Stability of Topological Semimetals against Strong Long-Range Interactions

Akihiko Sekine

Institute for Materials Research, Tohoku University

[AS & Nomura, Phys. Rev. B 90, 075137 (2014)]
[AS & Nomura, J. Phys. Soc. Jpn. 83, 094710 (2014)]

July 21, 2015

Outline

Are Dirac and Weyl semimetals stable against long-range interactions ?

Band gap opens by long-range electron-electron interactions ??

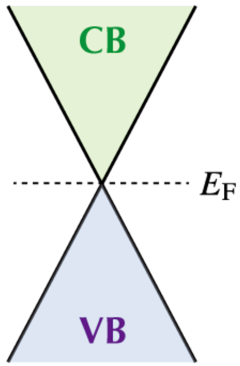
1. Introduction to Dirac & Weyl semimetals
2. Lattice-gauge-theoretical study of correlation effects in Dirac semimetals
3. Lattice-gauge-theoretical study of correlation effects in a Weyl semimetal
4. Summary

Dirac and Weyl Semimetals

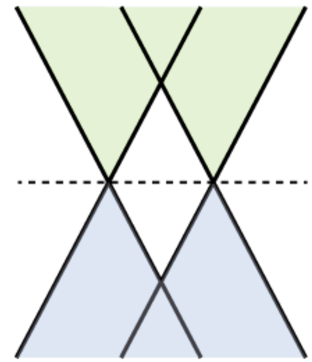
Dirac Semimetal

$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\alpha}$

(four-component)



Symmetry breaking
(time-reversal and/or parity)



Weyl Semimetal

$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\sigma}$

(two-component)

Theoretical predictions

[S. M. Young *et al.*, PRL **108** (2012)]
[Z. Wang *et al.*, PRB **85** (2012)]

Experimental observations

Na_3Bi [Z. K. Liu *et al.*, Science **343** (2014)]

Cd_3As_2 [M. Neupane *et al.*, Nat. Commun. **5** (2014)]

Theoretical predictions

[X. Wan *et al.*, PRB **83** (2011)]
[Burkov & Balents, PRL **107** (2011)]

Experimental observations

Photonic crystal [L. Lu *et al.*, arXiv:1502.03438]

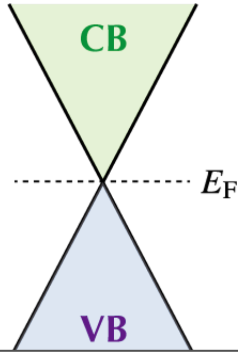
TaAs [S.-Y. Xu *et al.*, arXiv:1502.03807]
[B. Q. Lv *et al.*, arXiv:1502.04684]

Dirac and Weyl Semimetals

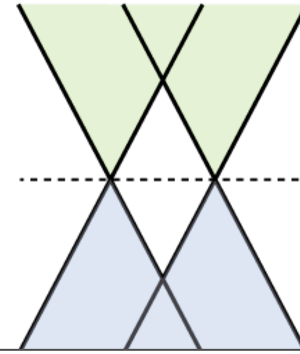
Dirac Semimetal

$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\alpha}$

(four-component)



Symmetry breaking (time-reversal and/or parity)



Weyl Semimetal

$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\sigma}$

(two-component)

Theoreti

[S. M. You

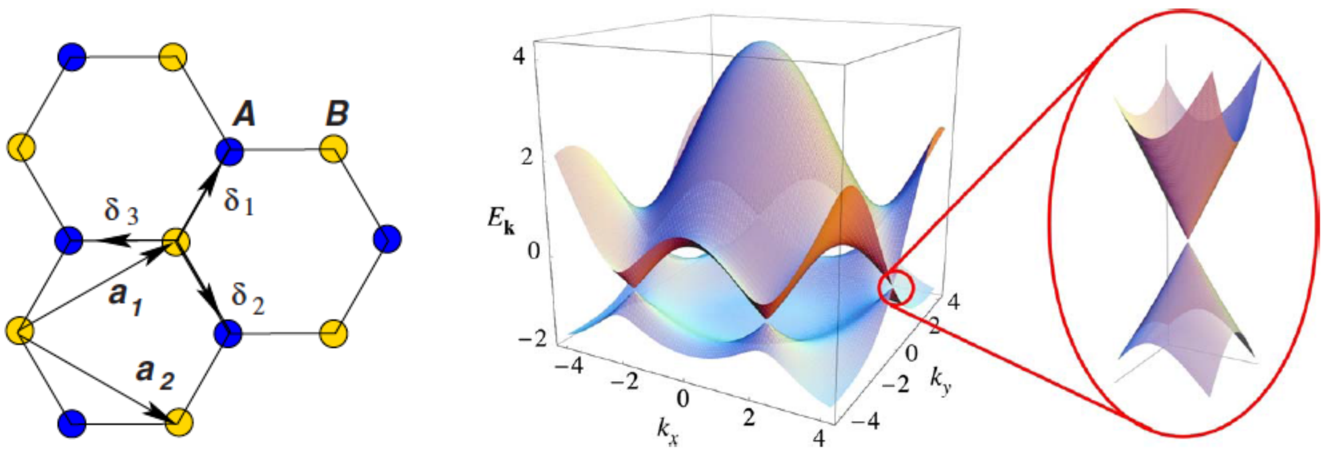
[Z. Wang

Experim

Na_3Bi [Z. … 502.03438]

Cd_3As_2 [I … 7]

… 4]



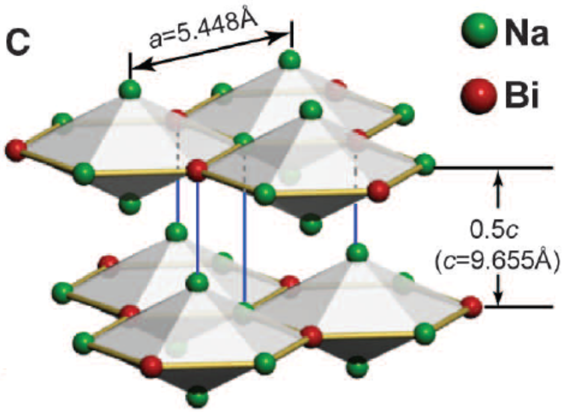
[A. H. Castro Neto *et al.*, RMP 81 (2009)]

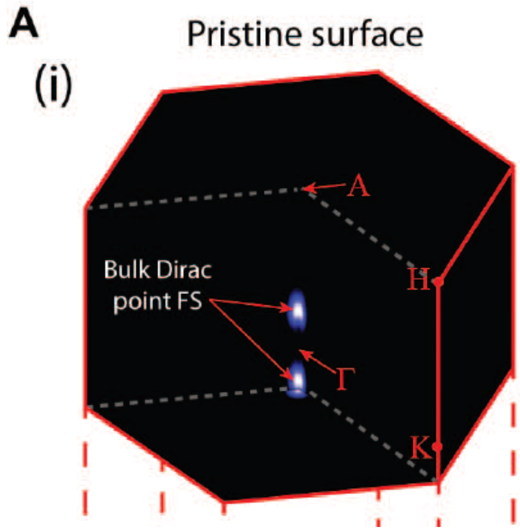
They can be regarded as 3D analogs of graphene.

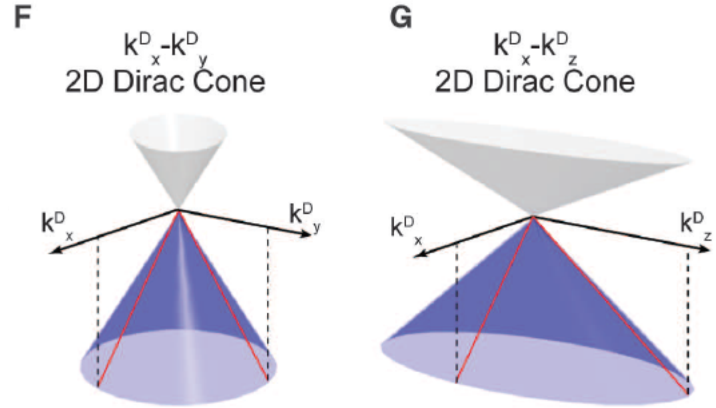
Dirac Semimetals

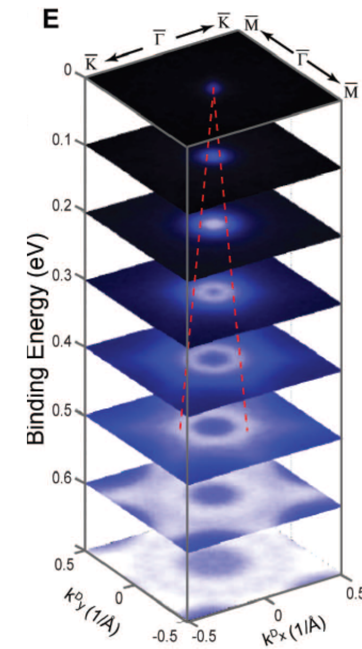
Na_3Bi [Z. K. Liu *et al.*, Science **343** (2014)]

$$\mathcal{H}_{\text{eff}}(\boldsymbol{k}) = v_{\text{F}} \boldsymbol{k} \cdot \boldsymbol{\alpha} \quad \text{(4 × 4 Hamiltonian)}$$









In both Na_3Bi and Cd_3As_2 …

- Two Dirac points (protected by crystalline symmetry)
- Large out-of-plane Fermi velocity anisotropy

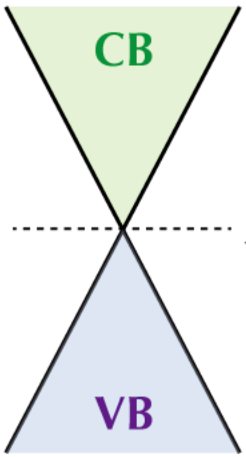
$$\boxed{v_{\text{F}\perp}/v_{\text{F}||} \sim 0.1 - 0.2} \quad (v_{\text{F}x} \approx v_{\text{F}y} \equiv v_{\text{F}||})$$

Three-Dimensional Topological Phases

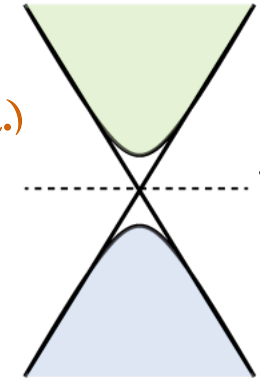
Dirac Semimetal

$$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\alpha}$$

(four-component)



parameter tuning
(element substitution etc.)



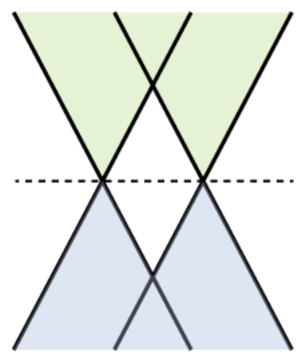
Topological Insulator

$$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\alpha} + m\beta$$

(four-component)

symmetry breaking
(time-reversal / inversion)

symmetry breaking
(time-reversal / parity)



Weyl Semimetal

$$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\sigma}$$

(two-component)

Weyl Semimetals

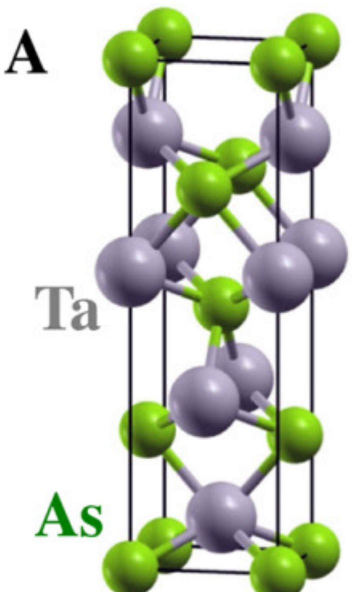
◆ **Time-reversal and/or parity (inversion) symmetry breaking is required.**

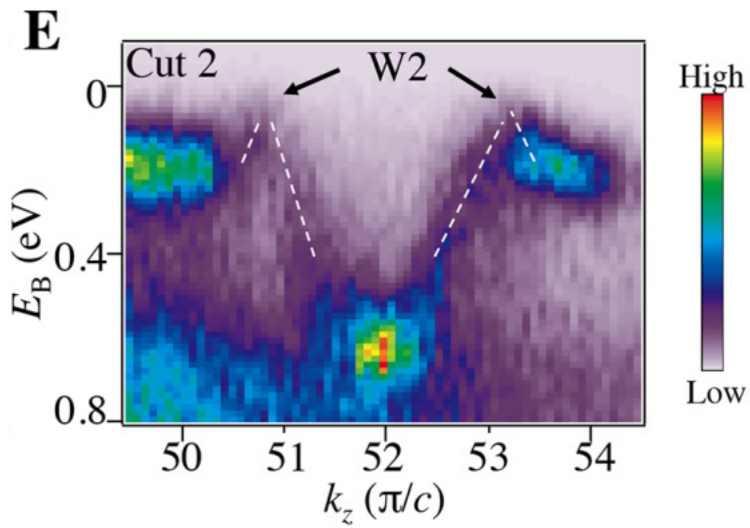
[G. E. Volovik, Lect. Notes Phys. 718 (2007)] [S. Murakami, New J. Phys. 9 (2007)]

TaAs (with broken parity symmetry) [S.-Y. Xu *et al.*, arXiv:1502.03807 (Science, in press)]

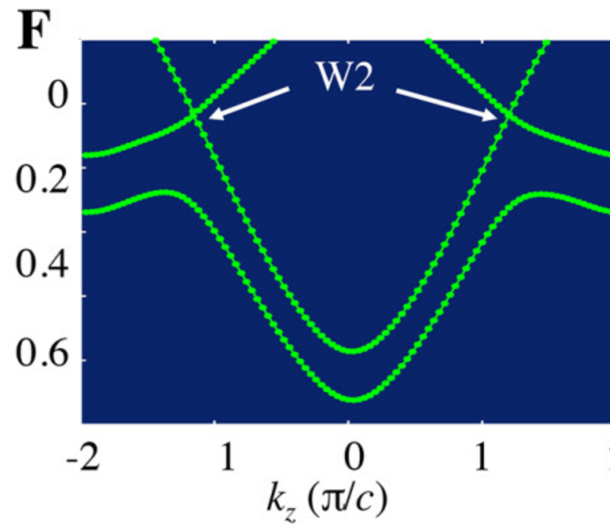
24 Weyl points!

$$\mathcal{H}_{\mathrm{eff}}(\boldsymbol{k}) = \pm v_{\mathrm{F}} \boldsymbol{k} \cdot \boldsymbol{\sigma} \quad \text{(2 × 2 Hamiltonian)}$$





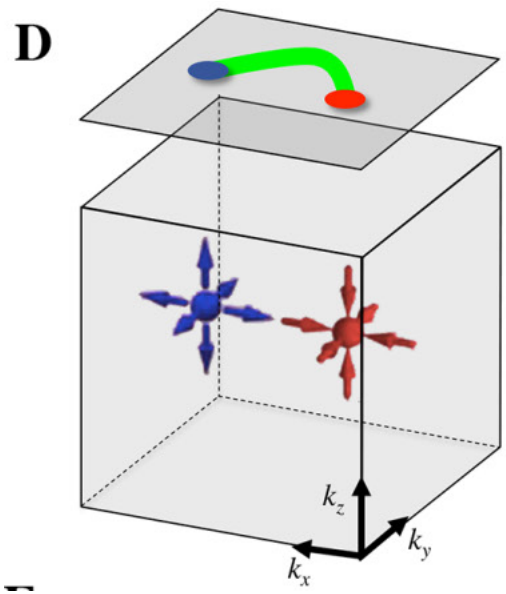
ARPES measurement of a Weyl cone



First principles calculation

Weyl Semimetals

◆ Time-reversal and/or parity (inversion) symmetry breaking is required.



[S.-Y. Xu *et al.*, arXiv:1502.03807]

Effective Hamiltonian around each Weyl node:

$$\mathcal{H}_{\mathrm{eff}}(\boldsymbol{k}) = \pm v_{\mathrm{F}} \boldsymbol{k} \cdot \boldsymbol{\sigma} \quad \text{(2 × 2 Hamiltonian)}$$

chirality ± 1

Each Weyl node can be regarded as a **"monopole"** of the Berry connection $\mathcal{A}(\boldsymbol{k}) = -i \sum_n \langle u_{n\boldsymbol{k}} | \nabla_{\boldsymbol{k}} | u_{n\boldsymbol{k}} \rangle$ in momentum space.

Energy gap opens *only when* Weyl nodes with opposite chirality meet each other.

➡ **Topological nature of Weyl semimetals**

Coulomb Interactions

TOHOKU UNIVERSITY

$\boldsymbol{H_U}$ (on-site int.) : orbital (*s*, *p*, *d*, *f*…) dependent

$\boldsymbol{H_{\text{long-range}}}$ (inter-site int.) : dielectric-constant dependent

$$H_{\text{long-range}} = \sum_{i,j} n_i \left[\frac{e^2}{4\pi\epsilon} \frac{e^{-k_0 r}}{r} \right] n_j \qquad \left(r = |\boldsymbol{r}_i - \boldsymbol{r}_j| \right)$$

where $k_0 \propto \sqrt{\rho(E_{\mathrm{F}})}$ $\begin{cases} \rho(E) \propto E & \text{(2D Dirac)} \\ \rho(E) \propto E^2 & \text{(3D Dirac)} \end{cases}$ ⇒ $\boldsymbol{k_0 = 0}$ at the Dirac point

3D Dirac fermions + $1/r$ Coulomb interactions (U(1) gauge field)

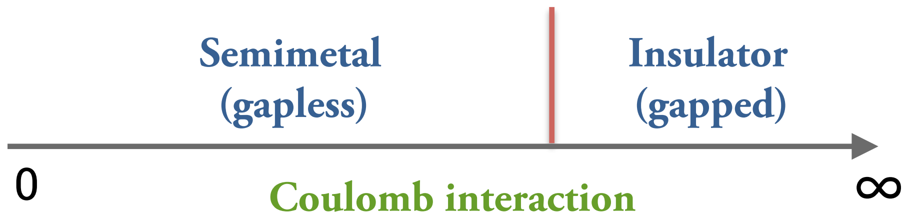
⇓ on a lattice

U(1) lattice gauge theory (≈ lattice QED)

Analysis from the strong coupling limit

Lattice Gauge Theory

In 2D systems (such as graphene)… Lattice gauge theory has been applied.



MC simulation [Hands & Strouthos, PRB **78** (2008)]
[Drut & Lähde, PRL **102** (2009)]
[Armour, Hands & Strouthos, PRB **81** (2010)]

Strong coupling expansion [Araki & Hatsuda, PRB **82** (2010)]
[Araki & Kimura, PRB **87** (2013)]

3D Dirac fermions + 1/r Coulomb interactions (U(1) gauge field)

on a lattice

U(1) lattice gauge theory (≈ lattice QED)

Analysis from the strong coupling limit

Outline

Are Dirac and Weyl semimetals stable against long-range interactions ?

Band gap opens by long-range electron-electron interactions ??

1. Introduction to Dirac & Weyl semimetals
2. Lattice-gauge-theoretical study of correlation effects in Dirac semimetals
3. Lattice-gauge-theoretical study of correlation effects in a Weyl semimetal
4. Summary

Purpose of This Study

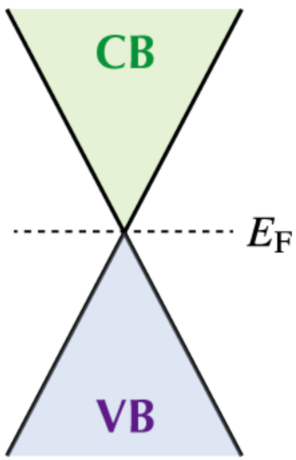
Are DSM phases *stable* against strong long-range correlations?

The semimetal-insulator transition in DSMs is discussed.

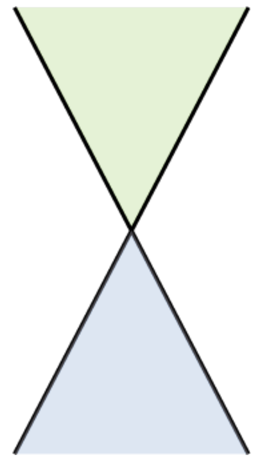
Dirac Semimetal

$$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\alpha}$$

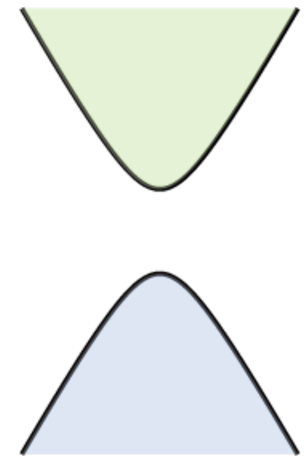
(four-component)



strong $1/r$ correlations



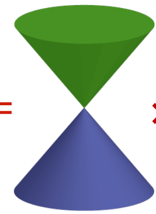
or



Effective continuum model for Dirac semimetals → Lattice regularization, Strong coupling expansion → Derivation of the free energy

Effective Continuum Model

TOHOKU UNIVERSITY

***N*-node Dirac semimetal** =  $\times N$

Four-component Dirac fermions of N flavors interacting via $1/r$ Coulomb interactions (scalar potential A_0):

$$S = \int d^4x \sum_{f=1}^{N} \bar{\psi}_f(x) \left[\gamma_0(\partial_0 + iA_0) + \xi_j \gamma_j \partial_j\right] \psi_f(x) + \frac{1}{2\boldsymbol{g^2}} \int d^4x (\partial_i A_0)^2$$

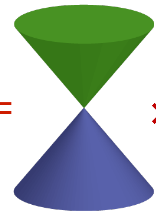
where $\xi_1 = \xi_2 = 1, \quad \xi_3 = v_{F\perp}/v_{F\parallel}$ **(Fermi velocity anisotropy)**

$$S_{\mathrm{Coulomb}} = \int d\tau d^3r ieA_0(x)n(x) + \frac{1}{2}\int d\tau d^3r \sum_j [\partial_j A_0(x)]^2$$

$$= \frac{T}{L^3} \sum_{\boldsymbol{q},\omega_n} ieA_{0,q} n_{-q} + \frac{1}{2}\frac{T}{L^3} \sum_{\boldsymbol{q},\omega_n} A_{0,q} \boldsymbol{q}^2 A_{0,-q}$$

$$\Rightarrow \int \mathcal{D}A_0 \exp\left[-\frac{1}{2}A_{0,q}\boldsymbol{q}^2 A_{0,-q} - ieA_{0,q}n_{-q}\right] = \boxed{\exp\left[-\frac{1}{2}\frac{e^2}{\boldsymbol{q}^2} n_q n_{-q}\right]}$$

Effective Continuum Model

***N*-node Dirac semimetal** =  × N

Four-component Dirac fermions of N flavors interacting via $1/r$ Coulomb interactions (scalar potential A_0):

$$S = \int d^4x \sum_{f=1}^{N} \bar{\psi}_f(x) \left[\gamma_0(\partial_0 + iA_0) + \xi_j \gamma_j \partial_j\right] \psi_f(x) + \frac{1}{2g^2} \int d^4x (\partial_i A_0)^2$$

where $\xi_1 = \xi_2 = 1, \quad \xi_3 = v_{F\perp}/v_{F\parallel}$ **(Fermi velocity anisotropy)**

$$g^2 = \frac{e^2}{v_{F\parallel}\epsilon}$$

(Strength of the $1/r$ Coulomb interactions)

ϵ **: dielectric constant**

$g^2 = \infty$ ⟺ **strong coupling limit**

$g^2 = 0$ ⟺ **noninteracting limit**

Cd_3As_2 ($g^2 \approx 0.5$)

vacuum = QED ($g^2 = e^2/(c\epsilon_0) \approx 0.1$)

Lattice Models (Lattice Gauge Theory)

The N=4 Dirac semimetal

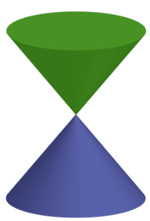
(staggered fermions)

[Kogut & Susskind, PRD 11 (1975)]

$$S^{(N=4)} = S_F^{(N=4)} + S_G$$

$$S_F^{(N=4)} = \frac{1}{2}\sum_n \eta_{n,0}\left[\bar{\chi}_n U_{n,0}\chi_{n+\hat{0}} - \bar{\chi}_{n+\hat{0}}U^\dagger_{n,0}\chi_n\right] + \frac{1}{2}\sum_{n,j}\xi_j\eta_{n,j}\left[\bar{\chi}_n\chi_{n+\hat{j}} - \bar{\chi}_{n+\hat{j}}\chi_n\right]$$

χ_n : single-component spinor



$\times 4$

The N=16 Dirac semimetal

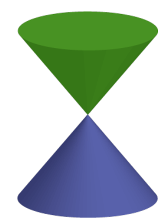
(naively discretized Dirac fermions)

[K. G. Wilson, PRD 10 (1974)]

$$S^{(N=16)} = S_F^{(N=16)} + S_G$$

$$S_F^{(N=16)} = \frac{1}{2}\sum_n \left[\bar{\psi}_n\gamma_0 U_{n,0}\psi_{n+\hat{0}} - \bar{\psi}_{n+\hat{0}}\gamma_0 U^\dagger_{n,0}\psi_n\right] + \frac{1}{2}\sum_{n,j}\xi_j\left[\bar{\psi}_n\gamma_j\psi_{n+\hat{j}} - \bar{\psi}_{n+\hat{j}}\gamma_j\psi_n\right]$$

ψ_n : four-component spinor



$\times 16$

$$S_G = \frac{1}{g^2}\sum_n\sum_{\mu>\nu}\left[1 - \frac{1}{2}\left(U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu} + \text{H.c.}\right)\right]$$

$$\begin{cases} U_{n,0} = e^{iA_{0,n}} \\ U_{n,j} = 1 \end{cases}$$

Strong Coupling Expansion

TOHOKU UNIVERSITY

We derive the effective action S_{eff}

$$Z^{(N=4)} = \int \mathcal{D}[\chi, \bar{\chi}, A_0] e^{-S^{(N=4)}} = \int \mathcal{D}[\chi, \bar{\chi}] e^{-S_{\text{eff}}^{(N=4)}}$$

with the use of U(1) group integral formula:

$$\int_{-\pi}^{\pi} \frac{dA_0}{2\pi} = 1, \quad \int_{-\pi}^{\pi} \frac{dA_0}{2\pi} e^{iA_0} = 0, \quad \int_{-\pi}^{\pi} \frac{dA_0}{2\pi} e^{iA_0} e^{-iA_0} = 1$$

$$\boldsymbol{U_{n,0} = e^{iA_{0,n}}}$$

The term in the strong coupling limit ($g^2 = \infty$)

$$\int \mathcal{D}A_0 e^{-S^{(N=4)}} = \prod_n \int_{-\pi}^{\pi} \frac{dA_{0,n}}{2\pi} \exp\left\{\frac{1}{2}\left[\bar{\chi}_n U_{n,0} \chi_{n+\hat{0}} - \bar{\chi}_{n+\hat{0}} U_{n,0}^{\dagger} \chi_n\right] - \cancel{S_G}\right\}$$

$$= \prod_n \left[1 - \frac{1}{4} \bar{\chi}_n \chi_{n+\hat{0}} \bar{\chi}_{n+\hat{0}} \chi_n\right]$$

$$\boxed{= e^{\frac{1}{4} \sum_n \bar{\chi}_n \chi_n \bar{\chi}_{n+\hat{0}} \chi_{n+\hat{0}}}}$$

$$\propto 1/g^2$$

Decoupling of the Interaction Terms

Exact action in the strong coupling limit ($g^2 = \infty$)

$$S_{\text{eff}}^{(N=4)} = \frac{1}{2}\sum_{n,j}\xi_j\eta_{n,j}\left[\bar{\chi}_n\chi_{n+\hat{j}} - \bar{\chi}_{n+\hat{j}}\chi_n\right] - \underline{\frac{1}{4}\sum_{n}\bar{\chi}_n\chi_n\bar{\chi}_{n+\hat{0}}\chi_{n+\hat{0}}}$$

We'd like to decouple $\bar{\chi}\chi\bar{\chi}\chi$ term to fermion bilinear form to compute the free energy $F = -\ln Z$ with the use of the Grassmann integral formula

$$Z = \int D[\chi,\bar{\chi}]e^{-S} \approx \int D[\chi,\bar{\chi}]e^{-\bar{\chi}\mathcal{M}\chi} = \det\mathcal{M}$$

Hubbard-Stratonovich transformation

$$e^{\frac{1}{4}\bar{\chi}_n\chi_n\bar{\chi}_{n+0}\chi_{n+0}} \sim \exp\left\{-\frac{1}{4}\left[\sigma\sigma' - \sigma\bar{\chi}_n\chi_n - \sigma'\bar{\chi}_{n+0}\chi_{n+0}\right]\right\}$$

with $\sigma = \langle\bar{\chi}_{n+0}\chi_{n+0}\rangle\,,\quad \sigma' = \langle\bar{\chi}_n\chi_n\rangle$

Order Parameter

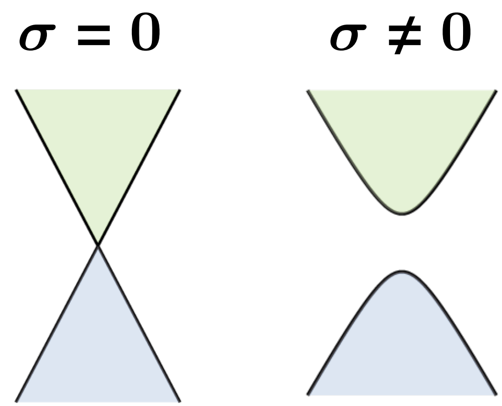
Mean-field effective action in the strong coupling limit

"mass term"

$$S_{\mathrm{eff}}^{(N=4)}(\sigma) = \frac{1}{4}\sum_n \sigma^2 + \frac{1}{2}\sum_{n,j}\xi_j\eta_{n,j}\left[\bar{\chi}_n\chi_{n+\hat{j}} - \bar{\chi}_{n+\hat{j}}\chi_n\right] + \underline{\frac{1}{2}\sigma\sum_n \bar{\chi}_n\chi_n}$$

$m_{\mathrm{eff}} = \frac{1}{2}\sigma$ (σ : chiral condensate)

σ is the order parameter
for the semimetal-insulator transition



$$\Psi_{n_0,\boldsymbol{k}} = \begin{bmatrix} \chi_{n_0}(k_1,k_2,k_3) \\ \chi_{n_0}(k_1-\pi,k_2,k_3) \\ \chi_{n_0}(k_1,k_2-\pi,k_3) \\ \chi_{n_0}(k_1,k_2,k_3-\pi) \\ \chi_{n_0}(k_1,k_2-\pi,k_3-\pi) \\ \chi_{n_0}(k_1-\pi,k_2,k_3-\pi) \\ \chi_{n_0}(k_1-\pi,k_2-\pi,k_3) \\ \chi_{n_0}(k_1-\pi,k_2-\pi,k_3-\pi) \end{bmatrix}$$

$$S_{\mathrm{eff}}^{(N=4)}(\sigma) = \frac{1}{4}\frac{V}{T}\sigma^2 + \sum_{n_0}\sum_{\boldsymbol{k}=0}^{\pi}\bar{\Psi}^T_{n_0,\boldsymbol{k}}\mathcal{V}(n_0,\boldsymbol{k};\sigma)\Psi_{n_0,\boldsymbol{k}}$$

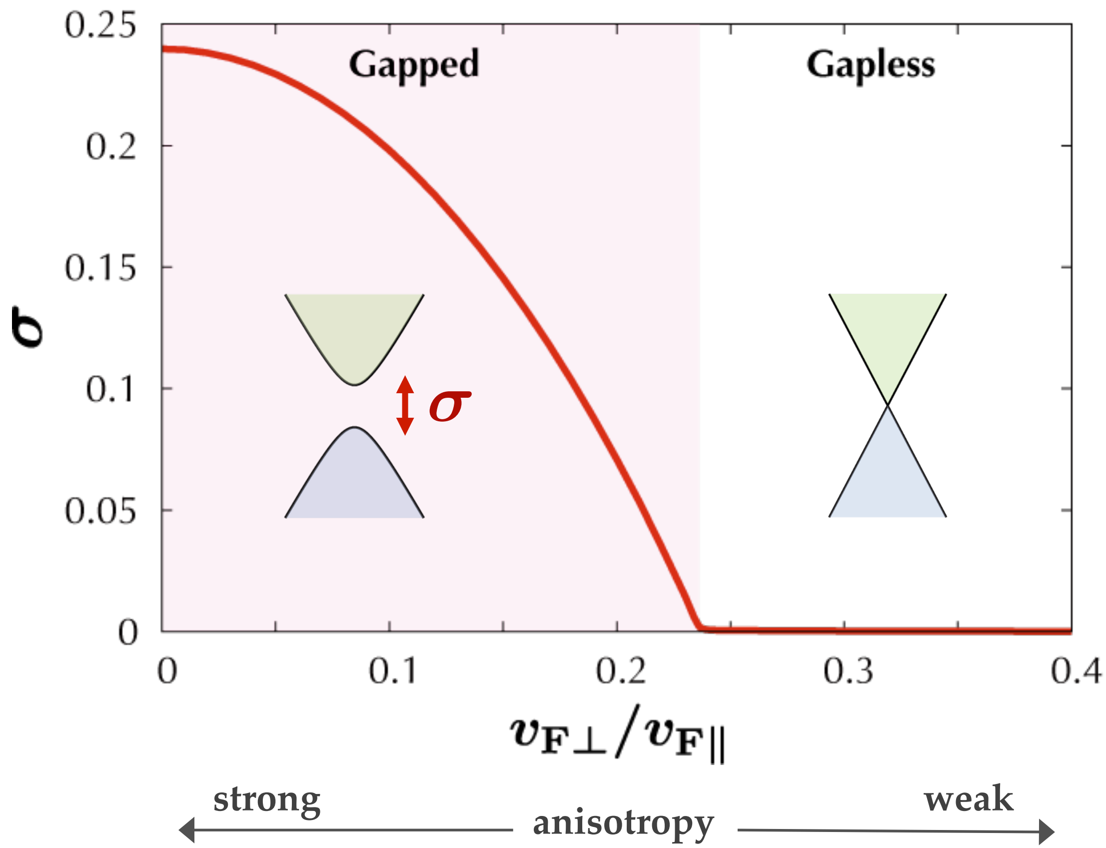
with $\det\mathcal{V} = \left[\sum_j \xi_j^2\sin^2 k_j + \frac{1}{4}\sigma^2\right]^4$

Numerical Results

Free energy at zero temperature in the strong coupling limit ($g^2 = \infty$)

$$\mathcal{F}^{(N=4)}(\sigma) = \frac{1}{4}\sigma^2 - \frac{1}{2}\int_{-\pi}^{\pi} \frac{d^3k}{(2\pi)^3} \ln\left[\sum_j \xi_j^2 \sin^2 k_j + \frac{1}{4}\sigma^2\right]$$

$$\xi_1 = \xi_2 = 1$$
$$\xi_3 = v_{\mathrm{F}\perp}/v_{\mathrm{F}\|}$$

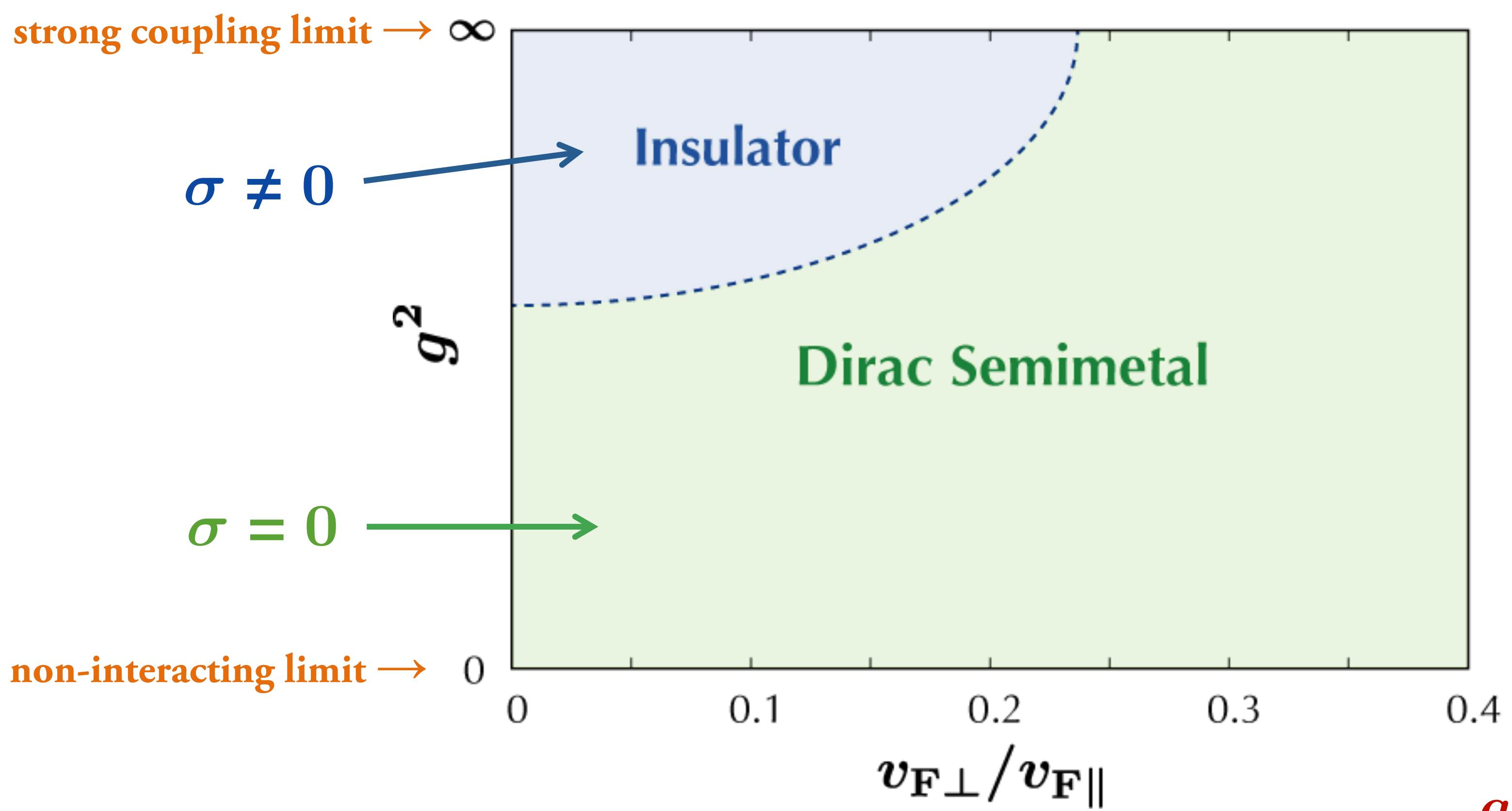


Dirac semimetal survives in the strong coupling limit when the Fermi velocity anisotropy is weak.

Dimensional crossover

Proposal for a Global Phase Diagram

A possible global phase diagram of a correlated Dirac semimetal with four nodes



$$g^2 = \frac{e^2}{v_{F\parallel}\epsilon}$$

ϵ : dielectric constant

Outline

Are Dirac and Weyl semimetals stable against long-range interactions ?

Band gap opens by long-range electron-electron interactions ??

1. Introduction to Dirac & Weyl semimetals
2. Lattice-gauge-theoretical study of correlation effects in Dirac semimetals
3. Lattice-gauge-theoretical study of correlation effects in a Weyl semimetal
4. Summary

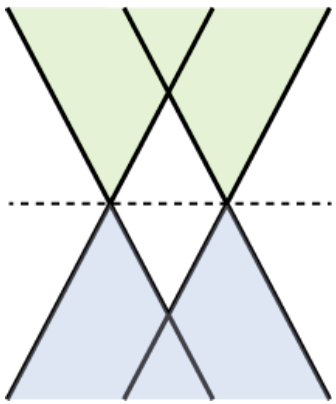
Purpose of This Study

Are WSM phases *stable* against strong long-range correlations?

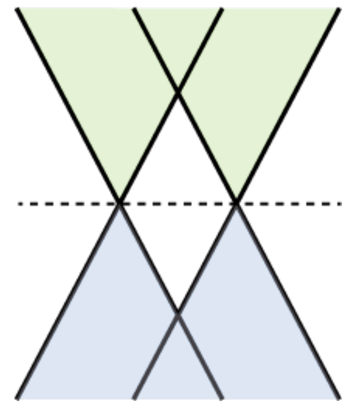
Weyl Semimetal

$\mathcal{H}(\boldsymbol{k}) = v_{\mathrm{F}}\boldsymbol{k}\cdot\boldsymbol{\sigma}$

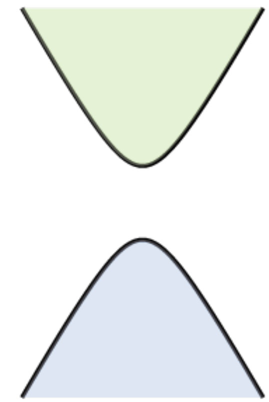
(two-component)



strong
$1/r$ correlations



or



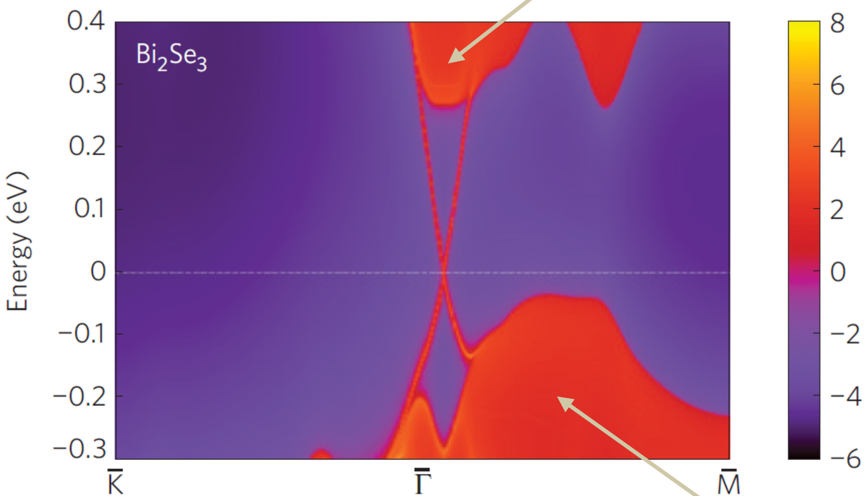
Lattice model
for a Weyl semimetal → Strong coupling expansion → Derivation of
the free energy

3D Topological Insulators (TIs)

3D topological insulators: bulk energy gap + gapless surface states

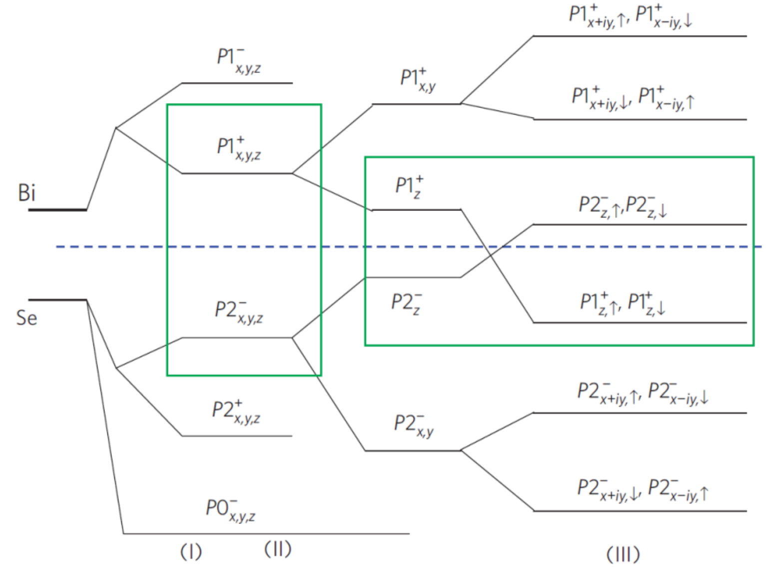
- **Bi_2Se_3** [H. Zhang *et al.*, Nat. Phys. 5 (2009)]

Bulk conduction band



[First principles calculation]

Bulk valence band



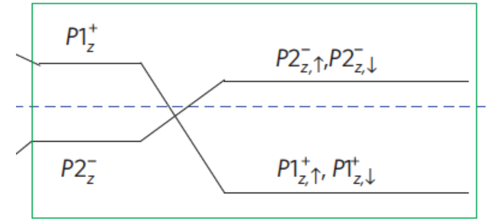
Chemical bonding | Crystal-field splitting | Spin-orbit coupling

Strong spin-orbit coupling is essential.

Effective Hamiltonian for a 3D TI

$$\mathcal{H}_{\mathrm{eff}}(\boldsymbol{k}) = \begin{array}{cc}
\begin{array}{cccc} |P1_z^+,\uparrow\rangle & |P1_z^+,\downarrow\rangle & |P2_z^-,\uparrow\rangle & |P2_z^-,\downarrow\rangle \end{array} & \\
\begin{bmatrix} \mathcal{M}(\boldsymbol{k}) & 0 & A_1 k_z & A_2 k_- \\ 0 & \mathcal{M}(\boldsymbol{k}) & A_2 k_+ & -A_1 k_z \\ A_1 k_z & A_2 k_- & -\mathcal{M}(\boldsymbol{k}) & 0 \\ A_2 k_+ & -A_1 k_z & 0 & -\mathcal{M}(\boldsymbol{k}) \end{bmatrix} & \begin{array}{c} |P1_z^+,\uparrow\rangle \\ |P1_z^+,\downarrow\rangle \\ |P2_z^-,\uparrow\rangle \\ |P2_z^-,\downarrow\rangle \end{array}
\end{array}$$

$$= A_2 k_x \alpha_x + A_2 k_y \alpha_y + A_1 k_z \alpha_z + \mathcal{M}(\boldsymbol{k})\alpha_4$$



[H. Zhang *et al.*, Nat. Phys. **5** (2009)]

On a cubic lattice

Effective lattice model (Wilson fermions)

$$\mathcal{H}_0(\boldsymbol{k}) = v_{\mathrm{F}} \sum_j \alpha_j \sin k_j + \left[m_0 + r \sum_j (1 - \cos k_j) \right] \alpha_4$$

with $\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}$

Lattice Model for a Weyl Semimetal

A 3D topological insulator (Bi_2Se_3 family) doped with magnetic impurities

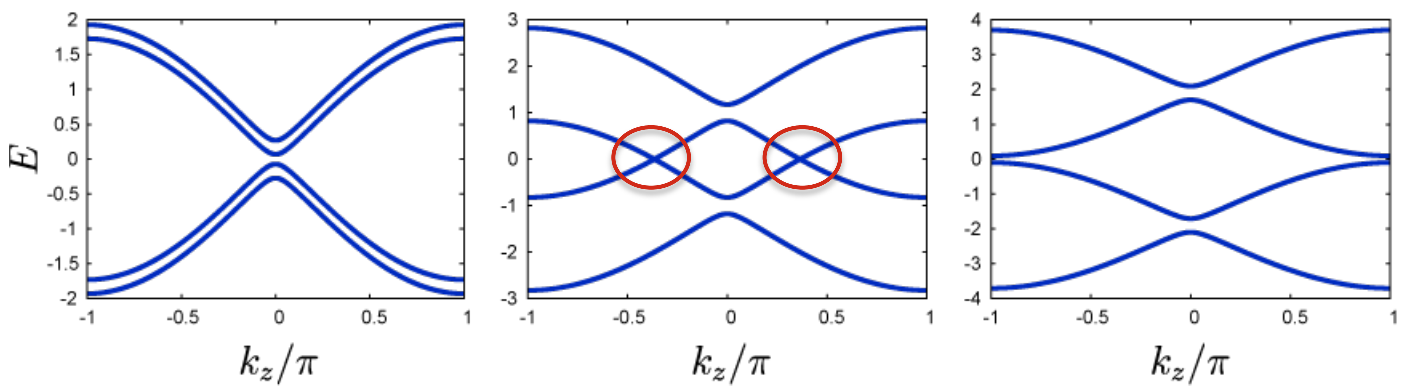
$$\mathcal{H}_0(\boldsymbol{k}) = v_\mathrm{F}\sum_j \alpha_j \sin k_j + \left[m_0 + r\sum_j (1-\cos k_j)\right]\alpha_4 + b\Sigma_3$$

$$\Sigma_3 = \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}$$

ferromagnetic exchange interaction with magnetic impurities

→ **breaks time-reversal symmetry**

$$\psi_{\boldsymbol{k}} = [c_{\boldsymbol{k}+\uparrow}, c_{\boldsymbol{k}+\downarrow}, c_{\boldsymbol{k}-\uparrow}, c_{\boldsymbol{k}-\downarrow}]^T$$



Magnetic Topological Insulator | **Weyl Semimetal** | **Anomalous Hall Insulator**

→ $\boldsymbol{b}$

[AS & Nomura, JPSJ 82 (2013)]

Interacting Weyl Semimetal

TOHOKU UNIVERSITY

Action of a WSM with $1/r$ Coulomb interactions: $S = S_F + S_G$

$$S_F = (m_0 + 4r)\sum_n \bar{\psi}_n\psi_n - \frac{1}{2}\sum_n\left[\bar{\psi}_n(r-\gamma_0)U_{n,0}\psi_{n+\hat{0}} + \bar{\psi}_{n+\hat{0}}(r+\gamma_0)U^\dagger_{n,0}\psi_n\right]$$

$$-\frac{1}{2}\sum_{n,j}\left[\bar{\psi}_n(r-\gamma_j)\psi_{n+\hat{j}} + \bar{\psi}_{n+\hat{j}}(r+\gamma_j)\psi_n\right] + b\sum_n \bar{\psi}_n\gamma_0\Sigma_3\psi_n$$

$$\begin{cases} U_{n,0} = e^{iA_{0,n}} \\ U_{n,j} = 1 \end{cases}$$

$$S_G = \frac{1}{g^2}\sum_n\sum_{\mu>\nu}\left[1 - \frac{1}{2}\left(U_{n,\mu\nu} + U^\dagger_{n,\mu\nu}\right)\right] \qquad U_{n,\mu\nu} = U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu}$$

$$g^2 = \frac{e^2}{v_F\epsilon}$$

(Strength of the $1/r$ Coulomb interactions)

ϵ : dielectric constant

$g^2 = \infty$	⟺	strong coupling limit
$g^2 = 0$	⟺	noninteracting limit

Cd_3As_2 ($g^2 \approx 0.5$)

Bi_2Se_3 ($g^2 \approx 0.3$)

Strong Coupling Expansion

We derive the effective action S_{eff}

$$Z = \int \mathcal{D}[\psi, \bar{\psi}, A_0] e^{-S} = \int \mathcal{D}[\psi, \bar{\psi}] e^{-S_{\text{eff}}}$$

with the use of U(1) group integral formula:

$$\int_{-\pi}^{\pi} \frac{dA_0}{2\pi} = 1, \quad \int_{-\pi}^{\pi} \frac{dA_0}{2\pi} e^{iA_0} = 0, \quad \int_{-\pi}^{\pi} \frac{dA_0}{2\pi} e^{iA_0} e^{-iA_0} = 1 \qquad \boldsymbol{U_{n,0} = e^{iA_{0,n}}}$$

The term in the strong coupling limit ($g^2 = \infty$)

$$\int \mathcal{D}A_0 e^{-S_F[A_0]} = \prod_n \int_{-\pi}^{\pi} \frac{dA_{0,n}}{2\pi} \exp\left[\bar{\psi}_n P_0^- U_{n,0} \psi_{n+\hat{0}} + \bar{\psi}_{n+\hat{0}} P_0^+ U_{n,0}^\dagger \psi_n + \cancel{S_G}\right]$$

$\propto 1/g^2$

$$= \prod_n \int_{-\pi}^{\pi} \frac{dA_{0,n}}{2\pi} \left[1 + \bar{\psi}_n P_0^- \psi_{n+\hat{0}} \bar{\psi}_{n+\hat{0}} P_0^+ \psi_n U_{n,0} U_{n,0}^\dagger\right]$$

$$P_\mu^\pm = \frac{r \pm \gamma_\mu}{2}$$

= 4×4 matrix

$$= \prod_n \left[1 + \bar{\psi}_n P_0^- \psi_{n+\hat{0}} \bar{\psi}_{n+\hat{0}} P_0^+ \psi_n\right]$$

$$\boxed{= e^{\sum_n \bar{\psi}_n P_0^- \psi_{n+\hat{0}} \bar{\psi}_{n+\hat{0}} P_0^+ \psi_n}}$$

Decoupling of the Interaction Terms

Effective action in the strong coupling limit ($g^2 = \infty$)

$$S_{\rm eff} = (m_0 + 4r)\sum_n \bar\psi_n\psi_n - \sum_{n,j}\left[\bar\psi_n P_j^- \psi_{n+j} + \bar\psi_{n+j}P_j^+\psi_n\right] + b\sum_n \bar\psi_n\gamma_0\Sigma_3\psi_n$$
$$+\underline{\sum_n \mathrm{tr}\left[\bar\psi_n\psi_n P_0^+\bar\psi_{n+0}\psi_{n+0}P_0^-\right]}$$

$$F = -\ln Z$$

We'd like to decouple $\bar\psi\psi\bar\psi\psi$ term to fermion bilinear form to compute the free energy by using the formula $Z = \int D[\psi,\bar\psi]e^{-S} \approx \int D[\psi,\bar\psi]e^{-\bar\psi\mathcal{M}\psi} = \det\mathcal{M}$

Hubbard-Stratonovich transformation to the trace of two arbitrary matrices:

$$e^{\kappa\,\mathrm{tr}AB} \sim \exp\left\{-\kappa\left[Q_{\alpha\beta}Q'_{\alpha\beta} - A_{\alpha\beta}Q_{\beta\alpha} - B^T_{\alpha\beta}Q'_{\beta\alpha}\right]\right\}$$

with

$$Q_{\alpha\beta} = \langle B^T\rangle_{\beta\alpha}, \quad Q'_{\alpha\beta} = \langle A\rangle_{\beta\alpha}$$

$$(\kappa, A, B) = (1, \bar\psi_n\psi_n P_0^+, -\bar\psi_{n+0}\psi_{n+0}P_0^-)$$

Decoupling of the Interaction Terms

TOHOKU UNIVERSITY

Effective action in the strong coupling limit ($g^2 = \infty$)

$$S_{\mathrm{eff}} = (m_0 + 4r)\sum_n \bar{\psi}_n\psi_n - \sum_{n,j}\left[\bar{\psi}_n P_j^- \psi_{n+j} + \bar{\psi}_{n+j} P_j^+ \psi_n\right] + b\sum_n \bar{\psi}_n \gamma_0 \Sigma_3 \psi_n$$
$$+ \underline{\sum_n \mathrm{tr}\left[\bar{\psi}_n\psi_n P_0^+ \bar{\psi}_{n+0}\psi_{n+0} P_0^-\right]}$$

$$F = -\ln Z$$

We'd like to decouple $\bar{\psi}\psi\bar{\psi}\psi$ term to fermion bilinear form to compute the free energy by using the formula $Z = \int D[\psi,\bar{\psi}]e^{-S} \approx \int D[\psi,\bar{\psi}]e^{-\bar{\psi}\mathcal{M}\psi} = \det\mathcal{M}$

$\langle\bar{\psi}_n\psi_n\rangle$ consists of 16 independent matrices

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$

Property	Matrix	# of modes
scalar	$\mathbf{1}$	1
vector	γ_μ	4
tensor	$\frac{i}{2}[\gamma_\mu, \gamma_\nu]$	6
pseudovector	$\gamma_\mu\gamma_5$	4
pseudoscalar	γ_5	1

Free Energy in the Strong Coupling Limit

$$\langle \bar{\psi}_n \psi_n \rangle = -\sigma \mathbf{1} + \rho_1 \gamma_0 \Pi_1 = \underbrace{-\sigma \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}_{\text{Bandgap renormalization}} + \rho_1 \underbrace{\begin{bmatrix} 0 & i\sigma_1 \\ i\sigma_1 & 0 \end{bmatrix}}_{\text{Parity symmetry breaking}}$$

Free energy at zero temperature in the strong coupling limit ($g^2 = \infty$):

$$\mathcal{F}(\sigma, \rho_1) = (1 - r_\tau^2)\sigma^2 + (1 + r_\tau^2)\rho_1^2 - \int_{-\pi}^{\pi} \frac{d^3k}{(2\pi)^3} \ln \left\{ \frac{I(\boldsymbol{k}, b, \tilde{\rho_1}) I(\boldsymbol{k}, -b, -\tilde{\rho_1}) - J(\boldsymbol{k}, b, \tilde{\rho_1})}{[\tilde{m}(\boldsymbol{k}) + r_\tau]^2 - b^2} \right\}$$

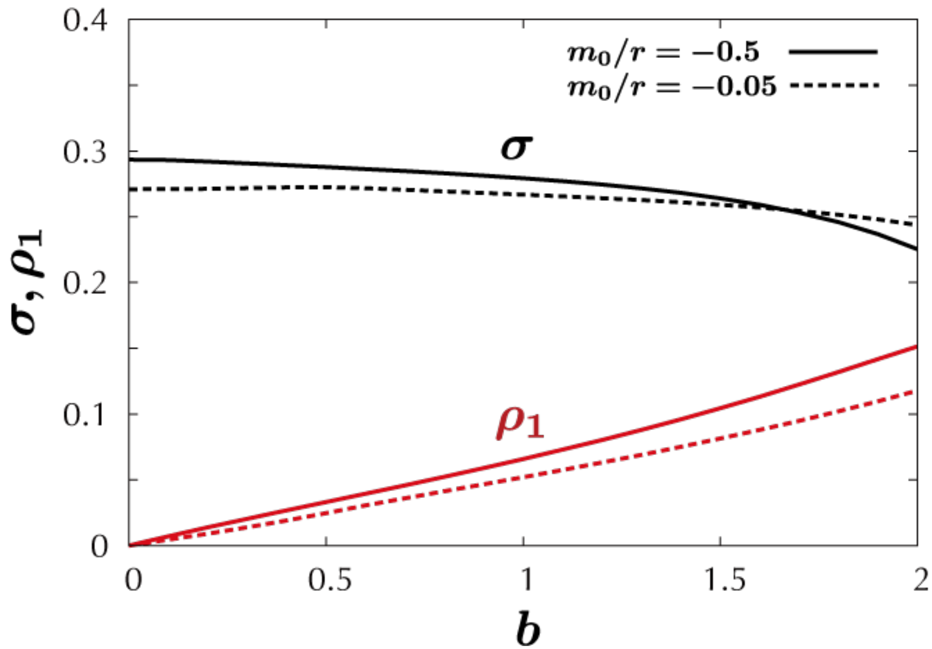
where

$$\begin{cases} I(\boldsymbol{k}, b, \tilde{\rho_1}) = [\tilde{m}(\boldsymbol{k}) + r_\tau - b]\{[\tilde{m}(\boldsymbol{k}) + r_\tau]^2 + \sin^2 k_3 - b^2\} + [\tilde{m}(\boldsymbol{k}) + r_\tau + b][\sin^2 k_1 + (\sin k_2 + \tilde{\rho_1})^2] \\ J(\boldsymbol{k}, b, \tilde{\rho_1}) = 4 \sin^2 k_3 (\{\tilde{\rho_1}[\tilde{m}(\boldsymbol{k}) + r_\tau] + b \sin k_2\}^2 + b^2 \sin^2 k_1) \end{cases}$$

The ground state is determined by the stationary condition

$$\frac{\partial \mathcal{F}(\sigma, \rho_1)}{\partial \sigma} = \frac{\partial \mathcal{F}(\sigma, \rho_1)}{\partial \rho_1} = 0$$

Numerical Results



$$\mathcal{H}' = b \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}$$

$\sigma \neq 0$ ⇨ **Bandgap is renormalized**

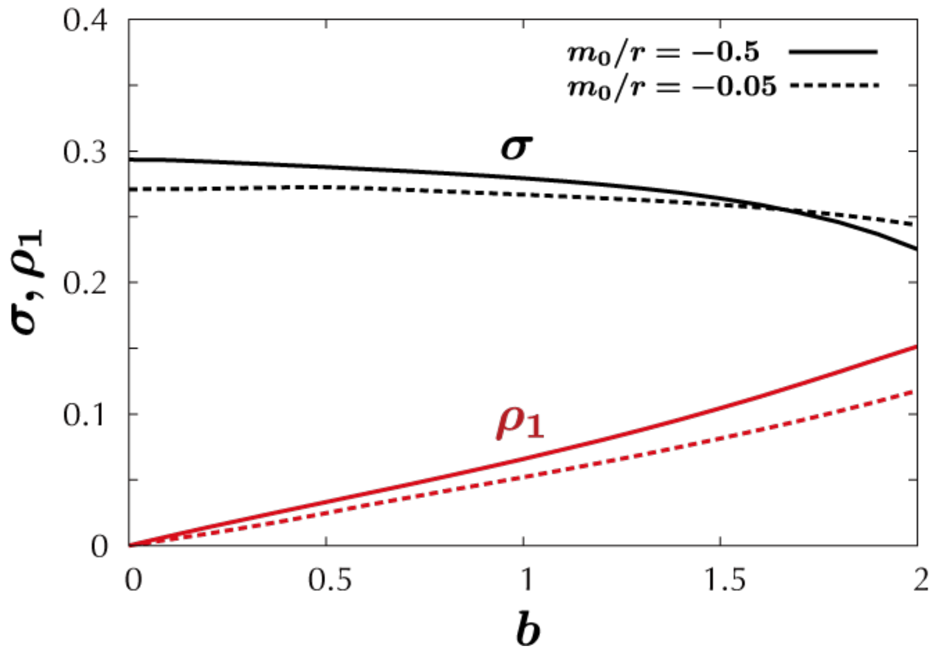
$\rho_1 \neq 0$ ⇨ **Parity symmetry is spontaneously broken**

$$\mathcal{H}_{\mathrm{MF}}(\boldsymbol{k}) = \alpha_j \sin k_j + \tilde{m}(\boldsymbol{k})\alpha_4 + b\Sigma_3 + \rho_1 \Pi_1$$

with $\tilde{m}(\boldsymbol{k}) = m_0 + \frac{1}{2}(1 - r_\tau^2)\sigma + r \sum_j \left(1 - \cos k_j\right)$

$$E(\boldsymbol{k}) = \pm \left\{ s^2(\boldsymbol{k}) + [\tilde{m}(\boldsymbol{k})]^2 + b^2 + \rho_1^2 \pm 2\sqrt{[\tilde{m}(\boldsymbol{k})b - \rho_1 \sin k_2]^2 + (b^2 + \rho_1^2)\sin^2 k_3} \right\}^{1/2}$$

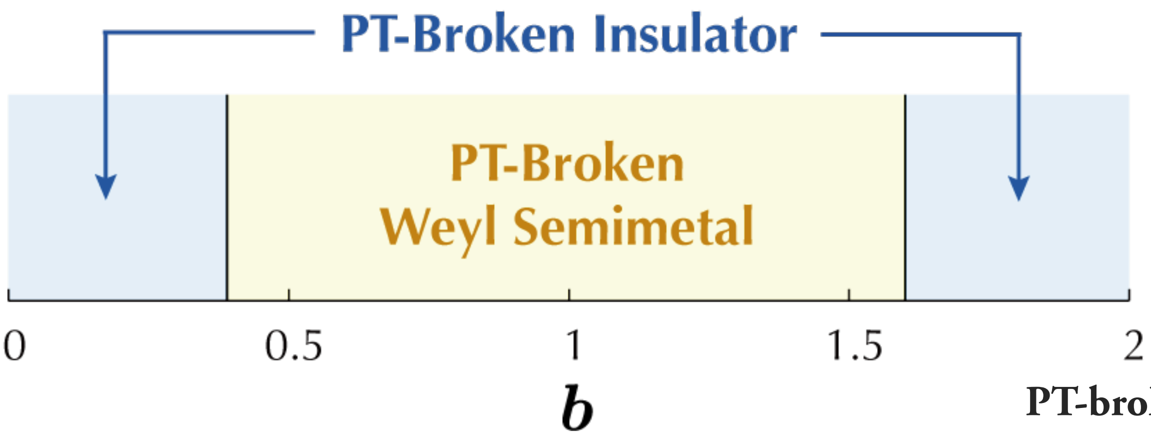
Numerical Results



$$\mathcal{H}' = b \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}$$

$\sigma \neq 0$ ⇨ **Bandgap is renormalized**

$\rho_1 \neq 0$ ⇨ **Parity symmetry is spontaneously broken**

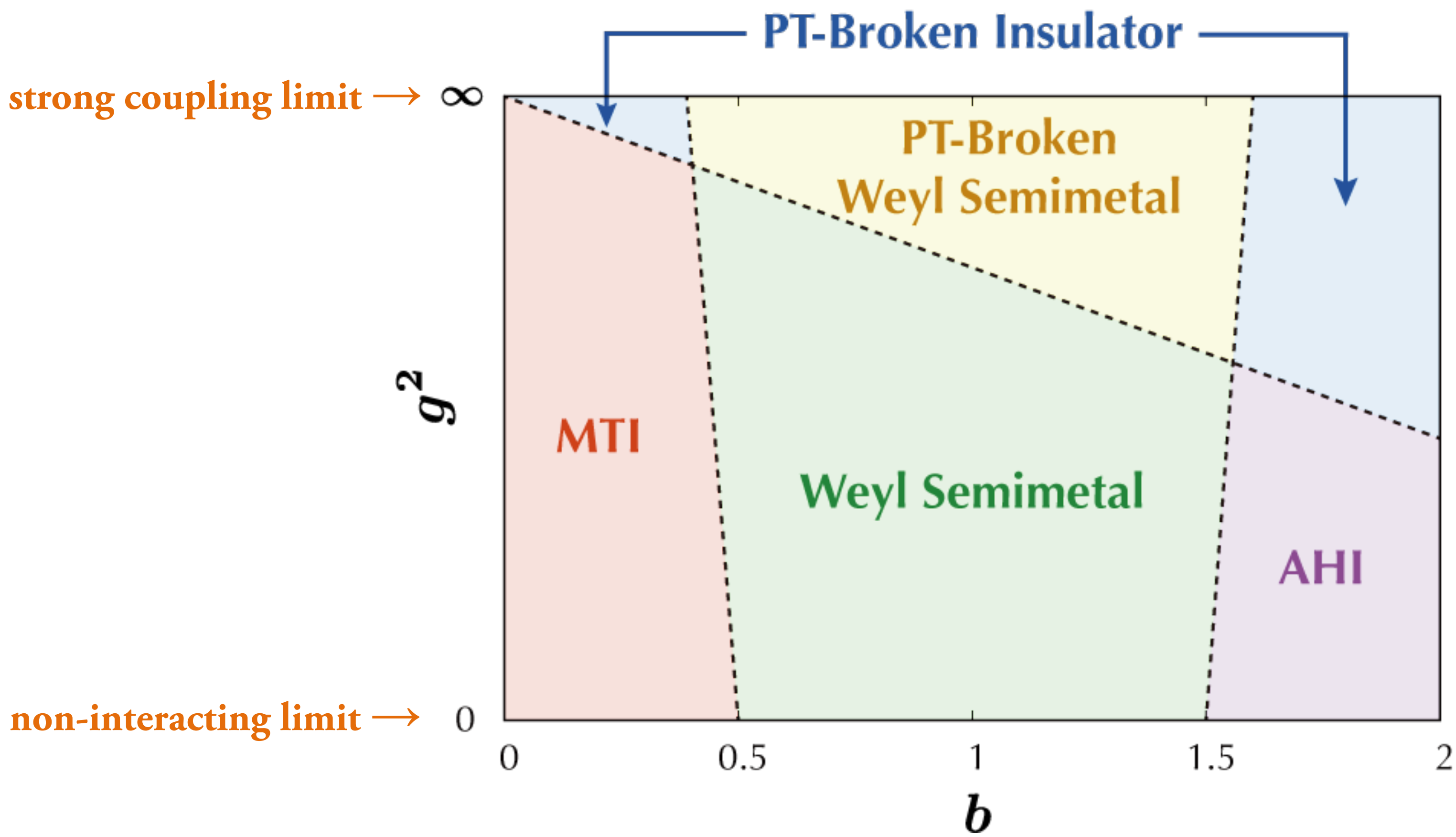


A Weyl semimetal phase survives in the strong coupling limit!

PT-broken = broken parity & time-reversal symmetries

Proposal for a Global Phase Diagram

A possible global phase diagram of a correlated Weyl semimetal with two nodes



$$g^2 = \frac{e^2}{v_F \epsilon}$$

MTI = Magnetic topological insulator

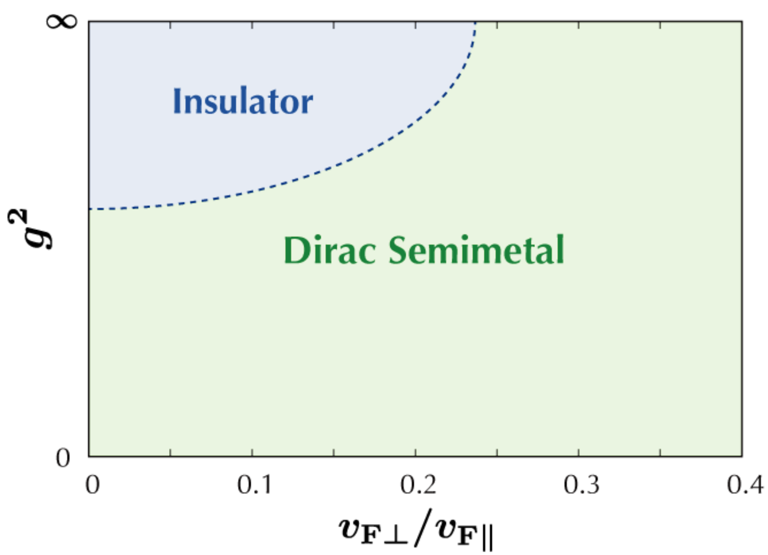
AHI = Anomalous Hall insulator

$$\mathcal{H}' = b \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}$$

ϵ : dielectric constant

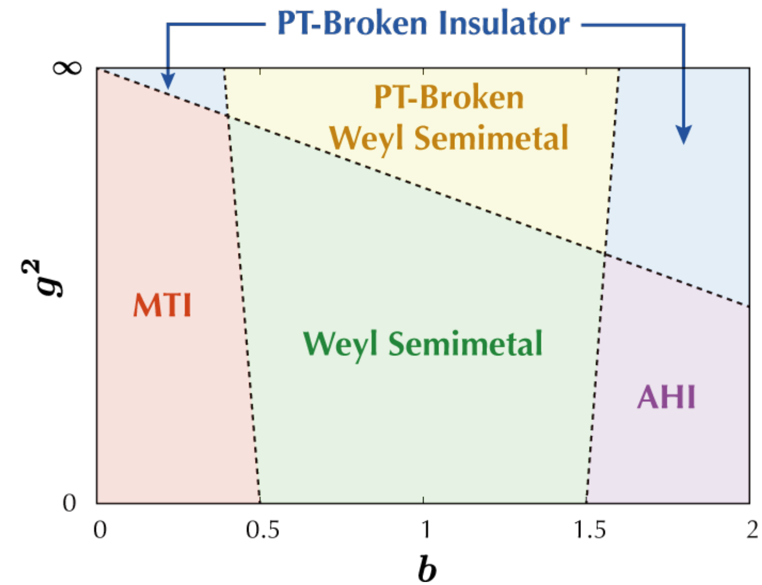
Summary

Effects of 1/*r* Coulomb interactions in Dirac and Weyl semimetals



- **The DSM phases survive in the strong coupling limit when the Fermi velocity anisotropy is weak.**

[AS & Nomura, Phys. Rev. B 90, 075137 (2014)]



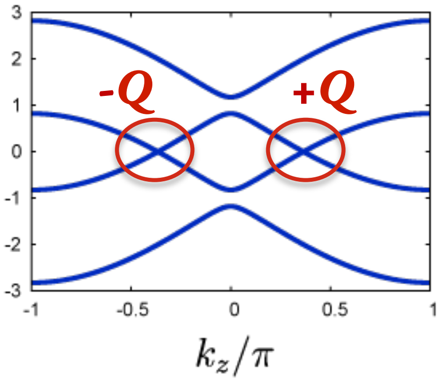
- **PT-broken WSM appears in the strong coupling limit.**

[AS & Nomura, J. Phys. Soc. Jpn. 83, 094710 (2014)]

Correlation Effects in DSM and WSM

Type of interactions	Weyl semimetals	Dirac semimetals
Short-range	gapped [Wei, Chao & Aji, PRL **109** (2012)] [AS & Nomura, JPSJ **82** (2013)] [Maciejko & Nandkishore, PRB **90** (2014)]	???
Long-range	gapped [Wei, Chao & Aji, PRB **89** (2014)] gapless [AS & Nomura, JPSJ **83** (2014)]	gapless [AS & Nomura, PRB **90** (2014)] [J. González, PRB **90** (2014)]

Inter-nodal Scattering



In the low-energy limit, the four-component spinor becomes

$$\psi_n \simeq \left(\int_{|\boldsymbol{k}-W_+|<\Lambda} \frac{d^3k}{(2\pi)^3} + \int_{|\boldsymbol{k}-W_-|<\Lambda} \frac{d^3k}{(2\pi)^3} \right) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_n} \sum_{\lambda=2,3} a_{k\lambda} |u_{k\lambda}\rangle$$

$$\equiv e^{iQz}\psi_{R,n} + e^{-iQz}\psi_{L,n}$$

Then the mean-field decoupled interaction term is written as

$$\begin{aligned} \bar{\psi}_n \langle N_n \rangle \psi_n \simeq\ & \bar{\psi}_{R,n}\langle\bar{\psi}_{R,n}\psi_{R,n}\rangle\psi_{R,n} + \boxed{\bar{\psi}_{R,n}\langle\bar{\psi}_{L,n}\psi_{R,n}\rangle\psi_{L,n}} \\ & + \bar{\psi}_{R,n}\langle\bar{\psi}_{L,n}\psi_{L,n}\rangle\psi_{R,n} + \bar{\psi}_{L,n}\langle\bar{\psi}_{R,n}\psi_{R,n}\rangle\psi_{L,n} \\ & + \boxed{\bar{\psi}_{L,n}\langle\bar{\psi}_{R,n}\psi_{L,n}\rangle\psi_{R,n}} + \bar{\psi}_{L,n}\langle\bar{\psi}_{L,n}\psi_{L,n}\rangle\psi_{L,n} \end{aligned}$$

$$H_{\mathrm{eff}} = \begin{bmatrix} \psi_R^\dagger & \psi_L^\dagger \end{bmatrix} \begin{bmatrix} \boldsymbol{k}\cdot\boldsymbol{\sigma} & \langle\bar{\psi}_{L,n}\psi_{R,n}\rangle \\ \langle\bar{\psi}_{R,n}\psi_{L,n}\rangle & -\boldsymbol{k}\cdot\boldsymbol{\sigma} \end{bmatrix} \begin{bmatrix} \psi_R \\ \psi_L \end{bmatrix}$$

Intra-nodal scattering process which lead to the gap opening is included.