Disorder Effects on Massive Dirac Fermions

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Outline

- Introduction
- Scattering Universality Classes: implications on side jump Hall conductivity
- Spin Flip Scattering on Massive Dirac Fermions: Weak Scattering Regime
- Spin Flip Scattering on Massive Dirac Fermions: Strong Scattering Regime

Massive Dirac Fermion: Introduction

Electron in vacuum:

Dirac, 1928

$$(-i\hbar c\boldsymbol{\alpha}\cdot\nabla+\beta mc^2)\Psi=i\hbar\frac{\partial\Psi}{\partial t}$$



Electron mass: m





Massive Dirac Fermion: Semiclassical view

a wavepacket in the upper band





Has a magnetic moment, and feels a Berry curvature which leads to spin Hall effect and spin Nernst effect

$$\begin{split} \hbar \dot{\mathbf{k}}_{c} &= -e\mathbf{E} - \frac{e}{c} \frac{\hbar \mathbf{k}_{c}}{\epsilon m} \times \mathbf{B}, \\ \dot{\mathbf{r}}_{c} &= \frac{\hbar \mathbf{k}_{c}}{\epsilon m} + \frac{e}{\hbar} \left(\mathbf{E} \times \mathbf{F} + \mathbf{B} \cdot \mathbf{F} \frac{\hbar \mathbf{k}_{c}}{\epsilon m c} \right), \end{split}$$

C.-P. Chuu, M.-C. Chang and Q. Niu, 2010

Massless Dirac Fermion



Topological insulators

Desire for Opening a Gap

- 1. Gap is essential for any logical device applications.
- 2. Nonzero Berry curvature leads to interesting physics.

staggered potential on graphene



Magnetically doped TI



Y. L. Chen et al., 2010

Massive Dirac Fermions from TI thin film

Hai Zhou Lu...SQ Shen: PHYSICAL REVIEW B **81**, 115407 2010

Yi Zhang ... QiKunXue: Nature Physics 6, 584-588 (2010)

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Binding energy (eV)

E.

-0.2

-0.4

-0.6

-0.8

-0.1



k,, (Å-1)

k// (Å-1)

Berry Curvature and Semiclassical Dynamics

Equation of motion for a electron wavepacket:

$$\dot{m{r}} = rac{\partial \mathcal{E}}{\partial m{k}} - \dot{m{k}} imes m{\Omega}$$

 $\dot{m{k}} = -em{E} - e\dot{m{r}} imes m{B}$

$$\Omega_z(\boldsymbol{k}) = -2\mathrm{Im}\left\langle \frac{\partial u}{\partial k_x} | \frac{\partial u}{\partial k_y} \right\rangle$$

For massive Dirac Fermion:

 $\mathcal{H}(k) = v \boldsymbol{k} \cdot \boldsymbol{\sigma} + \Delta \sigma_z$



Berry curvature (conduction band)

energy spectrum

Berry Curvature and Hall Transport

Intrinsic contribution to Hall conductivity:

$$\sigma_{xy}^{\text{int}} = -e^2 \int \frac{d\mathbf{k}}{(2\pi)^2} f_{\mathbf{k}} \Omega^z(\mathbf{k}) = -\frac{e^2}{4\pi} \frac{\Delta}{\mu} \qquad (\mu > \Delta)$$

Valley Hall effect in graphene:



Di Xiao, Wang Yao, and Qian Niu, 2007

Disorder Scattering, interplayed with Berry curvature, provides another important contribution.

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Scattering in Spin-Orbit Coupled System

- Disorder scattering strongly affects transport properties.
- Scattering has various origins: impurity, dislocation, surface roughness, phonon, magnon, ...

For spin-orbit coupled system, the effects of scattering sensitively depends on its spin structure.

Three universality classes of scattering for 2D systems:

Class A
$$\hat{V} = V^o \hat{1},$$

Class B $\hat{V} = V^o \hat{\sigma}_z,$
Class C $\hat{V} = V^o \hat{\sigma}_{\pm} / \sqrt{2},$

S. A. Yang et al., arXiv:1011.3239

Scattering Universality Classes

Class A
$$\hat{V} = V^o \hat{1}$$
,
Class B $\hat{V} = V^o \hat{\sigma}_z$,
Class C $\hat{V} = V^o \hat{\sigma}_{\pm} / \sqrt{2}$,
Spin-flip scattering

For ferromagnet: Class A: normal impurity, phonon ... Class B: magnetic impurity in the mean magnetization direction ... Class C: magnon ...

For graphene: Class A: on-site impurity, acoustic phonon ... Class C: optical phonon ...

Scattering Universality Classes

Different scattering class leads to different anomalous Hall conductivity.



Intrinsic + side jumps

It was believed that side jump Hall conductivity does not depend on the strength and range of scattering.

We found: side jump Hall conductivity depends strongly on the symmetry type of scattering. For mixed type scatterings, the result depends on the relative strength of different types of scatterings

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• Generalize the Berry curvature concept to disordered systems

For each eigenstate α , define Berry curvature for this state as

$$\Omega_{\alpha} \equiv -\sum_{\beta \neq \alpha} \frac{2 \mathrm{Im} \langle \alpha | v_x | \beta \rangle \langle \beta | v_y | \alpha \rangle}{(\omega_{\beta} - \omega_{\alpha})^2}$$

Its spectral distribution is described by density of Berry curvature, which is defined as

$$\Omega(\varepsilon) \equiv \frac{1}{A} \sum_{\alpha} \Omega_{\alpha} \delta(\varepsilon_{\alpha} - \varepsilon)$$

The density of Berry curvature completely determines the Hall conductivity

$$\sigma_{xy} = -e^2 \int d\varepsilon \langle \Omega(\varepsilon) \rangle_c f(\varepsilon)$$

Sum rule: integral of Berry curvature density between mobility edges is an integer



With spin-flip scattering, Berry curvature distribution is singularly compressed to band edges.



Flat Hall plateaus even for partially filled bands

Numerical evaluation from Kubo formula with disorder average,



These results agree with perturbative results in the thermodynamic limit.

Density of States and Spin Polarization



DOS and spin polarization are greatly enhanced at band edges, which can be explained by a self energy with a real part diverging at band edges.

$$\operatorname{Re}\Sigma^{R}(\varepsilon) = -\frac{n_{\operatorname{dis}}V^{2}}{2\pi v^{2}} \ln \left| \frac{\varepsilon^{2} - \varepsilon_{c}^{2}}{\varepsilon^{2} - \Delta^{2}} \right| (\varepsilon \sigma_{0} - \Delta \sigma_{z})$$

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$$H = \lambda(\sigma_x \sin k_x + \sigma_y \sin k_y) + (\cos k_x + \cos k_y + \Delta)\sigma_z$$
-2

In the non-interacting Dirac model, half integer quantum Hall conductance is not possible. So this means there must other contributions from the Brillouin zone to add or cancel this contribution, so that the total Hall conductance becomes an integer.

(1) Dirac contribution

(2) Conventional contribution



Averaged Two-Terminal Conductance

Landau-Buttiker formula + Green's function method



Spin-flip disorder

Spin-independent disorder

Real Space Calculation of Finite-Size Kubo Formula



Similar character as that of two-terminal conductance

Evolution of Berry Curvature Density



The Dirac component of the Berry Curvature Density of the electron regime moves towards the hole side, and vice versa (green arrow). While the conventional component moves towards the opposite direction (red arrow).

Evolution of Berry Curvature Density



Evolution of Berry Curvature Density



They are superposed when meet each other, but do not kill each other, just as the waves.

Evolution of Berry Curvature Density (Schematic)



Phase Diagram (preliminary result)



Conclusions

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Thank You!