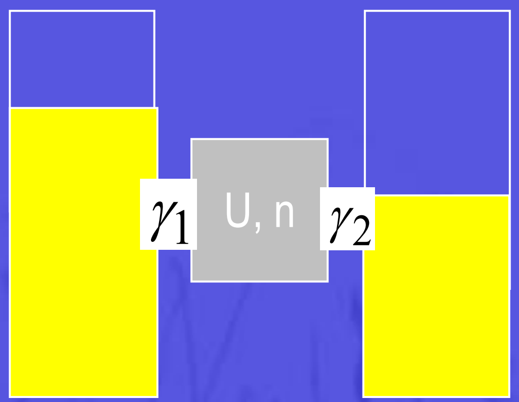
Therefore we have:

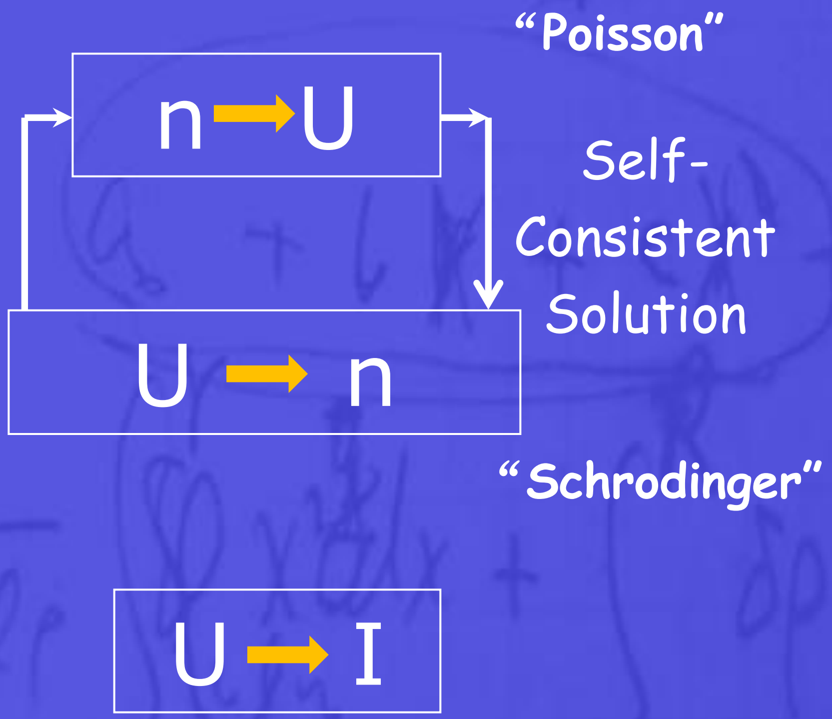
$$G_o = \frac{e^2}{h} = (25.8\,K\Omega)^{-1}$$

Including spin, the basic conductance quanta is twice this value.

Self-consistent theory:

Simplified flavor
of a very complicated problem





Semiconductors/Nanowires /Nanotubes / Molecules/metal/Magnetic/superconductors/…
Namely: real materials and read devices.

S. Datta, Nanotechnology, 15, S433 (2004)

Real systems have many levels, things become matrices:

$\varepsilon \to [H]$

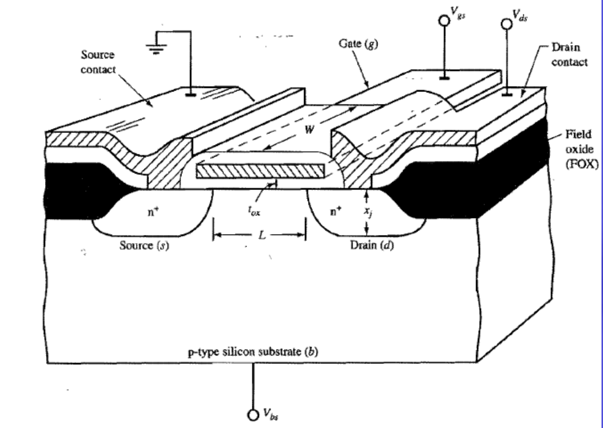
$U \to [U]$

$\gamma \to [\Gamma], [\Sigma]$

$N \to [\rho]$

$D(E) \to [A(E)]$

$n(E) \to [G^{<}(E)]$



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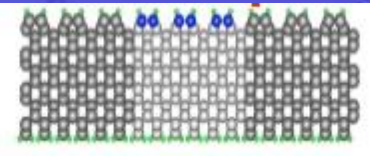
Picture from Taur and Ning, Fundamentals of Modern VLSI Devices

The Non-equilibrium Green's function (NEGF) method

Take home message 1: no contacts, no nonequilibrium transport.

Why NEGF ?

$$H = H_{leads} + H_{device} + H_{coupling}$$



- Calculating electric current flow driven by a finite bias voltage is a non-equilibrium problem, it is important to correctly determine non-equilibrium statistics of the device scattering region that is embedded in an open environment.

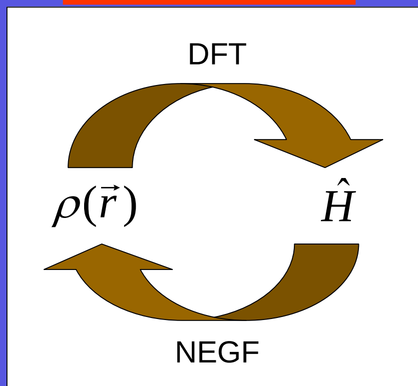
- A second consideration is the determination of device Hamiltonian H. H provides the energy levels of the device. How to fill these levels is given by the non-equilibrium statistics.

- Keldysh non-equilibrium Green's function (NEGF) is a natural approach to determine the non-equilibrium statistics. One may also evolve a non-equilibrium density matrix from some equilibrium initial condition.

- What kind of H to use is an issue of taste and level of accuracy: effective mass, kp, EH,TB, DFTB, HF, DFT, GW, higher-functionals, QMC, CI. In the end, one has to compare to experimental data without adjusting theoretical parameters.

NEGF-DFT: non-equilibrium density matrix

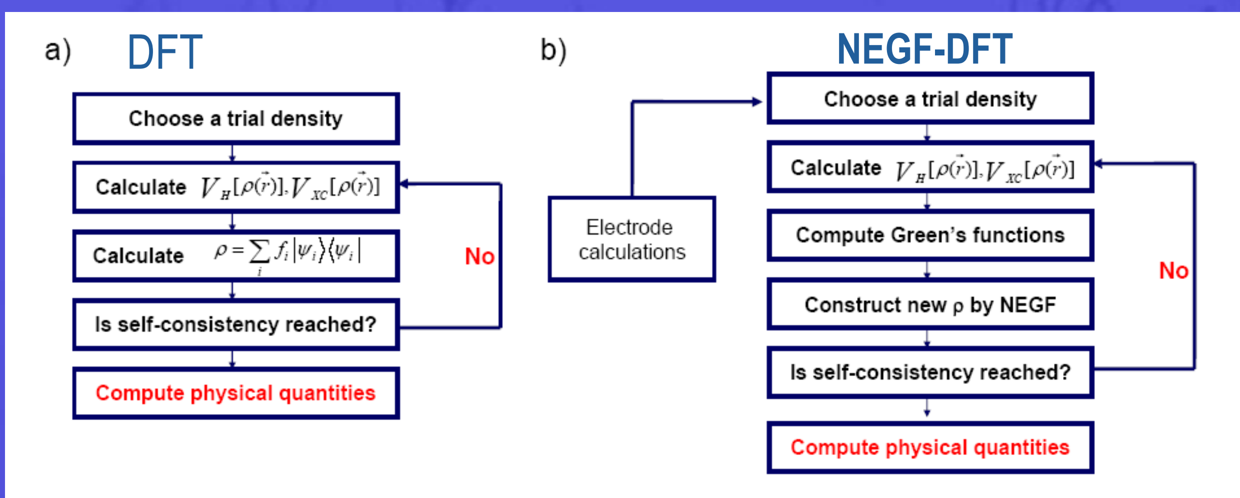
NEGF-DFT



DFT: density functional theory

NEGF: Keldysh nonequilibrium Green's function

$$\rho \sim \int G^{<}\, dE = \int G^{R}\Sigma^{<}G^{A}\, dE$$



`DFT' in NEGF-DFT is not the ground state DFT: because density matrix of NEGF-DFT is constructed at non-equilibrium.

No variation solution.

Taylor, Guo and Wang, PRB 63, 245401 (2001).

A technical point: computing density matrix via NEGF

The familiar way:

$$\hat{\rho} = \sum_b f_b |\Psi_b|^2 + \int dE \frac{f_k}{v_k} |\Psi_k|^2 + \int dE \frac{f_p}{v_p} |\Psi_p|^2$$

bound states **scattering states**

NEGF:

$$\hat{\rho} = \frac{1}{2\pi i} \int dE\, G^{\prec}$$

$$G^{\prec} = G^R \Sigma^{\prec} G^A$$

$$G^R(E,U) = \frac{1}{E - H_0 - eU - V_{ps} - V_{xc} - \Sigma_R}$$

$$\Sigma^{\prec} = i\, f_l(E;\mu_l)\Sigma^R_{l,l} + i\, f_r(E;\mu_r)\Sigma^R_{r,r}$$

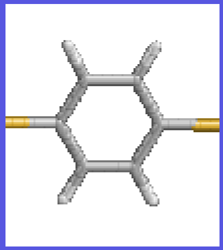
$$\nabla^2 U = -4\pi\rho$$

Many technical & numerical advantages for computing density matrix by NEGF.

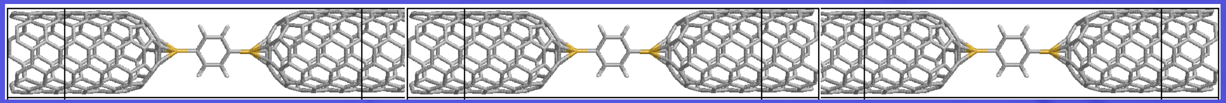
Math: need to invert a large matrix.
Implementation: LCAO, LMTO, Gaussian basis to control matrix size.

Book of Jauho; book of Datta; Wang et al. PRL 82, 398(1999)

Another technical issue - familiar DFT solves two kinds of problems:

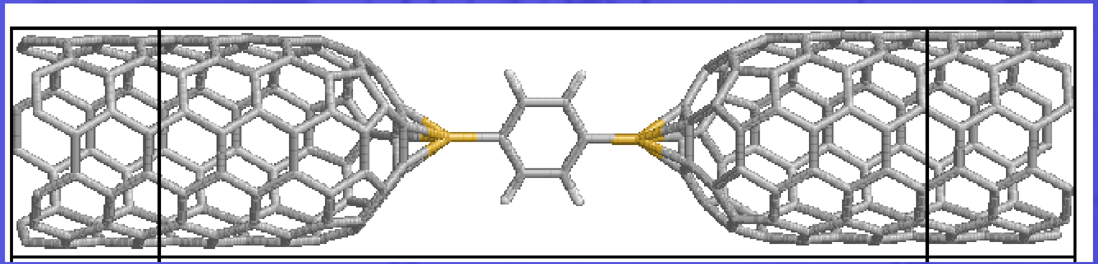


Finite isolated system



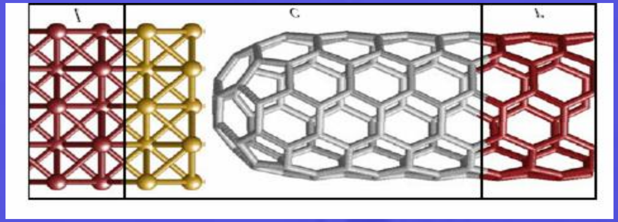
Periodic systems

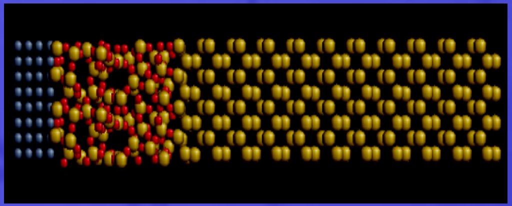
Quantum transport:



A device is neither finite nor periodic, and is in non-equilibrium

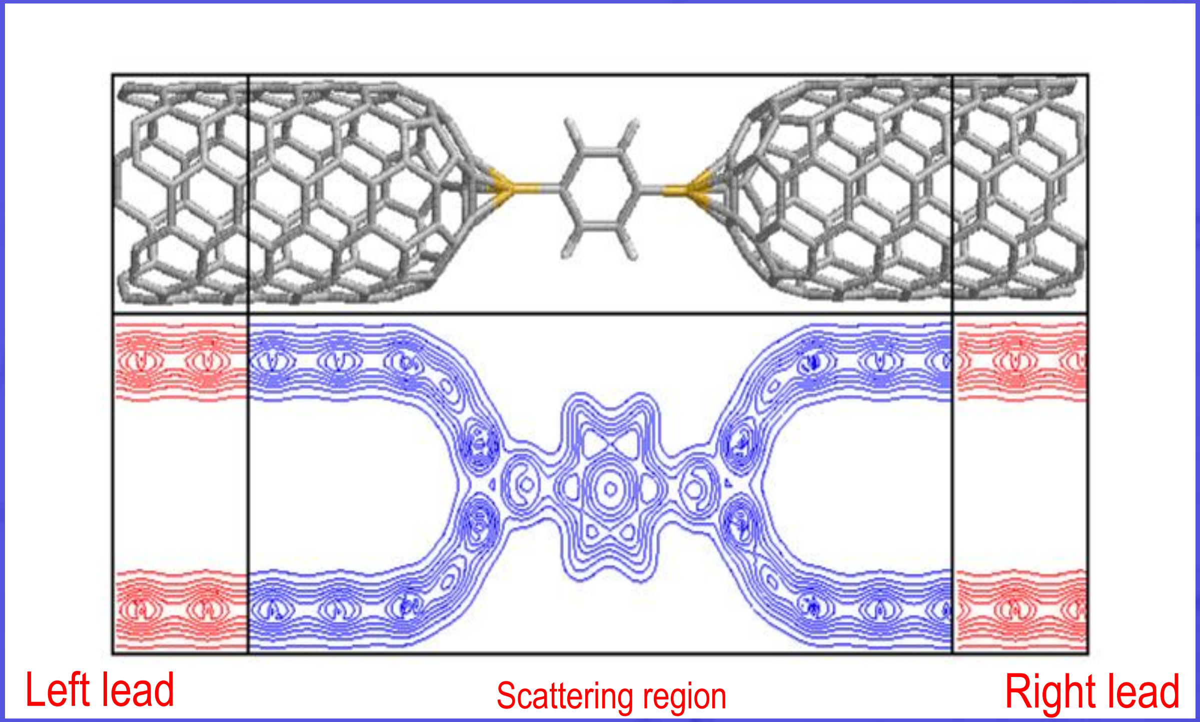
Need to solve **open** structures.





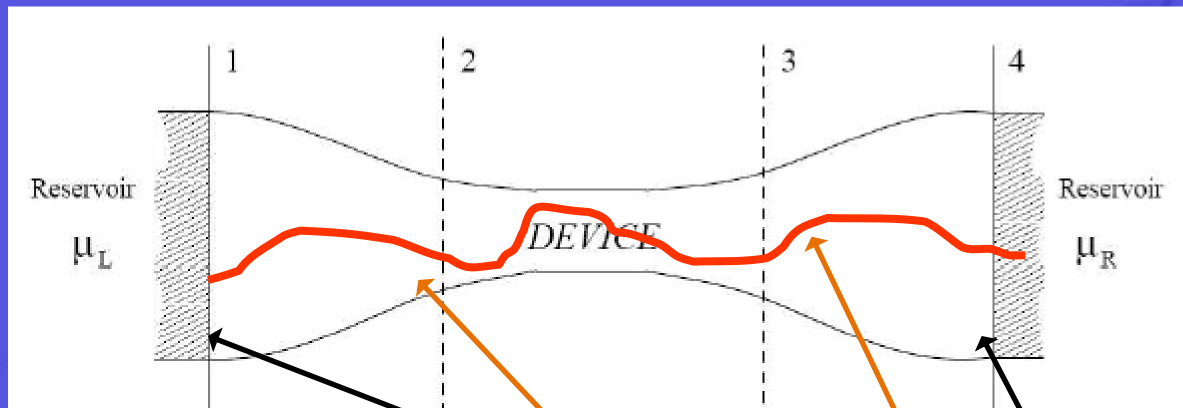
Screen approximation - reducing the infinitely large problem:

Within DFT, once the potential is matched at the boundary, charge density automatically goes to the bulk-electrode values at the boundaries:



Within screen approx., we only have to worry about a finite scattering region in the self-consistent iterations.

After self-consistency, compute transmission coefficients:



$$T(E,\Delta V) = Tr[G^r \Gamma_L G^a \Gamma_R]$$

$$I = \frac{e}{h}\int_{-\infty}^{+\infty} dE\, T(E)[f_1(E) - f_2(E)]$$

Take home message 2: essence of NEGF-DFT

- Using a self-consistent field (DFT-like) to compute the electronic structure and the Hamiltonian of the open device structure (the Hamiltonian).

- Using Keldysh NEGF to populate this electronic structure to obtain the nonequilibrium density matrix (the quantum statistical mechanics).

- Using real space numerical techniques to deal with the open device boundary, electrostatic boundary, and transport boundary conditions (the contacts).

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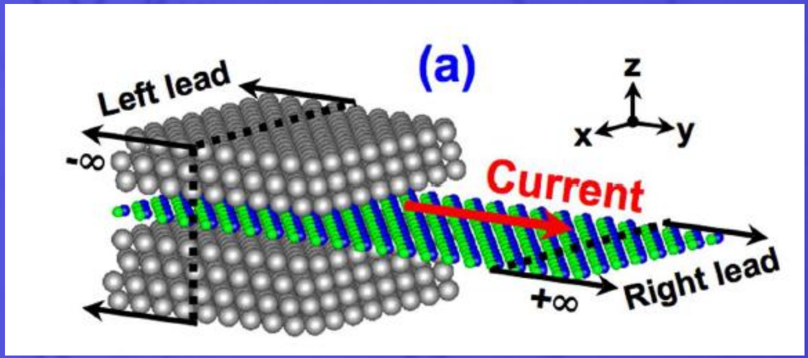

Taylor, Guo, Wang, PRB 63, 245407(2001)

Wide range of research has been done by NEGF-DFT

- Leakage current is MOSFET;
- Resistivity of Cu interconnects;
- Conductance, I-V curves of molecular transport junctions;
- Computation of capacitance, diodes, inductance, current density;
- TMR, spin currents, and spin injection in magnetic tunnel junctions;
- Transport in nanowires, rods, films, clusters, nanotubes;
- Resistance of surface, interface, grain boundary;
- STM image simulations;
- Atomic limit: transport within LDA+U;
- Transport in semiconductor devices;
- Transport through short peptides;
- ….

An example: topological insulator Bi_2Se_3

- Introduction: need for quantum transport from atomic first principles, crash course of quantum transport theory, NEGF-DFT method.
- **Spin-orbit: helical spin states in topological insulator Bi_2Se_3.**
- Disorder: non-equilibrium vertex correction theory. Roughness scattering.
- Other issues, large systems;
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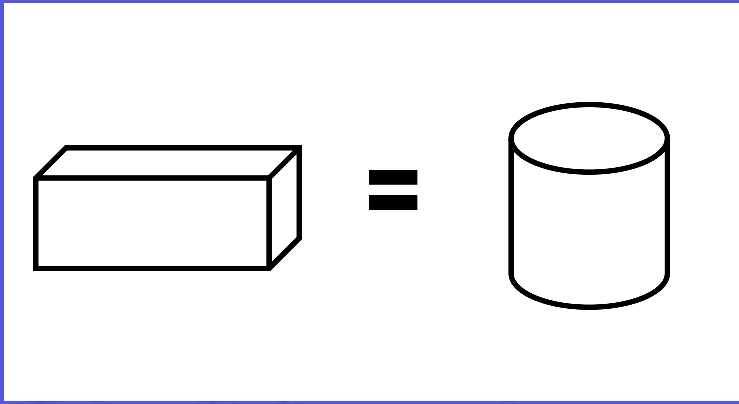
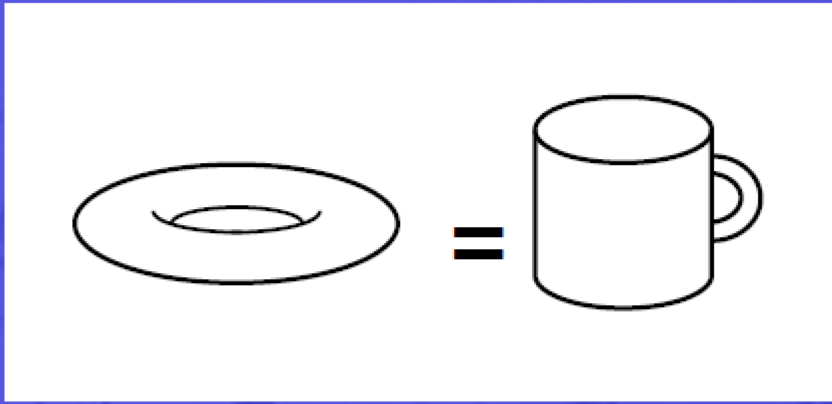
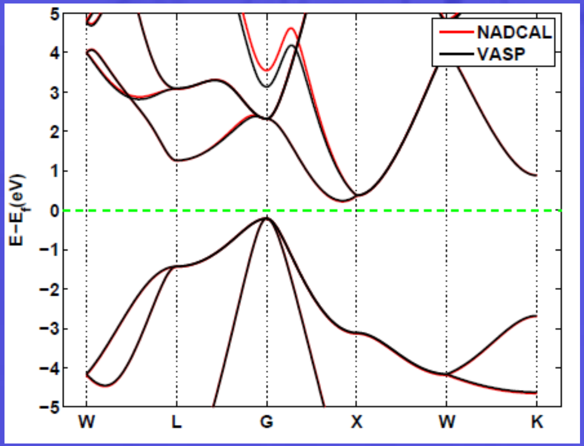
Topological point of view: high level classification







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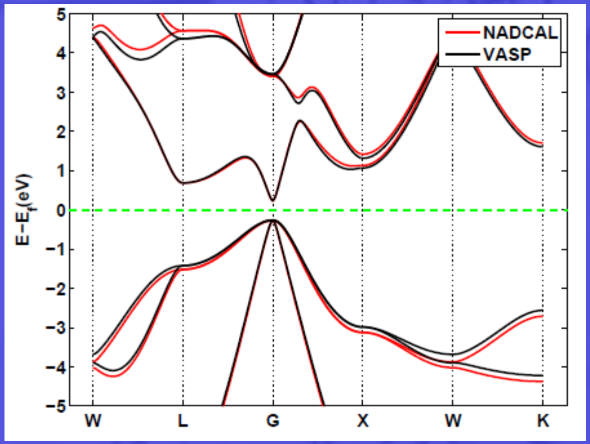
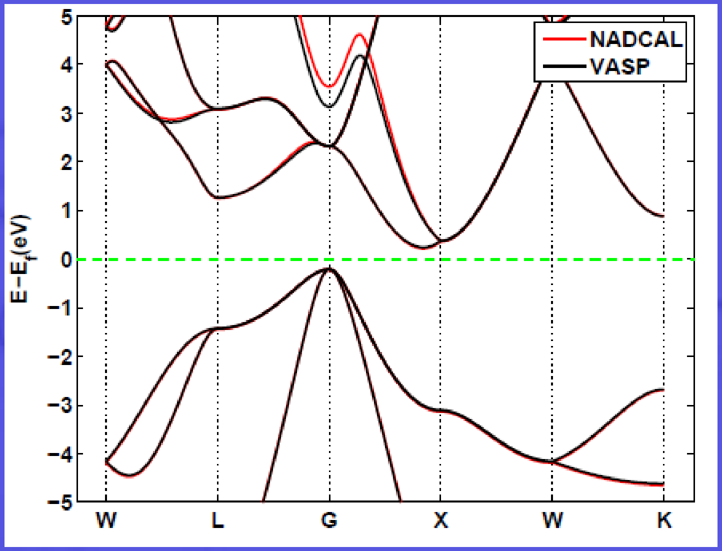


Turn one band structure into another without closing the gap

Topological insulators:

Band insulator



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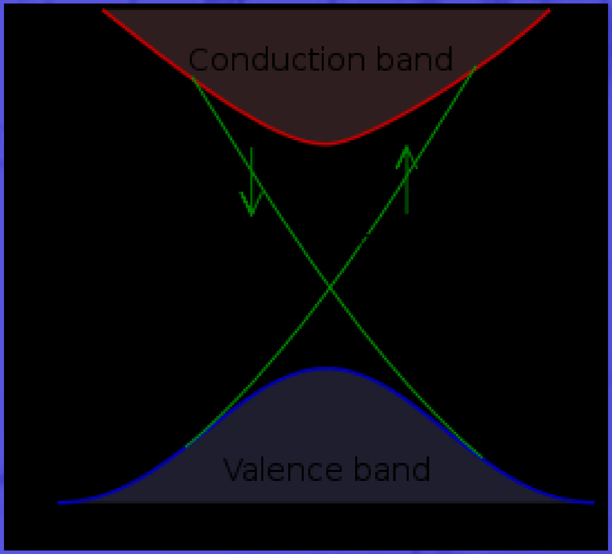
Topological insulator



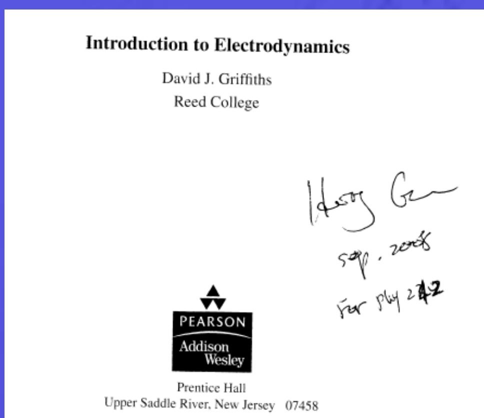
Spin-orbit interaction !

But why?

(1) Kane, C. L.; Mele, E. J. *Phys. Rev. Lett.* **2005**, *95*, 146802.
(2) Bernevig, B. A.; Hughes, T. L.; Zhang, S. C. *Science* **2006**, *314*, 1757.

David J. Griffiths' text book on E&M, page-544

Problem 12.62. A magnetic dipole moment m is located in an inertial system S' that moves with speed v with respect to inertial system S. … Show that the scalar potential in S is that of an ideal electric dipole p which equals to …



Introduction to Electrodynamics

David J. Griffiths
Reed College

PEARSON
Addison Wesley

Prentice Hall
Upper Saddle River, New Jersey 07458

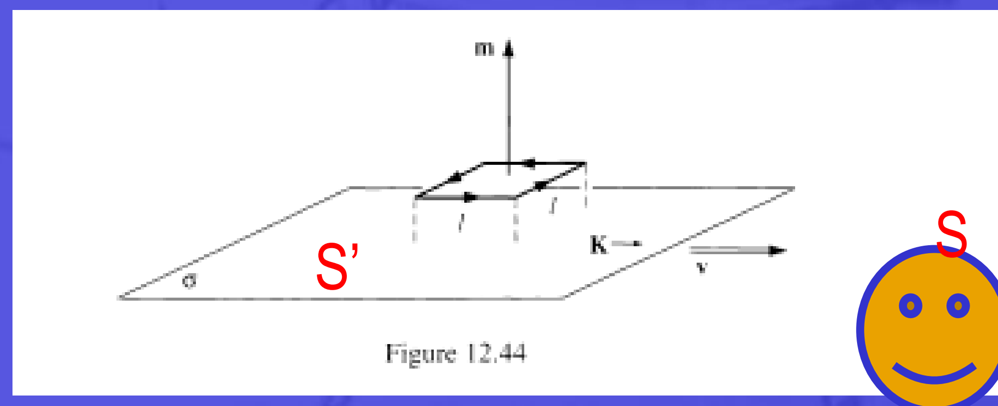
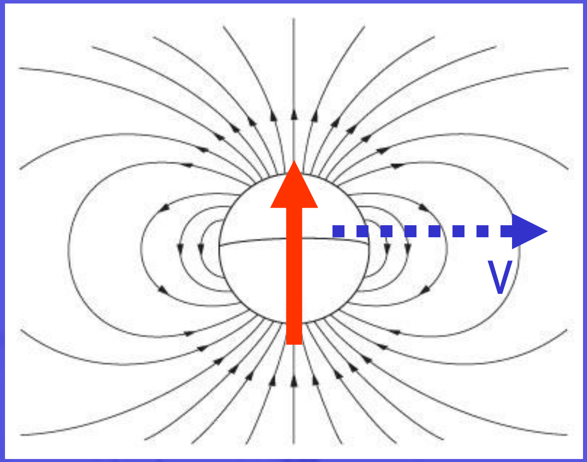


Figure 12.44

This problem appears to say that a moving magnetic dipole, somehow, can generate an electric field. Why?

Why a moving magnetic dipole generates an electric field E ?



A static magnetic moment generates a magnetic field B

If the spin moves with speed v, by special theory of relativity we will obtain a magnetic field B and an electric field E. Conclusion: spin current J_s produces an E !

$$\mathbf{E}' = \gamma(\mathbf{E} + \beta \times \mathbf{B}) - \frac{\gamma^2}{\gamma+1}\beta(\beta \bullet \mathbf{E})$$

$$\mathbf{B}' = \gamma(\mathbf{B} - \beta \times \mathbf{E}) - \frac{\gamma^2}{\gamma+1}\beta(\beta \bullet \mathbf{B})$$

Let’s do a bit more:

A pure spin-current generates an E-field.

What happens if a spin-current is put inside an external E-field ?

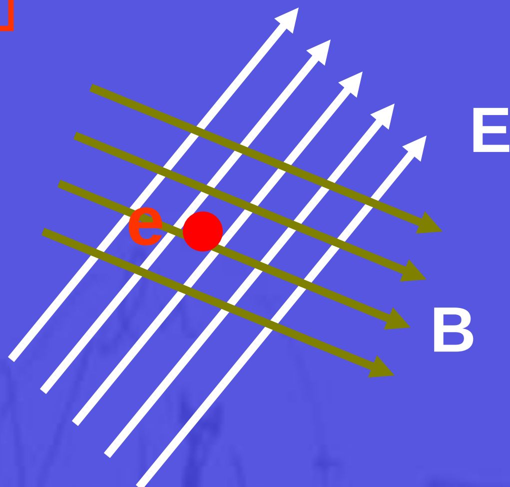
Let’s review the motion of electron inside external E, B fields.

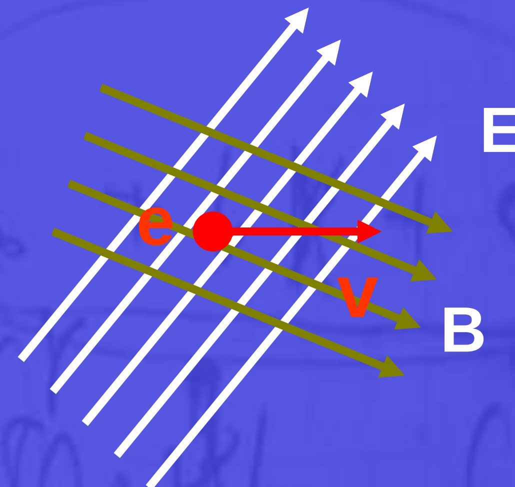
Namely, (e, s) inside (E, B).

Q.F. Sun, J. Wang and H.G. PRB 71, 165310 (2005).

Consider (e, s) in (E,B)

Charge e:





F = -eE

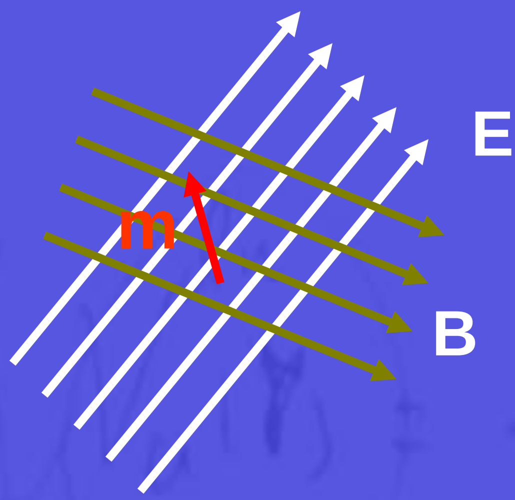
B has no effect on stationary charge

F = -e(E + v×B)

B has effect on moving charge

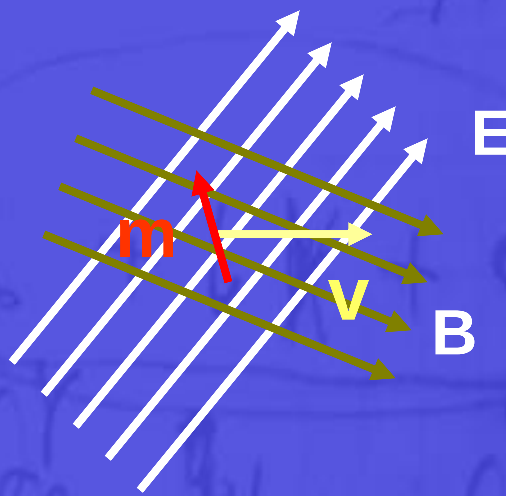
(e, s) in (E, B):   cont.

Spin s:



$$-m \bullet B$$

B acts on stationary spin

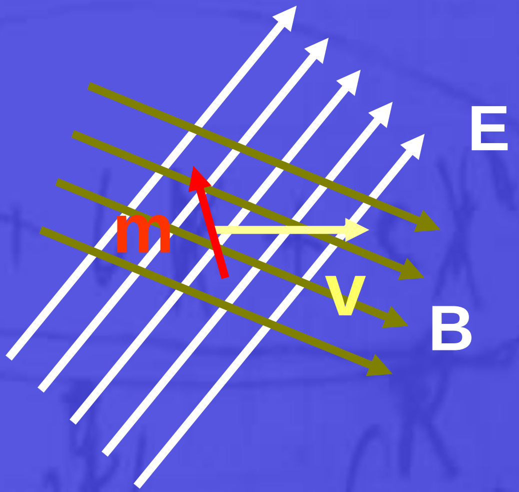


A moving spin inside an external electric field:

does E put a force on the moving spin ???

Moving spin inside external E field:

Since a spin current induces an E field, we expect an external E field to act on a spin current with a force.



This is like Onsager reciprocal relation.

Turns out:

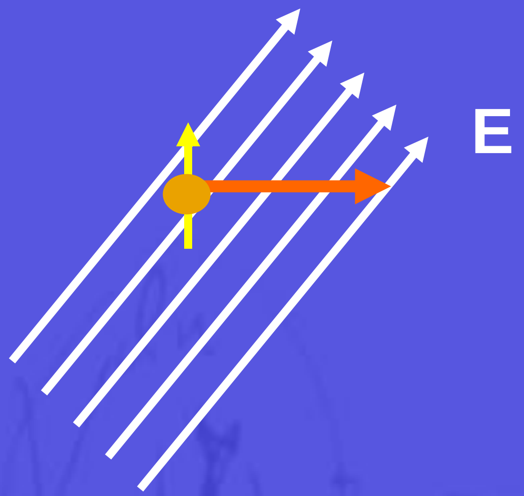
$$m \bullet (\mathrm{v} \times E)/c^2$$
$$= g\mu_B \sigma \bullet (\mathrm{v} \times E)/c^2$$

This is a small force but it pushes spin sideways.

Sun, Wang, H.G. PRB 69, 054409(2004); PRB 71 165310 (2005).

Let's do quantum mechanics: quantize this force

classical: electric field has action on moving spin



$$\alpha\sigma \bullet (\mathbf{v} \times \mathbf{E})$$

Quantum: we quantize the above formula:

$$\frac{\alpha}{2}\left[\sigma \bullet (p \times \nabla V(r)) - \sigma \bullet (\nabla V(r) \times p)\right]$$

$$= \frac{\alpha}{2}\left[(\sigma \times p) \bullet \nabla V(r) + \nabla V(r) \bullet (\sigma \times p)\right]$$

Spin-orbit interaction !

Usually one derives SOI from Dirac equation

SO = $\frac{\alpha}{2}\left[(\sigma \times \mathbf{p}) \bullet \nabla V(r) + \nabla V(r) \bullet (\sigma \times \mathbf{p})\right]$

If V is a central potential:

$$\nabla V(\mathbf{r}) = \frac{\mathbf{r}}{r}\frac{d}{dr}V(r)$$

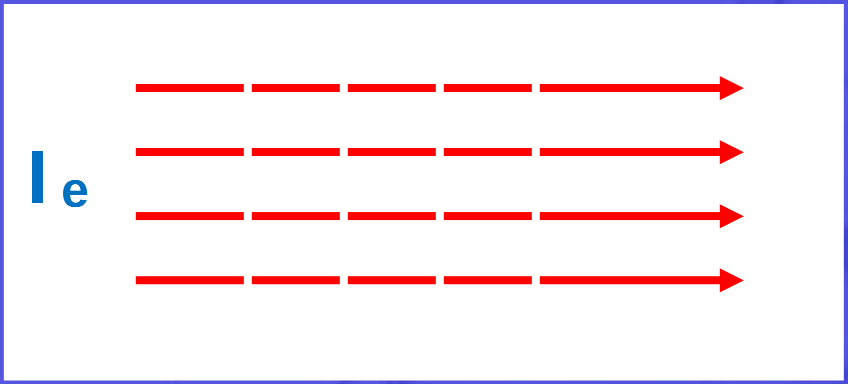
$$\begin{aligned}\nabla V(\mathbf{r}) \bullet (\sigma \times \mathbf{p}) &= \frac{\mathbf{r}}{r}\frac{d}{dr}V(r) \bullet (\sigma \times \mathbf{p}) \\ &= -\frac{1}{r}\frac{d}{dr}V(r)\sigma \bullet (\mathbf{r} \times \mathbf{p}) \\ &= -\frac{1}{r}\frac{d}{dr}V(r)\sigma \bullet \hat{l}\end{aligned}$$

a. Thomas spin-orbit: $\alpha(\mathbf{r})\hat{s} \bullet \hat{l}$

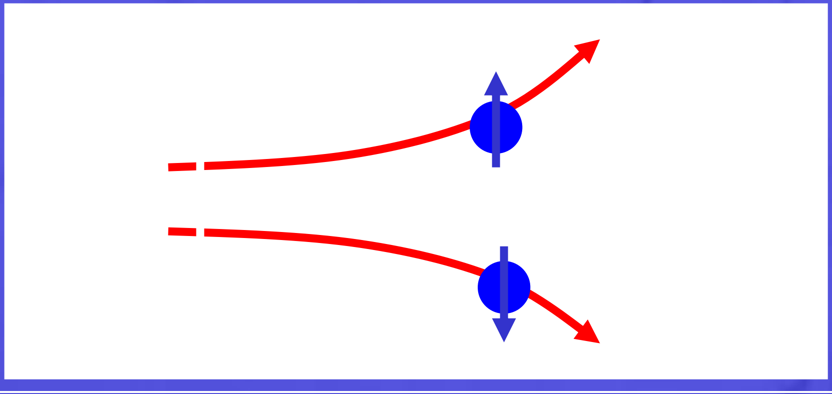
b. Darwin contact potential $\sim \nabla^2 V(\mathbf{r})$

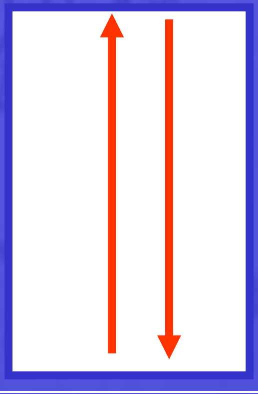
Take home message 3: SOI pushes spins side ways, linear in p

No SO interaction:
charges move forward



With SOI $\alpha \hat{z} \bullet (\sigma \times \mathbf{p})$ spin pushed sideways

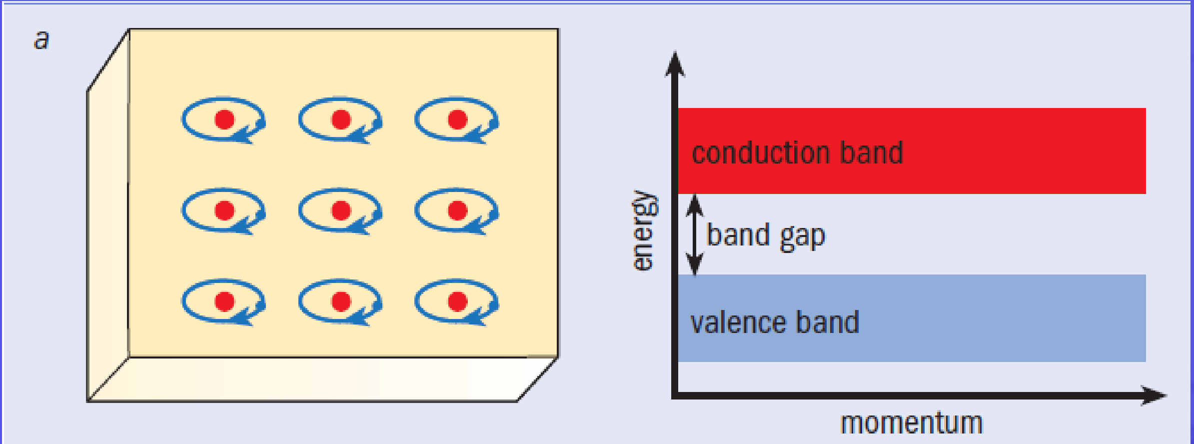




“No dissipation”

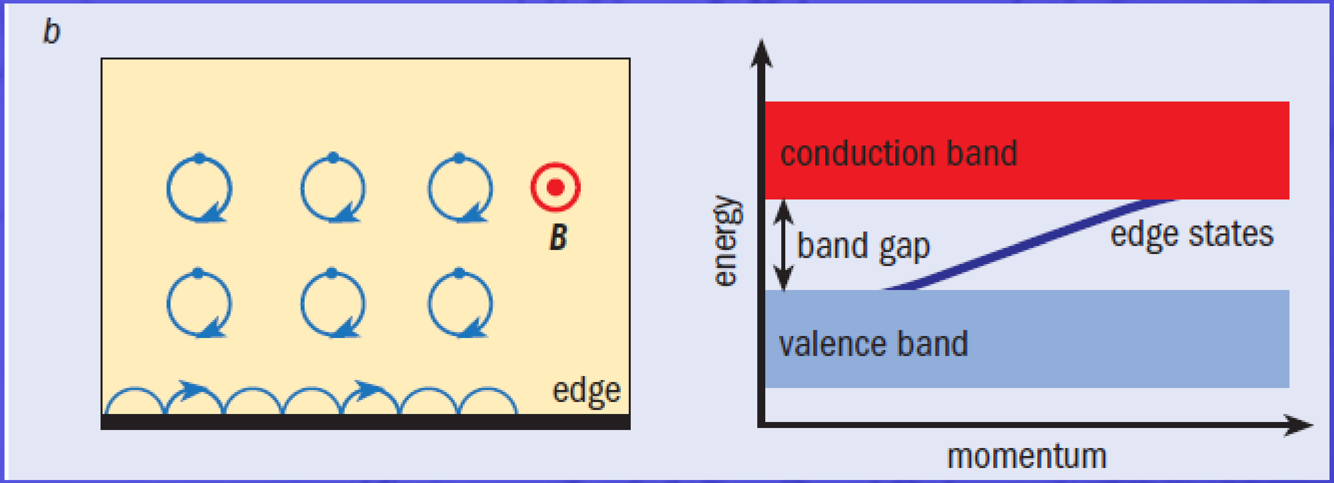
Murakami, etal. Science 301,1348 (2003).

Band insulator and quantum Hall effect



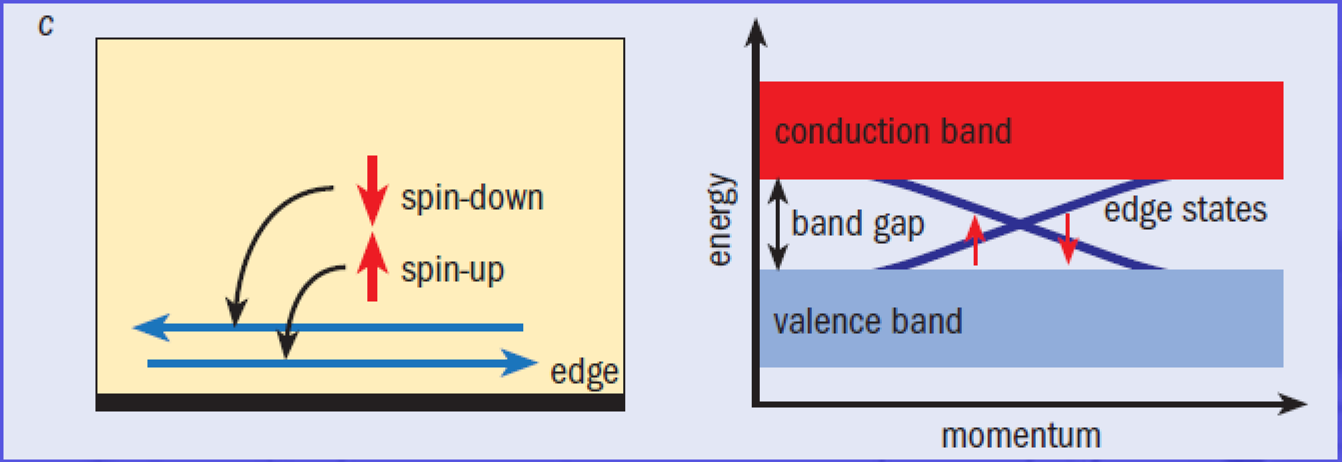
Insulator: Fermi level in the gap

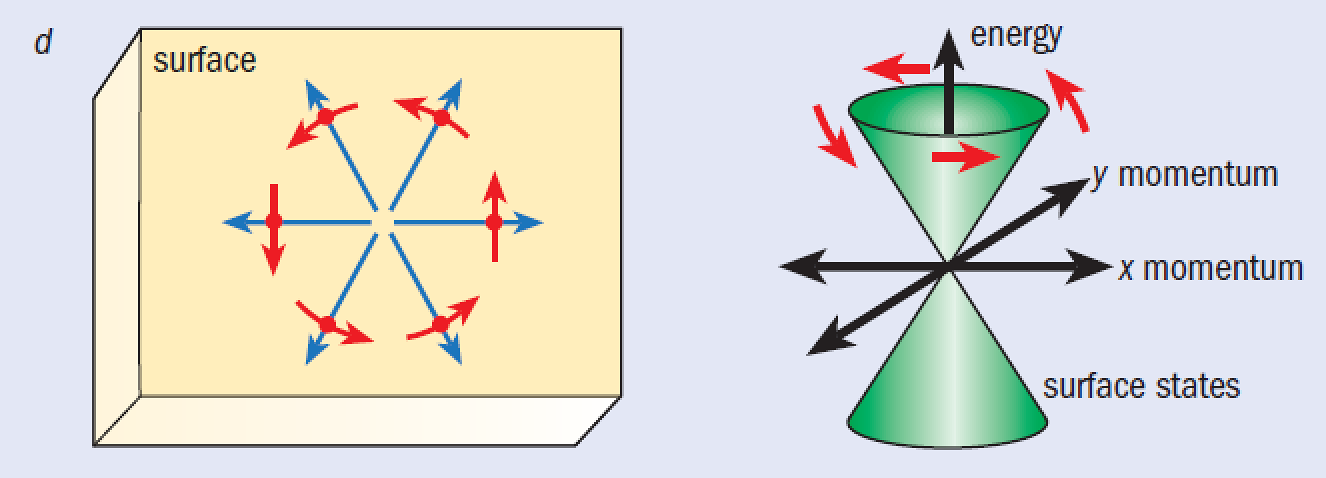
Quantum Hall: quantized skipping orbits conducts in 1d.



Picture from: C. Kane and J. Moore, Phys. World, Feb.2011

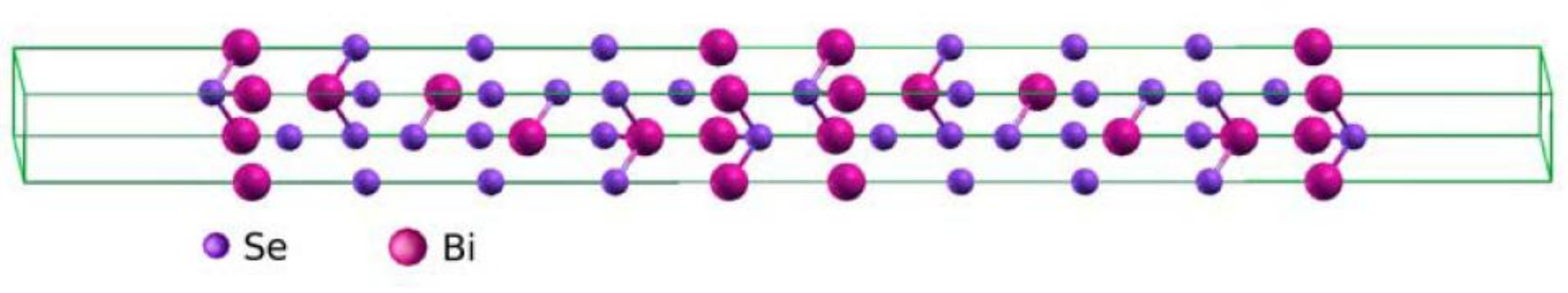
2d and 3d topological insulators





Picture from: C. Kane and J. Moore, Phys. World, Feb.2011

Bi_2Se_3 is believed to be a topological insulator



The crystal structure of Bi_2Se_3 is rhombohedral. The surface structure is a slab with six quintuple layers (QLs). Each surface terminates by a Se atomic layer.

The exchange correlation functional is local spin density approximation (LSDA).

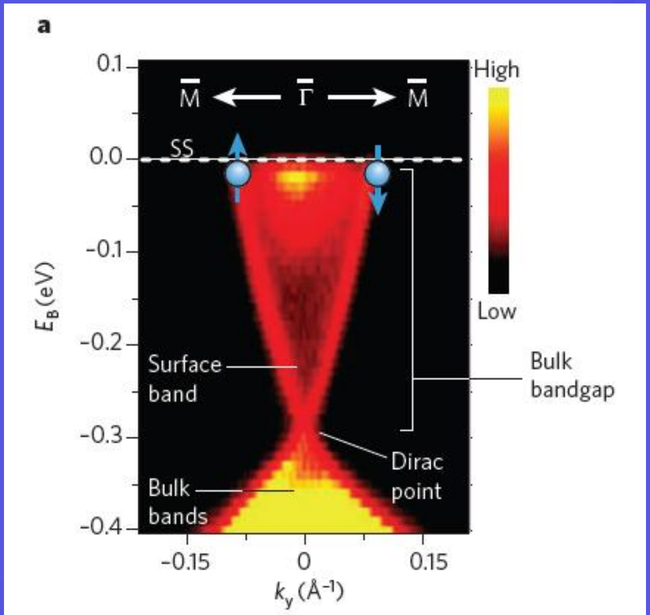
Electronic structure DFT with LCAO triple-zeta-double-polarization basis sets;

Quantum transport: NEGF-DFT as implemented in the nanodcal package (www.nanoacademic.ca).

SOI implementation:

(24) Theurich, G.; Hill, N. A. *Phys. Rev. B* **2001**, *64*, 073106.
(25) Fernández-Seivane, L.; Oliveria, M. A.; Sanvito, S.; Ferrer, J. *J. Phys: Condens. Matter* **2006**, *18*, 7999.

DFT band structure of 6QL slab calculated by our software



Hsieh D. *et al.*, *Nature* 460, 1101 (2009)

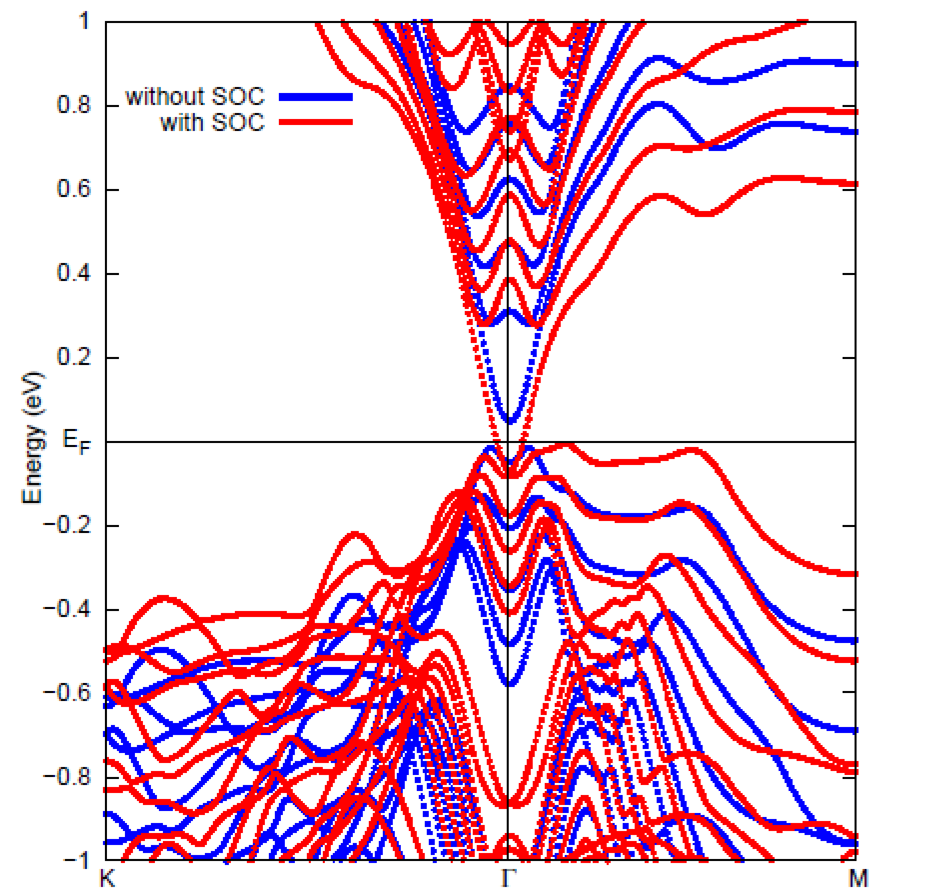


Figure 2: Band structures of the Bi_2Se_3 slab, where red and blue lines show those with and without spin-orbit coupling.

Our Dirac point is 72meV below E_f.

New experiment: 135meV below (http://arxiv.org/abs/1012.5716)

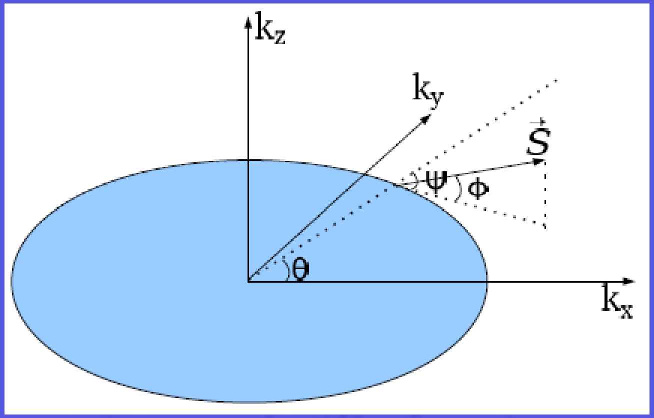
Surface states projection

$$\hat{\rho}_{\mathbf{nk}} = |\psi_{\mathbf{nk}}\rangle\langle\psi_{\mathbf{nk}}| = \begin{pmatrix} \left|\psi^{\uparrow}_{\mathbf{nk}}\right\rangle\left\langle\psi^{\uparrow}_{\mathbf{nk}}\right|, & \left|\psi^{\uparrow}_{\mathbf{nk}}\right\rangle\left\langle\psi^{\downarrow}_{\mathbf{nk}}\right| \\ \left|\psi^{\downarrow}_{\mathbf{nk}}\right\rangle\left\langle\psi^{\uparrow}_{\mathbf{nk}}\right|, & \left|\psi^{\downarrow}_{\mathbf{nk}}\right\rangle\left\langle\psi^{\downarrow}_{\mathbf{nk}}\right| \end{pmatrix}$$

$$Q_{\mathbf{nk}} = \frac{1}{2} Tr \begin{pmatrix} \rho^{\uparrow\uparrow}_{\mathbf{nk}} S_{\mathbf{k}} + S_{\mathbf{k}} \rho^{\uparrow\uparrow}_{\mathbf{nk}}, & \rho^{\uparrow\downarrow}_{\mathbf{nk}} S_{\mathbf{k}} + S_{\mathbf{k}} \rho^{\uparrow\downarrow}_{\mathbf{nk}} \\ \rho^{\downarrow\uparrow}_{\mathbf{nk}} S_{\mathbf{k}} + S_{\mathbf{k}} \rho^{\downarrow\uparrow}_{\mathbf{nk}}, & \rho^{\downarrow\downarrow}_{\mathbf{nk}} S_{\mathbf{k}} + S_{\mathbf{k}} \rho^{\downarrow\downarrow}_{\mathbf{nk}} \end{pmatrix}$$

$$Q_{\mathbf{nk}} = Q\mathbf{I} + P_x\sigma_x + P_y\sigma_y + P_z\sigma_z$$

Surface helical spin states of Bi_2Se_3



Polar angle θ is used to distinguish different surface states around the circle at Fermi level. Angle Ψ indicates azimuth angle, angle Φ indicates tilting angle, and they are used to characterize the spin directions.

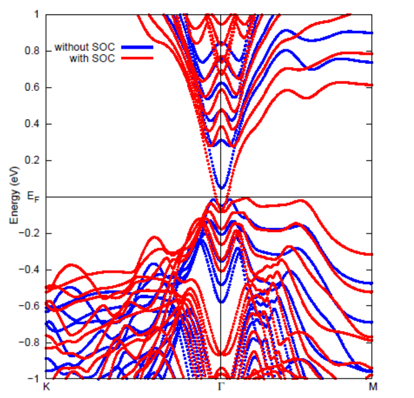
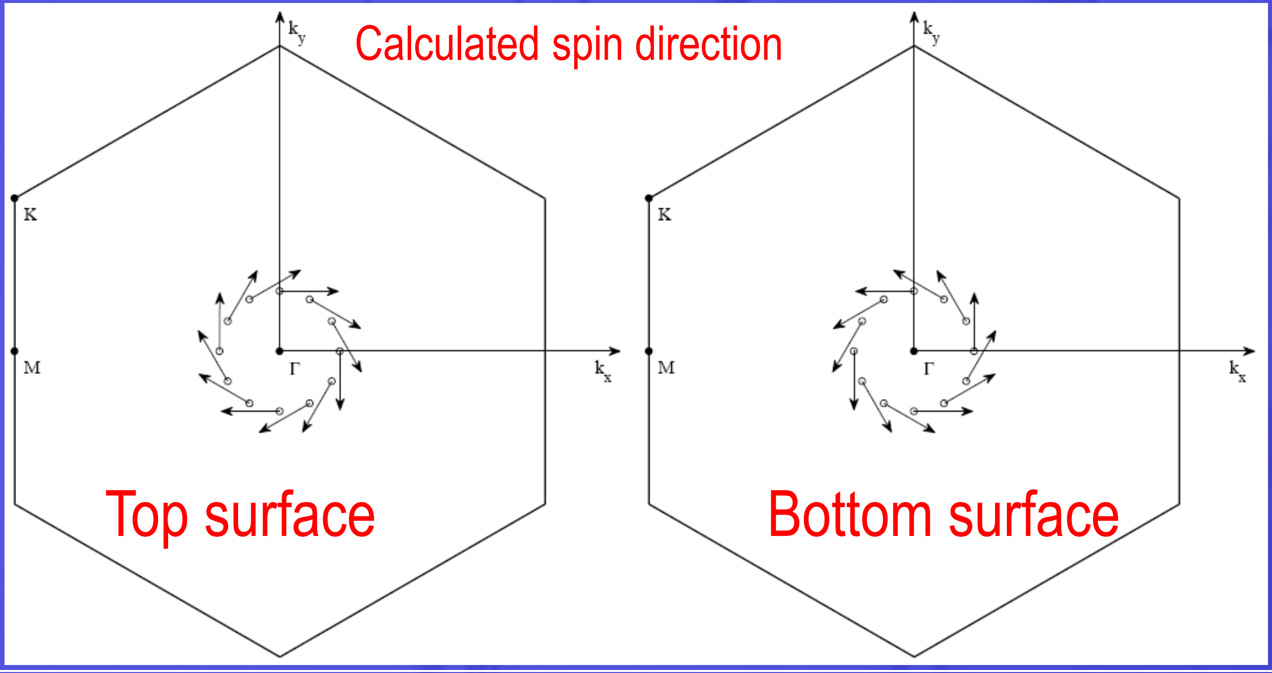
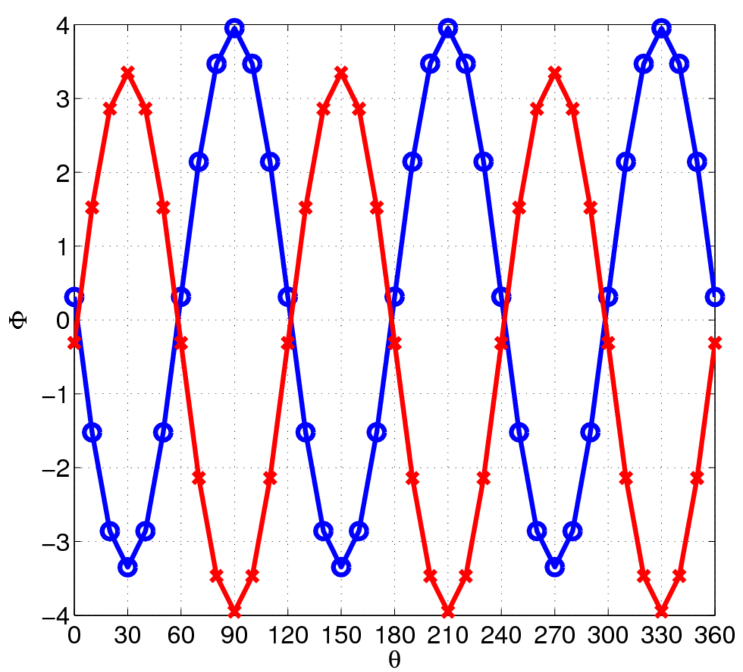
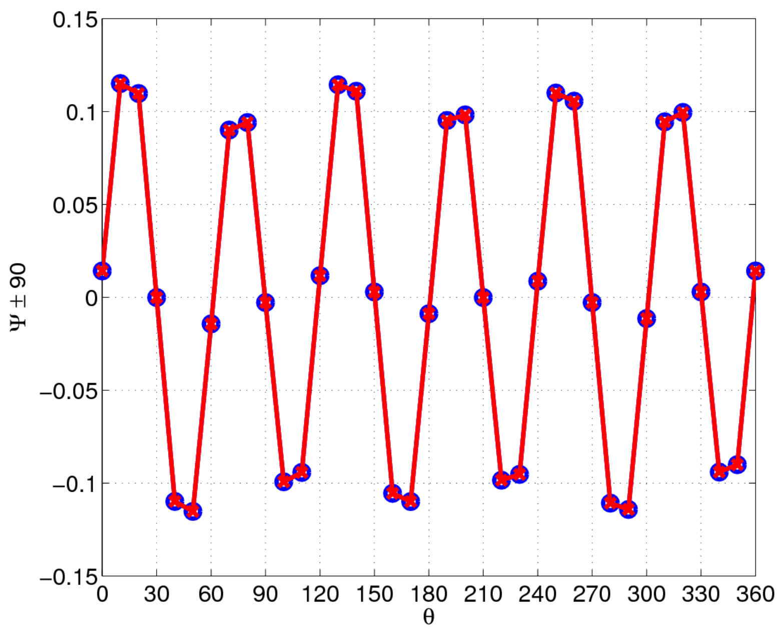


Figure 2: Band structures of the Bi_2Se_3 slab, where red and blue lines show those with and without spin-orbit coupling.



Surface helical spin states of Bi_2Se_3

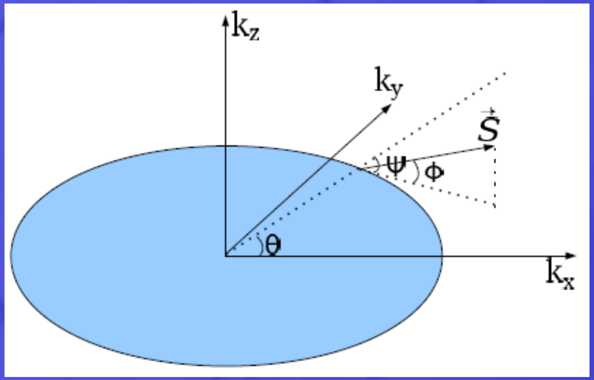




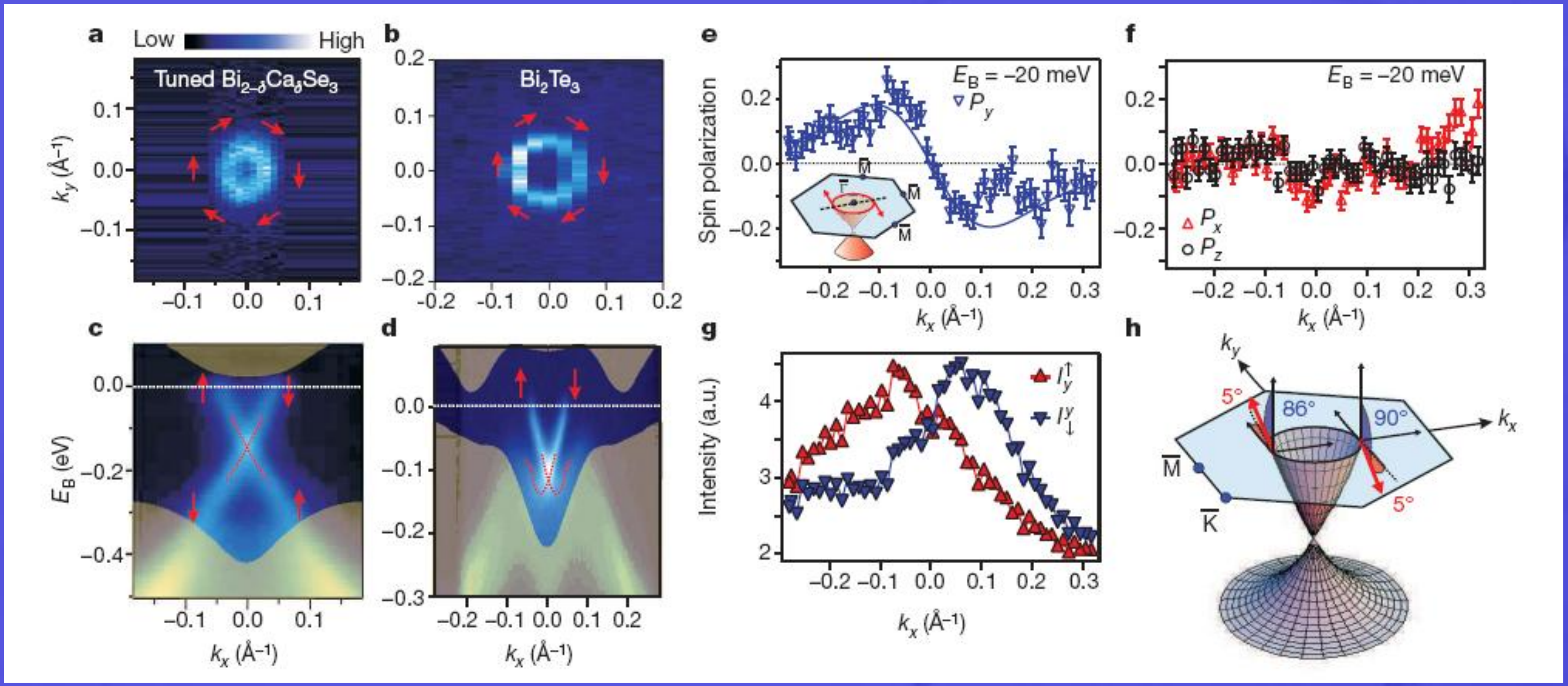
Left figure shows tilting Φ versus polar θ for the helical states.

Right figure shows azimuth Ψ versus polar.

They show oscillations periodically with a 3-fold symmetry which reflects the rotational symmetry of the Bi_2Se_3 slab.

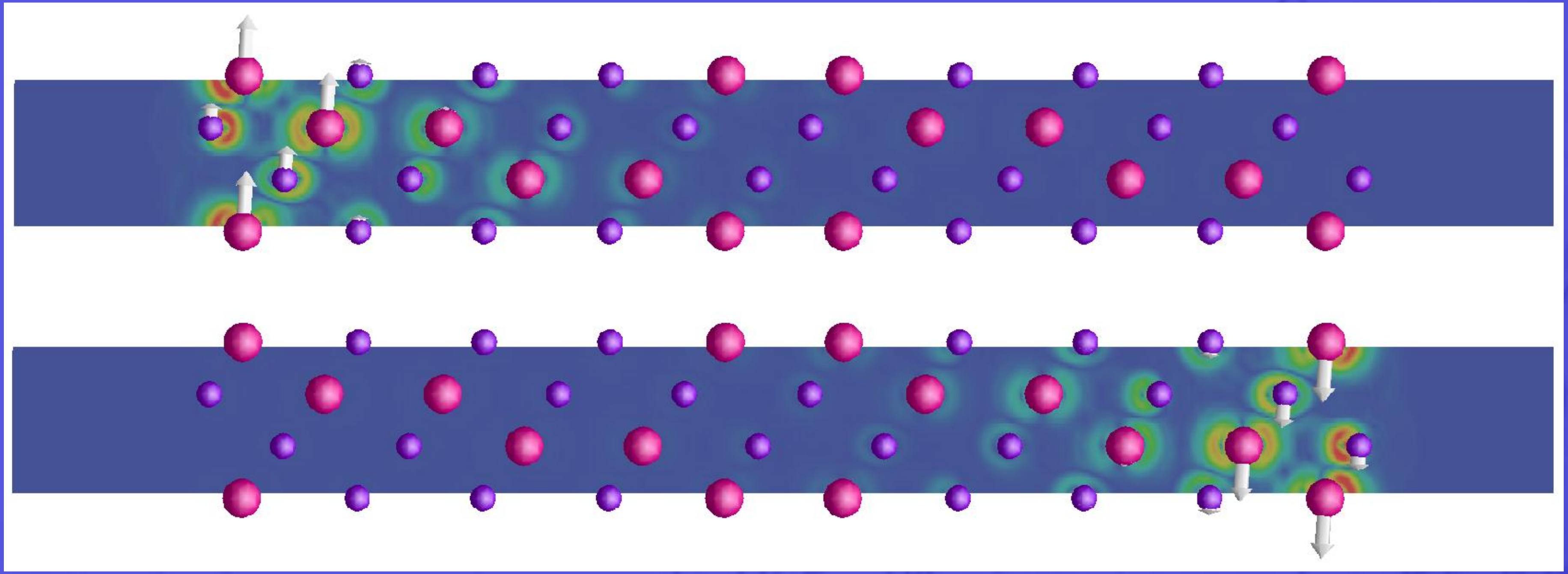


Experimentally, the tilting angle is 5 degrees



Hsieh D. *et al.*, *Nature* 460, 1101 (2009)

Surface states projected in real space



The charge density of the helical states for the top and bottom surfaces. White arrows indicate the spin polarization projected on each atom.

The charge density of the helical states on both surfaces are contributed 70% by the first QL, 22.3% by the second QL, and 5.6%, 1.4% 0.45%, 0.25% by the other inner QLs respectively.

Zhao etal. *Nano Lett.* 2011, 11, 2088–2091

Conductance of surface states

Zhao etal. *Nano Lett.* 2011, 11, 2088–2091

The conductance exhibits a 'V-shape' whose minimum is at the Fermi level, consistent to the Dirac dispersion.

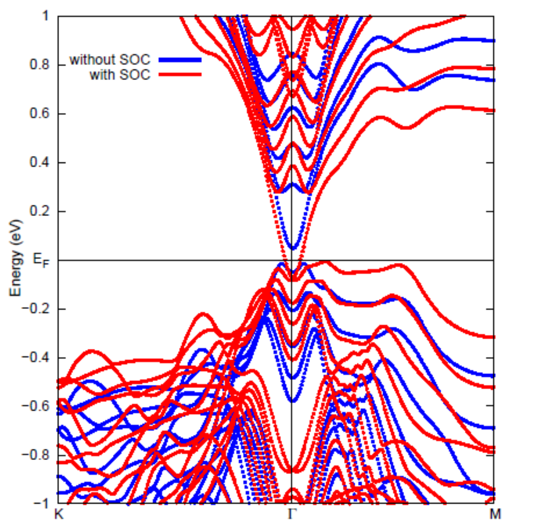
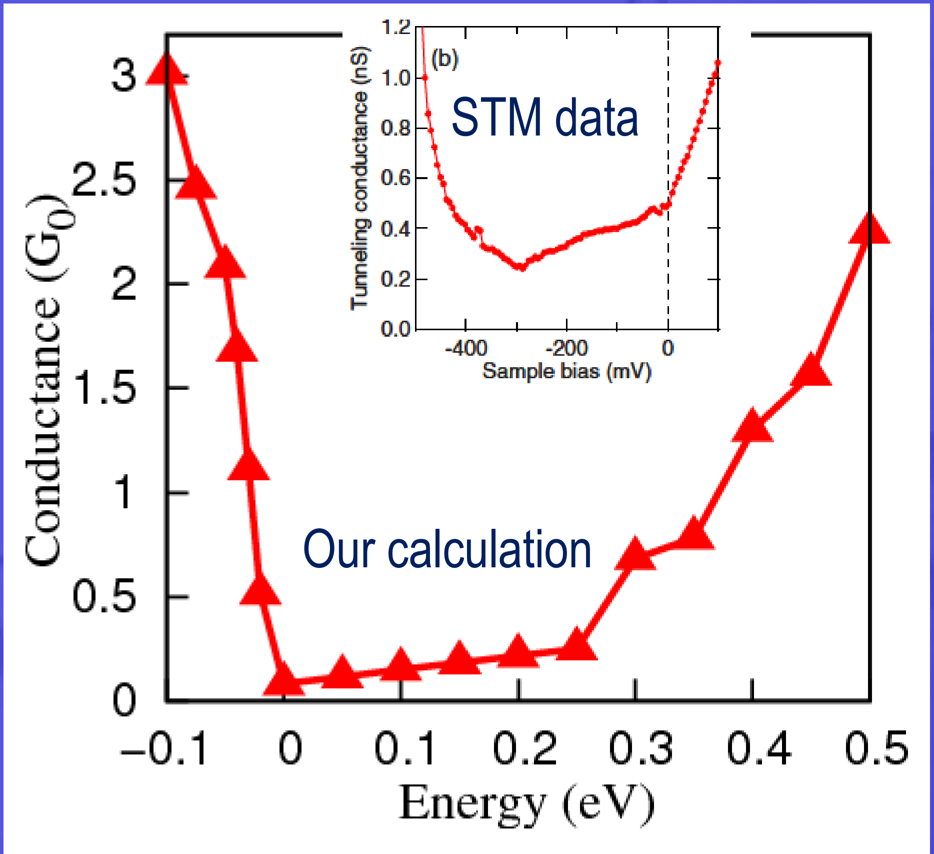
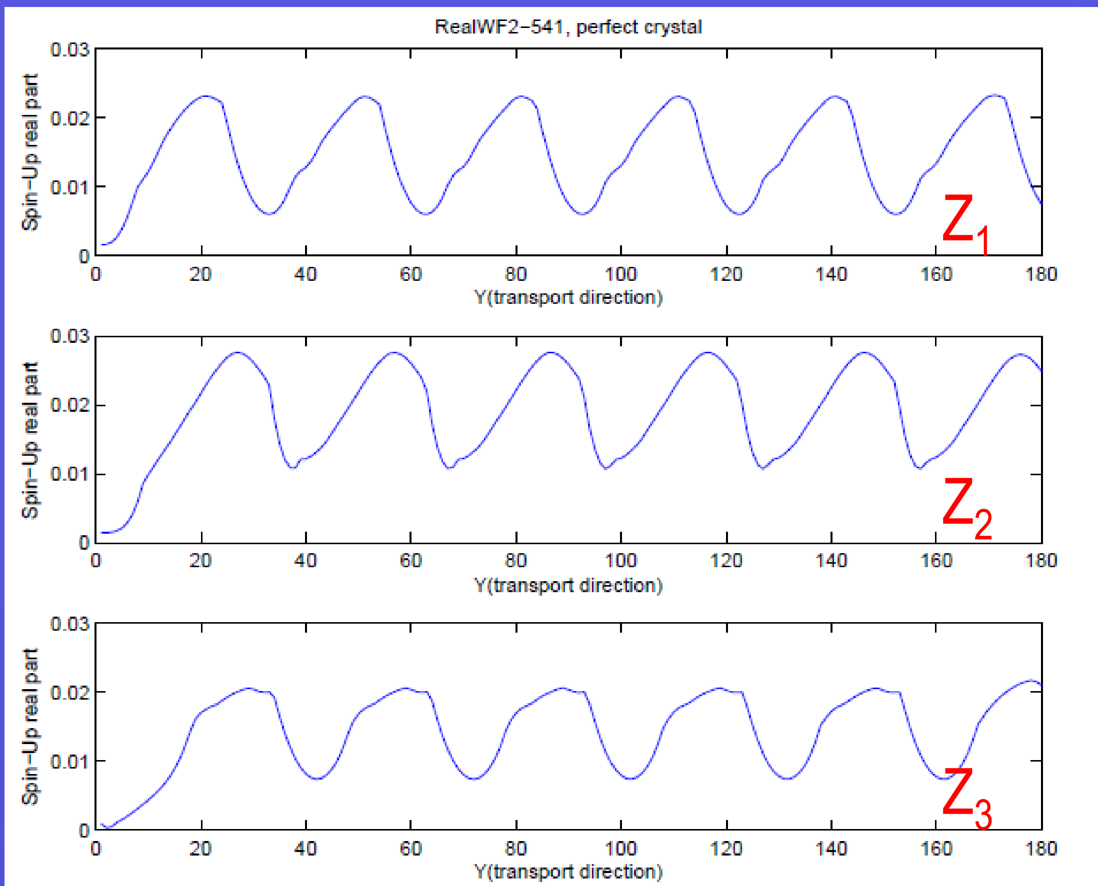


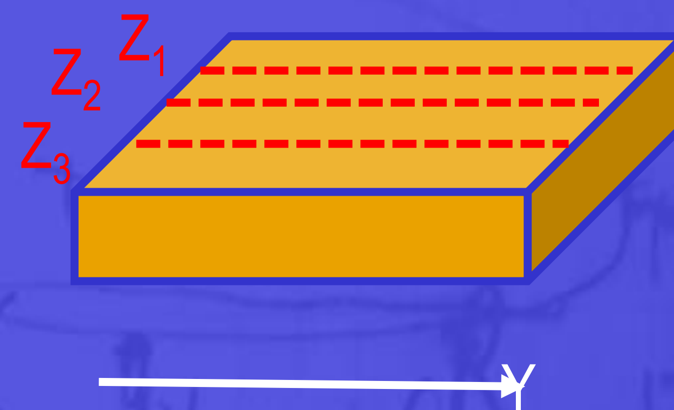
Figure 2: Band structures of the Bi_2Se_3 slab, where red and blue lines show those with and without spin-orbit coupling.



STM experiment: Hanaguri et al. PRB 82, 081305 (2010).

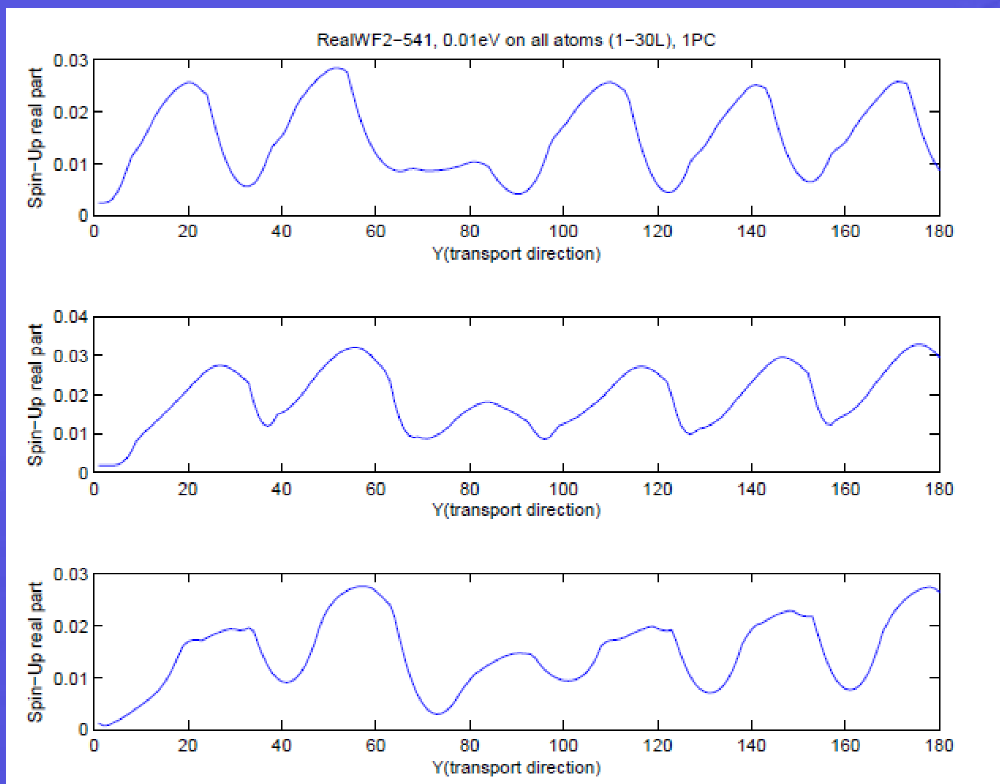
Norm of helical state: no disorder

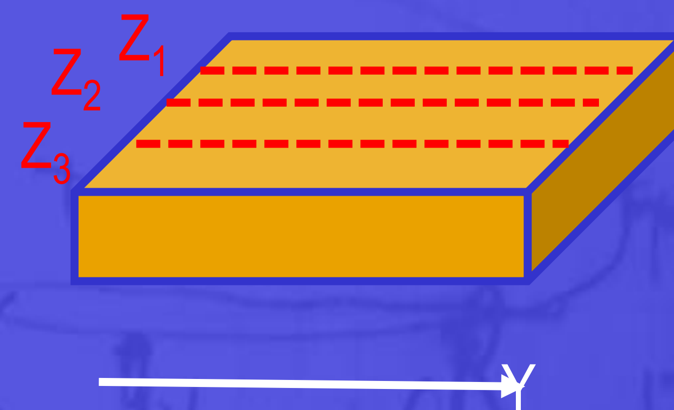




With Xuefeng Wang (Soochow Univ.), YB Hu. (2011).

Norm of helical state: with diagonal disorder





No backscattering;

spin-momentum locked perfectly.

Xuefeng Wang, Yibin Hu, H.G. (2011).

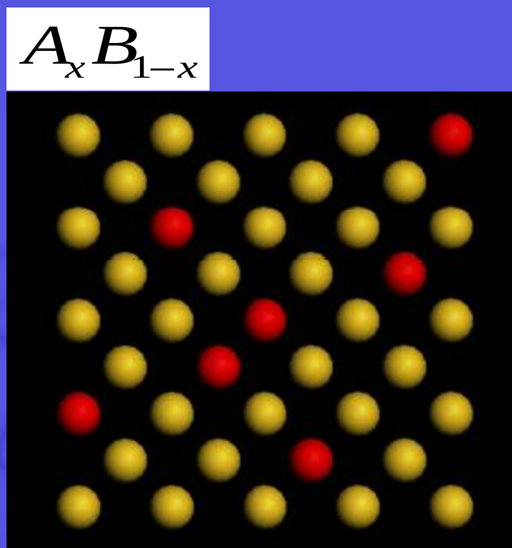
An example: topological insulator Bi_2Se_3

- Introduction: need for quantum transport from atomic first principles, crash course of quantum transport theory, NEGF-DFT method.
- Spin-orbit: helical spin states in topological insulator Bi_2Se_3.
- Disorder: non-equilibrium vertex correction theory. Roughness scattering.
- Other issues, large systems;
- Summary

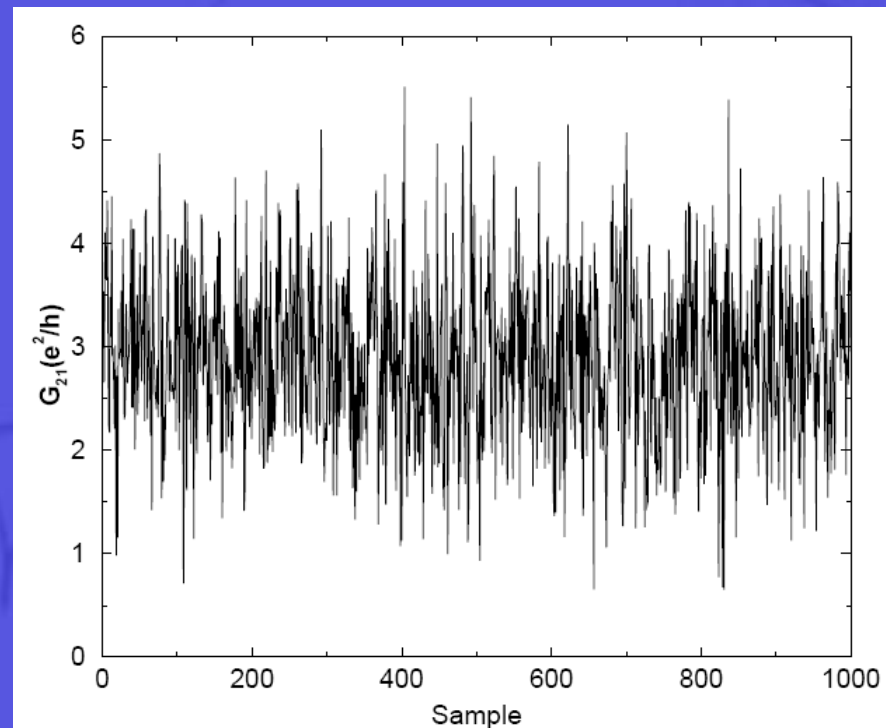
Collaborators: Dr. Youqi Ke (Princeton), Prof. Ke Xia (Beijing Normal U.)

Impurity: unavoidable in any realistic device

Conductance of a wire with impurities shows substantial sample to sample fluctuations:



T. Dejesus, Ph.D thesis, McGill University, 2002.



For any theoretical calculations, disorder averaging must be done.

How to do this in atomistic calculations at non-equilibrium?

Impurities can be very bad and very useful:

- Discrete doping atoms in semiconductor transistors;
- Surface roughness in Cu interconnect wires;
- Spin dependent scattering centers in spin transistors, spin injection pumps;
- Disorder effects reduce spin transfer torque;
- Dilute magnetic semiconductors;
- Microscopic physics of the anomalous Hall effect;
- $In_xGa_{1-x}N$ for solar cells;
- …..

Impurities play important roll in all these topics…

Disorder presents difficulty for atomic calculations:

Brute force averaging: generate many samples, compute every one, then average over the ensemble.

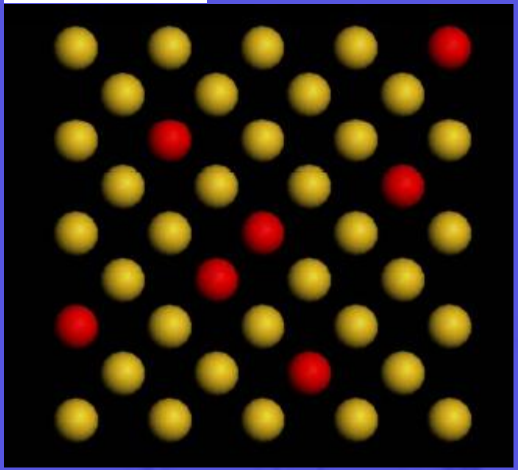
For atomistic calculations, brute force averaging suffers from:

- If impurity concentration is low, say 0.1%, one needs to compute 1000 host atoms to just accommodate 1 impurity atom.
- Cannot calculate arbitrary impurity concentration x, unless using very large supercells.
- Many configurations (1000 or more) must be averaged, too much work.

New approach: non-equilibrium vertex correction theory (NVC).

Average over H: CPA --- well established method

$A_x B_{1-x}$



When there are impurities, translational symmetry is broken. Coherent Potential Approximation (CPA) is an effective medium theory that averages over the disorder and restores the translational symmetry. So, an atomic site has x% chance to be occupied by A, and (1-x)% chance by B.

P. Soven, Phys. Rev. **156, 809 (1967).**

$$G = P + PVG.$$

$$\overline{G} = P + P\overline{V}P + P\overline{VPV}P + \cdots$$

$$\overline{T(E,\Delta V)} = Tr[\overline{G^r \Gamma_L G^a \Gamma_R}]$$

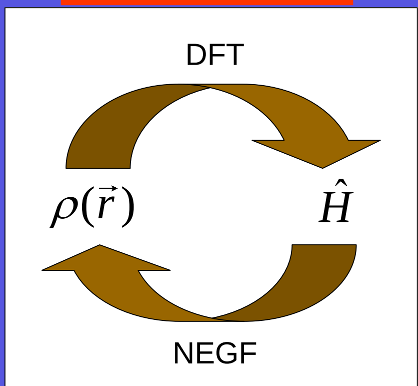
B. Velycky, Phys. Rev. 183 (1969).

Elliott, Krumhansl, and Leath: Randomly disordered crystals

Rev. Mod. Phys. 46, 466 (1974)

Non-equilibrium density matrix: nonequilibrium vertex

NEGF-DFT

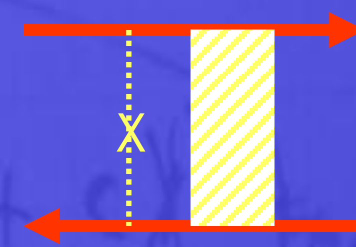


$$\rho \sim \int G^{<}\, dE = \int G^{R}\Sigma^{<}G^{A}\, dE$$

Average over random disorder:

$$\overline{\rho} \sim \int \overline{G^{<}}\, dE = \int \overline{G^{R}\Sigma^{<}G^{A}}\, dE$$

$$\overline{T} = \mathrm{Tr}\left(\overline{G^{R}\Gamma_{l}G^{A}\Gamma_{r}}\right)$$



$$\overline{G^{R}\Sigma^{<}G^{A}} \neq \overline{G^{R}}\ \overline{\Sigma^{<}}\ \overline{G^{A}}$$

$$\overline{T} = Tr\left[\Gamma_{l}\overline{g}^{\mathcal{R}}\Gamma_{r}\overline{g}^{\mathcal{A}}\right] + Tr\left[\Gamma_{l}\overline{g}^{\mathcal{R}}\Omega'_{VC}\overline{g}^{\mathcal{A}}\right]$$

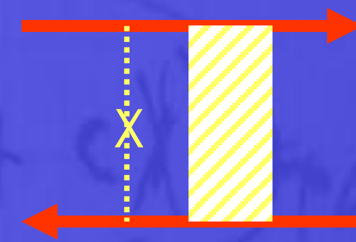
specular part   diffusive part

We found: the problem of correlated disorder scattering at non-equilibrium can be solved by a non-equilibrium vertex correction theory (NVC) and be implemented in a NEGF-DFT-NVC software.

Youqi Ke, Ke Xia and Hong Guo PRL **100**, 166805 (2008); PRL 105, 236801 (2010).

Essence of Nonequilibrium Vertex Correction (NVC)

$$\begin{aligned}\overline{g}^{\alpha,<} &= \overline{g^{\alpha,\mathcal{R}}\Sigma^{\alpha,<}g^{\alpha,\mathcal{A}}} \\ &= \overline{g}^{\alpha,\mathcal{R}}(\Sigma^{\alpha,<}+\Omega_{NVC})\overline{g}^{\alpha,\mathcal{A}}\end{aligned}$$



Conventional vertex correction, *i.e.* that appears in computing Kubo formula in disordered metal, is done at equilibrium.

NVC is done at non-equilibrium: it is related not only to multiple impurity scattering, but also to the non-equilibrium statistics of the device scattering region.

nanoDSIM

Implementation: LMTO with atomic sphere approximation for CPA and NVC, within NEGF-DFT.

Rather messy and complicated in technical details

$$
\begin{aligned}
\Omega_{NVC,R} &= \sum_{Q=A,B} C_R^Q t_R^{Q,\mathcal{R}} [\overline{g}^{\alpha,\mathcal{R}} \Sigma^{\alpha,<} \overline{g}^{\alpha,\mathcal{A}}]_{RR} t_R^{Q,\mathcal{A}} \\
&- \sum_{Q=A,B} C_R^Q t_R^{Q,\mathcal{R}} \overline{g}_{RR}^{\alpha,\mathcal{R}} \Omega_{NVC,R} \overline{g}_{RR}^{\alpha,\mathcal{A}} t_R^{Q,\mathcal{A}} \\
&+ \sum_{Q=A,B} C_R^Q t_R^{Q,\mathcal{R}} [\sum_{R'} \frac{1}{N_{k_\parallel}} \sum_{k_\parallel} \overline{g}_{RR'}^{\alpha,\mathcal{R}}(k_\parallel, E) \Omega_{NVC,R'} \\
&\times \overline{g}_{R'R}^{\alpha,\mathcal{A}}(k_\parallel, E)] t_R^{Q,\mathcal{A}} \qquad (23)
\end{aligned}
$$

See EPAPS Document No. E-PRLTAO-100-020817 for supplemental material. For more information on EPAPS, see http://www.aip.org/pubservs/epaps.html.

Youqi Ke, Ke Xia and Hong Guo PRL **100**, 166805 (2008); PRL 105, 236801 (2010).

Example 2: Resistance of Cu interconnects

Collaboration with Daniel Gall of RPI;

Dr. F. Zahid, Univ. of Hong Kong.

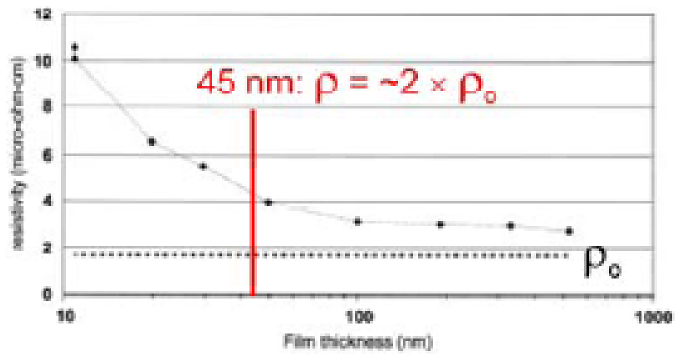
Dr. Youqi Ke, Princeton.

$: SRC

Size Effect

Cu-resistivity increases with decreasing line-width

Electron mean-free path at room temperature:
λ = 39 nm.



Cause for size effect:

electron scattering on

(1) surfaces

(2) grain boundaries

(3) surface roughness

Rossnagel & Kuan (2004)

E.g.: 45-nm-wide lines have a ~2x higher resistivity than bulk.

2

Fuchs-Sondheimer Model of surface diffusive scattering

FUCHS, K., 1938, *Proc. Camb. Phil. Soc.*, **34**, 100.

ADVANCES IN PHYSICS

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The Mean Free Path of Electrons in Metals

By E. H. SONDHEIMER*,
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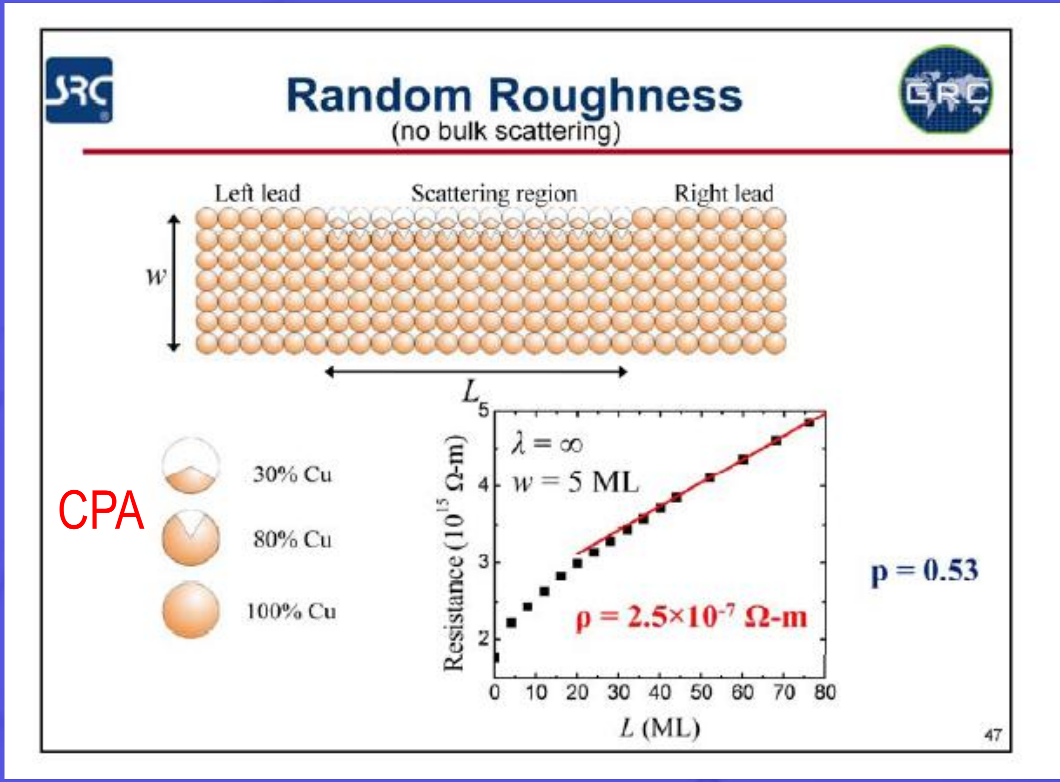
$$\rho = \rho_0 (1 + 0.375 \frac{\lambda}{d} (1 - p))$$

where ρ_0 = 1.67 μΩ–cm, $\rho = \rho_0 + \rho_s$, λ= 39 nm, d= thickness, p=specularity parameter

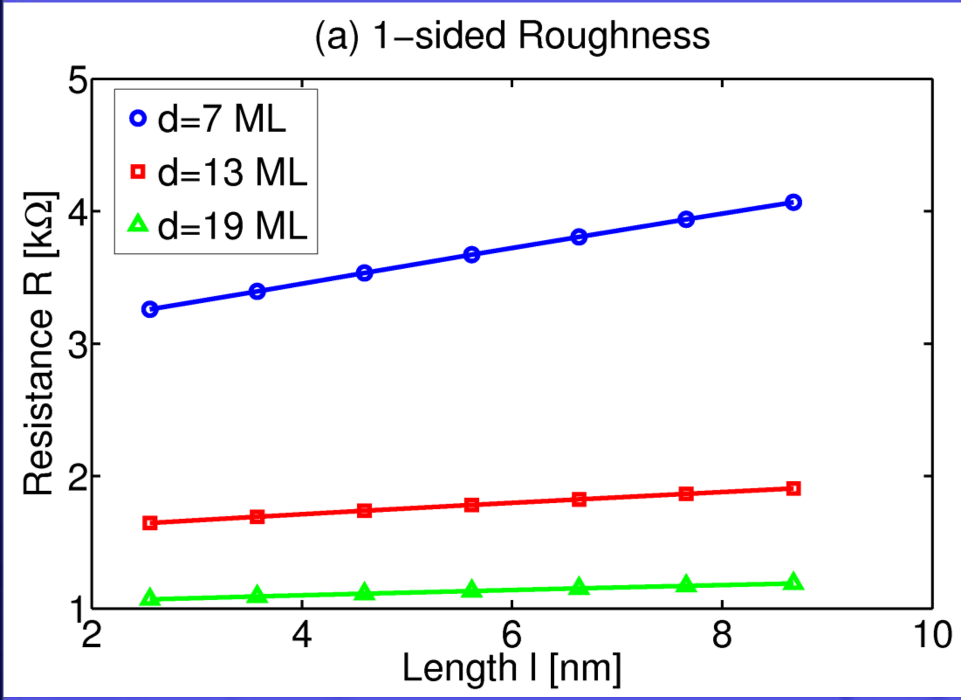
Surface roughness scattering:

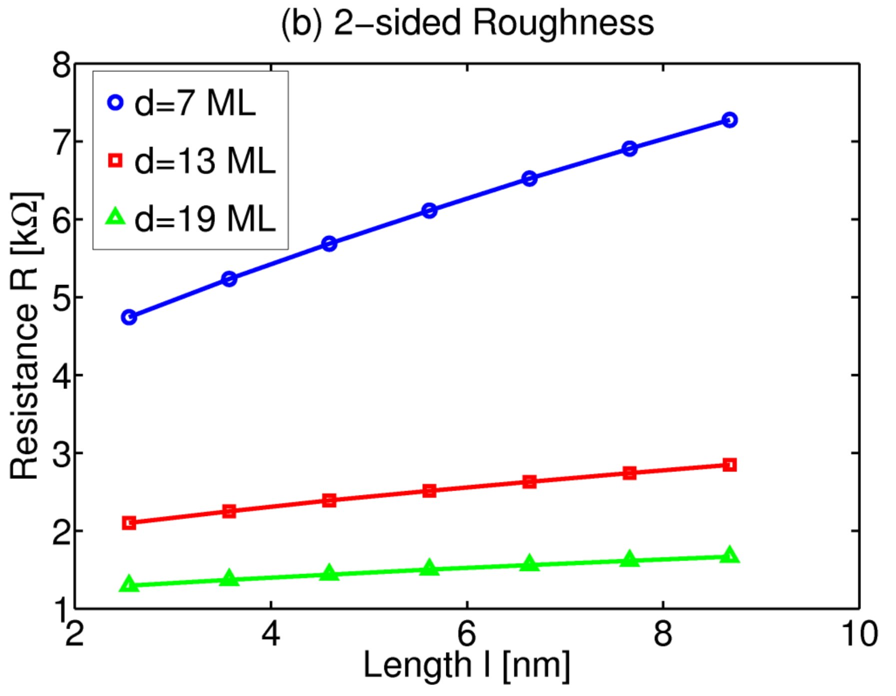


CPA

- Thin Cu film as a two probe device of specific length and thickness.
- Pure, single crystal, fcc, lattice constant = 3.61 A
- Two probe device size is 1800 atoms (maximum 8,000 atoms).

Results: R vs. L



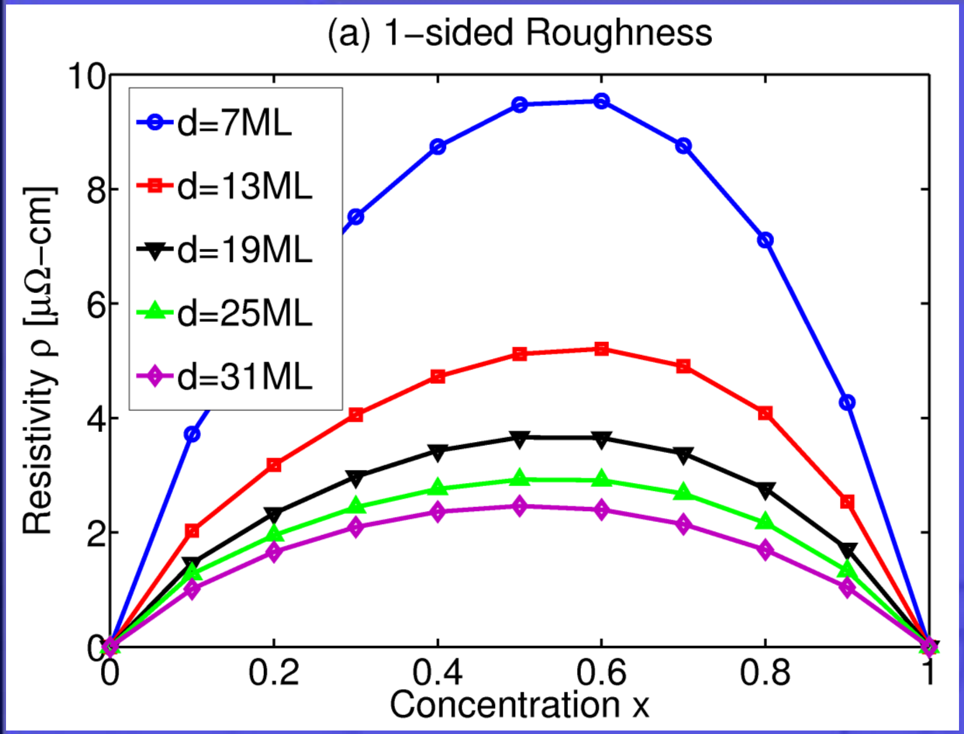


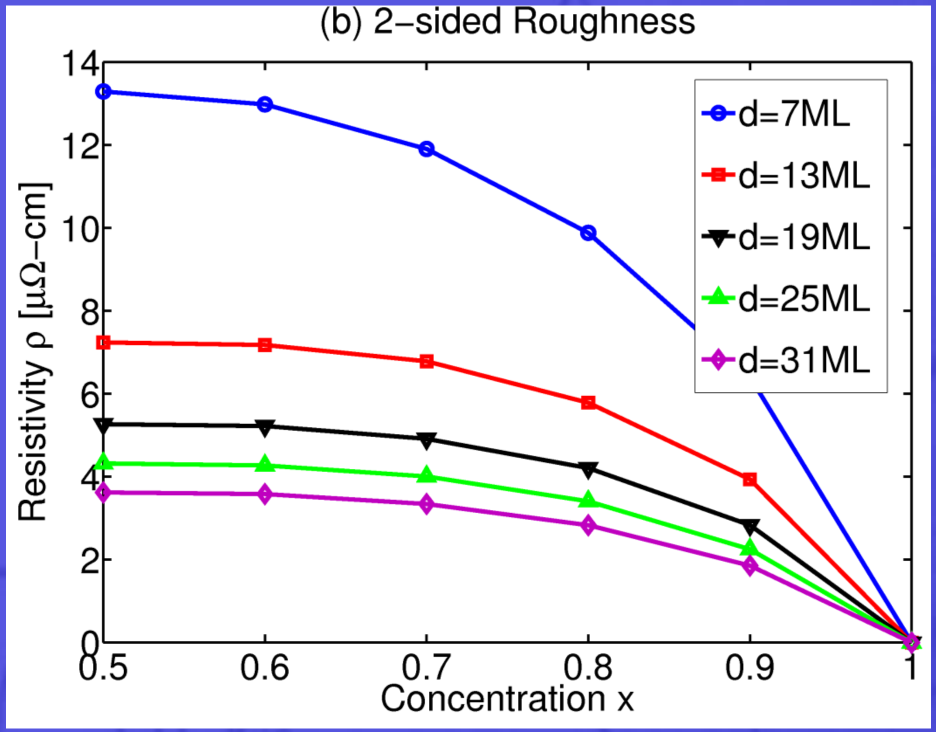
Linear behaviour – like Ohm's law for metal.

From the slope, we extract resistivity.

F. Zahid etal. Phys. Rev. B 81, 045406 (2010).

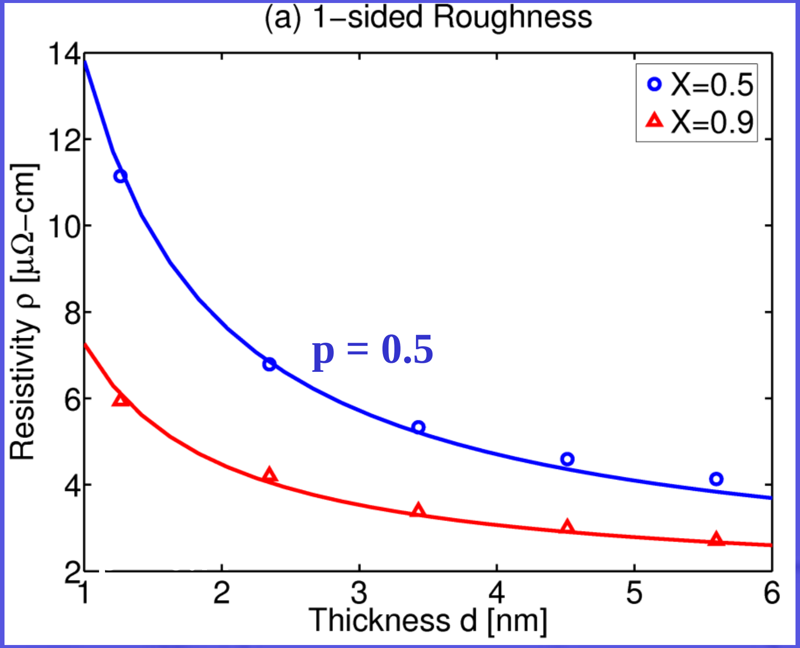
Results: ρ vs. x

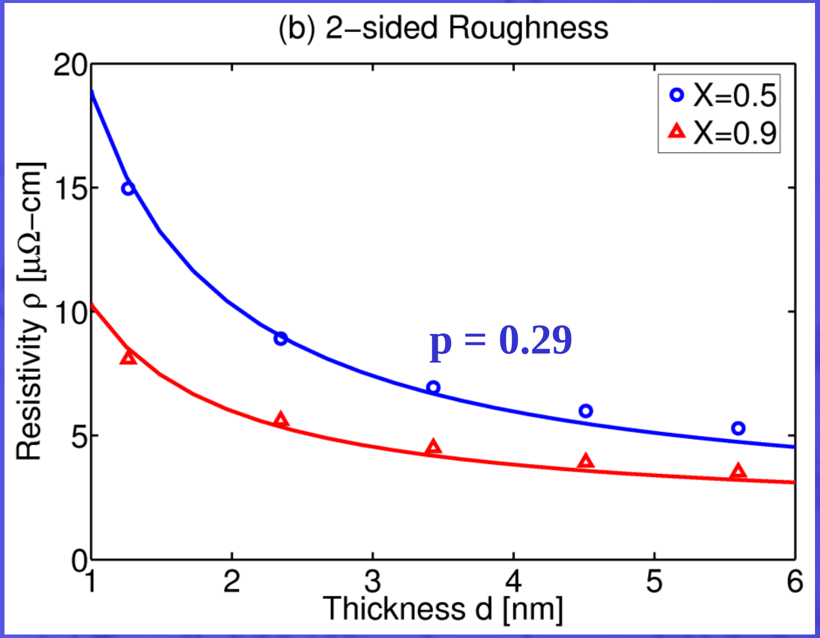




- No scattering (ρ = 0) at the perfect surface i.e. for x = 0 and 1
- Not symmetric for 1-sided roughness. Symmetric for 2-sided.

Results: ρ vs. d





Solid lines = F-S fit

Exp: ρ = 8.35 μΩ-cm at d = 6.6 nm

Theory: ρ = 5.30 μΩ-cm at d = 5.3 nm

Fuchs-Sondheimer Model:

$$\rho = \rho_0 (1 + 0.375 \frac{\lambda}{d}(1 - p))$$

where ρ_0 = 1.67 μΩ–cm, $\rho = \rho_0 + \rho_s$ (our values)
λ= 39 nm, d= thickness, p=specularity parameter

An example: topological insulator Bi_2Se_3

- Introduction: need for quantum transport from atomic first principles, crash course of quantum transport theory, NEGF-DFT method.
- Spin-orbit: helical spin states in topological insulator Bi_2Se_3.
- Disorder: the non-equilibrium vertex correction theory; Fe/MgO/Fe MTJ;
- Other issues, large systems;
- Summary

Large systems: principle underlying O(N) methods

Locality: the properties of a certain observation region comprising one or a few atoms are only weakly influenced by factors that are spatially far away from this observation region. S. Geodecker Rev. Mod. Phys. (1999)

Equilibrium density matrix exhibits decaying property:

$$\rho(\mathbf{r},\mathbf{r}') = \sum f(\epsilon_i)\psi_i^*(\mathbf{r})\psi_i(\mathbf{r}') \qquad f(\epsilon) = \frac{1}{1+\exp\frac{\epsilon-\mu}{k_BT}}$$

insulator

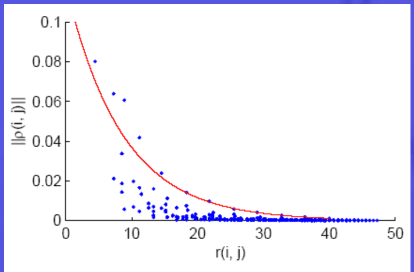
$$\rho(\mathbf{r},\mathbf{r}') \propto \exp(-c_1\cdot a\cdot\Delta\cdot|\mathbf{r}-\mathbf{r}'|) \text{ or } \exp\left(-c_2\cdot\sqrt{\Delta}\cdot|\mathbf{r}-\mathbf{r}'|\right)$$

metal

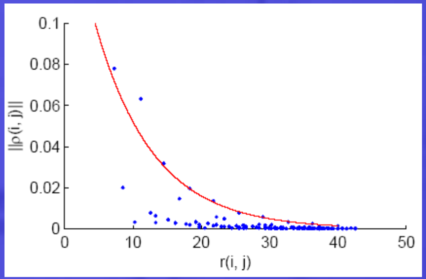
$$\rho(\mathbf{r},\mathbf{r}') \propto k_F\frac{\cos(k_F|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^2}\exp\left(-c_3\frac{k_BT}{k_F}|\mathbf{r}-\mathbf{r}'|\right)$$

Example: Si bulk

LMTO

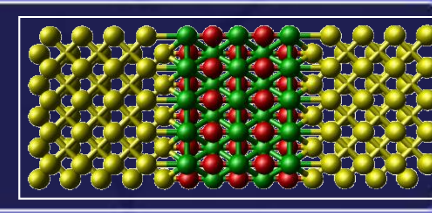


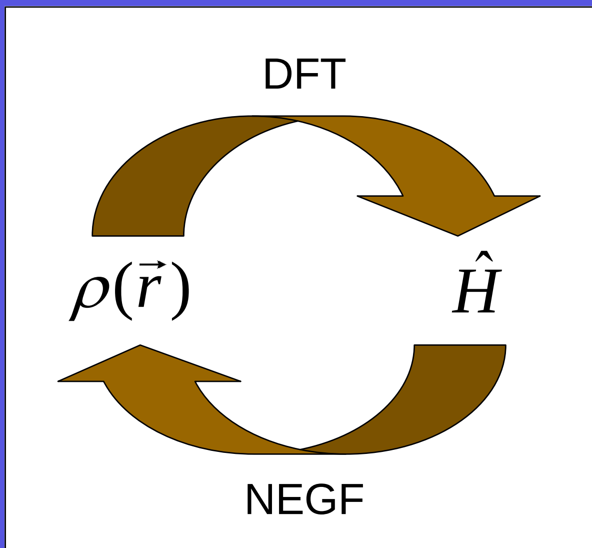
LCAO



Eric Zhu, H.G. (2011).

Density matrix computation:





DFT – computes potential and energy levels of the device;

NEGF – non-equilibrium statistics that fills levels;

The self-consistent loop – NEGF-DFT algorithm.

Practically, density matrix is divided into two parts: equilibrium and non-equilibrium parts:

$$\hat{\rho} = \frac{1}{\pi} Im \left[\int_{-\infty}^{\mu_L} dE \mathbf{G}^R(E) \right] + \frac{1}{2\pi} \left[\int_{\mu_L}^{\mu_R} dE \mathbf{G}^<(E) \right]$$

locality — no locality

Eric Zhu, H.G. (2011).

Summary: status and perspective:

Phonons, electron-phonon scattering, forces, current-triggered forces, LDA+U, spin-orbit, AC quantities, time-dependent currents… Many things have been done.

TCAD (SPICE): using ~hundreds of parameters to model – difficult to go on;

NEGF-DFT: no parameter but brute force atomic computation – costly.

Future:

Taking advantage of progress in electronic structure theory, more accurately predict quantum transport.

Far from equilibrium, high frequency quantum transport.

Strong correlation effects.

“Coarse grain” atomic computation to identify critical variables for nanoelectronic devices.

Take home message 4:

Progress in electronic structure theory has great impact to device physics and device modeling.

We are at the door of first principles based TCAD tool for device modeling.

Thank you !