'Topological' Transport in Topological Semimetals



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Collaborators



Hosur, SP, Vishwanath, Phys. Rev. Lett. 108, 046602 (2012)

SP, Grover, Pesin, Abanin, Vishwanath, Phys. Rev. X 4, 031035 (2014)

Baum, Berg, SP, Stern, arXiv:1508.03047 (2015)



SIMONS FOUNDATION

Basic goal of condensed matter: classifying phases

One simple way





Metals

Insulators

Images: http://wikipedia.com, http://www.androidspin.com, http://www.nauticexpo.com

Band theory connects transport with symmetry

Bloch's theorem + Schrödinger equation \Rightarrow energy bands





Metals: partially filled/gapless (semimetals~filled bands touch other bands) Insulators: filled/gapped (semiconductors~gap is narrow)

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How do we connect transport with topology?

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Electrons in a crystal + E and B fields

Solve Schrödinger equation with E, B=0, get Bloch bands $\hat{H}_0(\mathbf{k})|\psi_{0,n}(\mathbf{k})\rangle = \mathcal{E}_{0,n}(\mathbf{k})|\psi_{0,n}(\mathbf{k})\rangle$

<u>Semiclassics</u>: wavepacket for Bloch electron, position x & average momentum k

How does this evolve when $E, B \neq 0$?

[Bloch & Peierls, '33; Jones & Zener '34; see Ashcroft & Mermin for intro.]

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velocity = 'band' (group) velocity $\dot{\mathbf{x}} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_{0,n}(\mathbf{k})}{\partial \mathbf{k}}$ force = Lorentz force $\hbar \dot{\mathbf{k}} = -e \, \mathbf{E} - e \, \dot{\mathbf{x}} \times \mathbf{B}$

[Bloch & Peierls, '33; Jones & Zener '34; see Ashcroft & Mermin for intro.]

Define 'electric' field in k-space
$$\tilde{\mathbf{E}}(\mathbf{k}) \equiv \frac{\partial \mathcal{E}_{0,n}(\mathbf{k})}{\partial \mathbf{k}}$$

Then the semiclassical equations become $(\hbar=e=1)$

$$\begin{split} \dot{\mathbf{x}} &= -\tilde{\mathbf{E}}(\mathbf{k}) & \text{look similar, but} \\ \dot{\mathbf{k}} &= -\mathbf{E}(\mathbf{x}) - \dot{\mathbf{x}} \times \mathbf{B}(\mathbf{x}) \end{split}$$

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Key: Berry's phase

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 $|n(\mathbf{R}(0))\rangle \longrightarrow$

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Missing piece: Berry's Phase

Berry's Phase

How did we get the 'dynamical phase' $e^{i \int_0^t E_n(t') dt'}$? Between $t, t+\Delta t$, state n picks up phase $E_n\Delta t$ Add up that phase for each bit of time But the state itself changes in that time!

 $|n(\mathbf{R}(t))\rangle \neq |n(\mathbf{R}(t+\Delta t))\rangle$

Berry's phase is how we account for this change!

After some work, can show

$$\gamma_n(t) = i \int_{\mathbf{R}(0)}^{\mathbf{R}(t)} d\mathbf{R} \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle$$

(depends only on path R(t), not on details of how R changes with t)

Normally, overall phase unimportant

(can remove by suitable redefinition of kets at each point)

But in some cases, evolution is periodic R(t)=R(0)



Then, if Berry phase for a 'cycle' is nonzero $\gamma_{\mathcal{C}} = i \oint_{\mathcal{C}} d\mathbf{R} \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle$

no choice of phase can make it zero

One way to think about Berry phase is in terms of a 'vector potential'

 $\mathcal{A}_n(\mathbf{R}) = i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle$ $\gamma_n = \int \mathcal{A}_n(\mathbf{R}) \cdot d\mathbf{R}$

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Berry phase for loop = 'Berry flux' through it

Semiclassical Transport in Solids Bloch states live on 'torus' in k-space ($\mathbf{k} \equiv \mathbf{k} + 2\pi$) Their evolution is <u>always</u> periodic! $\hat{H}_0(\mathbf{k})|\psi_{0,n}(\mathbf{k})\rangle = \mathcal{E}_{0,n}(\mathbf{k})|\psi_{0,n}(\mathbf{k})\rangle$

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 $\tilde{B}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \left[i \langle \psi_{0,n}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi_{0,n}(\mathbf{k}) \rangle \right]$

[Karplus & Luttinger 1954; Niu & Sundaram 2000; Haldane 2004]

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Berry phases matter!

Berry flux ~ momentum-space magnetic field $\tilde{B}(\mathbf{k}) = \nabla_{\mathbf{k}} \times [i \langle \psi_{0,n}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi_{0,n}(\mathbf{k}) \rangle]$

$$\dot{\mathbf{x}} = -\tilde{\mathbf{E}}(\mathbf{k}) - \dot{\mathbf{k}} \times \tilde{\mathbf{B}}(\mathbf{k})$$
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additional contribution often called 'anomalous velocity' [Karplus & Luttinger 1954; Niu & Sundaram 2000; Haldane 2004]

An example: 'Intrinsic' Anomalous Hall Effect

Conventional Hall effect:

- charge carriers deflected due to external magnetic field
- additional voltage transverse to current



- important probe: gives sign of charge carriers, etc....

An example: 'Intrinsic' Anomalous Hall Effect no external magnetic field (B=0) microscopic time-reversal symmetry-breaking

<u>microscopic</u> time-reversal symmetry-breaking e.g. due to magnetism

'extrinsic': due to asymmetric scattering with TRSB 'intrinsic': due to <u>Berry phase</u> of energy bands

$$\sigma_{xy}^{\text{AH-int}} = -\frac{e^2}{\hbar} \sum_n \int \frac{d\mathbf{k}}{(2\pi)^d} \hat{\mathbf{z}} \cdot \tilde{B}_n(\mathbf{k}) f[\mathcal{E}_n(\mathbf{k})]$$

[Karplus & Luttinger 1954; Niu & Sundaram 2000; Haldane 2004; review: Nagaosa et al 2009]

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Berry flux of band n

[Karplus & Luttinger 1954; Niu & Sundaram 2000; Haldane 2004; review: Nagaosa et al 2009]

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Berry flux occupation of band n of band n

[Karplus & Luttinger 1954; Niu & Sundaram 2000; Haldane 2004; review: Nagaosa et al 2009]

Quantized Anomalous Hall Effect

$$\sigma_{xy}^{\text{AH-int}} = -\frac{e^2}{\hbar} \sum_n \int \frac{d\mathbf{k}}{(2\pi)^d} \hat{\mathbf{z}} \cdot \tilde{B}_n(\mathbf{k}) f[\mathcal{E}_n(\mathbf{k})]$$

$$\implies \ f=0 \qquad \text{Fermi energy in gap ~ insulator}$$

$$F \xrightarrow{\text{pick up total}} f=1 \qquad \text{Berry flux from each filled band}$$

 \mathcal{E}

total Berry flux of a band must be $2\pi \times integer$

 $\sigma_{xy}^{\text{QAH}} = \frac{e^2}{h} \times \text{integer} \quad \text{fixed} \text{ as long as Fermi energy in gap!}$

[expt. in (Bi, Sb)₂Te_{3:}C-Z Chang et al., Science **340**, 167 (2013)]

'Strong' TIs : no TRSB so $\sigma_{xy}=0$, but nonzero 'Z₂ invariant' \Rightarrow helical edge states

Why do we care?

Topological insulators and related systems* represent fundamentally new phases of matter

Topological properties are very universal: robust to disorder, sample imperfections, etc...

May be possible to engineer 'topologically protected' quantum computers



Exotic materials, with potential for unforeseen applications

*also quantum Hall states, topological superconductors, quantum spin liquids...

This Talk: Topological Semimetals

topological insulators \Rightarrow gapped in the bulk

only surface is 'interesting': Dirac cones, transport, WAL etc...



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Can band topology play a role even when bulk is gapless?

The Invisible Man, HG Wells, Signet Ed.; Son of Man, Rene Magritte

'<u>Weyl semimetals</u>' ~ 3D graphene

Two bands touch at a point node w/o fine-tuning in d=3

(needs broken inversion/time reversal)



[Herring, '37; Abrikosov, Beneslavskii '71; X.Wan et al. '11]

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all 3 Pauli matrices used \Rightarrow cannot gap single node Pairs of nodes separated in BZ \Rightarrow robust w/ transl. symmetry For 'topological' reasons, nodes come in pairs. Why? [Herring, '37; Abrikosov, Beneslavskii '71; X.Wan *et al.* '11]

BZ = torus, 'Berry-Gauss law' \Rightarrow zero <u>total</u> charge







BZ = torus, 'Berry-Gauss law' ⇒ zero <u>total</u> charge ⇒nodes created/destroyed in pairs



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Finite slab in z-direction: 'half' of a 2D Fermi surface on top 'other half' on bottom



top+bottom = 'legal' 2D Fermi surface

Where to look?

Original Candidate: Pyrochlore Iridates



 $A_2 I r_2 O_7 \qquad (A = Y, Eu)$

<u>Ir</u>: strong spin-orbit (Z~77) varying A: tunes interaction ('U') between Ir 5d

LDA+U DFT Results



[X.Wan, A. Turner, A Vishwanath, S. Savrasov, PRB 83, 205101 (2011)]

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Toy Model: TI/NI Heterostructures w/ Magnetism



TI-NI transition when $\Delta_d = \Delta_s$; split by magnetism (induced/spontaneous)

with TRS

broken TRS





Experimental Observation of WSM

ARPES: Fermi arcs on (001) surface in TaAs



[S.-Y. Xu et al., Science, July'15]



[B.Q. Lv et al., PRX '15]

Other examples: NbAs,... (many more!)

Typically, pair of Weyl nodes at same point 'gap out' (2x2 mass matrix impossible in 3D, 4x4 mass matrix allowed) Can remain gapless if crystal symmetry forbids mass term

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Proposed examples

- Na₃Bi [Z.Wang, et al., Phys. Rev. B 85, 195320 (2012)]
- Cd₃As₂ [Z.Wang, et al., Phys. Rev. B 88, 125427 (2013)]

stable, volatile

stable, high mobility

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[Z. Liu et al. Science '14; S.-Y. Xu et al. arXiv:1312.7624]



[M. Neupane et al. Nat. Comm. '14]

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Proposed examples



[Z. Liu et al. science 14; S.-Y. Xu et al. arXiv:1312.7624] **Detecting Topological Semimetals**

'quantum critical' resistivity

 $\rho \sim T^{-1}$

(assumes chemical potential at nodes)

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Conductivity Scaling $\rho \sim T^{-1}$ 'quantum critical' resistivity **Einstein relation** $\sigma_{\rm dc} \sim e^2 D \left. \frac{\partial n}{\partial \mu} \right|_T$

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Einstein relation $\sigma_{\rm dc} \sim e^2 D \left. \frac{\partial n}{\partial \mu} \right|_T$

Diffusion const.

 $D \sim v_F^2 \tau$

$\begin{array}{c|c} \mbox{Density of states} \\ \hline \partial n \\ \hline \partial \mu \\ T \end{array} \sim \frac{NT^2}{v_F^3} \end{array}$

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Scattering rate

 $\tau^{-1} \sim N \alpha^2 T$

(assumes chemical potential at nodes)

Experimental Signatures

'quantum critical' resistivity



[Th.: Hosur, SP, Vishwanath, PRL 'II)]

 $\rho \sim T^{-1}$

[Expt.:Yanagashima & Maeno,JPSJ '01)]

Topological signatures?

	Topological Insulators	Topological Semimetals
Boundary	<section-header><section-header><text></text></section-header></section-header>	
Bulk	$magnetoelectric effect$ $S = S_{em} + \frac{\alpha}{4\pi} \int \boldsymbol{E} \cdot \boldsymbol{B}$	

Topological signatures?

	Topological Insulators	Topological Semimetals
Boundary	protected Dirac node ARPES, STM, surf. transport	'Fermi arcs' ARPES Quantum Oscillations
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Bulk	$magnetoelectric effect$ $S = S_{em} + \frac{\alpha}{4\pi} \int \boldsymbol{E} \cdot \boldsymbol{B}$	Quantum Anomalous Hall Eff. Adler-Bell-Jackiw Anomaly

Boundary Effects

I. "Seeing" Arcs in ARPES



[S.-Y. Xu et al., Science, July '15]

[S.-Y. Xu et al., Science, Jan '15]
2. Quantum Oscillations

Semiclassical orbits on nonlocal Fermi surface \Rightarrow quantum oscillations



[Theory: A.C. Potter, I. Kimchi, A.Vishwanath, Nat. Comm. '14]

Quantum Oscillations: Experiments



Quantum Oscillations: Experiments

Angle-dependence

Thickness-dependence + Interference



3. Current-at-a-Distance & Resonant Transparency

Weyl cyclotron orbits transfer charge between surfaces parallel to B

DC: Nonlocal resistance between surfaces



[Baum, Berg, S.P., Stern, arXiv:1508.03047]

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AC: resonant transmission of microwaves in anomalous skin regime



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Bulk Effects











[Th.: K.-Y.Yang, Y.-M. Lu, Y. Ran, PRB'11)]





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to verify quantization, need input: location of nodes in BZ contributions from several pairs of nodes can cancel

2. Adler-Bell-Jackiw Anomaly [Adler '69; Bell & Jackiw, '69]

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'valley' current (' $j^{\mu 5}$ ') $j^{\mu}_{R} - j^{\mu}_{L}$ not conserved







WSM: <u>two</u> Weyl fermions, opposite chirality:



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WSM: *two* Weyl fermions, opposite chirality:

Measurable consequences?

Unlike TIs, here 'generic' metallic transport masks topology

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<u>additional</u> anomaly current for $E \| B \Rightarrow$ negative MR, anisotropic σ_{ij}

[Nielsen, Ninomiya, Phys. Lett. B**130**, 389 ('83); Aji, PRB **85**, 241101 ('12); Son & Spivak, PRB **88**, 104412 ('12)]

anomaly + scattering \Rightarrow negative 'classical' MR

[Son & Spivak, PRB 88, 104412 ('12)]

T-breaking WSM from magnetic order \Rightarrow anom. magnon-plasmon coupling [Liu, Ye & Qi, arXiv:1204.6551]

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Ideally: qualitative (yes vs. no) not quantitative (big vs. small) signature!

'Seeing' the Anomaly via Nonlocal Transport

Valley charge not conserved:
$$\partial_{\mu}(j_{R}^{\mu} - j_{L}^{\mu}) = \frac{e^{2}}{2\pi^{2}}\boldsymbol{E}\cdot\boldsymbol{B}$$



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Valley

relaxing 'valley' imbalance requires inter-node scattering but charge imbalance can relax at single node!

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relaxing 'valley' imbalance requires inter-node scattering but charge imbalance can relax at <u>single</u> node!

⇒ 'topological' transport ~ valley imbalance ~ slow relaxation
'boring' bulk transport ~ charge imbalance ~ fast relaxation



Proposed Experiment



Generating Valley Imbalance



[SP, et al., PRX 4, 031035 (2014)]

Z ▲

Generating Valley Imbalance










Detecting Valley Imbalance



[SP, et al., PRX 4, 031035 (2014)]

Detecting Valley Imbalance



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Aside: Modeling Disorder



$$\frac{\tau_c}{\tau_v} \approx \frac{|v(2\mathbf{K}_0)|^2}{|v(0)|^2} \approx \left(\frac{k_F}{2K_0}\right)^2 \sim x^{4/3}$$
(x = doping level)

For x ~ 1%, and mean free path ~ 10 nm, $\ell_v \sim 5 \, \mu {
m m}$

Aside: Impurity Scattering in Dirac Semimetals

 τ_c , τ_v as before; but new 'isospin' relaxation time τ_i need τ_i to be long or else mixing destroys valley imbalance



 τ_i depends on isospin mixing due to curvature terms in H_{eff}

$$\begin{split} |\mathbf{k},+,\uparrow\rangle_c &\approx |\mathbf{k},+,\uparrow\rangle + \frac{\beta k}{2v_F} \sin^2\theta_{\mathbf{k}} e^{-2i\phi_{\mathbf{k}}} |\mathbf{k},-,\downarrow\rangle \\ |\mathbf{k},+,\downarrow\rangle_c &\approx |\mathbf{k},+,\downarrow\rangle + \frac{\beta k}{2v_F} \sin^2\theta_{\mathbf{k}} e^{+2i\phi_{\mathbf{k}}} |\mathbf{k},-,\uparrow\rangle \end{split}$$

(analogous to Elliot-Yafet spin relaxation)

Estimate for Na₃Bi yields $au_i \sim 10^3 au_c$

Experiments?





Small field-induced nonlocal contribution in Cd₃As₂?

Possible alternative explanations? (early days yet...)

[C. Zhang et al., arXiv:1504.07698]

Summary

Topological phenomena don't need a bulk gap! Weyl/Dirac Semimetals: robust topological transport phenomena surface: Fermi arcs + effects on cyclotron orbits bulk: anomaly, chiral charge pumping, ...

Many proposed effects (only discussed a few)...

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Experimentalists: We Need You!

Thanks for listening!