Transport at strong and weak topological insulator surfaces

NewSpin2, College Station, 15 December 2011

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Outline

I. Transport in some unusual 2D "metals" in the Dirac approximation

Ordinary 2D non-magnetic metals, and also graphene, are ultimately localized by even weak disorder.

Strong TI surface: single Dirac cone that should be very stable
How does the Berry phase show up in transport experiments?

Weak TI surface: two Dirac cones with T^2 = -1
Is this ever delocalized?

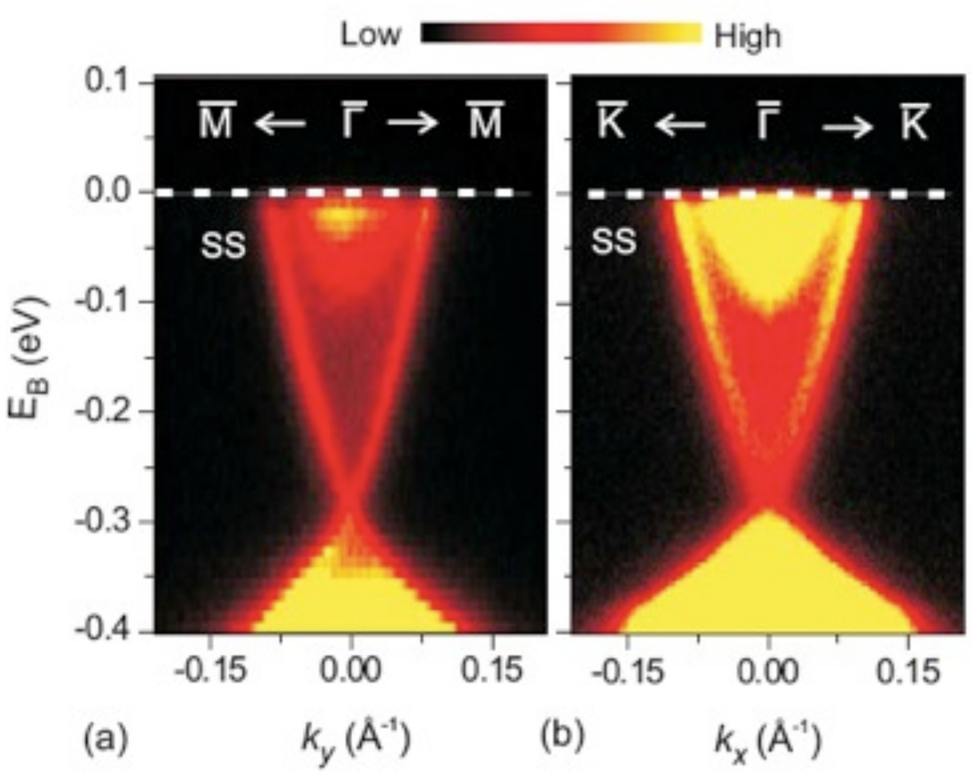
with Jens Bardarson (UCB), Piet Brouwer (Cornell), Roger Mong (UCB)

II. An example of electronic structure calculations for surfaces of a strong TI slab
with Oleg Yazyev (EPFL), Steven Louie (UCB)

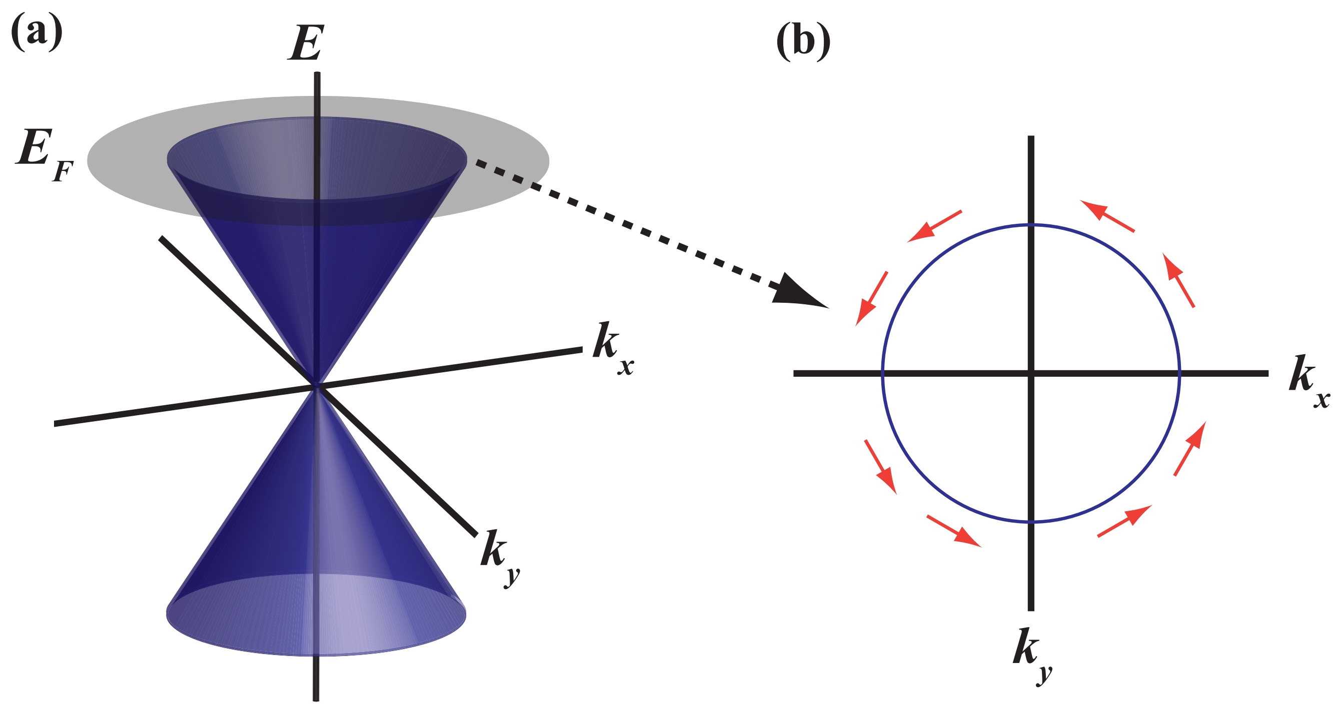
III. How can we understand the Dirac surface of the strong TI at a deeper level?
Effective field theory of TIs with Gil Young Cho (UCB)

Strong topological insulator surface

First observation by D. Hsieh et al. (Z. Hasan group), Princeton/LBL, 2008. This is later data on Bi_2Se_3 from the same group in 2009:



Odd number of Dirac cones
Spin locked to momentum
Stable to non-magnetic disorder



Relation to classification scheme of TIs (neglecting interactions)

Cartan nomenclature	TRS	PHS	SLS	Hamiltonian	NLSM (ferm. replicas)	$d=1$	$d=2$	$d=3$
A (unitary)	0	0	0	$U(N)$	$U(2n)/U(n)\times U(n)$	-	$\mathbb{Z}$	-
AI (orthogonal)	+1	0	0	$U(N)/O(N)$	$Sp(2n)/Sp(n)\times Sp(n)$	-	-	-
AII (symplectic)	−1	0	0	$U(2N)/Sp(2N)$	$O(2n)/O(n)\times O(n)$	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
AIII (chiral unit.)	0	0	1	$U(N+M)/U(N)\times U(M)$	$U(n)$	$\mathbb{Z}$	-	$\mathbb{Z}$
BDI (chiral orthog.)	+1	+1	1	$SO(N+M)/SO(N)\times SO(M)$	$U(2n)/Sp(n)$	$\mathbb{Z}$	-	-
CII (chiral sympl.)	−1	−1	1	$Sp(2N+2M)/Sp(2N)\times Sp(2M)$	$U(2n)/O(2n)$	$\mathbb{Z}$	-	$\mathbb{Z}_2$
D	0	+1	0	$SO(2N)$	$O(2n)/U(n)$	$\mathbb{Z}_2$	$\mathbb{Z}$	-
C	0	−1	0	$Sp(2N)$	$Sp(n)/U(n)$	-	$\mathbb{Z}$	-
DIII	−1	+1	1	$SO(2N)/U(N)$	$O(2n)$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
CI	+1	−1	1	$Sp(2N)/U(N)$	$Sp(n)$	-	-	$\mathbb{Z}$

What is the effect of topological term on the Anderson localization?

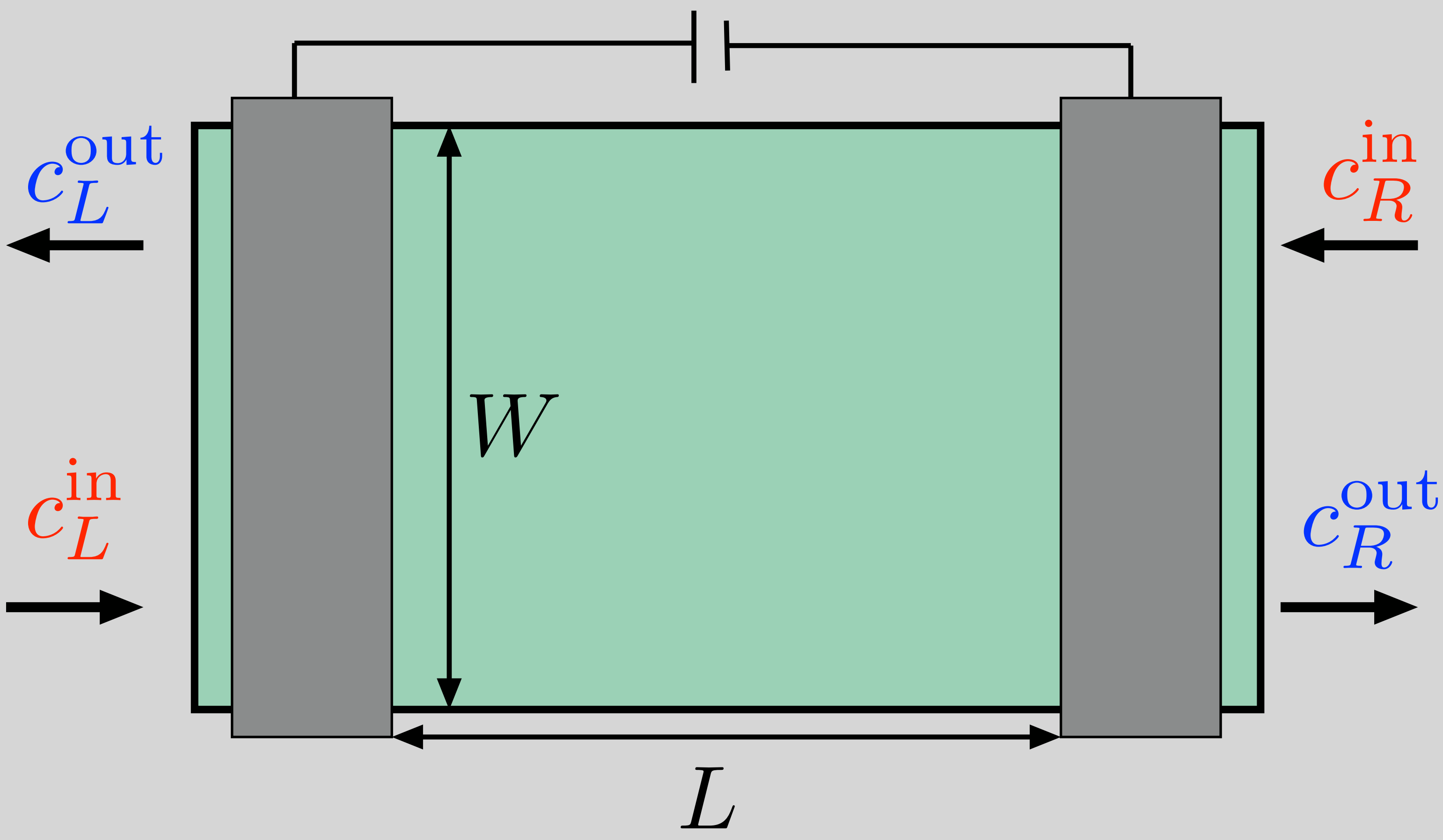
Symplectic class in 3D: Strong vs. weak topological insulators

Schnyder, Ryu, Furusaki and Ludwig, (Landau Memorial Conf.;arXiv:0905.2029), AIP Conf. Proc. 1134, 10 (2009).

Symplectic class (AII) -- Consequences of time reversal

Time reversal: $T^2 = -1 \qquad THT^{-1} = H$

Schematic setup and basic definitions



$$\begin{pmatrix} c_L^{out} \\ c_R^{out} \end{pmatrix} = S \begin{pmatrix} c_L^{in} \\ c_R^{in} \end{pmatrix}$$

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

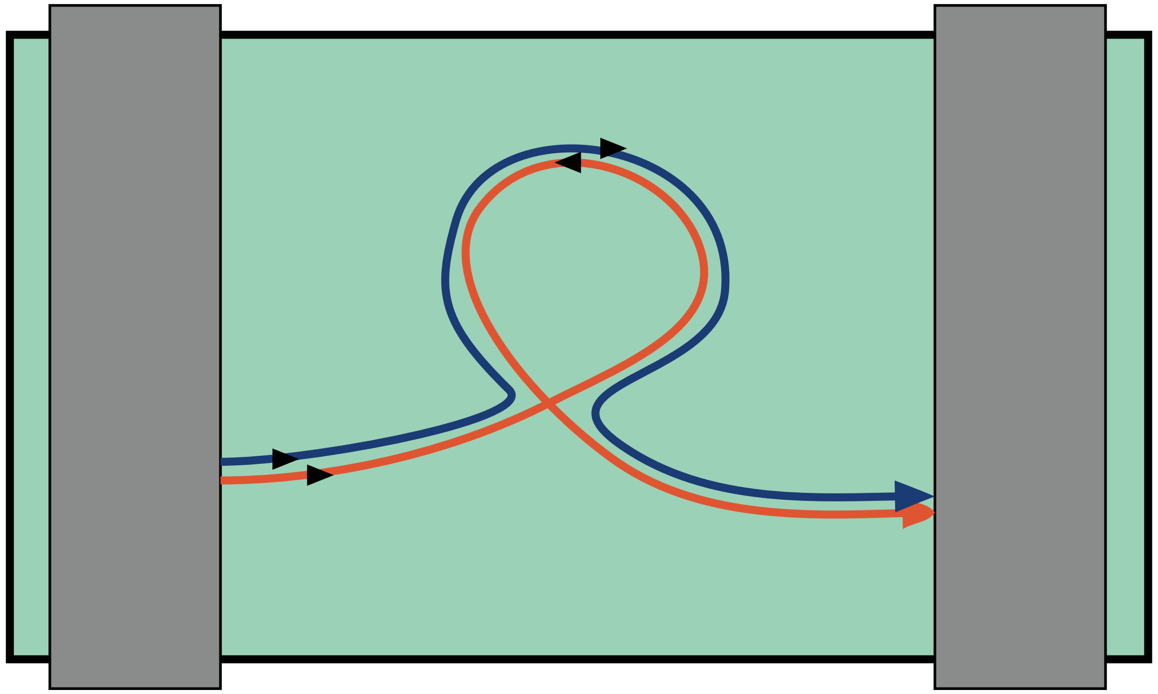
Landauer conductance: $G = \mathrm{tr}\, t^\dagger t = \mathrm{tr}\,(1 - r^\dagger r) = \sigma W/L$

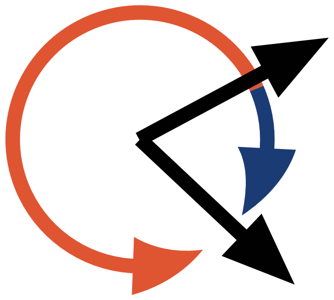
Symplectic class (AII) -- Consequences of time reversal

Time reversal: $T^2 = -1$ $THT^{-1} = H$

i) $S^T = -S \Rightarrow$
- Absence of backscattering (also for multiple scattering)
- Kramers' degeneracy of transmission eigenvalues
- Perfectly transmitted mode if odd number of modes (minimum conductance of e^2/h)

ii) Weak anti-localization $\sigma = \sigma_0 + \frac{1}{\pi} \ln L$





Single parameter scaling and non-linear sigma model

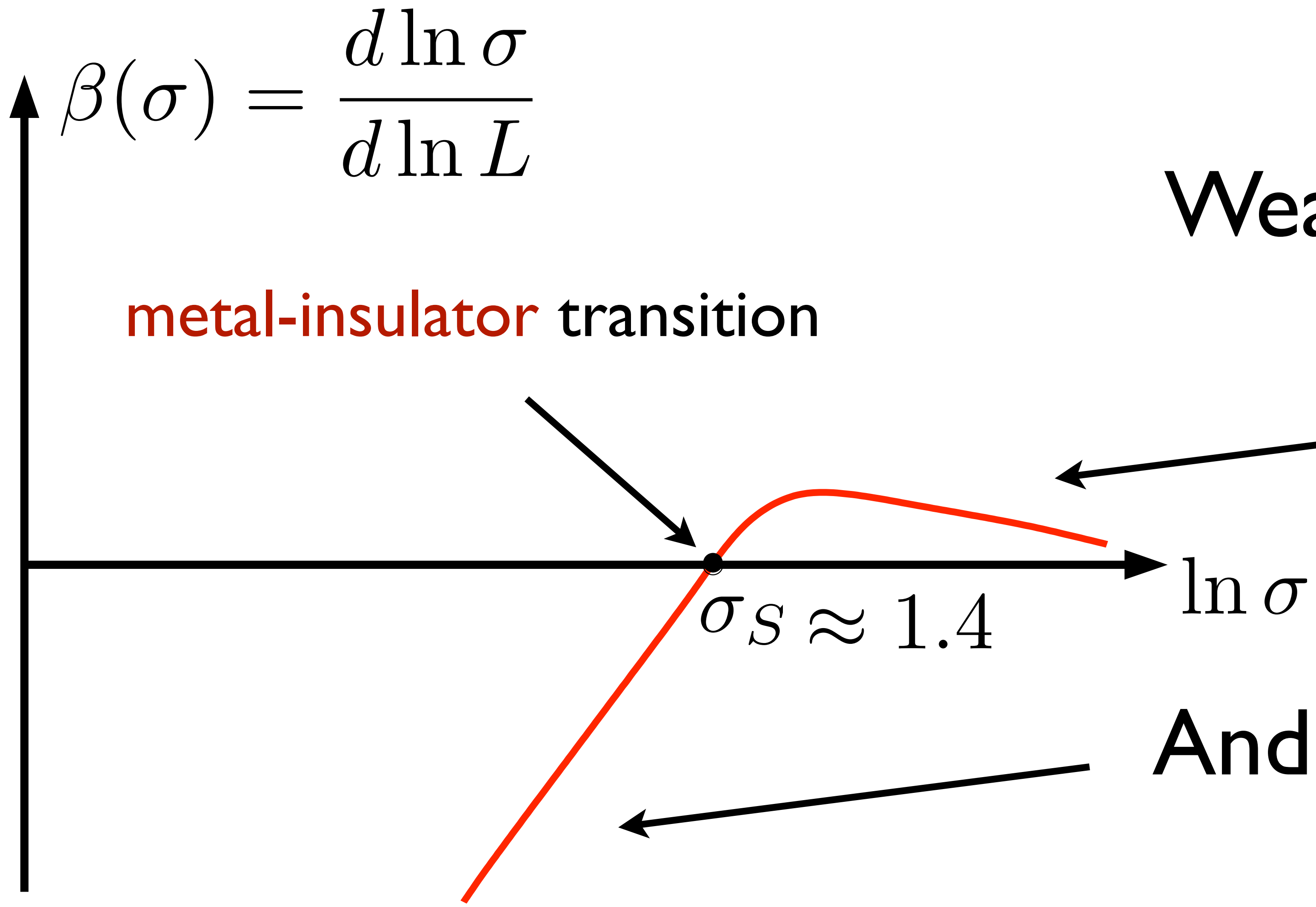
Effective low energy field theory of a strong TI:

S. Ryu, C. Mudry, H. Obuse, and A. Furusaki, Phys. Rev. Lett. **99**,116601 (2007).
P. M. Ostrovsky, I. V. Gornyi, and A. D. Mirlin, Phys. Rev. Lett. **98**, 256801 (2007).

$$S = S^{\mathrm{NL}\sigma\mathrm{M}}_{\mathrm{symp}} + S_{\mathrm{topological}}$$

Without topological term:

S. Hikami, A. I. Larkin and Y. Nagaoka (1980)
P. Markoš and L. Schweitzer (2006)



Weak anti-localization:

$$\beta(\sigma) \sim \frac{1}{\pi\sigma}$$

Anderson-localization

$$\beta(\sigma) \sim -\ln \sigma$$

Single parameter scaling and non-linear sigma model

Effective low energy field theory of a strong TI:

S. Ryu, C. Mudry, H. Obuse, and A. Furusaki, Phys. Rev. Lett. **99**,116601 (2007).
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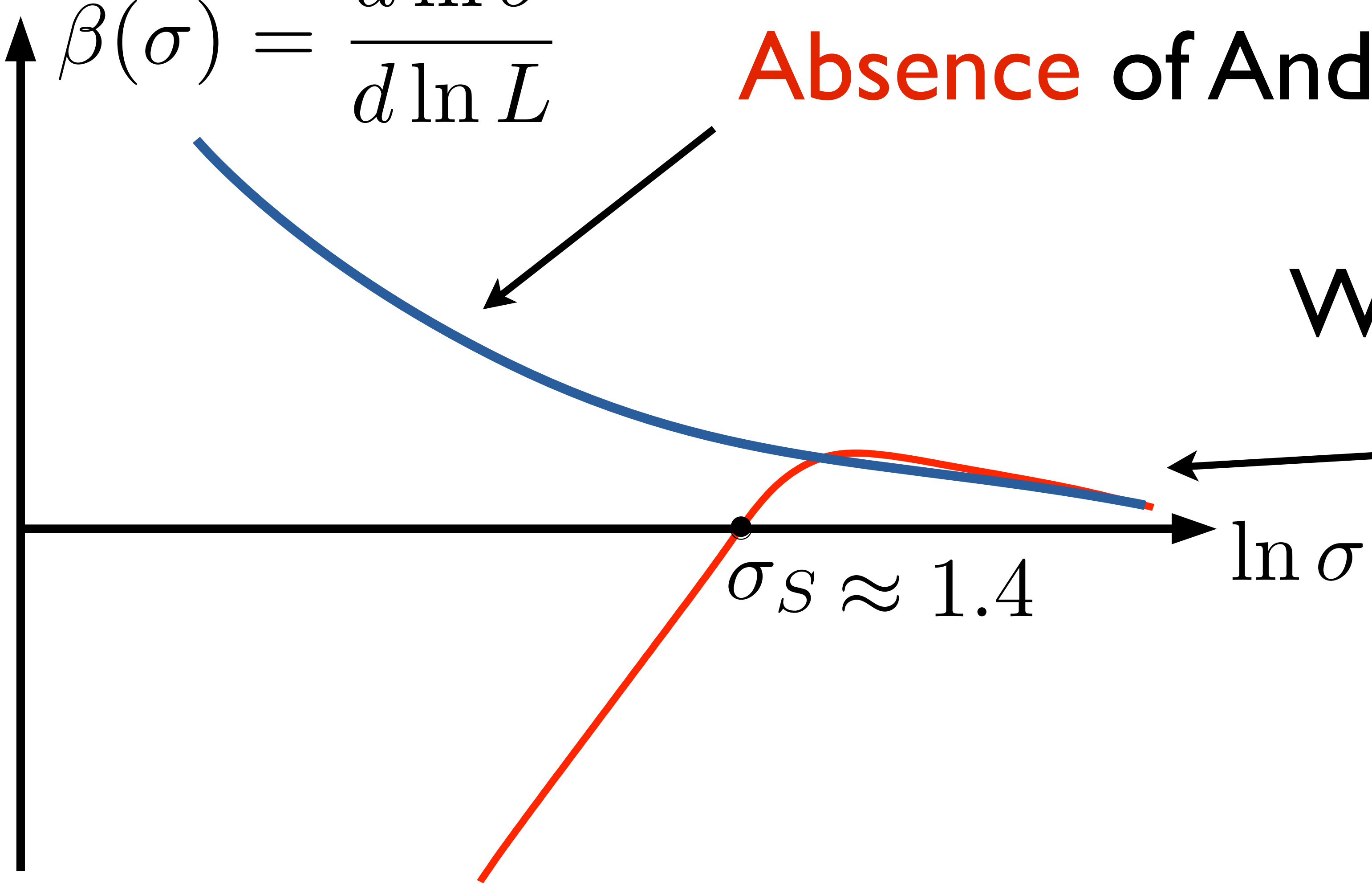
$$S = S_{\mathrm{symp}}^{\mathrm{NL}\sigma\mathrm{M}} + S_{\mathrm{topological}}$$

With topological term:

J. H. Bardarson, J. Tworzydlo, P.W. Brouwer, C.W.J. Beenakker, PRL **99**, 106801, (2007)

$$\beta(\sigma) = \frac{d \ln \sigma}{d \ln L}$$



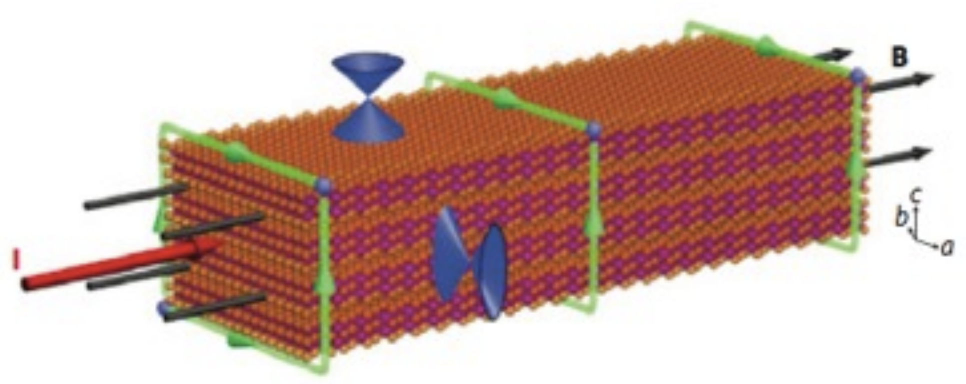
Absence of Anderson localization

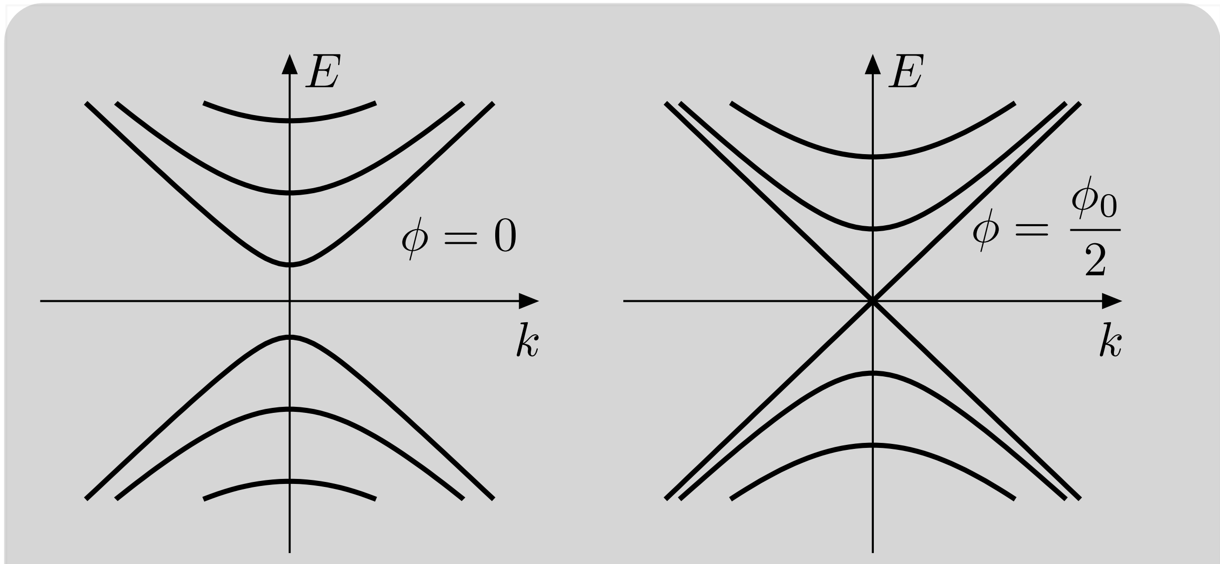
Weak anti-localization:

$$\beta(\sigma) \sim \frac{1}{\pi\sigma}$$

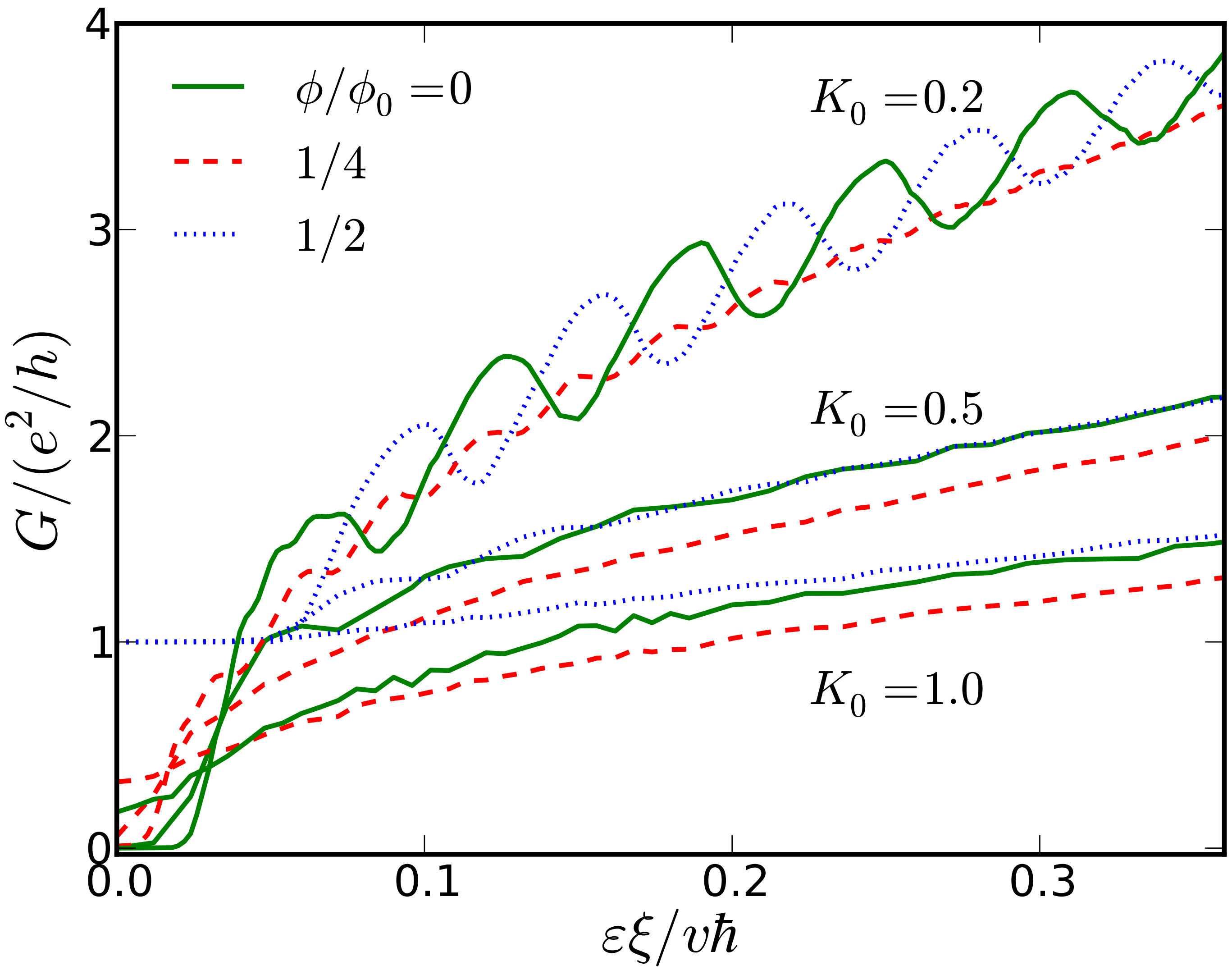
Aharonov-Bohm oscillations in nanowires

J.H. Bardarson, P.W. Brouwer, and J.E. Moore, PRL (2010)





Perfectly transmitted mode at nonzero flux due to Berry phase



Three regimes:

i) Dirac point. period h/e, min G

ii) Weak disorder, away from Dirac point, period h/e, min or max G

iii) Strong disorder, away from Dirac point, period h/2e (WAL)

nature materials
LETTERS
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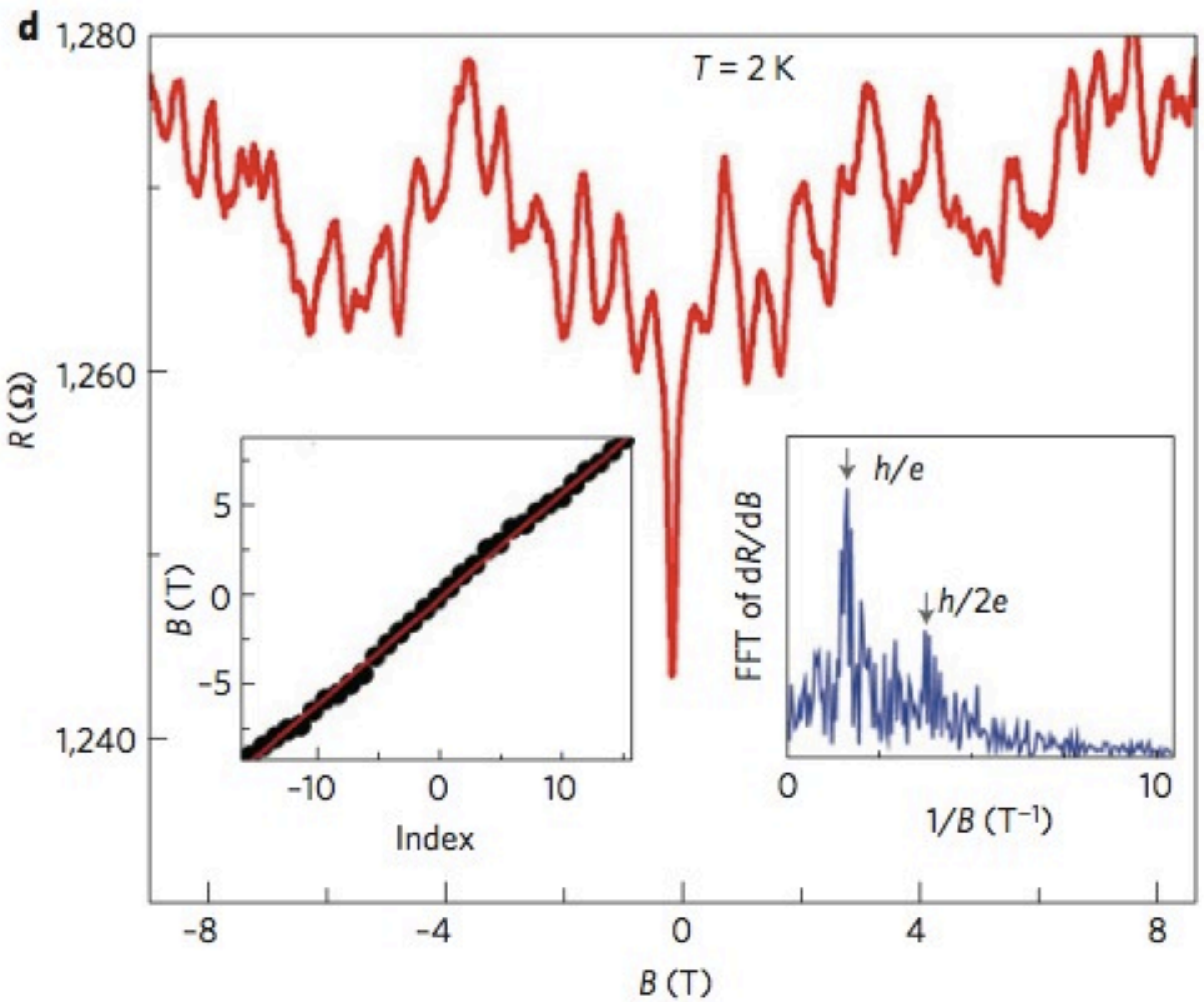
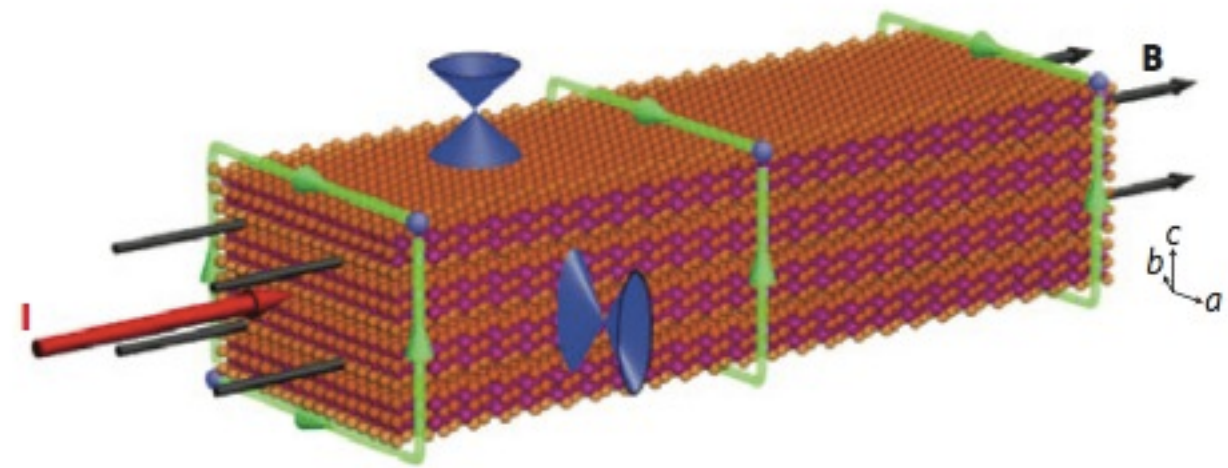
Aharonov–Bohm interference in topological insulator nanoribbons

Hailin Peng[1,2]★, Keji Lai[3,4]★, Desheng Kong[1], Stefan Meister[1], Yulin Chen[3,4,5], Xiao-Liang Qi[4,5], Shou-Cheng Zhang[4,5], Zhi-Xun Shen[3,4,5] and Yi Cui[1†]





- Oscillations of the magnetocondutance with period h/e (one flux quantum)
- Maximum conductance at zero flux
- No periodic oscillations in wide ribbons

Quantum transport in weak TI's

R. S. K. Mong, J.H.Bardarson, J.E. Moore, arXiv: 1109.3201

$$H = \hbar v_D \tau^0 (\sigma^x k_x + \sigma^y k_y) + V(\mathbf{r})$$

$$V(\mathbf{r}) = \sum_{\alpha\beta} V_{\alpha\beta}(\mathbf{r})\, \tau^\alpha \otimes \sigma^\beta$$

$$\langle \delta V_{\alpha\beta}(\mathbf{r})\, \delta V_{\alpha\beta}(\mathbf{r}') \rangle = g_{\alpha\beta} K(\mathbf{r} - \mathbf{r}')$$

Disorder structure	Disorder type	Notation
$V_{x0} \cdot \tau^x$	scalar potential (2×AII)	
$V_{yx} \cdot \tau^y \sigma^x$	gauge potential (2×AIII)	
$V_{yy} \cdot \tau^y \sigma^y$	gauge potential (2×AIII)	
$V_{yz} \cdot \tau^y \sigma^z$	mass (2×D)	$m = \langle V_{yz} \rangle$
$V_{z0} \cdot \tau^z$	scalar potential (2×AII)	
$V_{00} \cdot \mathbb{1}$	scalar potential (2×AII)	$\mu = -\langle V_{00} \rangle$

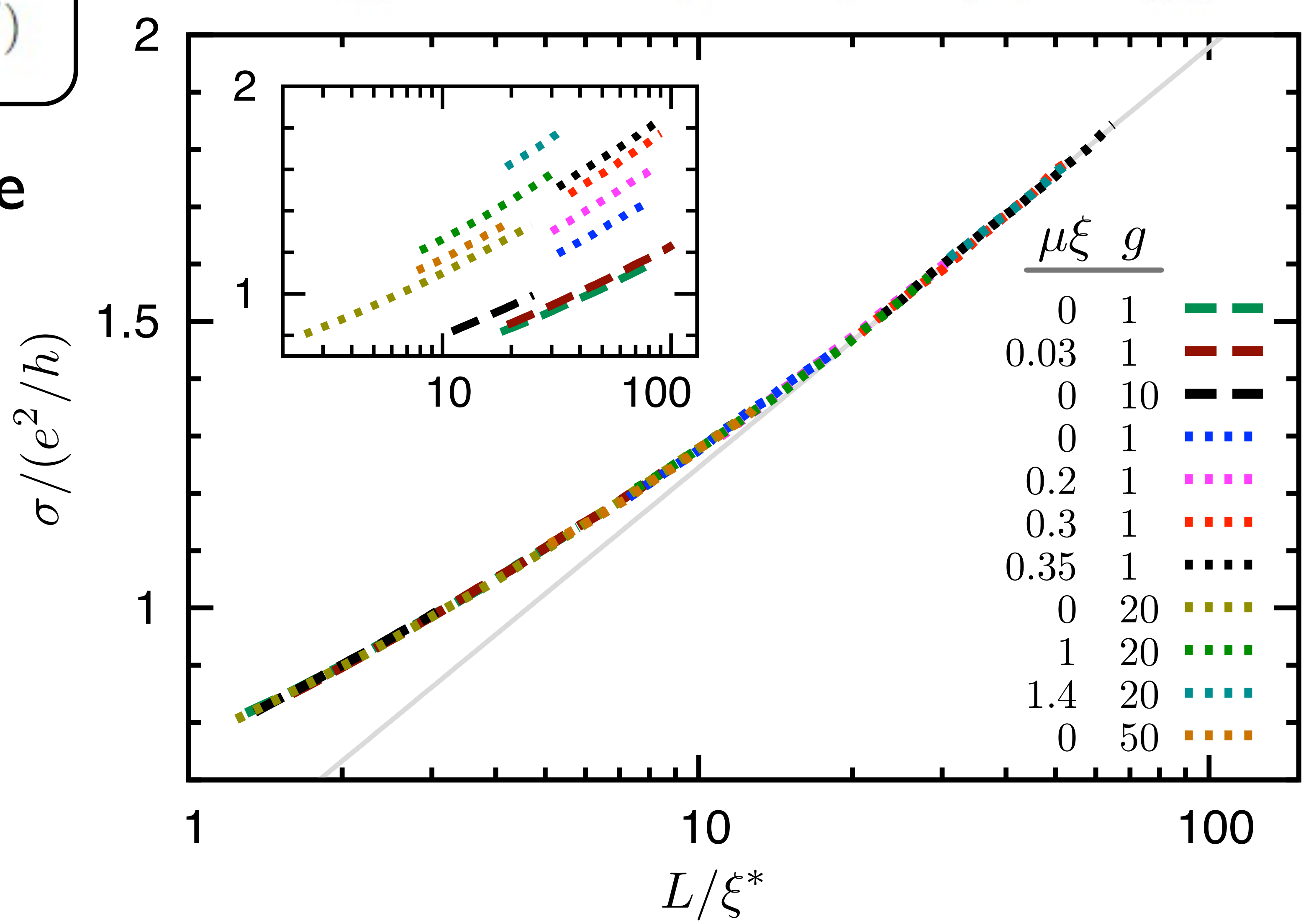
No topological term in the NLσM!

but

for $m = 0$

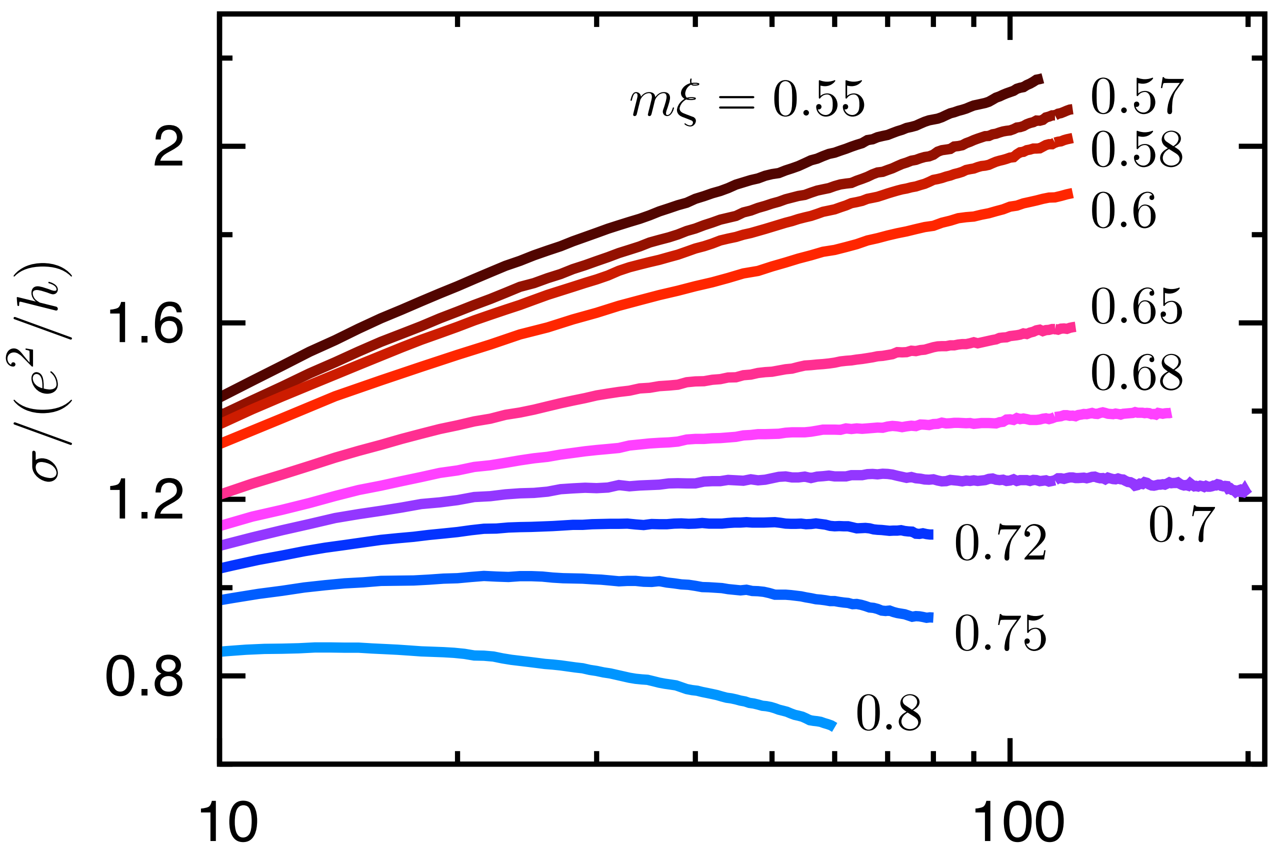
Single parameter scaling.

Flow to symplectic metal.

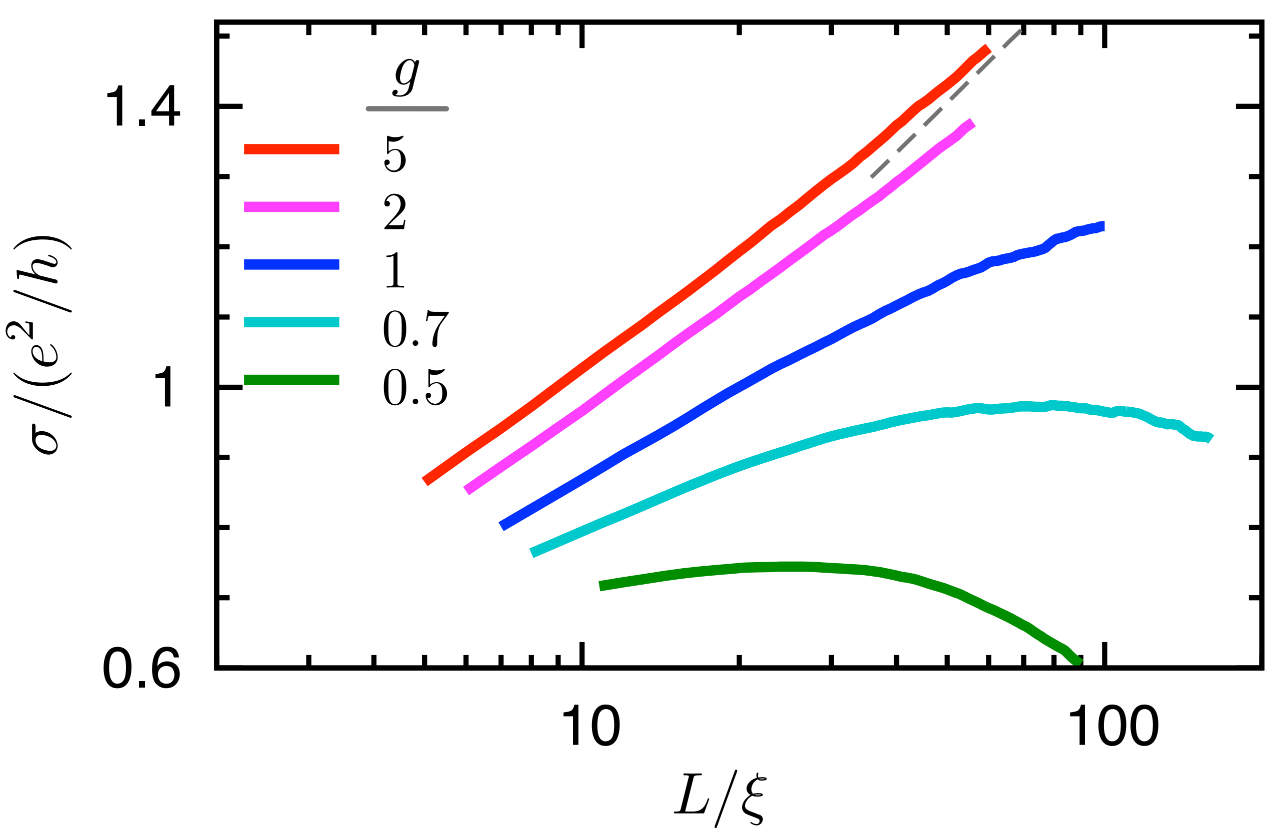


See also: Ringel, Kraus and Stern, arXiv:1105.4351

Effect of nonzero mass m

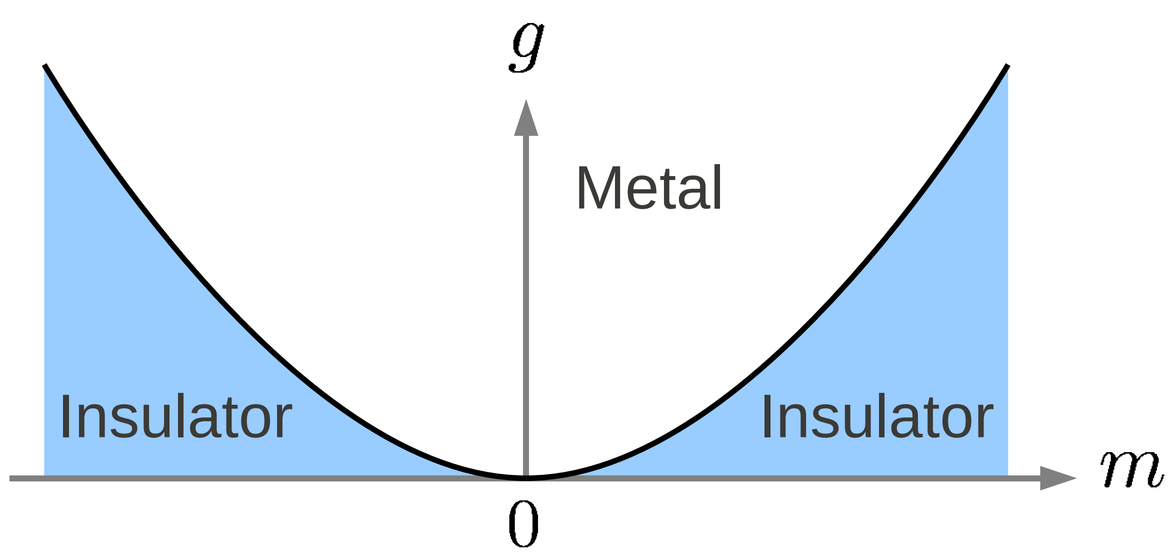


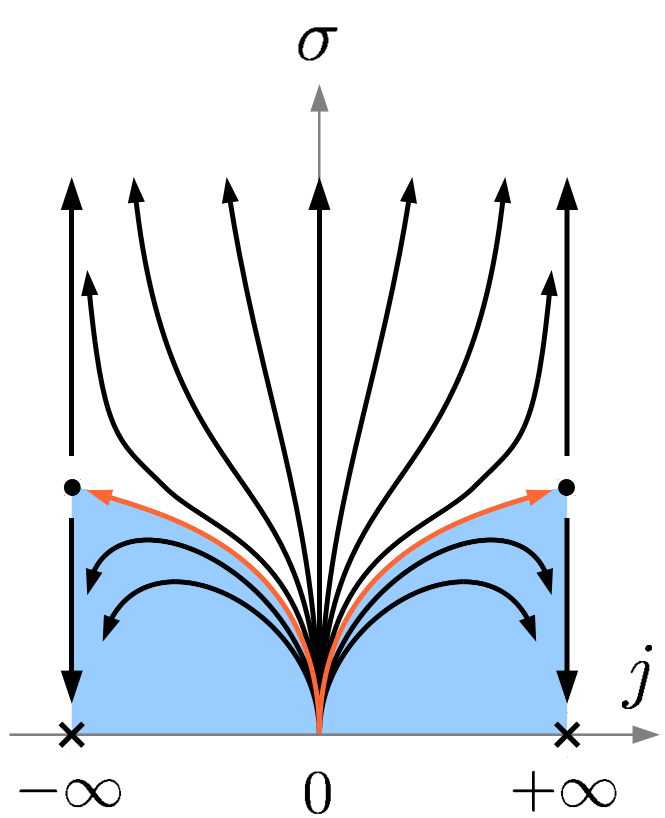
Increasing mass drives the system insulating

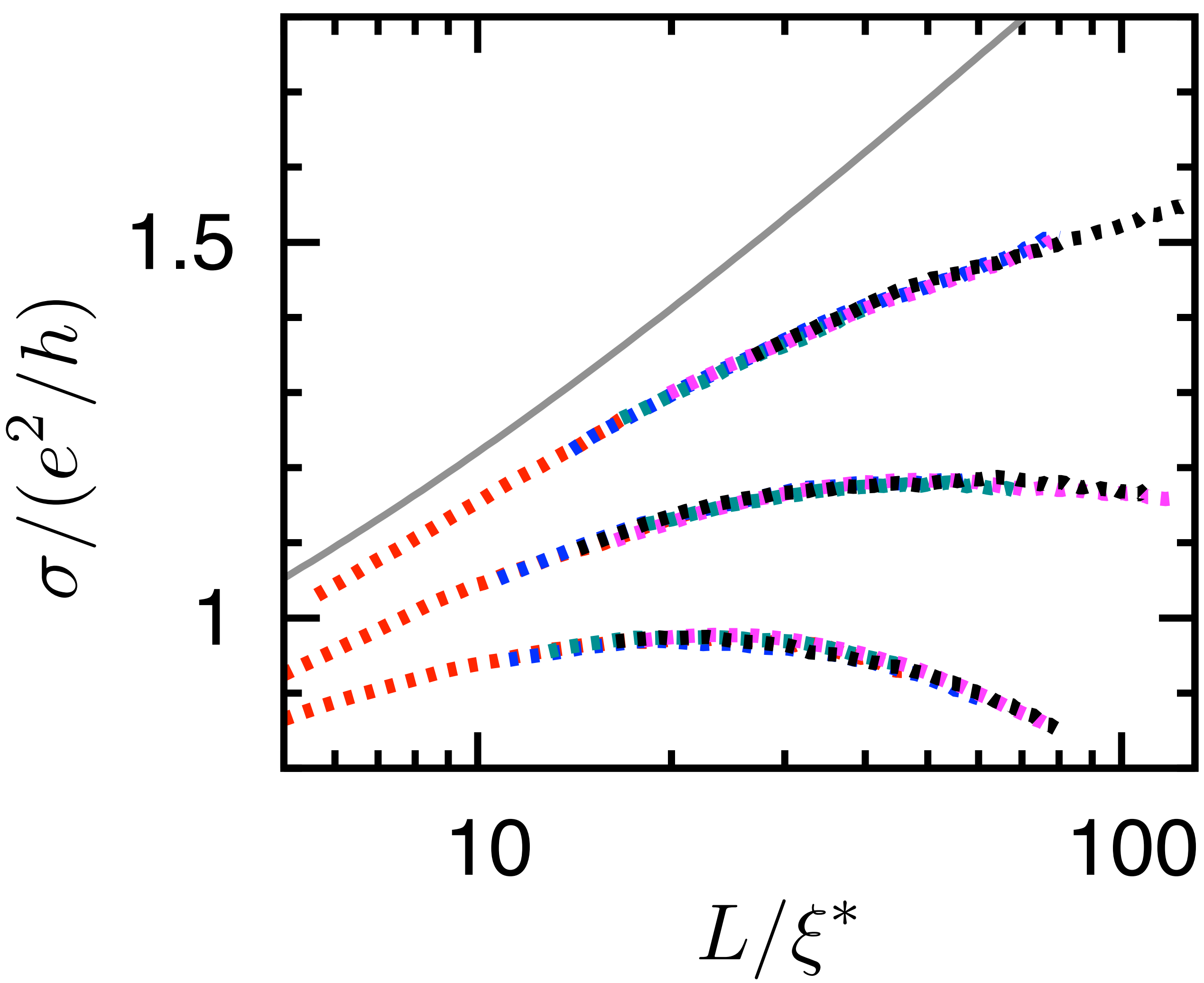


Increasing disorder drives the system metallic

Phase diagram and numerical two parameter scaling



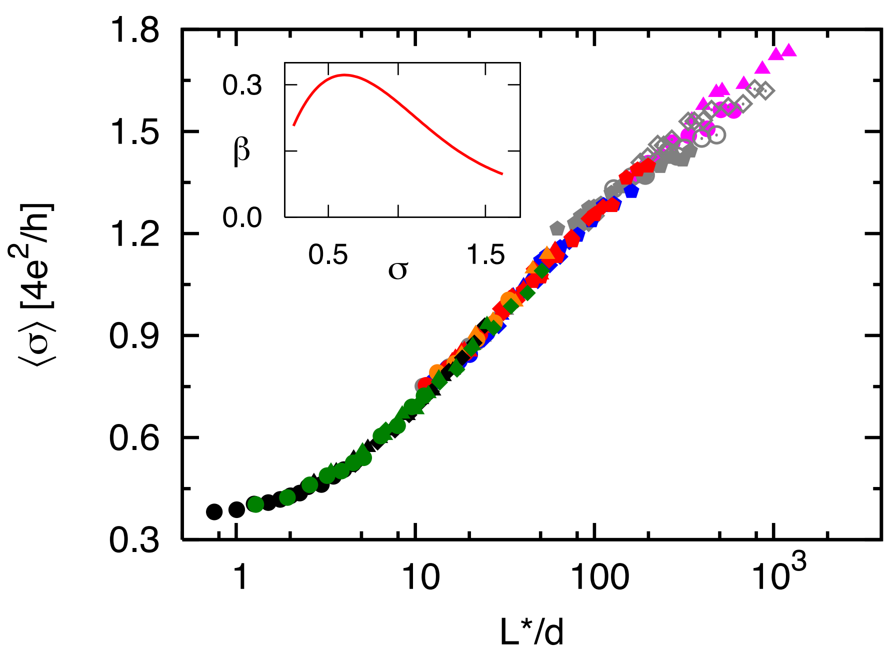




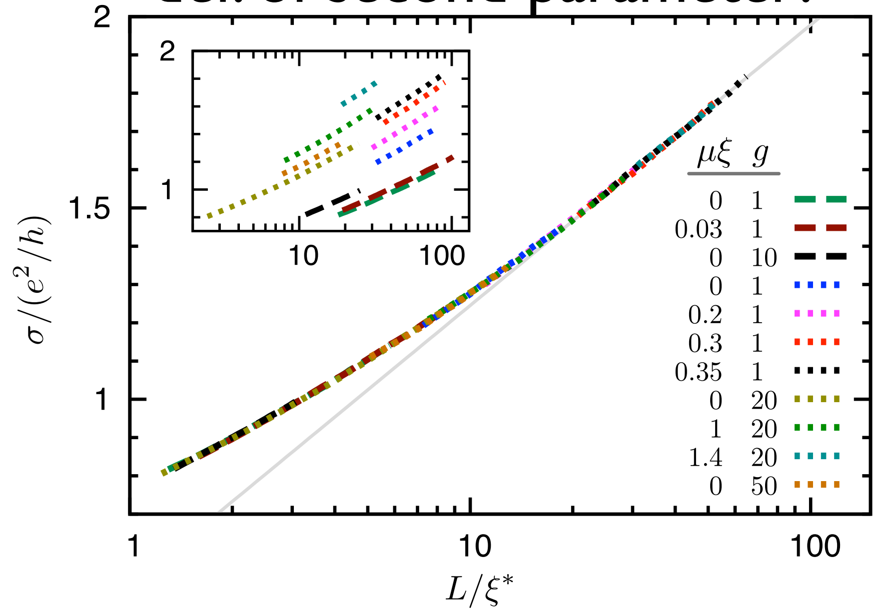
See also: Obuse, Furusaki, Ryu and Mudri PRB, 2007
Essin and Moore, RRB 2007, Shindou and Murakami PRB 2009

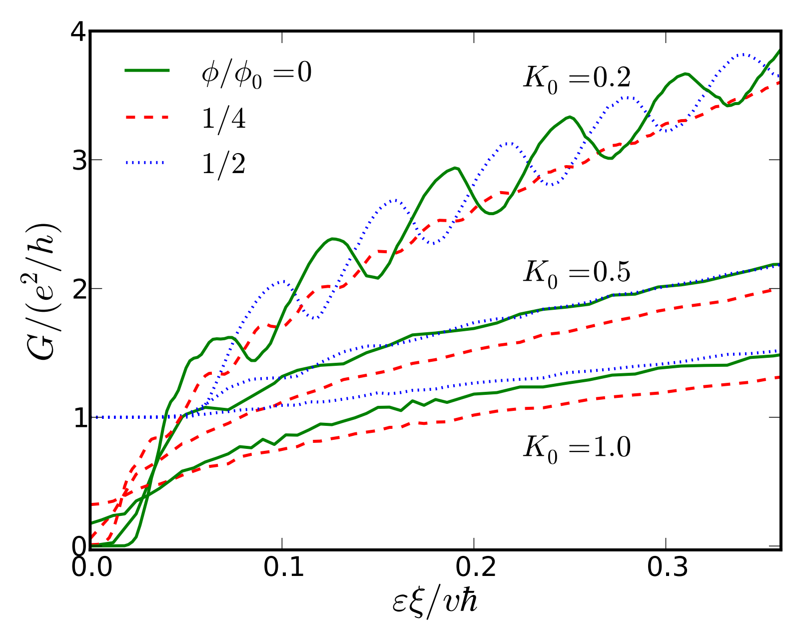
Conclusions: surface transport

Disorder always drives the strong insulator surface into the symplectic metal phase, characterized by weak anti-localization



In weak topological insulators, similar behavior is observed in the absence of mass. Including mass gives rise to two parameter scaling--but what is general def. of second parameter?





WAL also obtained in wires, expect close to the Dirac point (dominated by perfectly transmitted mode) or at very weak disorder

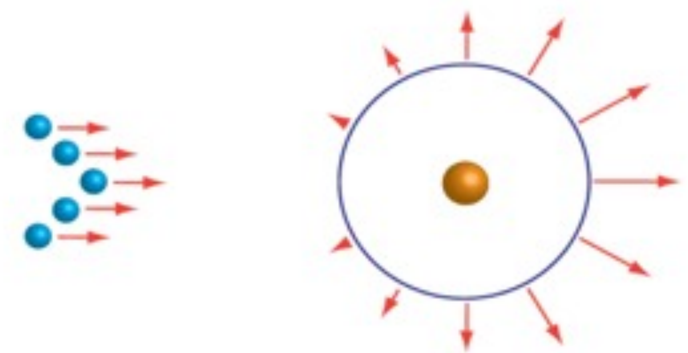
Part II: "Spintronic" applications with current materials

•Observation of giant spin-charge coupling?

Spin-charge coupling

Charge current = spin density
About 100 times larger than QWs

Align 10 **spins/micron^2** $\Rightarrow$ **1 microamp**



The locking of spin and momentum at a TI surface means that a charge *current* at one surface generates a spin *density*.

Similarly a charge *density* is associated with a spin *current.*

While these effects could cancel out between the top and bottom surfaces of an unbiased thin film, any asymmetry (such as electrical bias or substrate effects) leads to a net spin-charge coupling.
(O. Yazyev, JEM, S. Louie, PRL 2011)

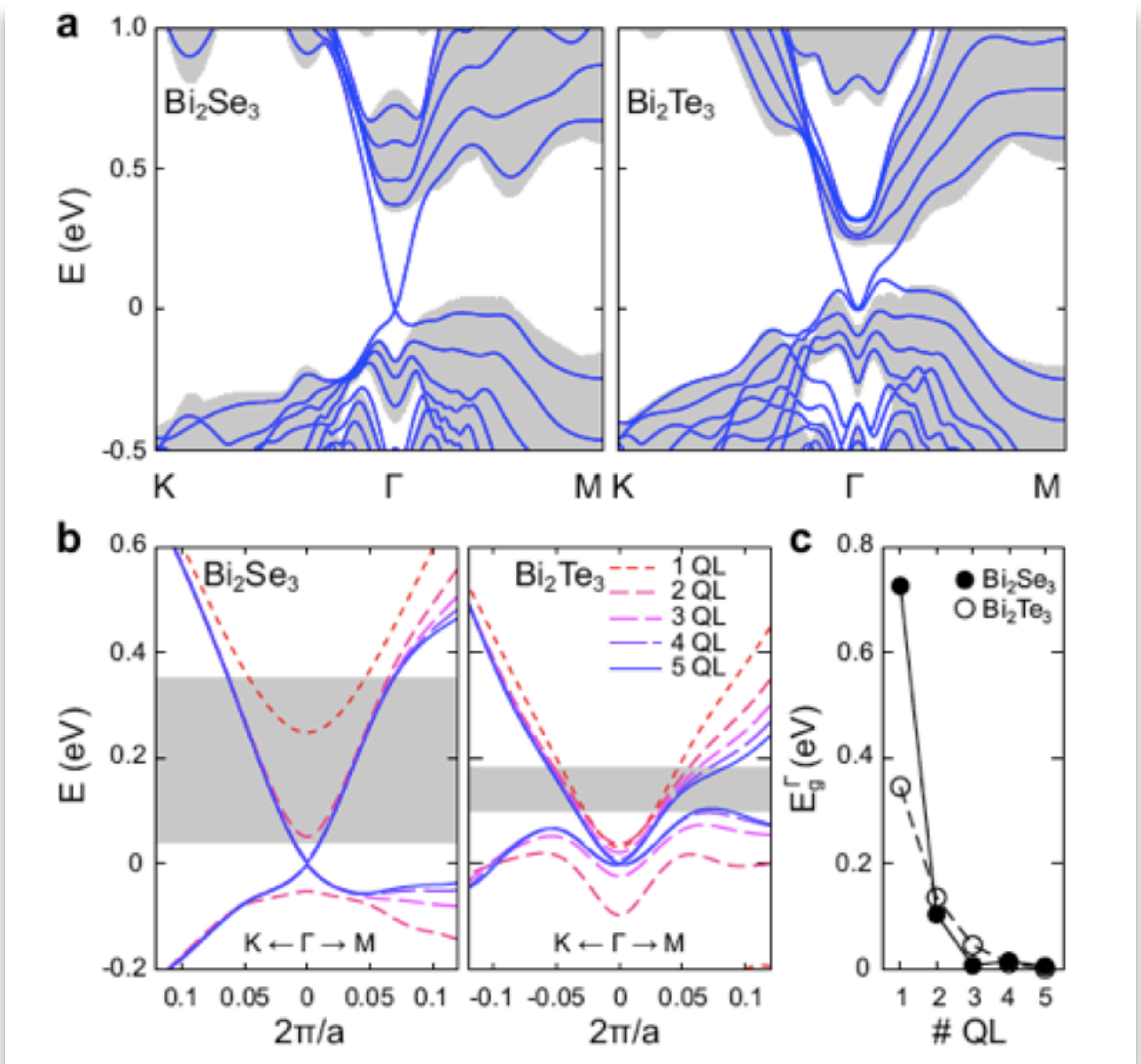
“Spintronic” applications with current materials

•Observation of giant spin-charge coupling

First-principles calculations of surface states, including reduced spin polarization (O. Yazyev, JEM, S. Louie, PRL 2011)

Can incorporate GW corrections (arXiv preprint + Kioupakis).

Some aspects (e.g., g-factor) remain difficult to calculate.



1. Gives numerical strength of spin-charge coupling, e.g., in “inverse spin-galvanic effect’ (Garate and Franz): use TI surface current to switch an adsorbed magnetic film

2. Can bias electrically so that *combination of* surfaces has net spin-charge coupling

Topological order

What type of order causes the precise quantization in the Integer Quantum Hall Effect (IQHE)?

Definition I:

In a topologically ordered phase, some physical response function is given by a "topological invariant".

What is a topological invariant? How does this explain the observation?

Definition II:

A topological phase is insulating but always has metallic edges/surfaces when put next to vacuum or an ordinary phase.

What does this have to do with Definition I?

Definition III (Wen): A topological phase is defined by a topological QFT, just as Ginzburg-Landau theory defines a symmetry-breaking phase.

Topological insulators and energy

Big question:
Does knowing that Bi_2Te_3 has these unusual surface states help with thermoelectric applications?

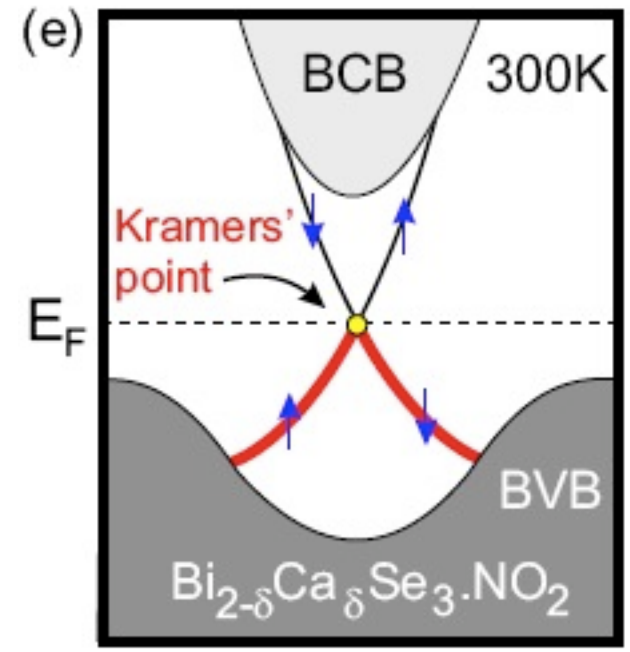
Yes, at least for low temperature (10K - 77K), where ZT=1 is not currently possible. We hope to double ZT.
P. Ghaemi, R. Mong, JEM, PRL, 2010.
For 2D, see R. Takahashi and S. Murakami, PRB 2010.

Thermoelectrics work best when the band gap is about 5 times kT.
Gap of Bi_2Te_3 = 1800 K = 0.15 eV.

Idea: in a thin film, the top and bottom surfaces of a topological insulator "talk" to each other, and a controllable thickness-dependent gap opens.

Key: good thickness and Fermi-level control

Recent development: exfoliated thin films (Balandin et al., UC Riverside, APL)



Fermi-level control
in crystals (Hsieh et al., 2009)

Part III: BF Theory of TIs

Motivation:

For superconductors, Ginzburg-Landau theory captures the "universal" properties defining the phase. It is also useful for many computations.

What is the equivalent for topological insulators?

1. Essential properties of topological insulators that a theory should capture.

2. Review of Chern-Simons description of fractional quantum Hall effect.

3. Topological insulators: axion electrodynamics and surface Dirac fermion

4. Pathway to fractional 3D topological insulators

Details: Cho and JEM, arXiv: 1011.3485, Annals of Physics, Jan. 2011

Model: field theory of QHE

How can we describe the topological order in the quantum Hall effect, in the way that Landau-Ginzburg theory describes the order in a superconductor?

Standard answer: Chern-Simons theory

$$L_{CS} = -\frac{k}{4\pi}\varepsilon^{\mu\nu\lambda}a_\mu\partial_\nu a_\lambda + j^\mu a_\mu, \qquad j^\mu = \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda}\partial_\nu A_\lambda$$

There is an "internal gauge field" *a* that couples to electromagnetic *A*.

Integrating out the internal gauge field *a* gives a Chern-Simons term for *A*, which just describes a quantum Hall effect:

$$L_{QHE} = -\frac{1}{4k\pi}\varepsilon^{\mu\nu\lambda}A_\mu\partial_\nu A_\lambda$$

There is a difference in principle between the topological field theory and the topological term generated for electromagnetism; they are both Chern-Simons terms.

Topological field theory of QHE

What good is the Chern-Simons theory? (Wen)

$$L_{CS} = -\frac{k}{4\pi}\varepsilon^{\mu\nu\lambda}a_\mu\partial_\nu a_\lambda + j^\mu a_\mu, \qquad j^\mu = \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda}\partial_\nu A_\lambda$$

The bulk Chern-Simons term is not gauge-invariant on a manifold with boundary.

It predicts that a quantum Hall droplet must have a chiral boson theory at the edge:

$$S = \frac{k}{4\pi}\int \partial_x\phi(\partial_t\phi - v\partial_x\phi)\,dx\,dt$$

For fractional quantum Hall states, the chiral boson is a "Luttinger liquid" with strongly non-Ohmic tunneling behavior.

Experimentally this is seen qualitatively--perhaps not quantitatively.

Topological field theory of TIs

We believe that in both 2D and 3D the appropriate topological field theory of TIs is a "BF" theory. (G.Y. Cho and JEM, Annals of Physics, 2011)

In 2D this is essentially two copies of Chern-Simons theory. (see also J. Goryo and collaborators for BF terms in 2D TIs, but slightly different).

In 3D, it is a bulk topological theory that predicts a single Dirac fermion at the edge.

When the edge is gapped, the magnetoelectric effect results.

$$L_{BF} = \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda\rho} a_\mu \partial_\nu b_{\lambda\rho} + \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda\rho} A_\mu \partial_\nu b_{\lambda\rho} + C\varepsilon^{\mu\nu\lambda\rho}\partial_\mu a_\nu \partial_\lambda A_\rho$$

Just as in the QHE, one can change coefficients in the topological field theory to obtain a "fractional topological insulator" with a non-Fermi-liquid surface state.

There are fractional statistics of pointlike and linelike excitations.

More details in 2D

For the two-dimensional topological insulator, we know that an example of the state is provided by a pair of integer quantum Hall states for "spin-up" and "spin-down".

We can write the resulting combination of two Chern-Simons theories in a basis of two fields *a* and *b* with different time-reversal properties:

$$L_{BF} = \frac{1}{\pi} \varepsilon^{\mu\nu\lambda} (b_\mu \partial_\nu a_\lambda + A_\mu \partial_\nu b_\lambda)$$

This is known as 2D "BF theory", since the topological part couples the field *b* and the field strength *F* of *a*. It is time-reversal even, unlike CS theory.

Its edge has two oppositely propagating boson modes. In the above we have written the coupling to electromagnetism, and indeed we obtain the localized states around a pi flux.

The sources of a and b are charge density and spin density.

This theory was previously studied in CM in other contexts (Hansson, Oganesyan, Sondhi 2004; Diamantini, Trugenberger, Sodano, several papers 1996-present).

What about 3D?

Unlike Chern-Simons theory, BF theory exists in 3D and still describes time-reversal-invariant systems.

$$L_{BF} = \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda\rho} a_\mu \partial_\nu b_{\lambda\rho} + \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda\rho} A_\mu \partial_\nu b_{\lambda\rho} + C\varepsilon^{\mu\nu\lambda\rho}\partial_\mu a_\nu \partial_\lambda A_\rho$$

Now b is a two-form and there are two possible couplings to the EM field.

One is T-invariant and the other is not; we expect it to be generated by a T-breaking perturbation at a surface, and indeed it is a boundary term.

The electromagnetic current contains both contributions from a and b.

$$J^\mu_{EM} = J^\mu_b + J^\mu_a = \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda\rho}\partial_\nu b_{\lambda\rho} + \frac{1}{8\pi^2}\varepsilon^{\mu\nu\lambda\rho}\partial_\nu(\theta\partial_\lambda a_\rho)$$

The two-form b contains information about electric and magnetic polarizations, which can be viewed as a density of intrinsically line-like objects (think about field lines). Derivatives give ordinary charge and current.

Topological field theory of TIs

When the edge is gapped, the magnetoelectric effect results. We can view the surface T-breaking coupling as arising from a bulk polarization tensor (in addition to normal current piece)

$$L_{\rm surf} = \frac{1}{8\pi}\varepsilon^{\mu\nu\lambda\rho}\partial_\mu a_\nu \partial_\lambda A_\rho = \frac{1}{2}P^{\mu\nu}\partial_\mu A_\nu = \frac{1}{2}(\overrightarrow{P}\cdot\overrightarrow{E} + \overrightarrow{M}\cdot\overrightarrow{B})$$

What does it mean to "bosonize the surface state"? We can canonically represent a Dirac fermion using the emergent surface fields (first-order scalar and vector bosons):

$$\tilde{\psi}(y,\hat{n}) = C\exp(i\sqrt{\pi}\left[\tilde{A}(y,\hat{n}) + \tilde{B}(y,\hat{n})\right])$$

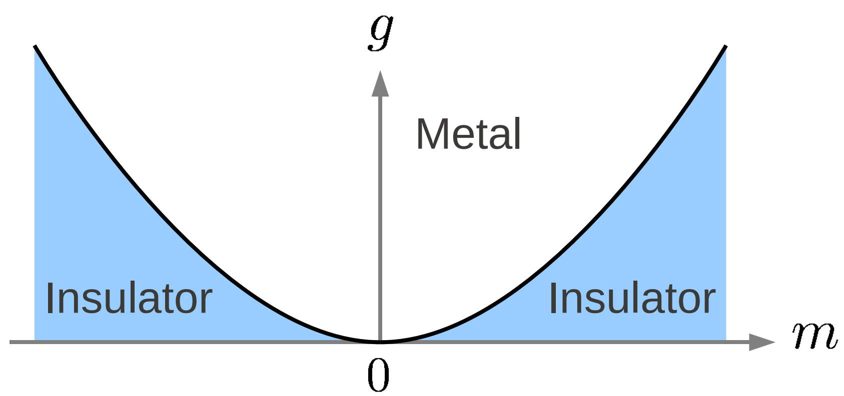
$$\begin{aligned} O_{\hat{n}} &= \exp\left(\frac{i\sqrt{\pi}}{2}\int_0^\theta d\theta'\,\left[\alpha(\hat{n}(\theta')) + \beta(\hat{n}(\theta'))\right]\right) \\ \alpha(\hat{n}) &= \int_{-\infty}^{\infty} \partial_0 \tilde{A}(y,\hat{n}) \\ \beta(\hat{n}) &= \int_{-\infty}^{\infty} \partial_0 \tilde{B}(y,\hat{n}). \end{aligned}$$

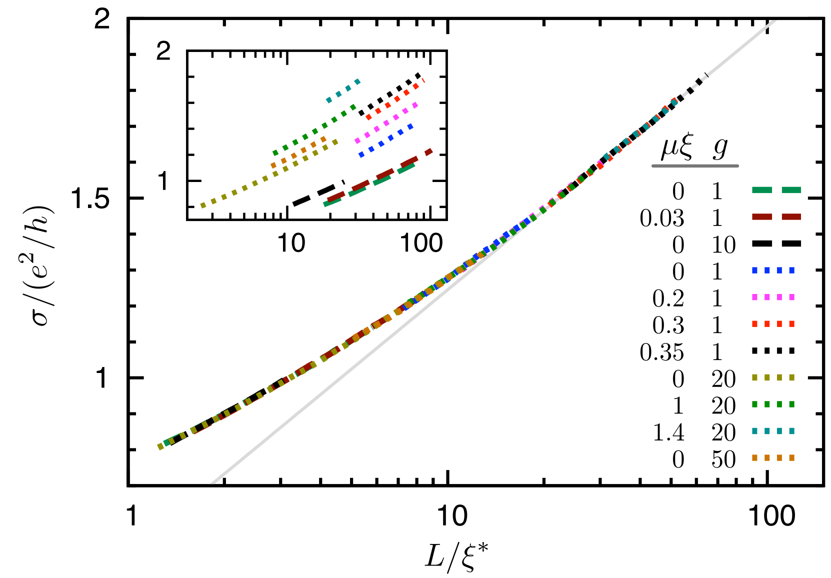
A difference from the FQHE case: there the surface details set the velocity, but the chemical potential is essentially irrelevant; here the surface still determines the velocity and chemical potential, and *both* matter for the low-energy theory.

Conclusions

1. Both weak and strong topological insulator surfaces are interesting exceptions to conventional Anderson localization.

Consistent with Ringel et al., the weak TI surface is only localized when there is a nonzero average of the potential causing scattering between two Dirac cones, e.g., a period-doubling reconstruction of the crystal.





2. Some properties of surfaces in real materials can be calculated efficiently by electronic structure methods, including effects of electrical bias.

3. The combination of *symmetry* and *topology* probably has more surprises in store. BF theory is an effective description of some such states.

Connection to 3D partons? (Maciejko et al., Swingle et al., Levin et al., Walker-Wang)