Topological Electronic States & Materials

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Acknowledgement:

Theory: H. M. Weng, X. Dai, Z. J. Wang (IoP),
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Exp: Yulin Chen's group (Oxford),
X. J. Zhou, Li Lu, Hong Ding, Y. Q. Li (IoP)
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Ming Shi, N. Xu (PSI)

Outline:

1. **Introduction: Topological States**

2. **Computational Method: Wilson Loop Method**

3. **Realization & Materials:**

   (1) Dirac Semimetal: Na_3Bi & Cd_3As_2

   (2) Weyl semimetal: $HgCr_2Se_4$ & TaAs (TaP, NbAs, NbP)

4. **New Fermions:**

5. **Detecting CME by lattice dynamics**

   (Z. D. Song, et.al, PRB 94, 214306 (2016). Talk: E44.00005)

1. Introduction:

Topo-States: State (wave-function) with topological characters
Description: Topological Invariants
Significance: (1) Robust against local perturbation
(2) Protected boundary states (usually gapless)

Extension of concept in Condensed Matter Physics:

Real Space (r)	⇒	Parameter Space (k or q)
Real EM field ($F_{\mu\nu}$)	⇒	Emergent Gauge field ($f_{\mu\nu}$)
Fundamental particles:	⇒	Emergent Quasi-particles
Low energy state:	⇔	Quantum State in lattice

Topological States in Momentum (k) Space:
Z or Z2 Insulators, Dirac/Weyl Semimetal, and etc.

1. Introduction: K-space as parameter space

Bloch State:

$$\begin{cases} H(\vec{r})\psi_{nk}(\vec{r}) = \varepsilon_{nk}\psi_{nk}(\vec{r}) \\ \psi_{nk}(\vec{r}) = e^{ik\cdot r}u_{nk}(\vec{r}) \end{cases} \Rightarrow \begin{cases} H_k(\vec{r})u_{nk}(\vec{r}) = \varepsilon_{nk}u_{nk}(\vec{r}) \\ H_k = e^{-ik\cdot r}He^{ik\cdot r} \end{cases}$$

Gauge Freedom:

$$|u'_{nk}\rangle = e^{i\phi(k)}|u_{nk}\rangle \Rightarrow H_k|u'_{nk}\rangle = \varepsilon_{nk}|u'_{nk}\rangle$$

Berry Connection:

$$\vec{A}_n(k) = i\langle u_{nk}|\vec{\nabla}_k|u_{nk}\rangle$$

Gauge dependent

$$\vec{A}'_n(k) = i\langle u'_{nk}|\vec{\nabla}_k|u'_{nk}\rangle = \vec{A}_n(k) - \vec{\nabla}_k\phi(k)$$

Berry Curvature:

$$\vec{\Omega}_n(k) = \vec{\nabla}_k \times \vec{A}_n(k) = i\langle\vec{\nabla}_k u_{nk}|\times|\vec{\nabla}_k u_{nk}\rangle$$

Gauge invariant

$$\vec{\Omega}_n(k) = \vec{\nabla}_k \times \vec{A}'_n(k) = \vec{\nabla}_k \times \vec{A}_n(k)$$

Symmetry:

$\vec{\Omega}_n(k) = \vec{\Omega}_n(-k)$ for IS

$\vec{\Omega}_n(k) = -\vec{\Omega}_n(-k)$ for TRS

$\vec{\Omega}_n(k) \equiv 0$ for IS and TRS

1. Introduction: Magnetic (gauge) Field in K-space

Key quantity: $$\vec{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \vec{\mathbf{A}}(\mathbf{k}) = \nabla_{k} \times i\langle u_{nk} | \nabla_{k} | u_{nk} \rangle$$

$\mathbf{A}(\mathbf{k})$: Berry connection, $u_{n\mathbf{k}}$: periodic part of Bloch function

can be viewed as magnetic field in k-space

[Sundaram & Niu, et.al, PRB (1999); Jungwirth & Niu, et.al, PRL (2002); Fang, et.al, Science (2003); Y. Yao & Niu, et.al. PRL (2004)]

Analogies

Berry curvature $\vec{\Omega}(\vec{k})$	Magnetic field $\vec{B}(\vec{r})$
Berry connection $\vec{A}(\vec{k}) = \langle\psi\| i\frac{\partial}{\partial\vec{k}}\|\psi\rangle$	Vector potential $\vec{A}(\vec{r})$
Geometric phase $\oint d\vec{k}\bullet\vec{A}(\vec{k}) = \iint d^2k\ \Omega_z(\vec{k})$	Aharonov-Bohm phase $\oint d\vec{r}\bullet\vec{A}(\vec{r}) = \iint d^2r\ B_z(\vec{r})$
Chern number $\oiint d^2k\ \ \Omega_z(\vec{k}) = \text{integer}$	Dirac monopole $\oiint d^2r\ \ B_z(\vec{r}) = \text{integer}\ h/e$

Equation of motion:

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\frac{\partial\varepsilon(\mathbf{k})}{\mathbf{k}} - \dot{\mathbf{k}}\times\mathbf{\Omega}(\mathbf{k})$$

$$\hbar\dot{\mathbf{k}} = -e\mathbf{E}(\mathbf{r}) - e\dot{\mathbf{r}}\times\mathbf{B}(\mathbf{r})$$

Anomalous velocity

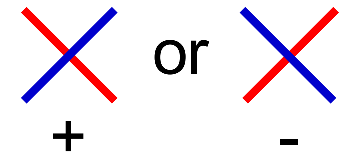
$$x_i = i\frac{\partial}{\partial k_i} - \tilde{A}_i(\vec{k}), \quad [x, y] = -i\Omega_z(\vec{k})$$

Observable:
Anomalous Hall Effect

1. Introduction: Monopoles (Weyl nodes) in 3D

Weyl representation (2x2):
(Irreducible !!)
Left-hand + right-hand

$$H(\vec{k}) = \pm \vec{k}\cdot\vec{\sigma} = \pm\begin{bmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{bmatrix} \Rightarrow$$



Note: (1) No way to have mass term: **Weyl conditions:** $\left|\vec{f}(\vec{k})\right| = 0$

(2) + and – nodes have to appear in pairs in lattice.

Magnetic Monopole in K-space $\Leftrightarrow$ Topological Weyl Semimetal

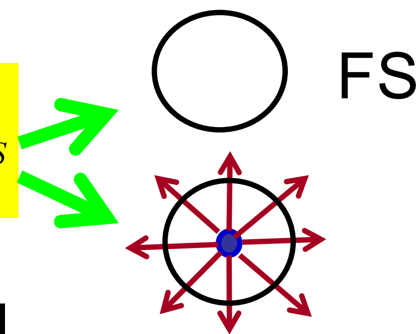
$$\vec{\Omega}(k) = \vec{\nabla}_k \times \vec{A}(k) = \pm\frac{\vec{k}}{2|k|^3} \qquad \vec{\nabla}\cdot\vec{\Omega} \neq 0$$

$$\frac{1}{2\pi}\oint_S \vec{\Omega}(k)\cdot dS(k) = Q$$

"Monopole Charge"

Z. Fang, et.al, Science (2003).

$$\frac{1}{2\pi}\oint_{FS} \vec{\Omega}(k)\cdot dS(k) = C_{FS}$$



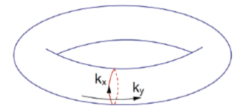
C_{FS}=0, Normal

C_{FS}≠0, Topological

Volovik, JETP (2003).
X.G.Wan, et.al. PRB (2011).
Z. J. Wang, et.al., PRB (2012)

1. Introduction: Various topo. states in terms of $\boldsymbol{\Omega}$(k)

2D: $k_z = m$ $\quad H = \begin{bmatrix} m & k_x - ik_y \\ k_x + ik_y & -m \end{bmatrix}$



$$\oint_{BZ} \vec{\Omega}(\boldsymbol{k}) \cdot d\boldsymbol{S} = 2\pi Z$$

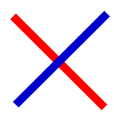
(Chern Insulator)

TRS: $\begin{bmatrix} m & k_x - ik_y \\ k_x + ik_y & -m \end{bmatrix}$ and $\begin{bmatrix} m & k_x + ik_y \\ k_x - ik_y & -m \end{bmatrix}$

$$\oint_{BZ} \vec{\Omega}(\boldsymbol{k}) \cdot d\boldsymbol{S} = 0$$

(QSHI, need Z2=Z mod 2)

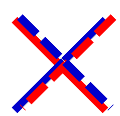
3D: $H = \pm \vec{k} \cdot \vec{\sigma}$



$$\oint_{FS} \vec{\Omega}(\boldsymbol{k}) \cdot d\boldsymbol{S} = 2\pi Z$$

(Weyl Semimetal)

$H = \begin{bmatrix} \vec{k} \cdot \vec{\sigma} & 0 \\ 0 & -\vec{k} \cdot \vec{\sigma} \end{bmatrix}$

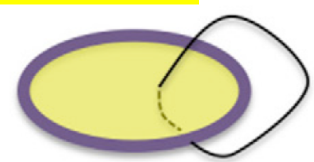


$$\oint_{FS/2} \vec{\Omega}(\boldsymbol{k}) \cdot d\boldsymbol{S} = 2\pi Z$$

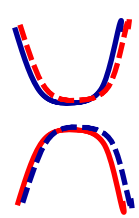
(Dirac Semimetal)

TRS + others

Or nodal-line semimetal:



$H = \begin{bmatrix} \vec{k} \cdot \vec{\sigma} & M \\ M & -\vec{k} \cdot \vec{\sigma} \end{bmatrix}$

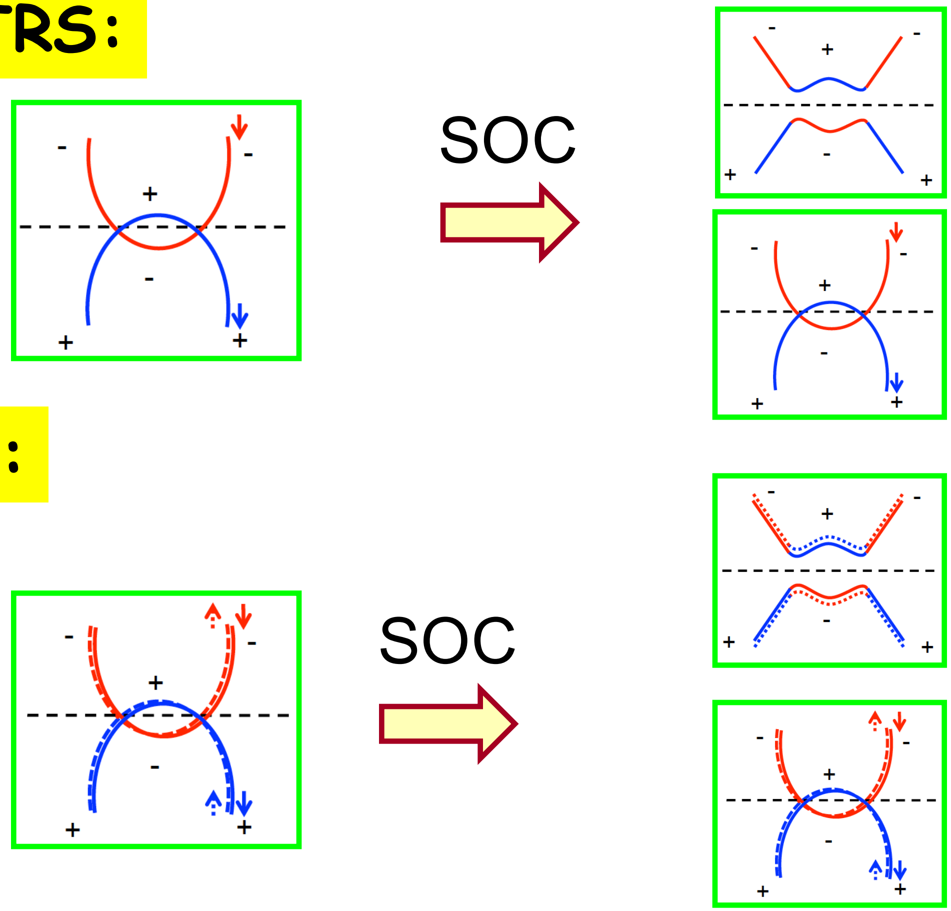


(3D TIs, need Z2 in 3D)

1. Introduction: Band Inversion Mechanism

Without TRS:

With TRS:



Gapped in 2D
Chern Insulator

Gapless in 3D
Weyl semimetal

Gapped in both 2D & 3D
Z2 TIs

Gapless if + Crystal symmetry
3D Dirac semimetal

- Intermetallic compounds or narrow-gap semiconductors
- Band inversion between s-p, p-d, p-p, d-d
- Strong SOC
- Symmetry: either I or T should be broken for Weyl

2. Method: Predictive roles by first-principles calculations

See our reviews: **Advance in Physics, <u>64</u>, 227 (2015); MRS Bulletin, <u>39</u>, 849 (2014).**

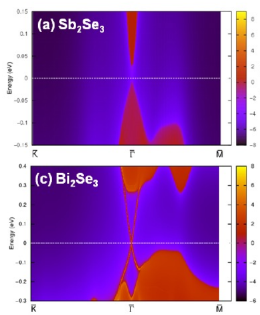
$\rho = \langle \Psi | \Psi \rangle$ VS. $|\Psi\rangle = e^{i\phi(k)} |\psi\rangle$ **Phase is important.**

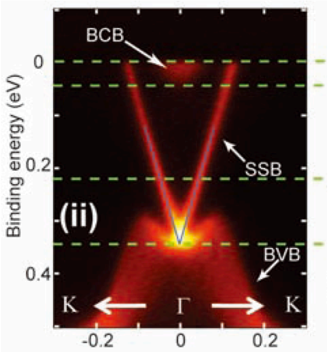
- **Berry phase can be well described by band-theory**
- **Topological States are robust against small errors**
- **Challenging for calculations of topological invariant**

Examples:

3D TI: Bi_2Se_3, Bi_2Te_3, Sb_2Te_3

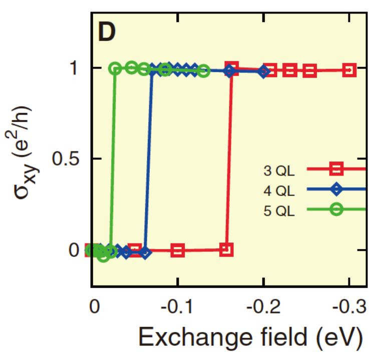
Theory: H. J. Zhang, et.al, Nature Phys. (2009),
Exp: Y. Xia, et.al, Nature Phys. (2009)
Y. L. Chen, et.al, Science (2009).

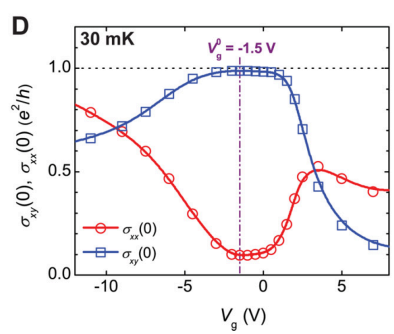




QAHE: Cr-doped Bi_2Te_3 family (Van-Vleck)

Theory: R. Yu, et.al, Science. (2010),
Exp: C. Z. Chang, et.al, Science (2013).





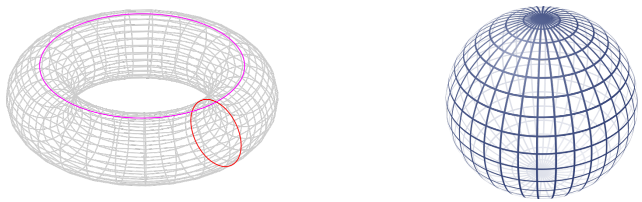
2. Methods: Difficulties

Connection: $\vec{A}_n(\boldsymbol{k}) = i\langle u_{n\boldsymbol{k}}|\vec{\nabla}_{\boldsymbol{k}}|u_{n\boldsymbol{k}}\rangle$

Curvature: $\vec{\Omega}_n(\boldsymbol{k}) = \vec{\nabla}_{\boldsymbol{k}}\times\vec{A}_n(\boldsymbol{k})$

Invariants: $\oint_S \vec{\Omega}_n(\boldsymbol{k})\cdot d\boldsymbol{S} = 2\pi Z$

Manifolds



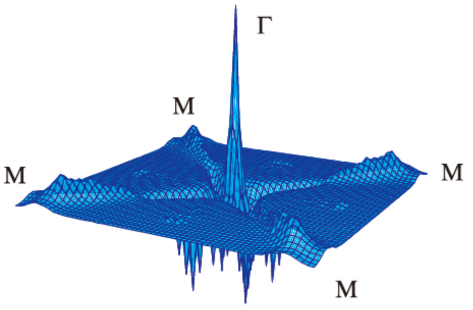
2D BZ   FS

Problems: (1) Fine k-points. (Wannier interpolation)
(2) Smooth gauge, non-abelian $U(N_b)$ (Kubo formula)
(3) Not work for Z_2

Matrix Elements: $\langle\psi_{m\boldsymbol{k}}|\hat{\boldsymbol{v}}|\psi_{n\boldsymbol{k}}\rangle = \omega_{nm,\boldsymbol{k}}\left\langle u_{m\boldsymbol{k}}\middle|\frac{\partial}{\partial\boldsymbol{k}}\middle|u_{n\boldsymbol{k}}\right\rangle$

$$\Omega_n^z(k) = -\sum_{m\neq n}\frac{2\mathbf{Im}\langle\psi_{n\boldsymbol{k}}|v_x|\psi_{m\boldsymbol{k}}\rangle\langle\psi_{m\boldsymbol{k}}|v_y|\psi_{n\boldsymbol{k}}\rangle}{\omega_{mn,\boldsymbol{k}}^2}$$

$$\sigma_{xy} = -\frac{e^2}{\hbar}\int_{BZ}\frac{d^2\boldsymbol{k}}{(2\pi)^2}\sum_{n(occ)}\Omega_n^z(\boldsymbol{k}) = Z\frac{e^2}{\hbar}$$

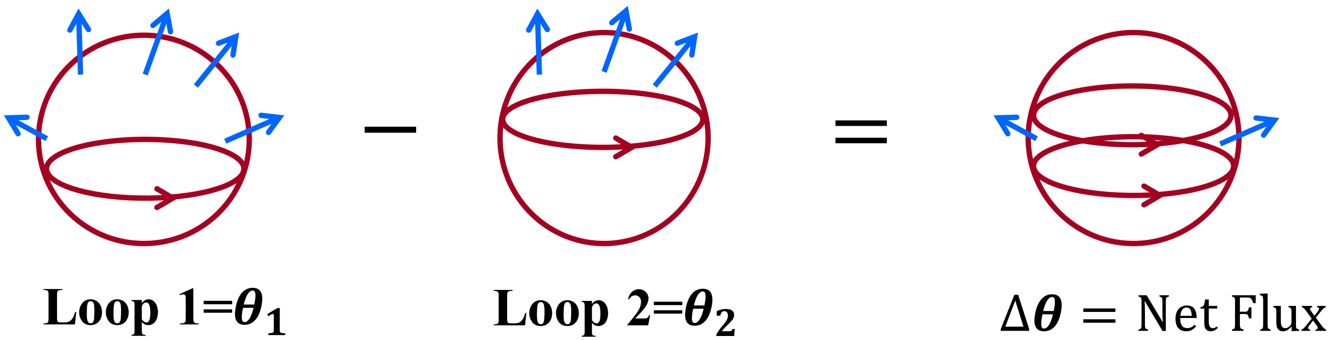


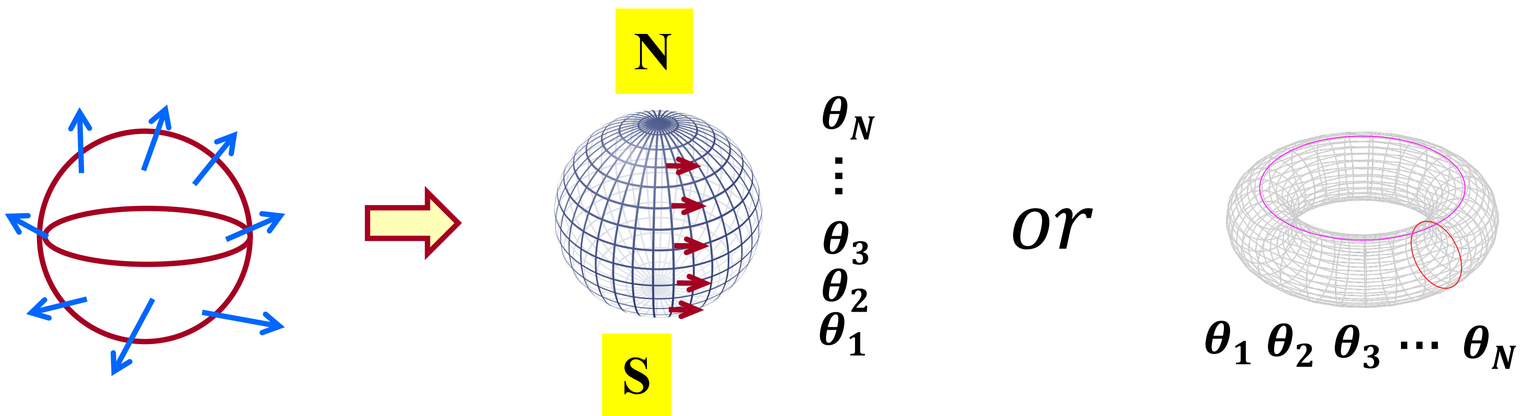
$\Omega^z(k)$ Of $SrRuO_3$
(Fang, et.al, Science 2003)

2. Methods: Loop Method

Stocks' theorem:

$$\text{Flux}=\int_S \vec{\Omega}_n(\boldsymbol{k})\cdot d\boldsymbol{S}=\int_S \vec{\nabla}_{\boldsymbol{k}}\times\vec{A}_n(\boldsymbol{k})\cdot d\boldsymbol{S}=\oint_{\partial S}\vec{A}\cdot d\boldsymbol{l}=\theta$$



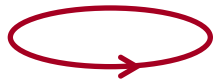


$$\text{Total Flux}=\oint_S \vec{\Omega}(\boldsymbol{k})\cdot d\boldsymbol{S}=\sum\Delta\theta=\int_{l_\perp} d\theta$$

where $\theta=\oint_{l_\parallel}\vec{A}\cdot d\boldsymbol{l}$

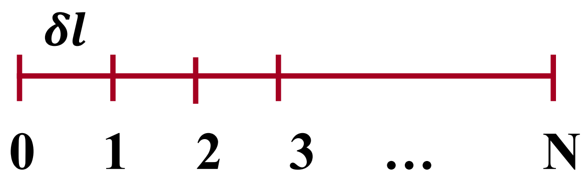
2. Methods: Wilson Loop integration

$$\theta = \oint_{l_{\parallel}} \vec{A} \cdot d\boldsymbol{l}$$



Loop $\boldsymbol{l}_{\parallel}$

Discretize



Periodic: site N= site 0

$$F_{i,i+1}^{mn} = \langle u_{m,i} | u_{n,i+1} \rangle \approx e^{-iA_{i,i+1}^{mn}\delta l}$$

$$A_{i,i+1}^{mn} = i\langle u_{m,i} | (| u_{n,i+1} \rangle - | u_{n,i} \rangle) \rangle / \delta l$$

$N_b \times N_b$ **Matrix:** $D^{mn} = F_{0,1} F_{1,2} F_{2,3} \dots F_{N-1,0} = \prod_{i=0}^{N-1} F_{i,i+1}$

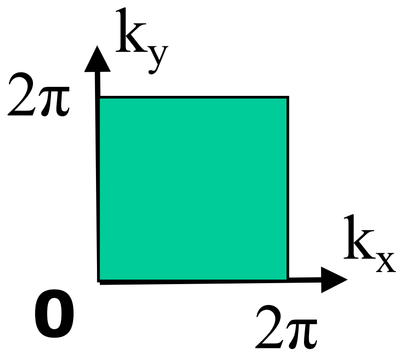
$U(N_b)$ **Wilson Loop:** $D = \left\{ Pexp\left[\oint_C -i\vec{A} \cdot d\boldsymbol{l} \right] \right\}$

Eigen Values of D^mn: $\lambda_m^D = |\lambda_m^D| e^{i\theta_m}$

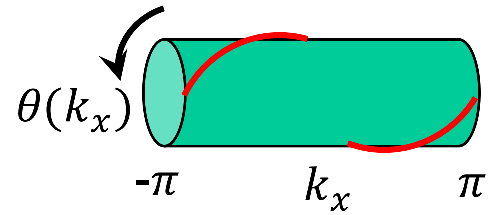
No need for gauge-fixing.
Good for both Z and Z2.

R. Yu, et.al, PRB 84, 075119 (2011)

2. Methods: Plots for Z and Z2 invariant

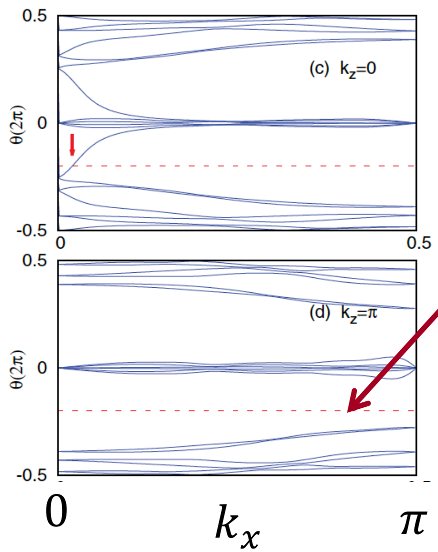


$$\theta_n(k_x) = \oint_{C_y} \vec{A}_n \cdot d\boldsymbol{k}_y$$



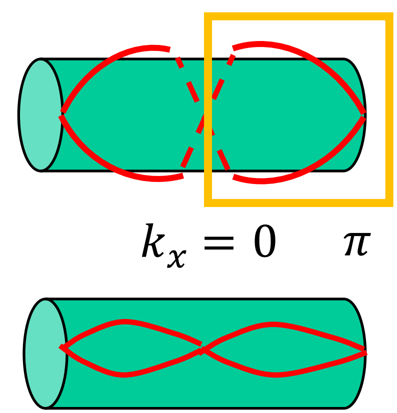
Z=1

Z=0



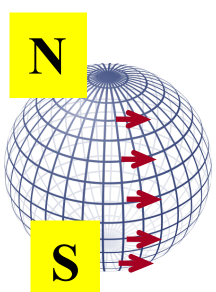
Reference line in gap.

Results for Bi_2Se_3



Z_2=1

Z_2=0



$\boldsymbol{\theta}_N$

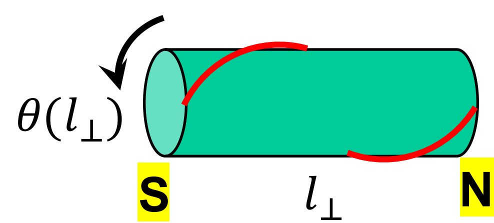
⋮

$\boldsymbol{\theta}_3$

$\boldsymbol{\theta}_2$

$\boldsymbol{\theta}_1$

$$\theta(l_\perp) = \oint_{l_\parallel} \vec{A} \cdot d\,l_\parallel$$

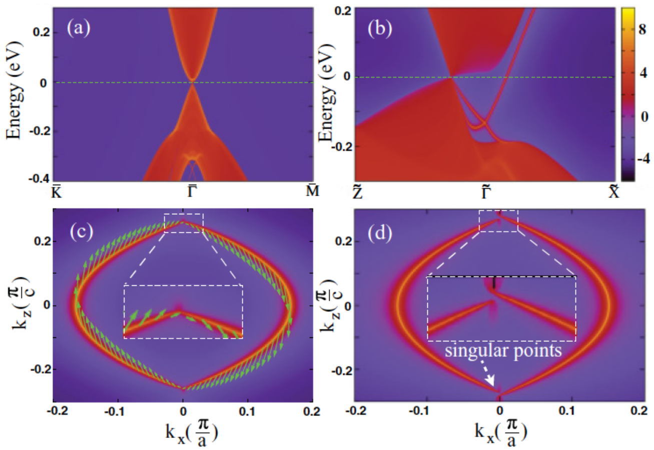


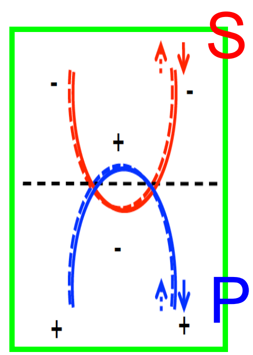
Fermi Surface
Chern number
Z=1

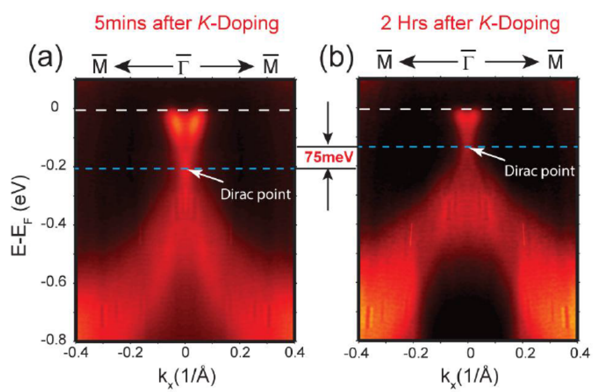
3. Materials: Dirac Semimetals

Na_3Bi

Z. J. Wang, PRB 85, 195320 (2012)







A single pair of Dirac points,

PT symmetry

+

C3 or C4

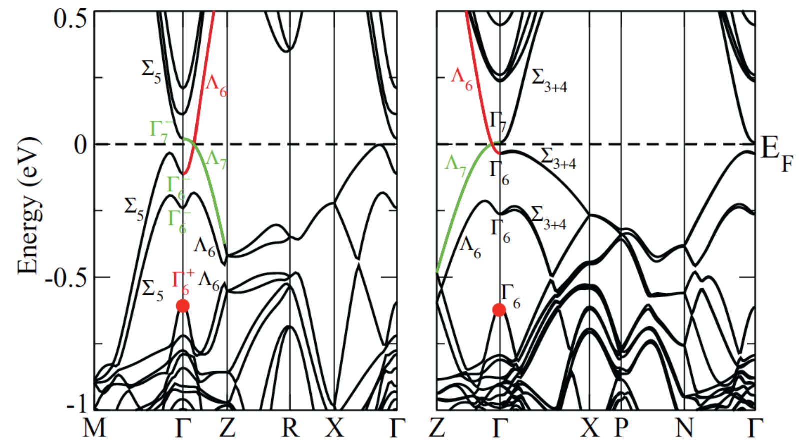
ARPES:

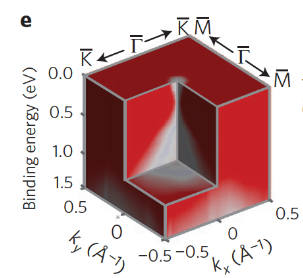
Z. K. Liu, Science (2014).

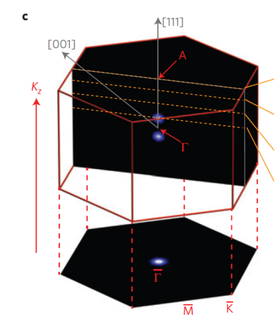
S. Y. Xu, Science (2014).

Cd_3As_2

Z. J. Wang, PRB 88, 125423 (2013)







ARPES:

Z. K. Liu, Nature Mater. (2014).

M. Neupane, Nature Comm. (2014).

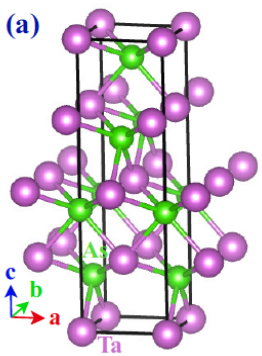
S. Borisenko, PRL (2014).

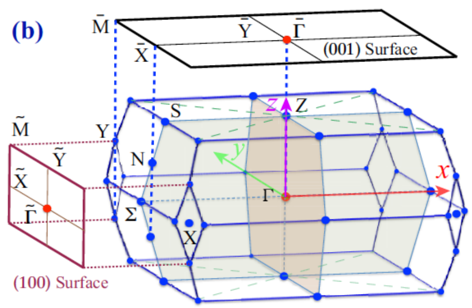
Cd_3As_2 mobility, up to 10^7 cm^2/Vs at 5K!

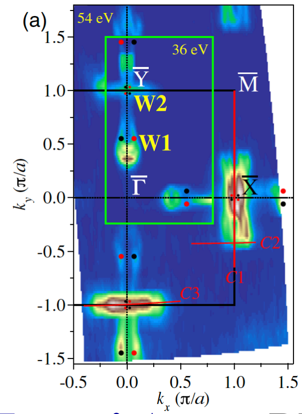
3. Materials: Weyl semimetals: TaAs family

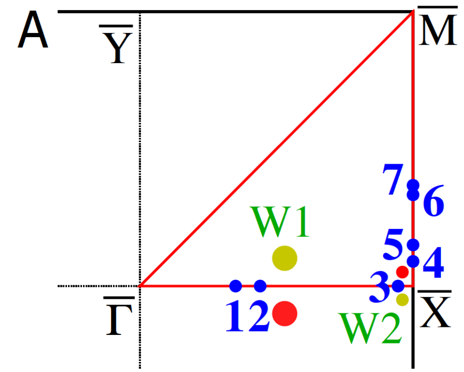
Family: TaAs, TaP, NbAs, NbP ($I4_1md$, 109, C4v)

Weng, et.al, PRX 5, 011029 (2015); S. M. Huang, et.al, Nature Comm. 6, 7373 (2015).

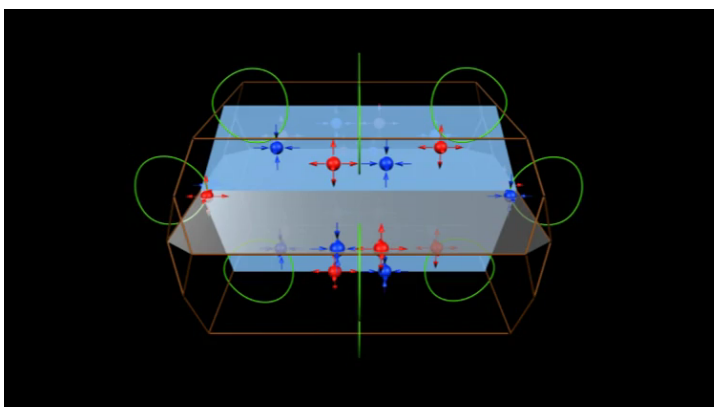




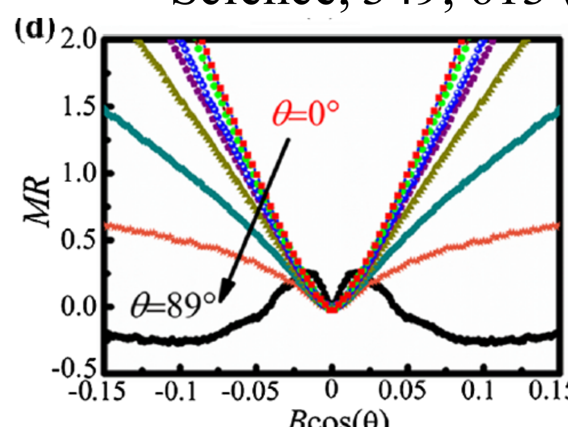




Fermi Arcs: PRX, 5, 031013 (2015)
Science, 349, 613 (2015).



Theory



Negative MR: PRX, 5, 031013 (2015)
Science, 349, 613 (2015).

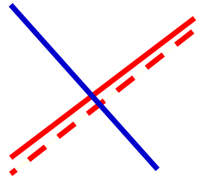
4、New Fermions:

- Fermions are spinor representation of Lorentz symmetry.
- No Lorentz symmtery in a crystal. Instead, we have crystal symmetry.
- New fermions are expected as representation of crystal symmetry.

3-fold point：between Weyl（2）and Dirac（4）？

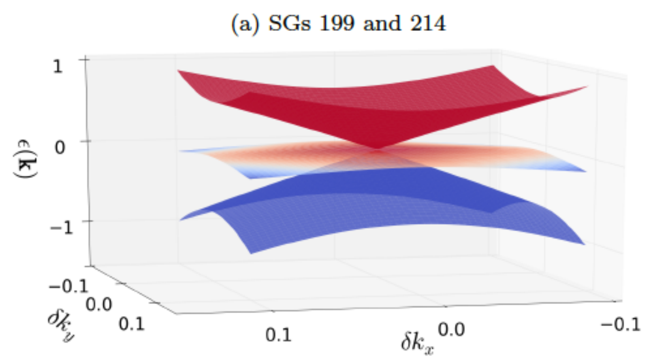
Scheme 1: 2-fold band＋1 band, anti-crossing

（Weng, et.al, PRB 93, 241202 (2016).）



Scheme 2: 3d-irrep, high symmetry point.

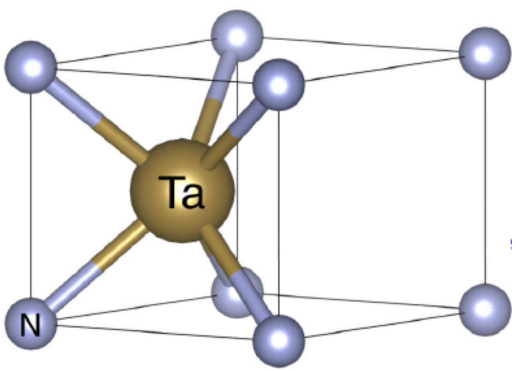
（B. Bradlyn, et.al. Science (2016).）

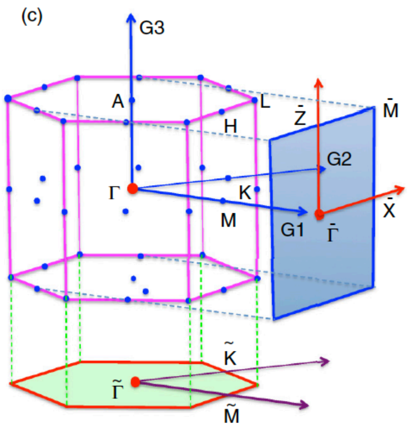


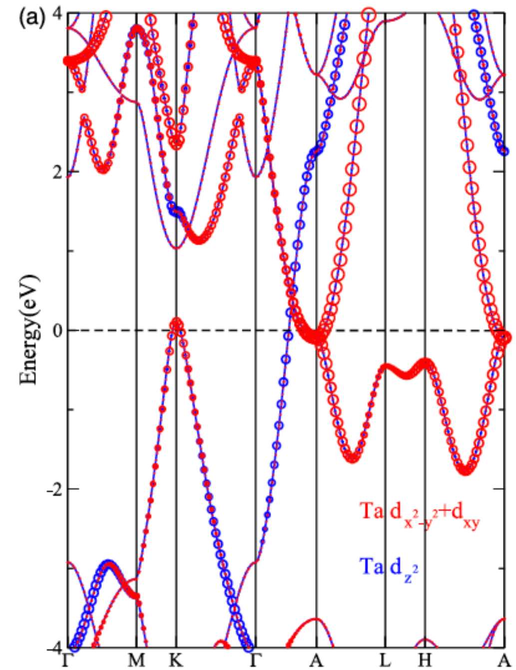
4、New Fermions:

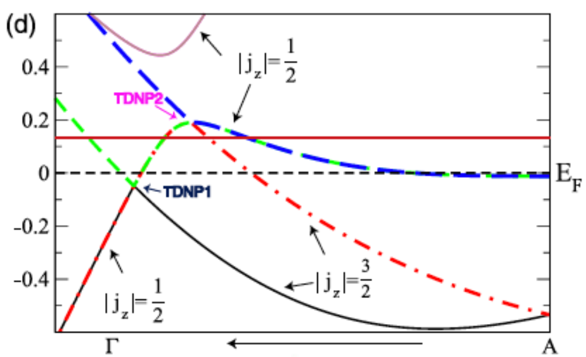
TaN: Weng, et.al, PRB 93, 241202 (2016).

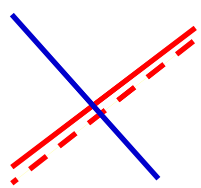
ZrTe: Weng, et.al, PRB 94, 165201 (2016)











$$j_z = \pm\frac{1}{2}$$

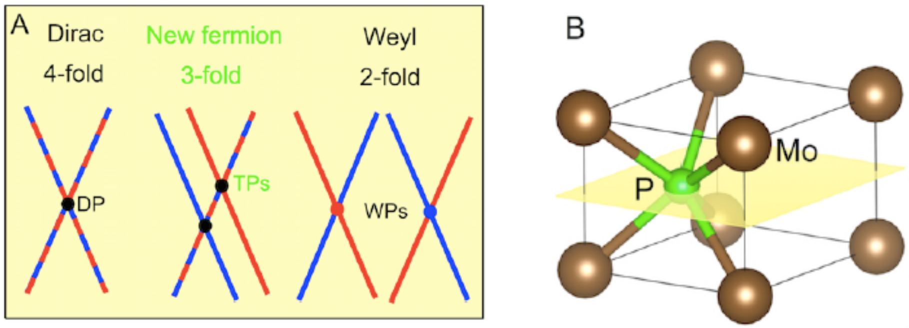
$$j_z = \frac{3}{2}$$

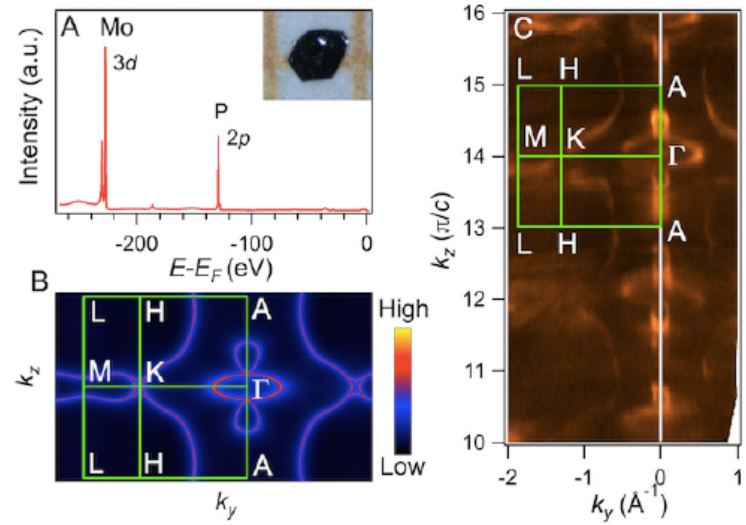
$$H_3(\mathbf{q}) = \begin{bmatrix} u_{1/2}q_z & \lambda_1 q_+^2 & \lambda_2 q_+ \\ \lambda_1 q_-^2 & u_{1/2}q_z & \lambda_2 q_- \\ \lambda_2 q_- & \lambda_2 q_+ & u_{3/2}q_z \end{bmatrix}$$

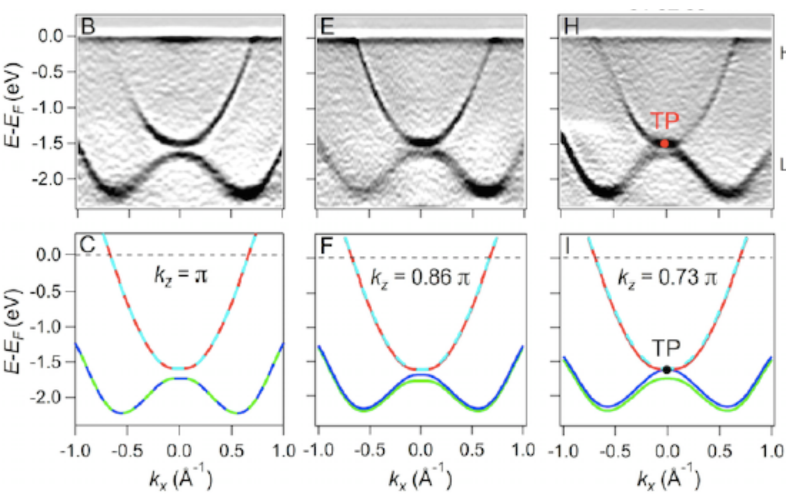
物理结果：Chiral Anomaly ➡ Helical Anomaly

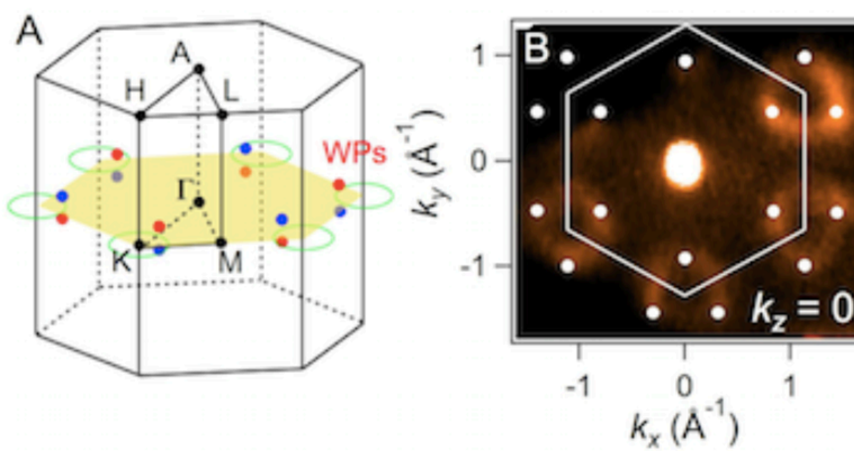
4、New Fermions:

MoP:　实验，B. Q. Lv. et.al,　Arxiv:1610.08877 (2016).





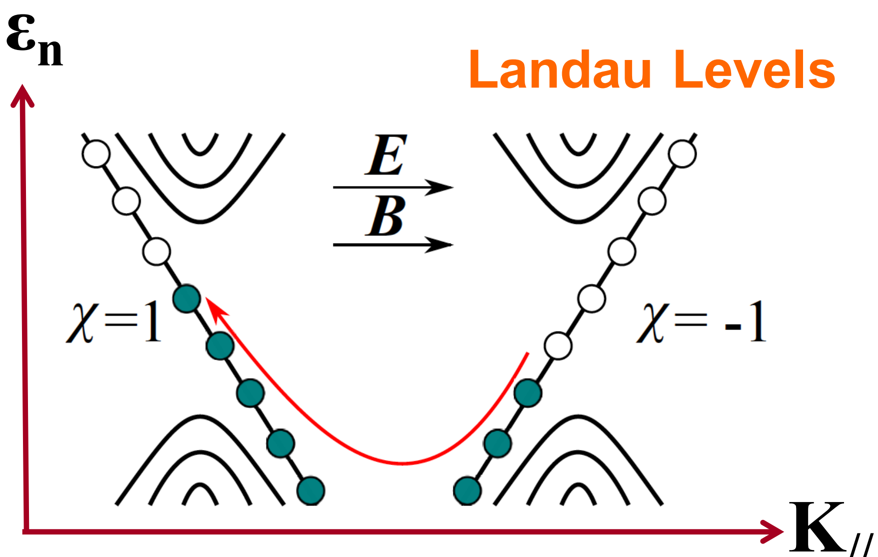




5、Detecting CME:

Chiral Anomaly

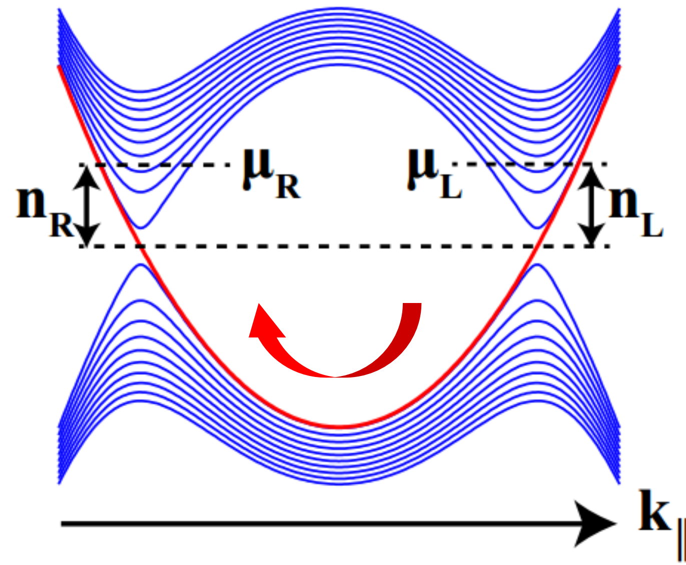
(Nielsen & Ninomiya, Phys. Lett. 2011)



- Negative MR for E//B .

Chiral Magnetic Effect

(K. Fukushima, et.al. PRB (2008)



$$\frac{\partial n_a}{\partial t} = \frac{e^2 N_W}{4\pi^2\hbar^2}\mathbf{E}\cdot\mathbf{B} - \frac{n_a}{\tau_{\mathrm{inter}}}$$

$$\mathbf{J}_{\mathrm{CME}} = \frac{e^2\mathbf{B}}{4\pi^2\hbar^2}\sum_{\mathbf{K}_i}\chi_i\mu_i$$

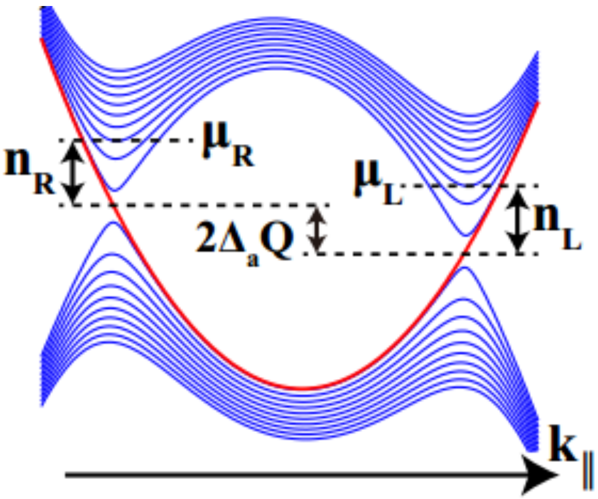
5、Detecting CME:

Deformation potential in longwave limit

$$\hat{H}_{ep} = \frac{1}{V}\sum_{\mathbf{K}_i\mathbf{p}} \hat{\psi}^{\dagger}_{\mathbf{K}_i+\mathbf{p}} \Delta_{\mathbf{K}_i,Q} \hat{\psi}_{\mathbf{K}_i+\mathbf{p}} Q$$

$$\mu_i = \Delta_{\mathbf{K}_i,Q} Q$$

$$\mathbf{J}_{\mathrm{CME},Q} = \frac{N_W e^2 \mathbf{B}}{4\pi^2\hbar^2} \Delta_{a,Q} Q$$



Symmetry of phonon mode

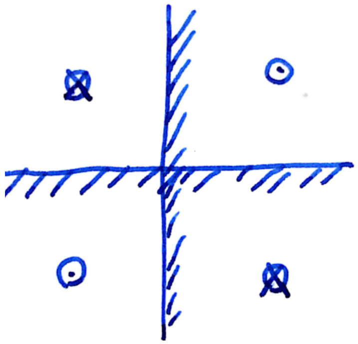
$$\Delta_{a,Q} = \frac{1}{N_W}\sum_{\mathbf{K}_i} \chi_i \Delta_{\mathbf{K}_i,Q}$$

$$= \frac{1}{N_W}\sum_{\mathbf{K}_i}{}' \chi_i \Delta_{\mathbf{K}_i,Q} \frac{1}{|H^{\mathbf{K}_i}|} \sum_{g\in G} \det g \cdot D_Q(g)$$

Sum over non-equivalent Weyl points

little group of K

Representation of the phonon mode



Example for C_{2v}

The phonon mode must behave like a pseudo scalar (Not Raman, and not infra-red active)

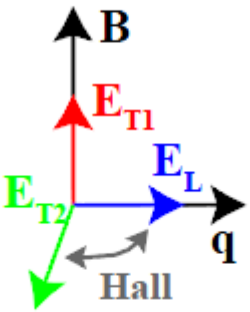
5、Detecting CME:

Pseudo scalar phonon in materials

Materials			Space Group	Little Group at Γ	Relevant Wyckoff Sites	SSGs	Pseudo Scalar Phonon [a]	Polarised
Weyl	non magnetic	$ABi_{1-x}Se_xTe_3$ [1]	160	C_{3v}	-	-	-	-
		BiTeI under pressure [1]	156	C_{3v}	-	-	-	-
		Se/Te under pressure [2]	152/153	D_3	$3a$	C_2	A_1	No
		TaAs [3, 4]	109	C_{4v}	-	-	-	-
	magnetic	$A_2Ir_2O_7$ [5]	227.131 [b]	$\mathcal{O}_h$ [c]	-	-	-	-
		$HgCr_2Se_4$ [6]	141.557 [b]	$\mathcal{D}_{4h}$ [c]	$8c$, $16h$	C_{2h}, C_s	$2 \times A_{1u}$	No
Dirac	Class I [d]	Cu_3PdN [7]	221	O_h	-	-	-	-
		A_3Bi [8]	194	D_{6h}	-	-	-	-
		BaAuBi-family [9]	194	D_{6h}	-	-	-	-
		LiGaGe-family [9]	186	C_{6v}	-	-	-	-
		$SrSn_2As_2$[9]	160	C_{3v}	-	-	-	-
		Cd_3As_2 [10]	137	D_{4h}	$3 \times 8g$, $8f$	C_s, C_2	$4 \times A_{1u}$	No
		Cd_3As_2 [10]	110	C_{4v}	$9 \times 16b$, $2 \times 8a$	C_1, C_2	$29 \times A_2$	No
	Class II	β-cristobalite BiO_2 [11]	227	O_h	-	-	-	-
		HfI_3 [9]	193	D_{6h}	-	-	-	-
		AMo_3X_3-family [9]	176	C_{6h}	$2 \times 6h$, $2c$	C_s, C_{3h}	$3 \times A_u$	Yes
		Distorted Spinel [12]	74	D_{2h}	$4a$, $4d$, $8h$, $8i$	C_{2h}, C_{2h}, C_s, C_s	$4 \times A_u$	No

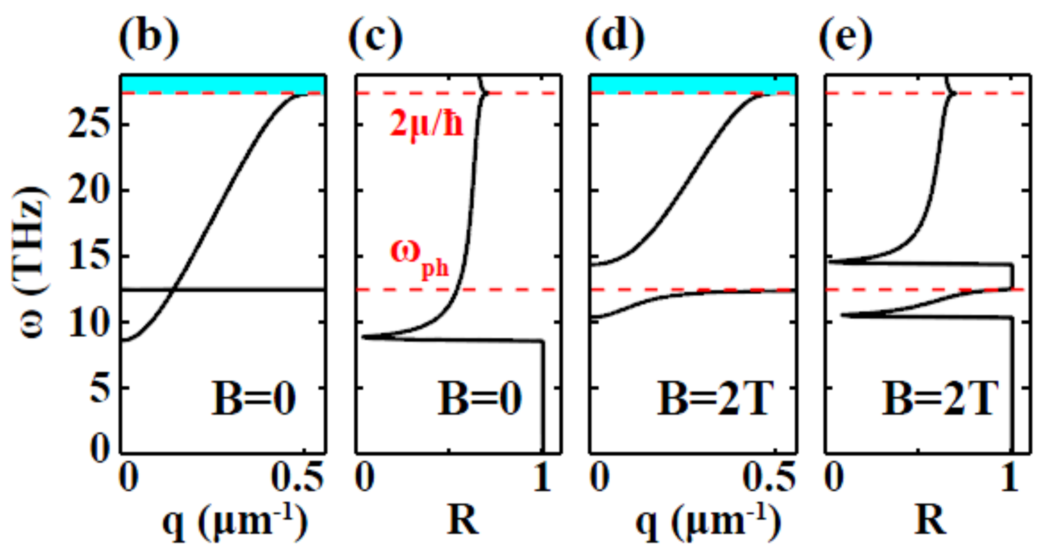
5、Detecting CME:

Transversal EM fields (non-polarized phonon)



$$-\kappa\omega^2 E_{T1} - i\frac{\omega}{\epsilon_0}\sigma_T(\omega\mathbf{q})E_{T1} + \frac{1}{\mu\epsilon_0}\mathbf{q}^2 E_{T1} - i\frac{\omega e^2 B}{4\pi^2\epsilon_0\hbar^2}\left(N_W\Delta_a Q + \frac{n_a}{\nu_D}\right) = 0$$

$$\Delta\omega \approx \frac{e^2 N_W \Delta_a |\mathbf{B}|}{\pi^2\hbar^2} \times \sqrt{\frac{\Omega}{8\epsilon_0 M_{ph}\omega_{ph}^3\left(\frac{2\epsilon^0_{r,T}}{\omega_{ph}} + \frac{\partial\epsilon^0_{r,T}}{\partial\omega}\right)_{\omega_{ph},\mathbf{q}_0}}}$$



Song, et.al,
PRB 94, 214306 (2016).

Talk: E44.00005

Summary:

1. Topological States (Insulators & Semimetals) in K-space.
2. Efficient Wilson Loop Method.
3. Dirac SM: Na_3Bi, Cd_3As_2
4. Weyl SM: $HgCr_2Se_4$, TaAs, NbAs, TaP, NbP
5. Detecting CME by lattice dynamics
6. Open questions:

   (1) MR is very complicated?

   (2) Superconductivity in doped WSM?

   (3) A single pair of Weyl nodes?

   (4) Controlling of Chiral Anomaly

   (5) ……