中国科学技术大学
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# Anomalous Hall effect in topological insulators

Dimitrie Culcer

Culcer and Das Sarma, PRB 83, 245441 (2011)
D. Culcer, arXiv: 1108.3076 – review on TI transport

合肥微尺度物质科学国家实验室(筹)
HEFEI NATIONAL LABORATORY FOR PHYSICAL SCIENCES AT THE MICROSCALE

# Outline

- Brief historical introduction to AHE
  - Long history – many mechanisms contribute
- Magnetic TI
  - Quantum AHE in 2D
  - Quantum AHE in 3D
- Our work – AHE in doped TI (metallic)
  - Density-matrix formulation of transport
  - Liouville equation ➔ kinetic equation
  - Scattering terms – absence of backscattering
  - Intrinsic mechanisms contributing to AHE
  - Extrinsic mechanisms contributing to AHE
  - Prediction for real materials
- Conclusions

D. Culcer and S. Das Sarma, PRB 83, 245441 (2011)

D. Culcer, arXiv: 1108.3076 – review on TI transport

# History of AHE

- AHE theory has a long history – over 50 years
- Controversy started with J. M. Luttinger PR 112, 739 (1958)
  - Identified band structure contribution (intrinsic)
  - Later recognized to be related to Berry curvature
- J. Smit, Physica 24, 39 (1958)
  - Transport not possible without scattering
  - Introduced skew scattering
- L. Berger, PRB 2, 4559 (1970)
  - Introduced side jump
- P. Nozieres and C. Lewiner, J. Phys 34, 901 (1973)
  - Put all terms together – classic paper
- Other mechanisms: cf. Burkov and Balents, PRL 2003

AHE review: N. Nagaosa *et al*, RMP 82, 1539 (2010)

# Spin-orbit: Dirac equation

$$H = \begin{pmatrix} m \cdot I & \sigma \cdot p \\ \sigma \cdot p & -m \cdot I \end{pmatrix} = \alpha \cdot p + \beta m,$$

$$\psi \equiv \begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix}$$

$$i\hbar \frac{\partial \varphi}{\partial t} = \left[ \frac{1}{2m} \left( \mathrm{p} - \frac{e}{c} \mathbf{A} \right)^2 - \frac{e\hbar}{2mc} \boldsymbol{\sigma} \cdot \mathbf{B} + e\Phi \right] \varphi$$

This is the Pauli equation. Spin appears after you separate particles from antiparticles.

The next relativistic correction gives the spin-orbit interaction.

$$-\frac{e}{4m^2} \sigma \cdot (E \times p)$$

Here **E** = - ∇V

# Position operator

- Spin-orbit is a relativistic correction
- Dirac Hamiltonian – Foldy-Wouthuysen transformation
  - Yields *effective* Hamiltonian
- Apply this transformation to the position operator
  - Gives spin-orbit correction to r
  - Physical position operator

$$\hat{r}_{\mathrm{phys}} = \hat{r} + \lambda \hat{\sigma} \times \hat{k}$$

- Everything that contains r is modified
  - Interaction with an electric field
  - Scattering potential

J. Smit, Physica 24, 39 (1958); P. Nozieres and C. Lewiner, J. Phys 34, 901 (1973)

# New interaction terms

- The position operator is modified

$$\hat{\boldsymbol{r}}_{\text{phys}} = \hat{\boldsymbol{r}} + \lambda \hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{k}}$$

- Interaction with electric field – in crystal momentum representation

$$H^{sc}_{E,\boldsymbol{k}\boldsymbol{k}'} = (e\boldsymbol{E} \cdot \hat{\boldsymbol{r}})_{\boldsymbol{k}\boldsymbol{k}'} \mathbb{1} = ie\boldsymbol{E} \cdot \frac{\partial}{\partial \boldsymbol{k}} \delta(\boldsymbol{k} - \boldsymbol{k}') \mathbb{1}$$

$$H^{sj}_{E,\boldsymbol{k}\boldsymbol{k}'} = e\lambda \boldsymbol{\sigma} \cdot (\boldsymbol{k} \times \boldsymbol{E}) \delta_{\boldsymbol{k}\boldsymbol{k}'}$$

- Scattering potential – in crystal momentum representation

$$\bar{U}_{\boldsymbol{k}\boldsymbol{k}'} = \mathcal{U}_{\boldsymbol{k}\boldsymbol{k}'} \left(1 - i\lambda \boldsymbol{\sigma} \cdot \boldsymbol{k} \times \boldsymbol{k}'\right) \quad \lambda k_F^2 \ll 1$$

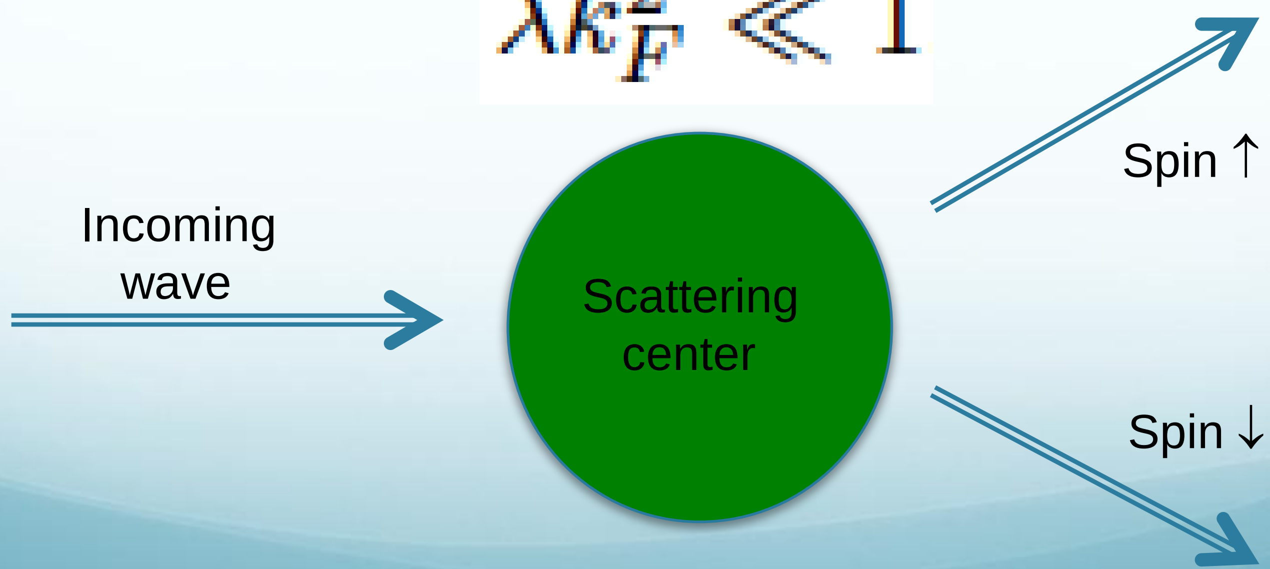
Culcer, Hankiewicz, Vignale, Winkler, PRB 81, 125332 (2010)

# Skew scattering

- Asymmetric scattering of spin ↑,↓
  - Spin ↑ scatter predominantly in one direction
  - Spin ↓ predominantly in the other direction
- Must go beyond first Born approximation
  - Typically 3rd order in scattering potential
  - cf. $U^4$ term in Sinitsyn JPCM 20, 023201 (2008)

$$\bar{U}_{\mathbf{k}\mathbf{k}'} = \mathcal{U}_{\mathbf{k}\mathbf{k}'}\left(1 - i\lambda\boldsymbol{\sigma}\cdot\mathbf{k}\times\mathbf{k}'\right).$$

$$\lambda k_F^2 \ll 1$$




J. Smit, Physica 24, 39 (1958); P. Nozieres and C. Lewiner, J. Phys 34, 901 (1973)

# Side-jump: *Seitensprung*

- Relativistic modification of position operator
  - Alters energy of interaction with an electric field

$$H^{sj}_{E,\mathbf{k}\mathbf{k}'} = e\lambda\,\boldsymbol{\sigma}\cdot(\mathbf{k}\times\mathbf{E})\,\delta_{\mathbf{k}\mathbf{k}'}$$

  - Causes sideways displacement during scattering

$$\hat{j}^{Born}(f_{\mathbf{k}}) = \langle \int_0^\infty \frac{dt'}{\hbar^2}[\hat{U}, e^{-\frac{i\hat{H}t'}{\hbar}}[\hat{U},\hat{f}]e^{\frac{i\hat{H}t'}{\hbar}}]\rangle,$$


- All terms together for SO-coupled semiconductors/ferromagnets
  - N. A. Sinitsyn *et al*, PRB 75, 045315 (2007); A. A. Kovalev *et al,* PRB 79, 195129 (2009); S. Onoda *et al*, PRB 77, 165103 (2008); Crepieux & Bruno, PRB 64, 014416 (2001).

# TI: Magnetic doping

- Consider doped TI – no worries about interface with ferromagnet
- Total Hamiltonian describing magnetic interactions

$$H_{\mathrm{mag}}(\boldsymbol{r}) = \boldsymbol{\sigma} \cdot \sum_I V(\boldsymbol{r} - \boldsymbol{R}_I)\, \boldsymbol{s}_I$$

- k-diagonal part gives Zeeman interaction with magnetization M

$$H_{\mathrm{mag}}^{\boldsymbol{k}=\boldsymbol{k}'} = n_{\mathrm{mag}} J\, s\sigma_z \equiv M\,\sigma_z$$

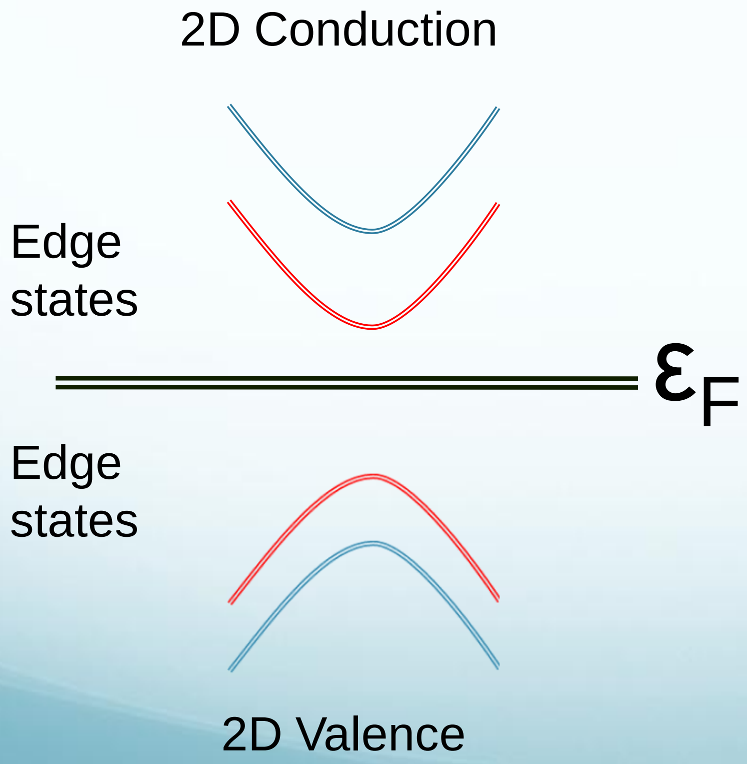
- k-off-diagonal part contributes to spin-dependent scattering

$$H_{\mathrm{mag}}^{\boldsymbol{k}\neq\boldsymbol{k}'} = \frac{Js}{V}\sigma_z \sum_I e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_I}.$$

  - This also gives asymmetric scattering of spin ↑,↓
  - Contributes to AHE in Born approximation

# 2D magnetic TI

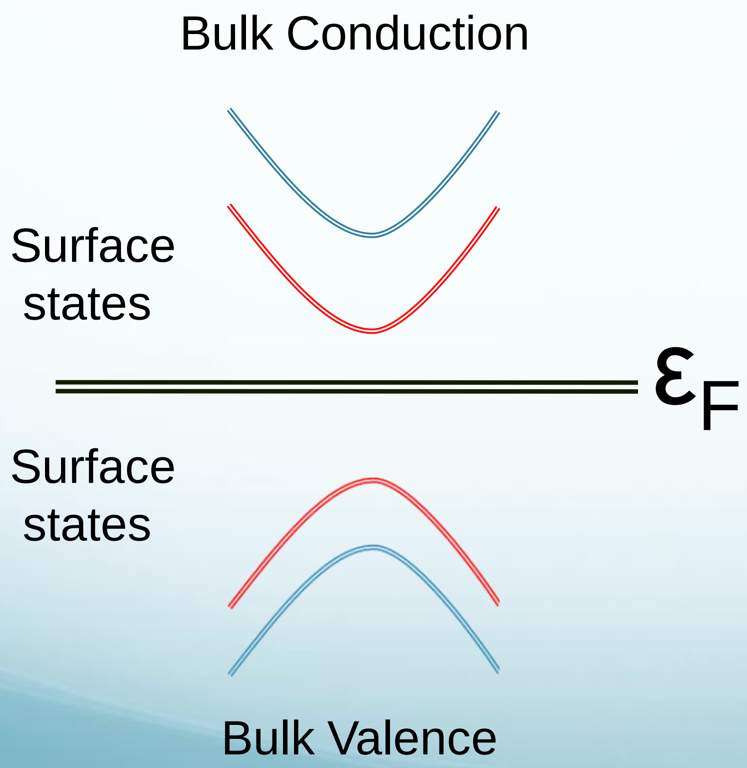
- 2D TI, chemical potential in gap
  - Edge states 4 = 2 + 2: quantized AHE
  - Yu *et al*, Science 329, 61 (2010)
  - Chern number




$$\sigma_{xy} = \frac{e^2}{h}$$

# 3D magnetic TI

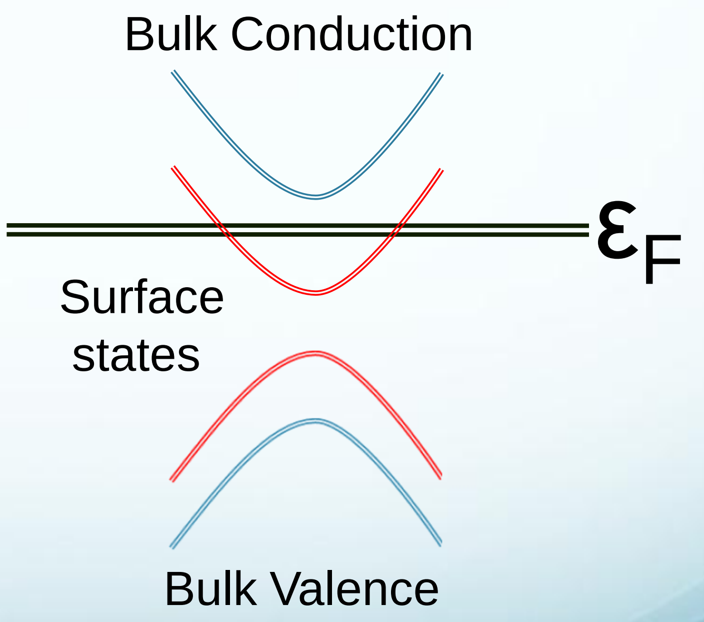
- 3D TI, chemical potential in gap
  - Half-quantized AHE
  - Zang and Nagaosa PRB 81, 245125 (2010)
  - Berry curvature




$$s_{xy} = \frac{e^2}{2h}$$

# 3D magnetic TI

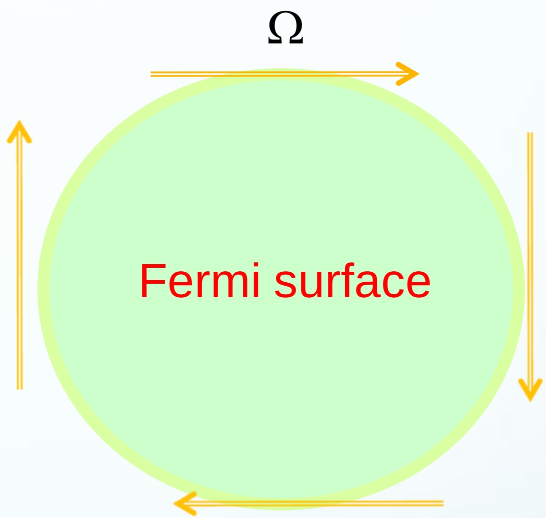
- Chemical potential in surface conduction band
  - QAHE is an exciting phenomenon
  - However, current TIs are doped
  - Half-quantized AHE – one contribution
  - Steady-state problem
  - Electric field drives electrons
  - Impurities scatter electrons
  - Must deal with scattering
  - Determine Hall current
  - Intrinsic and extrinsic AHE
  - Which term is dominant?
  - Is it still universal?
  - How big is it?
  - What will be observed?



# TI band structure

- Effective Zeeman field

$$H_{0\boldsymbol{k}} = -Ak\,\boldsymbol{\sigma}\cdot\hat{\theta} + \boldsymbol{\sigma}\cdot\boldsymbol{M} \equiv \frac{\hbar}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\Omega}_{\boldsymbol{k}},$$




- But no spin precession – only one band
- Ω slightly tilted out of the plane by M
  - Small $s_z$ component
- Typically $M \ll \varepsilon_F$
- Remember current operator = spin

$$\boldsymbol{j} = \frac{eA}{\hbar}\boldsymbol{\sigma}\times\hat{z},$$

- This will help explain band structure term

# Full Hamiltonian

- $H = H_0 + H_E + U$
  - $H_E$ = Electric field
    - Includes correction to position operator
  - U = Scattering potential
    - Includes correction to position operator
    - Impurity average

$$(n_i |\bar{U}_{\mathbf{k}\mathbf{k}'}|^2 \delta_{ss'})/V$$

  - $\varepsilon_F \tau_p >> 1$
  - $\tau_p$ = momentum relaxation time
  - $\varepsilon_F$ in bulk gap – electrons
  - T=0 ➔ no phonons, no e-e scattering
  - Scattering due to charged impurities, roughness, magnetic
  - Perturbation theory in $\lambda$

# Density matrix

- Density operator $\hat{\rho}$
- Project onto states of definite wave vector k and spin s

Density matrix

$$\rho_{\mathbf{k}\mathbf{k}'} \equiv \rho_{\mathbf{k}\mathbf{k}'}^{ss'} = \langle \mathbf{k} s | \hat{\rho} | \mathbf{k}' s' \rangle$$

- $H_0$ , $H_E$ diagonal in wave vector, off-diagonal in spin
- U off-diagonal in wave vector, diag./off-diag. in spin

$$U_{\mathbf{k}\mathbf{k}'} = \bar{U}_{\mathbf{k}\mathbf{k}'} \sum_J e^{i(\mathbf{k}-\mathbf{k}')\cdot \mathbf{R}_J}$$

- Divide DM into parts diagonal and off-diagonal in k

$$\rho_{\mathbf{k}\mathbf{k}'}^{ss'} = f_{\mathbf{k}}^{ss'} \delta_{\mathbf{k}\mathbf{k}'} + g_{\mathbf{k}\mathbf{k}'}^{ss'}$$

# Liouville equation

- Apply electric field ~ study density matrix
  - Starting point: Liouville equation

$$\frac{d\hat{\rho}}{dt} + \frac{i}{\hbar}[\hat{H}_0 + \hat{H}_E + \hat{U}, \hat{\rho}] = 0,$$

  - Method of solution – Nakajima-Zwanzig projection (中島二十)

- Project onto k and s ➔ kinetic equation

- Divide into equations for diagonal and off-diagonal parts

$$\rho_{\mathbf{k}\mathbf{k}'}^{ss'} = f_{\mathbf{k}}^{ss'}\delta_{\mathbf{k}\mathbf{k}'} + g_{\mathbf{k}\mathbf{k}'}^{ss'}.$$

$$\frac{df_{\mathbf{k}}}{dt} + \frac{i}{\hbar}[H_{0\mathbf{k}}, f_{\mathbf{k}}] = -\frac{i}{\hbar}[H_{\mathbf{k}}^{E}, f_{\mathbf{k}}] - \frac{i}{\hbar}[\hat{U}, \hat{g}]_{\mathbf{k}\mathbf{k}}$$

$$\frac{dg_{\mathbf{k}\mathbf{k}'}}{dt} + \frac{i}{\hbar}[\hat{H}, \hat{g}]_{\mathbf{k}\mathbf{k}'} = -\frac{i}{\hbar}[\hat{U}, \hat{f} + \hat{g}]_{\mathbf{k}\mathbf{k}'},$$

# Kinetic equation

- Reduce to equation for f – like Boltzmann equation

$$\frac{df_{\boldsymbol{k}}}{dt} + \frac{i}{\hbar}[H_{\boldsymbol{k}}, f_{\boldsymbol{k}}] + \hat{J}(f_{\boldsymbol{k}}) = -\frac{i}{\hbar}[H^E_{\boldsymbol{k}}, f_{\boldsymbol{k}}],$$

Spin precession — Scattering — Driving term due to the electric field

- Scattering term in the simplest case

$$\hat{J}(f_{\boldsymbol{k}}) = \frac{n_i}{\hbar^2}\lim_{\eta\to 0}\int \frac{d^2k'}{(2\pi)^2}|\bar{U}_{\boldsymbol{k}\boldsymbol{k}'}|^2 \int_0^\infty dt'\, e^{-\eta t'}\left\{e^{-iH_{\boldsymbol{k}'}t'/\hbar}(f_{\boldsymbol{k}} - f'_{\boldsymbol{k}})\, e^{iH_{\boldsymbol{k}}t'/\hbar} + h.c.\right\}.$$

Scattering in — Scattering out

  - This is 1st Born approximation – Fermi Golden Rule
  - 2nd Born approximation for spin-dependent scattering

# Scattering term

- Density matrix = Scalar + Spin

$$f_{\boldsymbol{k}} = n_{\boldsymbol{k}} \mathbb{1} + S_{\boldsymbol{k}};$$

- Spin = Conserved spin + Precessing spin

$$S_{\boldsymbol{k}} = S_{\boldsymbol{k}\parallel} + S_{\boldsymbol{k}\perp}$$

Conserved spin – most important

Precessing spin – expect only singular contribution

- Look at scattering term again (simplest Born approx.)

$$\int d\theta' \, |\bar{U}_{\boldsymbol{k}\boldsymbol{k}'}|^2 \, (s_{\boldsymbol{k}\parallel} - s_{\boldsymbol{k}'\parallel})(1 + \cos\gamma) \, \sigma_{\boldsymbol{k}\parallel}$$

- Suppression of backscattering
- Need all delta-functions including –ve energy

# Kinetic equation

- Conserved spin density

$$\frac{dS_{\mathbf{k}\parallel}}{dt} + P_{\parallel}\hat{J}(f_{\mathbf{k}}) = \mathcal{D}_{\parallel}$$

- Non-conserved spin density (also rotations &c)

$$\frac{dS_{\mathbf{k}\perp}}{dt} + \frac{i}{\hbar}[H_{\mathbf{k}}, S_{\mathbf{k}\perp}] + P_{\perp}\hat{J}(f_{\mathbf{k}}) = \mathcal{D}_{\perp}$$

- Solution – expansion in $1/(\varepsilon_F\tau)$
  - Fermi energy x momentum scattering time
  - Assumes $(\varepsilon_F\tau) \gg 1$ – in this sense it is semiclassical
  - Conserved spin gives leading order term linear in $\tau$
  - Precessing spin gives next-to-leading term independent of $\tau$

Culcer, Hwang, Stanescu, Das Sarma, PRB 82, 155457 (2010)

# Skew scattering

- Scattering potential ~ spin-orbit coupling
  - In TI band structure SO strong
  - Therefore extrinsic SO should be strong
- Asymmetric scattering of spin ↑,↓

$$\bar{U}_{\boldsymbol{k}\boldsymbol{k}'} = \mathcal{U}_{\boldsymbol{k}\boldsymbol{k}'}\left(1 - i\lambda\boldsymbol{\sigma}\cdot\boldsymbol{k}\times\boldsymbol{k}'\right).$$

- Typically 3rd order in scattering potential
  - In TI can appear in Born approximation

$$\hat{J}^{Born}(f_{\boldsymbol{k}}) = \langle\int_0^\infty \frac{dt'}{\hbar^2}[\hat{U}, e^{-\frac{i\hat{H}t'}{\hbar}}[\hat{U}, \hat{f}]e^{\frac{i\hat{H}t'}{\hbar}}]\rangle,$$

$$\hat{J}^{3rd}(f_{\boldsymbol{k}}) = -i\langle\int_0^\infty \frac{dt'dt''}{\hbar^3}[\hat{U}, e^{-\frac{i\hat{H}t'}{\hbar}}[\hat{U}, e^{-\frac{i\hat{H}t''}{\hbar}}[\hat{U}, \hat{f}]e^{\frac{i\hat{H}t''}{\hbar}}]e^{\frac{i\hat{H}t'}{\hbar}}]\rangle,$$

- We do not know λ for TI
  - But that is of no consequence

$$\lambda k_F^2 \ll 1$$

J. Smit, Physica 24, 39 (1958); P. Nozieres and C. Lewiner, J. Phys 34, 901 (1973)

# Side-jump

$$\hat{\boldsymbol{r}}_{\rm phys} = \hat{\boldsymbol{r}} + \lambda \hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{k}}$$

- Interaction with electric field

$$H^{sj}_{E,\boldsymbol{k}\boldsymbol{k}'} = e\lambda\, \boldsymbol{\sigma} \cdot (\boldsymbol{k} \times \boldsymbol{E})\, \delta_{\boldsymbol{k}\boldsymbol{k}'}$$

- Causes sideways displacement during scattering

$$\hat{j}^{Born}(f_{\boldsymbol{k}}) = \langle \int_0^\infty \frac{dt'}{\hbar^2} [\hat{U}, e^{-\frac{i\hat{H}t'}{\hbar}} [\hat{U}, \hat{f}]\, e^{\frac{i\hat{H}t'}{\hbar}}] \rangle,$$

- When band structure SO is present
  - Extra term – Tse & Das Sarma PRB 74, 245309 (2006)

$$-\frac{i}{\hbar} [H^{sj}_{E}, \rho_{0\boldsymbol{k}}]$$

  - This is effectively an intrinsic side-jump term
  - Also related to spin precession/rotation
  - Side-jump is not necessarily related to scattering

# Solving kin. eq. for AHE

- Driving terms
  - Bare driving term $(eE/\hbar)\cdot\frac{\partial f_{0k}}{\partial k}$
  - Side-jump driving term $-\frac{ie\lambda}{\hbar}[\sigma\cdot(k\times E), f_{0k}]$
- Perturbation theory in $\lambda$
  - Skew scattering also appears as a driving term
  - Side-jump scattering gives another driving term
- Terms to leading and next-to-leading order in $(1/\varepsilon_F\tau)$
  - Transport – leading term linear in $\tau$
  - Second term independent of $\tau$
  - Appears to be disorder-independent but is NOT
- Project repeatedly between conserved, precessing spin distributions – tedious

# Main question

- We know there will be a band structure contribution (Nagaosa)
  - It will be of the order of the conductivity quantum
- Contributions from skew scattering and side jump
  - Skew scattering, side jump give extra driving terms
  - H is spin-dependent
  - U is spin-dependent
  - Spin structure of SS, SJ driving terms not obvious
  - Either of them could contribute to the parallel driving term
  - In that case it will give something $\propto M\tau$
  - We are in the weak momentum scattering regime
  - Although M is small, such a term would dominate
  - It would overwhelm the band structure contribution
  - Does such a term exist?
    - A lot of algebra
- What is the dominant term?

# Dominant term in AHE

$$\sigma_{yx} = -\frac{e^2}{2h}(1-\alpha),$$

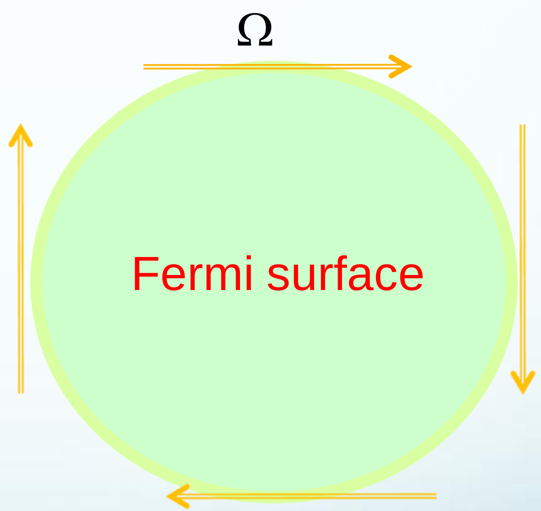
- This is the contribution from the conduction band.
  - Band structure
  - Disorder renormalization.
  - The bare term has no α.
- Remember there is an extra term – offset
- $\frac{e^2}{2h}$ from surface valence band
- What is observed is the disorder renormalization

See also: Zang & Nagaosa, PRB 81, 245125 (2010); Tse & MacDonald, PRL 105, 057401 (2010); Garate & Franz, PRL 104, 146802 (2010); Yokoyama *et al,*PRB 81, 121401 (2010).

# Band structure AHE

- $\Omega$ tilted out of the plane by M
  - Small $s_z$ component
- Coupled charge-spin dynamics
- Apply E//x
  - $k_x$ changes adiabatically
  - $\Omega_y$ changes adiabatically
  - Small rotation of $s_z$ about new $\Omega_y$
  - Small non-equilibrium $s_x$
  - SO $\rightarrow$ small non-equilibrium component of $k_y$
  - This component $\propto$ M
  - Total independent of M
  - Because of monopole at k=0

$$j = \frac{eA}{\hbar}\sigma \times \hat{z},$$




J. M. Luttinger PR 112, 739 (1958)

# Other terms in AHE

- Extrinsic AHE

$$\sigma_{yx}^{\text{ext}} = \frac{e^2}{2h} b_F \left(\lambda k_F^2\right) \left(9 - \frac{8\tau}{\tau_\mu} + \frac{\tau}{\tau_{ss}^{\text{Born}}} + \frac{\tau^2}{2\tau_{ss}^{3rd}\tau_{c+}}\right).$$

- Skew scattering and side jump are negligible
- Why? SS, SJ give rise to effective magnetic field out of the plane

$$\bar{U}_{\boldsymbol{k}\boldsymbol{k}'} = \mathcal{U}_{\boldsymbol{k}\boldsymbol{k}'} \left(1 - i\lambda\boldsymbol{\sigma}\cdot\boldsymbol{k}\times\boldsymbol{k}'\right).$$

$$H^{sj}_{E,\boldsymbol{k}\boldsymbol{k}'} = e\lambda\,\boldsymbol{\sigma}\cdot\left(\boldsymbol{k}\times\boldsymbol{E}\right)\delta_{\boldsymbol{k}\boldsymbol{k}'}$$

- This wants to rotate the spin away from Ω (which is in-plane)
- It counteracts spin-momentum locking
- Therefore it can never give rise to a parallel term
- Similar conclusion holds for magnetic impurities

# Dominant contribution

- Band structure contribution dominant as long as $\varepsilon_F \tau >> 1$
  - Expect it to be independent of magnetization
  - Therefore it overwhelms all terms proportional to M, J
  - No skew scattering, side jump terms linear in $\tau$
- Also overwhelms extrinsic SO since $\lambda k_F^2 << 1$
  - This is why we do not care about the size of $\lambda$
- In TI the wave vector determines the spin AND vice versa.
- Elastic scattering reduces this contribution – renormalization
  - Cf. Molenkamp PRB 2006 for Rashba model
- Not included
  - Electric field correction to skew scattering – 3rd order term in U

$$\int_0^{k_F} \frac{AkM}{(A^2k^2+M^2)^{3/2}} = \frac{1}{A}\left(1-\frac{M}{\sqrt{A^2k_F^2+M^2}}\right).$$

# Observation of AHE

- Bi2Se3, $r_s$~0.14 (assuming permittivity ~ 100)
- Disorder renormalization ~ same order of magnitude as intrinsic
  - Still topological – depends on the same Berry curvature term
- Overall sign depends on type of scattering
  - Coulomb and short-range scattering give opposite signs
  - For Coulomb scattering

$$\sigma_{yx}^{int} \approx -0.53\,(e^2/2h) \approx -e^2/4h$$

  - For short-range scattering

$$\sigma_{yx}^{int} \approx 0.18\,(e^2/2h)$$

  - In principle it could be zero – but only for one sample
- Surfaces increase in quality charged impurities should be dominant
  - There will still be variation depending on $r_s$
  - As $r_s \rightarrow 0$, 0.53 $\rightarrow$ 0.61
  - As $r_s \rightarrow \infty$, 0.53 $\rightarrow$ 0.12

# Summary

- Topological term dominates AHE
  - As long as $\varepsilon_F \tau >> 1$ independent of magnetization
  - Disorder renormalization – non-universal
  - We expect 0.1-0.25 of conductivity quantum
  - Different signs for Coulomb, short-range scattering
- AHE explained by spin-charge coupling in TI
  - What is observed is the disorder renormalization
- Problem – surfaces connected – observe one signal?

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**Anomalous Hall response of topological insulators**

Dimitrie Culcer
*ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, Anhui, China*

S. Das Sarma
*Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA*
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