Berry curvature dipole in Weyl materials

Binghai Yan
Weizmann Institute of Science, Israel
www.weizmann.ac.il/condmat/Yan/

Topological insulators and topological metals

More commonly existing in materials than thought.
Weyl SemiMetal (WSM)

\[
\begin{align*}
(\beta mc^2 + c\sum_{n=1}^{3} \alpha_n p_n) \psi(x,t) &= i\hbar \frac{\partial \psi(x,t)}{\partial t} \\
\end{align*}
\]

\[
\begin{align*}
m &= 0 \\
i \frac{\partial \psi}{\partial t} &= \pm c \vec{p} \cdot \vec{\sigma} \psi \\
H &= \pm \sigma \cdot \vec{p}
\end{align*}
\]

Hermann Weyl 1929'

\[X. \text{ Wan et al PRB 83, 205101 (2011).} \]
\[S. \text{ Murakami, New Journal of Physics 10, 029802 (2008).} \]
Quantum Hall effect or Chern insulator

C=0

C=1

\[ AHE = \frac{k_z}{\pi} G_0 \]

\[ SHE = \frac{k_z}{\pi} G_0 \frac{\hbar}{2e} \]
Topological Insulator

$\nu_0=0$

$Z_2 \nu_0=1$

$\nu_0=0$

$k_x$

$k_z$

Increasing $k_z$ dispersion

Time-Reversal Symmetry (TRS)

$$AHE = 0$$

$$SHE = \frac{k_z}{\pi} G_0 \frac{\hbar}{2e} \times 2$$

Murakami 2008'.

Weak TI

Weyl

Strong TI
WSM materials

Pyrochlore $Y_2\text{Ir}_2\text{O}_7$ (noncollinear AFM)
X. Wan, et al.

Super lattice: TI + FM
A. Burkov and L. Balents,

HgCr$_2$Se$_4$ (FM)
G. Xu et al.

Physically interesting,
Chemically more interesting!
The spin Hall effect (SHE) in a quantum spin Hall insulator and a Weyl semimetal based on simple analytical models. In a QSHE, the effective model Hamiltonians, the quantum spin Hall effect (QSHE) insulator and the Weyl semimetal. For the QSHE, the noninteger anomalous Hall conductivity (AHC) appears. In a 3D WSM, we adopt a minimal Hamiltonian for the WSM. The resultant SHC is a third-order tensor and represents the spin current. The Berry curvature is obtained by substituting the velocity operator in the Fermi-Dirac distribution. The correlation between spin Berry curvature and its ordinary counterpart is understood. The SHE in two simple systems is demonstrated. The band anticrossing leads to Berry curvature in the Weyl points. The energy dependent SHC for the WSM is shown, where the maximum value appears at the Weyl points. The SHC is zero as long as the SOC is turned off, but it is nonzero when the SOC is turned on. The nodal line is fully gapped out and a nonzero SHC appears. The band touching points in the Brillouin zone center, where the bands get inverted near the Fermi energy, are not necessarily quantized any more. In the two-dimensional (2D) Brillouin zone, the SHC is dominantly contributed by the band anticrossing. For a 3D WSM, we adopt a minimal Hamiltonian with the chemically well-known Bernevig-Hughes-Zhang model. The separation and reported in Refs. 

*TaAs, TaP, NbAs, NbP*

A family photo of four compounds

Theory

NbP  NbAs  TaP  TaAs

ARPES

Y. Sun, S.-C. Wu, B. Yan, PRB 92, 115428 (2015)

Magneto-transport of WSMs

Large MR and high mobility in NbP

Chiral anomaly, Negative LMR in TaP, NbP

Axial-gravitational anomaly in NbP

(MPI Dresden)

Spin Hall Conductivity

\[ J_S \hat{y}_z = \sigma_{xy} \hat{z} J_x \]

Anisotropic
\[ \sigma_{xy} \approx 800 \text{ (TaAs)} \]
\[ \approx 2000 \text{ (Pt)} \]

Spin Hall Angle
\[ \sigma_{\text{spin}} / \sigma_{\text{charge}} \]
Two types of Weyl points

A. A. Soluyanov et al. Nature 527, 495 (2015). (WTe2)
- MoTe2 -

Stacking 2D TI layers into a WSM
MoTe₂ ARPES

ARPES:
AFM WSMs from AHE materials

**Room-temperature** non-collinear AFM in the Kagome lattice

---

Observation of strong **AHE**:

Observation of strong **SHE**
AFM Weyl, AHE and SHE

Mn$_3$Sn  •  AFM WSMs
Mn$_3$Ge  •  Anomalous Hall and Nernst effects (AHE & ANE) at room temperature
  •  Intrinsic spin Hall effect due to spin texture (without SOC)

Weyl materials

Linear response to a *dc* electric field

**SHE & AHE**

- Both Weyl and ordinary bands contribute to AHC.
- Conventional materials work well.

*Are there some properties for which a WSM is unique or better than ordinary materials?*

Yes, possibly the nonlinear optical response.
Nonlinear optical response

Second-order nonlinear response to the oscillating E-field of light
- Circular photogalvanic effect (CPGE)
- Second harmonic generation (SHE)

\[ E_c(t) = \text{Re}\{\mathcal{E}_c e^{i\omega t}\} \]
\[ j_a = \text{Re}\{j_a^{(0)} + j_a^{(2\omega)} e^{2i\omega t}\} \]

\[ j_a^{(2\omega)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c \]
\[ j_a^{(0)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c^* \]

Experiment on WSM TaAs: Orenstein 17’, Gedik 17’, Wang 17’
Nonlinear optical response

\[ j_a = j_a^{(2\omega)} \Big|_{\omega \to 0} = 2\chi_{abb}|\mathcal{E}_b|^2 \]

At dc limit comes a nonlinear Hall effect.

Semiclassical theory

Current
\[ j_a = -e \int k f(k) v_a \]

Anomalous velocity
\[ v_a = \partial_a e(k) + \varepsilon_{abc} \Omega_b \hat{k}_c, \quad \hat{k}_c = -e E_c(t), \quad E_c(t) = \text{Re}\{\mathcal{E}_c e^{i\omega t}\} \]

Light field

Solve the Boltzmann equation to the second order
\[ -e \tau E_a \partial_a f + \tau \partial_t f = f_0 - f. \]

\[ j_a = \text{Re}\{j_a^{(0)} + j_a^{(2\omega)} e^{2i\omega t}\} \]

\[ j_a^{(0)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c^* \]

\[ j_a^{(2\omega)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c \]

\[ \chi_{abc} = \varepsilon_{abc} \frac{e^3 \tau}{2(1 + i\omega \tau)} \int_k (\partial_b f_0) \Omega_d \]

\[ \sigma_{ab} = -\varepsilon_{abc} \frac{e^2}{\hbar} \int_k f_0 \Omega_c = 0 \]

\[ \int_k f_0 \Omega_c = 0 \quad \int_k (f_0 + \partial_k f_0) \Omega_c = \int_k \partial_k f_0 \Omega_c \neq 0 \]

Semiclassical theory

Current
\[ j_a = -e \int_k f(k) v_a \]
Anomalous velocity
\[ v_a = \partial_a \epsilon(k) + \varepsilon_{abc} \Omega_b \hat{k}_c, \quad \hat{k}_c = -e E_c(t), \quad E_c(t) = \text{Re}\{\mathcal{E}_c e^{i\omega t}\} \]

Light field
\[ \text{Solve the Boltzmann equation to the second order} \quad -e \tau E_a \partial_a f + \tau \partial_t f = f_0 - f. \]
\[ j_a = \text{Re}\{j_a^0 + j_a^{2\omega} e^{2i\omega t}\} \quad j_a^{(0)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c^* \quad j_a^{(2\omega)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c \]
\[ \chi_{abc} = \varepsilon_{adc} \frac{e^3 \tau}{2(1 + i\omega \tau)} \int_k (\partial_b f_0) \Omega_d = -\varepsilon_{adc} \frac{e^3 \tau}{2(1 + i\omega \tau)} \int_k f_0 (\partial_b \Omega_d) \]

Berry curvature dipole
\[ D_{ab} = \int_k f_0 (\partial_a \Omega_b). \]
- Intrinsic to the band structure
- Inversion symmetry breaking
- A Fermi surface property

Ab initio calculations

Interband transitions are extensively studied for insulators, e.g. Rappe 12’, Sipe and Shkrebtii 00’

Current work on intraband contributions in the Berry curvature dipole formalism

1. DFT (GGA) band structure and Bloch wave functions two representative family's: Tpe-I TaAs, type-II MoTe2
2. Highly symmetric Wannier functions for a single-particle Hamiltonian
3. Berry curvature $\Omega$

$$
\Omega^{n}_a (k) = 2i \sum_{m \neq n} \frac{< n | \partial_{k_b} \hat{H} | m > < m | \partial_{k_c} \hat{H} | n >}{(\epsilon_n - \epsilon_m)^2}
$$

Xiao 10’

4. Berry curvature dipole $D$, a tensor

$$
D_{bd} = \int_k f_0 \frac{\partial \Omega_d}{\partial k_b}
$$

Fu 15’
Start with toy models

A single Weyl cone

\[ H_{Weyl}(\mathbf{q}) = \hbar v_t q_\tau \sigma_0 + \hbar v_F \mathbf{q} \cdot \sigma, \]

(a) Type-I

Berry curvature

\[ \Omega(\mathbf{q}) = \frac{\mathbf{q}}{2q^3} \]

(b) Type-I (titled)

Berry curvature dipole

\[ d_{xy} = \frac{\partial \Omega_y}{\partial q_x} = \frac{3q_x q_y}{2q^5} \]

(c) Type-II

Note that \( d_{xy} = \partial \Omega_y / \partial k_x \) is even to \( Mx, My \) or TRS. So a pair of Weyl points contribute the same \( D_{xy} \).
Berry curvature dipole for TaAs

- Point group C4v: M_x, M_y, C_4

  E.g. M_x: \( k_x \rightarrow -k_x, \Omega_x \rightarrow \Omega_x \) so \( d_{xx} \rightarrow -d_{xx} \) then \( D_{xx} = 0 \)

  Finally we have only one independent element \( D_{xy} = -D_{yx} \)
Berry curvature dipole for MoTe$_2$ and WTe$_2$

- Point group C2v

Finally we have two independent elements $D_{xy}$ and $D_{yx}$.

(a) MoTe$_2$

(b) WTe$_2$

No Weyl Points
Berry curvature dipole

<table>
<thead>
<tr>
<th>Material</th>
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<td>0.849</td>
<td>-0.703</td>
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- WSM is better than non-WSM
- Type–II is generally better than type–I
- $D_{xy}$ is not scaled by SOC, different from SHE
- A pair of Weyl points related by $M_{x,y}$ or TRS contribute the same $D_{xy}$

Estimation for the nonlinear Hall effect

\[
\begin{array}{c|cc|c|cc}
\text{Material} & D_{xy} & \text{Material} & D_{xy} & D_{yx} \\
\hline
\text{TaAs} & 0.39 & \text{MoTe}_2 & 0.849 & -0.703 \\
\text{TaP} & 0.029 & \text{WTe}_2 & 0.048 & -0.066 \\
\text{NbAs} & -9.88 & & & \\
\text{NbP} & 20.06 & & & \\
\end{array}
\]

\[
\begin{align*}
\mathbf{D}_{xy} &= \left( \begin{array}{cc} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{array} \right) \\
\mathbf{D}_{y}^z &= \left( \begin{array}{c} 0 \\ D_{y}^z \end{array} \right)
\end{align*}
\]

\[
\chi_{abc} = -\varepsilon_{adce} \frac{e^3 \tau}{2 \hbar^2 (1 + i \omega \tau)} D_{bd}
\]

\[
D_{xy} \text{ corresponds to } \chi_{zxx} \text{ and } \chi_{xxz}
\]

\[
\begin{align*}
j_z &= 2\chi_{zxx} \mathcal{E}_x^2 \\
j_x &= \sigma_{xx} \mathcal{E}_x
\end{align*}
\]

\[
\gamma = \frac{j_z}{j_x} = 2\left( \frac{\chi_{zxx}}{\sigma_{xx}} \right) \mathcal{E}_x
\]

\[
\tau \sim 10 \text{ ps and } \sigma_{xx} \sim 10^6 \text{ } \Omega^{-1} \text{m}^{-1}
\]

\[
\mathcal{E}_x \sim 10^2 \text{ V/m}
\]

\[
\chi_{zxx} \sim 10^{-1} D_{xy}
\]

\[
\gamma \sim 10^{-5} - 10^{-4}
\]

AHE systems \( \gamma \sim 10^{-3} \)

For TaAs, NbPAs, NbP, MoTe2

Fermi surface is tunable by gating, doping or strain.

Y. Zhang, Y. Sun, B. Yan, \textit{arXiv:1708.08589.}
Estimation for the nonlinear Hall effect

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\[
\begin{align*}
  j_z &= 2\chi_{zxx}\mathcal{E}_x^2 \\
  j_x &= \sigma_{xx}\mathcal{E}_x
\end{align*}
\]
Signatures in earlier experiments

Kerr rotation image of a single-layer MoS2 device

Valley magnetoelectricity in single-layer MoS2


WTe2?
Inversion breaking
Weyl, QSH Superconductor

NMR, Spin current
Summary

Topological materials

Berry curvature
Linear response

Berry curvature dipole
Nonlinear response

• Topological materials
• Experiments

• Berry phase induced electric and optical properties
• Develop ab initio tools

Mn₃Ge and Mn₃Sn

AFM Weyl
AHE, ANE
SHE w/o SOC
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Thanks for your attention!