ランダムな 3 次元トポロジカル物質の相図とスケーリング則

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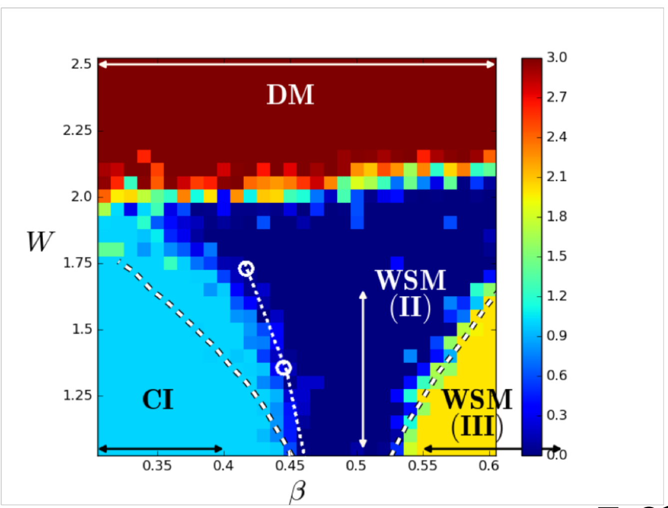
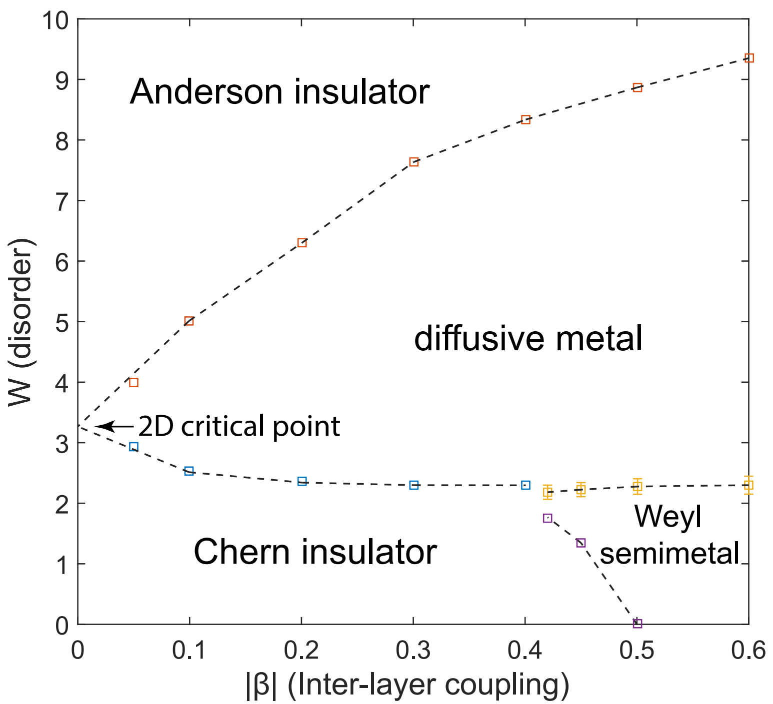


統計物理学懇談会(第 7 回)
2019/3/5

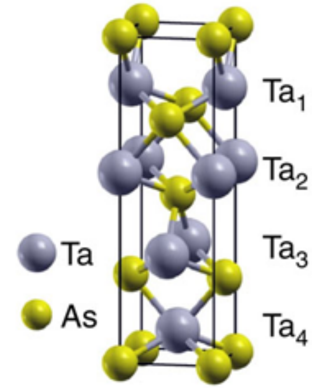
- T. Ohtsuki and T. Ohtsuki: J. Phys. Soc. Jpn, **85**, 123706 (2016), **86**, 044708 (2017).
- T. Mano and T. Ohtsuki: J. Phys. Soc. Jpn., **86**, 113704 (2017).
- S. Liu, T. Ohtsuki, R. Shindou: Physical Review Letters **116**, 066401 (2016).
- X. Luo, B. Xu, T. Ohtsuki, R. Shindou: Physical Review B **97**, 045129 (2018).
- X. Luo, T. Ohtsuki, R. Shindou: Physical Review B **98**, 020201 (2018).

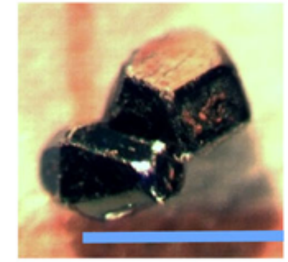
Outline

- What are Chern insulators (CI)?→2D quantum Hall system
- Construction of 3D Weyl semimetal from 2D CI
- Phase diagram of 3DWSM
  - Transfer matrix method
  - Machine learning (cf. previous talk)
- Scaling behaviors
  - Density of state scaling
  - Unconventional scaling



Weyl semimetal

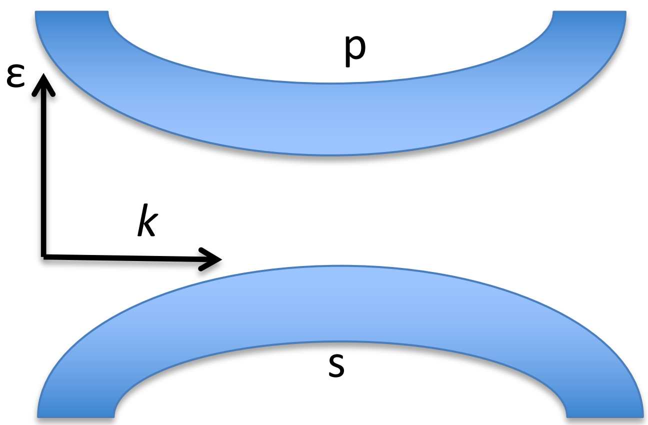




- $H=v\,(\mathbf{p}-\mathbf{p}_0)\cdot\sigma$, $E=v\,|\mathbf{p}-\mathbf{p}_0|$
- Many 3D examples have been discovered in the last few years. One possible realization is to stack two dimensional Chern insulator → today's talk
- Effect of randomness?
- Scaling theory of semi-metal to metal transition induced by disorder
- Other unconventional scaling behaviors

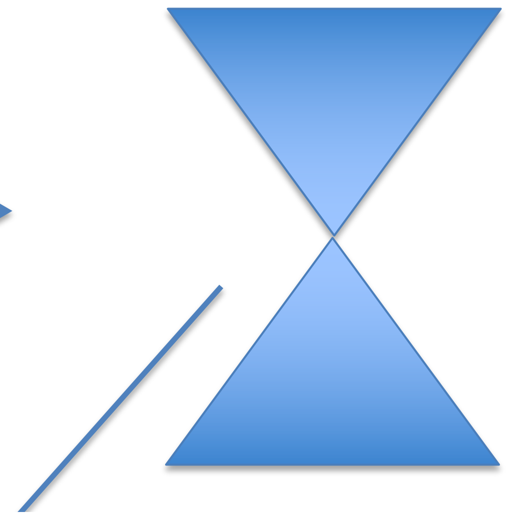
Phase transition for layered Chern insulator

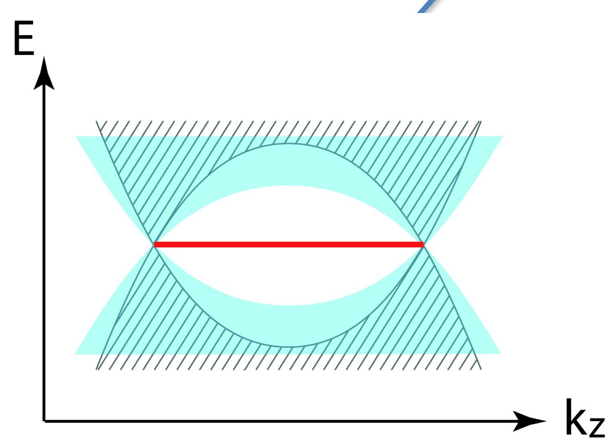
2D Chern Insulator



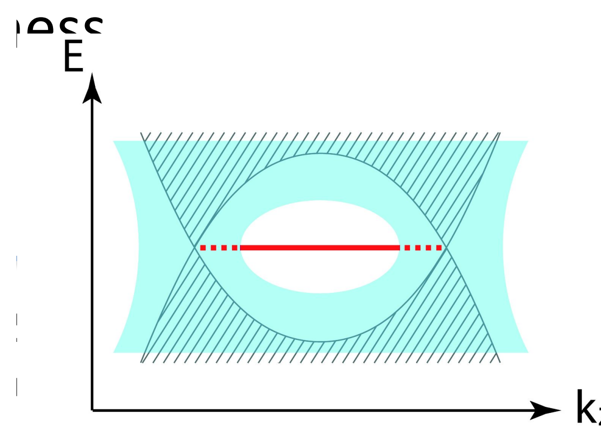
Stacking

Weyl semimetal
E=vk





$W \leq W_c$ ($K \leq K_c$)

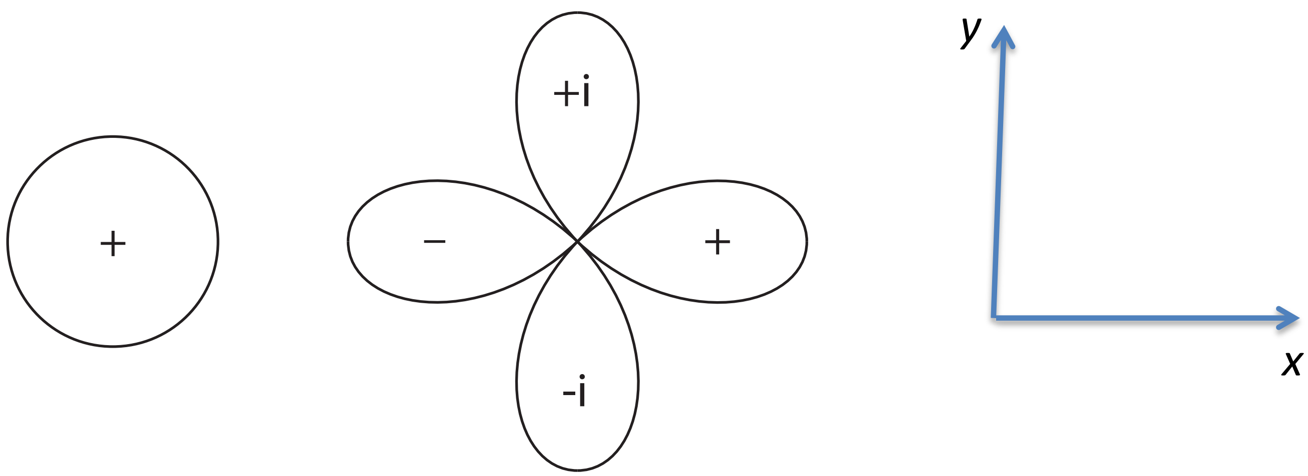


What are Chern insulators?

- **Band gap insulator with peculiar edge states.**
- **(pseudo) magnetization is present, time reversal symmetry is broken.**
- **quantized Hall conductivity**
  - **Belong to the quantum Hall universality class but without Landau levels.**
- **When stacked to the 3rd direction, it shows rich phase diagram.**

Model

- We start with a 2D spinless tight-binding model on a cubic (square) lattice, which comprises of s-orbital and $p_+ \equiv p_x + \mathrm{i}p_y$ orbital. (is a Chern insulator with suitable parameters)
- We then pile it up along z-direction with an inter-layer coupling amplitude β.



2D Chern insulator

- proposed by Haldane, PRL. 61, 2015 ('88).
- Qi-Wu-Zhang model,PRB. 74, 085308 ('06)

$$\mathcal{H} = \sum_{\boldsymbol{x}} ([\epsilon_s + v_s(\boldsymbol{x})] c^\dagger_{\boldsymbol{x},s} c_{\boldsymbol{x},s} + [\epsilon_p + v_p(\boldsymbol{x})] c^\dagger_{\boldsymbol{x},p} c_{\boldsymbol{x},p})$$
$$+ \sum_{\boldsymbol{x}} \Big(- \sum_{\mu=x,y} (t_s c^\dagger_{\boldsymbol{x}+\boldsymbol{e}_\mu,s} c_{\boldsymbol{x},s} - t_p c^\dagger_{\boldsymbol{x}+\boldsymbol{e}_\mu,p} c_{\boldsymbol{x},p})$$
$$+ t_{sp}(c^\dagger_{\boldsymbol{x}+\boldsymbol{e}_x,p} - c^\dagger_{\boldsymbol{x}-\boldsymbol{e}_x,p}) c_{\boldsymbol{x},s}$$
$$- i t_{sp}(c^\dagger_{\boldsymbol{x}+\boldsymbol{e}_y,p} - c^\dagger_{\boldsymbol{x}-\boldsymbol{e}_y,p}) c_{\boldsymbol{x},s} \text{ +h.c. } \Big)$$

$-W/2 < v_{s,x}$, $v_{p,x} < W/2$

$\varepsilon_s=-0.5$

$\varepsilon_p=0.5$

$t_s=t_p=0.25$

$t_{sp}=1/3$

$$H_{\mathbf{k}} = a_\mu \sigma^\mu \text{ with } \begin{cases} a_0 = 0 \\ (a_1, a_2) = -\frac{2}{3}(\sin k_y, \sin k_x) \\ a_3 = \frac{1}{2} - \frac{1}{2}(\cos k_x + \cos k_y) \end{cases}$$

Pseudo spin: *s* and *p* orbitals

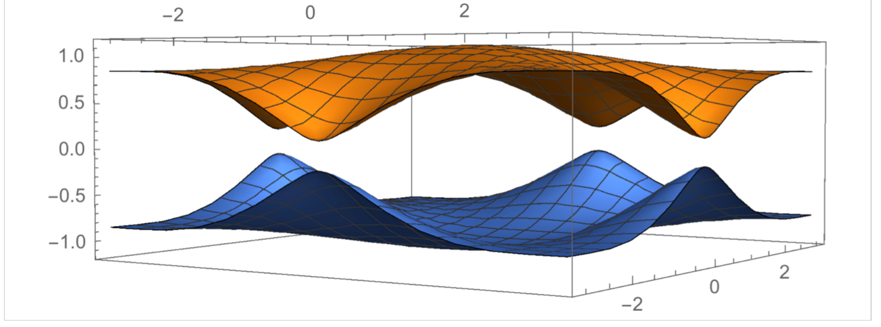
$$Ch = \frac{1}{4\pi} \iint dk_x\, dk_y \frac{(\partial_x a \times \partial_y a) \cdot a}{|a|^3}$$

Hall conductivity

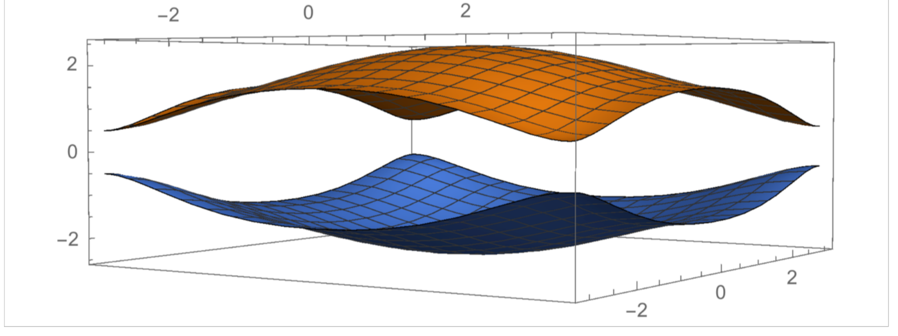
- $G_{xy}/(e^2/h)$

= $\text{sgn}((\varepsilon_p-\varepsilon_s)/4t_{sp})$ for $|(\varepsilon_p-\varepsilon_s)/2(t_s+t_p)|<2$

= 0 for $|(\varepsilon_p-\varepsilon_s)/2(t_s+t_p)|>2$



$G_{xy}/(e^2/h) = 1$

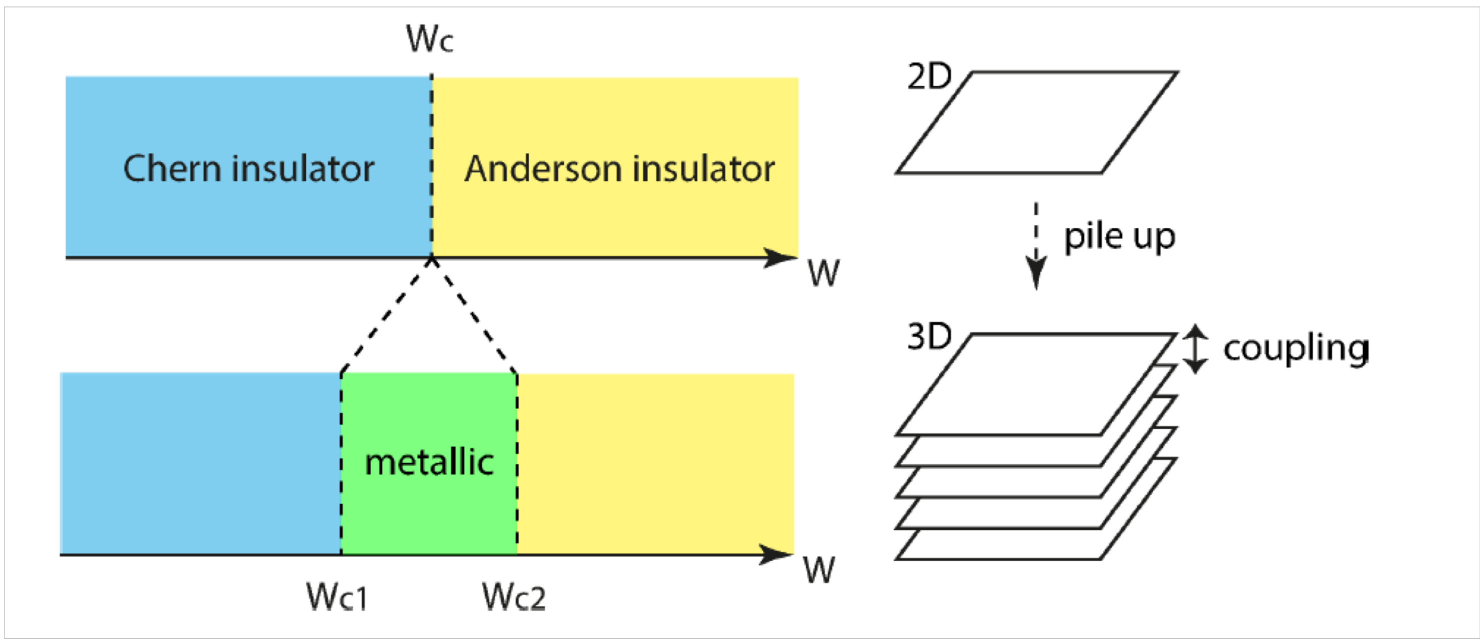


$G_{xy}/(e^2/h) = 0$

Introduce disorder→Chern insulator to Anderson insulator transition

Stacking 2D Chern insulators

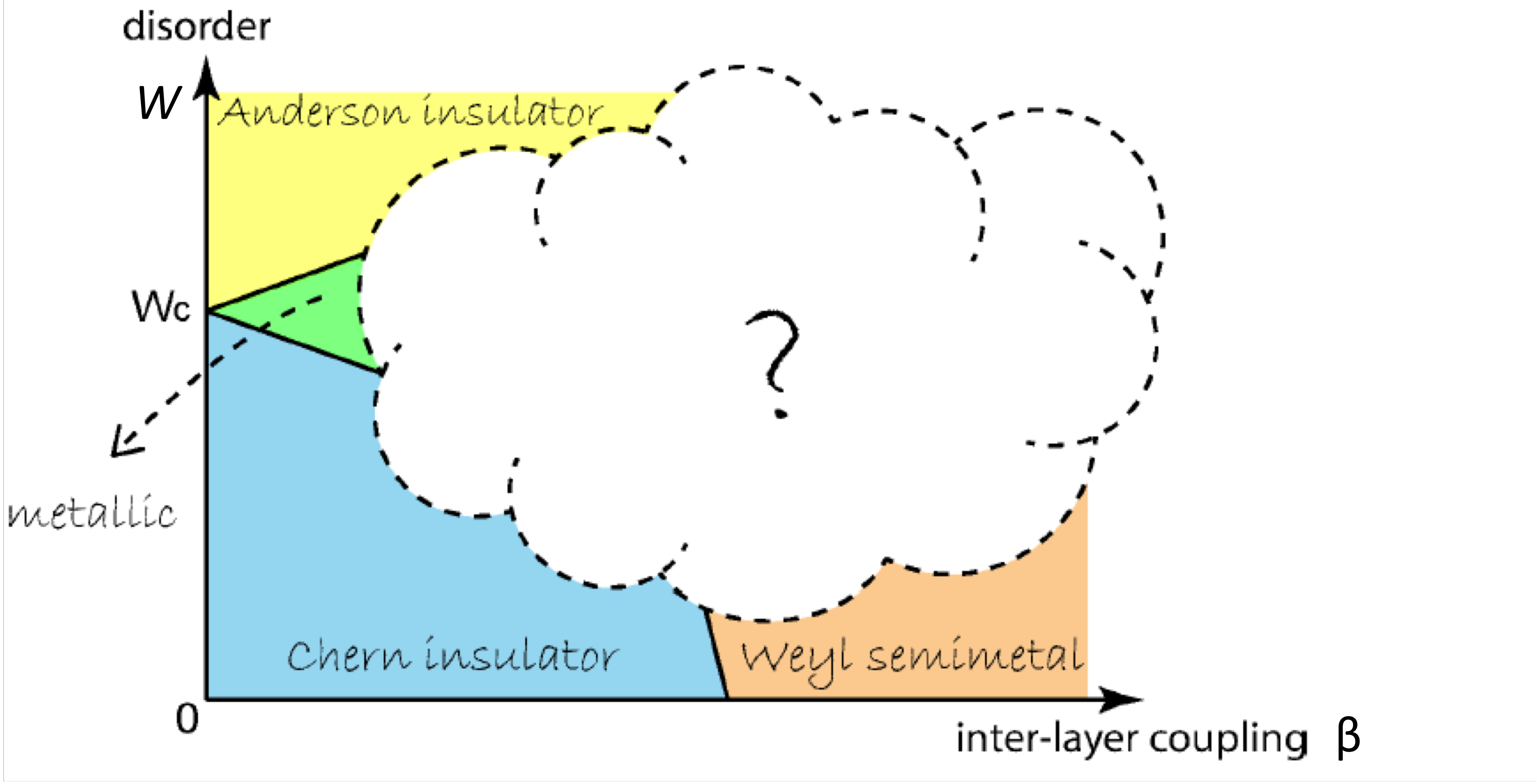
- finite region of diffusive metal regime appears with the increase of interlayer coupling



Cf. Layered quantum Hall system:
T. Ohtsuki et al., J. Phys. Soc. Jpn. 62, 224 (1993).
J. T. Chalker et al., Phys. Rev. Lett. 75, 4496 (1995).

phase diagram w.r.t. interlayer coupling and disorder

Liu, Ohtsuki, Shindou, PRL ‘16



Layered Chern Insulator

$$\boldsymbol{H}(\boldsymbol{k}) = a_0\sigma_0 + \boldsymbol{a}\cdot\boldsymbol{\sigma} \quad (7)$$

with $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices and

$$a_0(\boldsymbol{k}) = \frac{\epsilon_s + \epsilon_p}{2} + (t_p - t_s)(\cos k_x + \cos k_y) - (t'_s + t'_p)\cos k_z,$$

$$a_3(k) = \frac{\epsilon_s - \epsilon_p}{2} - (t_p + t_s)(\cos k_x + \cos k_y) - (t'_s - t'_p)\cos k_z,$$

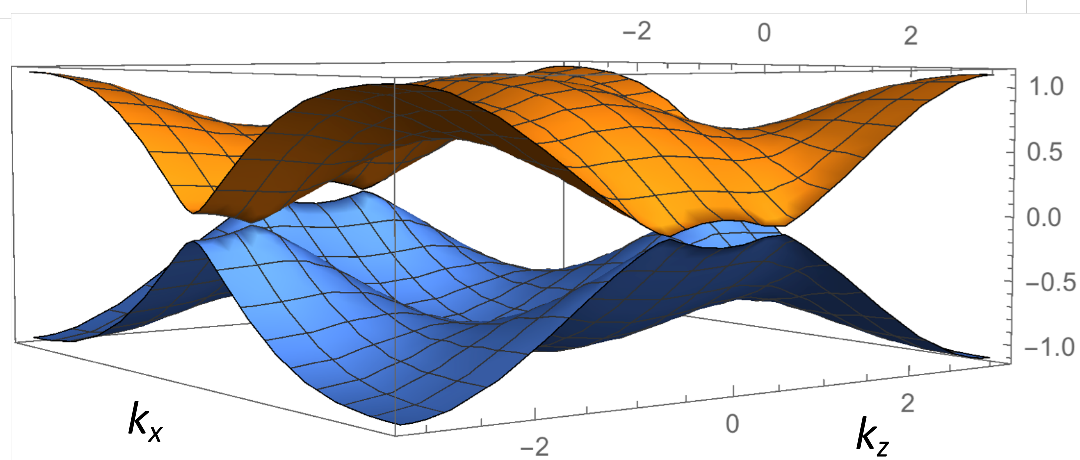
$$a_2(k) = -2t_{sp}\sin k_y,$$

$$a_1(k) = -2t_{sp}\sin k_x,$$

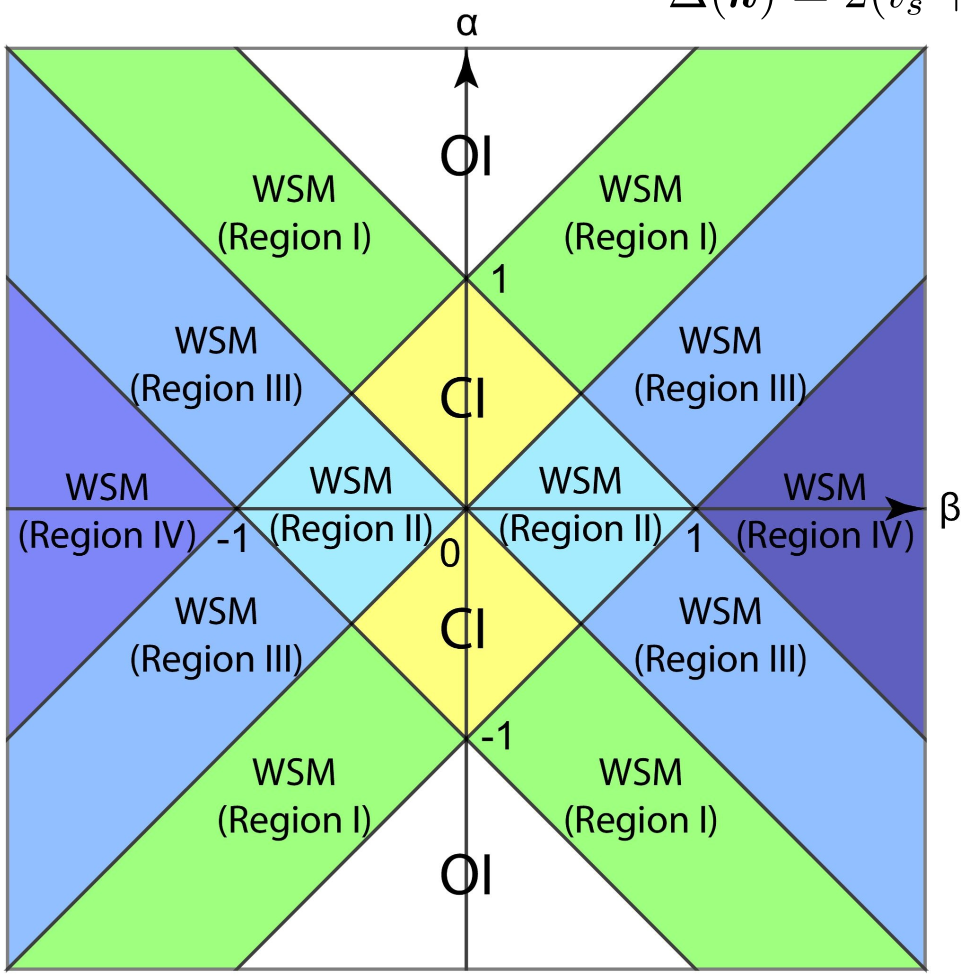
For simplicity,

$t_s' + t_p' = 0$, $t_s - t_p = 0$ $\varepsilon_s - \varepsilon_p = -2(t_s + t_p) = -4t_s$

$E = \pm(a_1^2 + a_2^2 + a_3^2)^{1/2}$



clean system



$$\Delta(\boldsymbol{k}) = 2(t_s + t_p) \cdot \left|\alpha - \frac{\cos k_x + \cos k_y}{2} + \beta \cos k_z\right|,$$

$k_x, k_y = 0, \pi$

$$\alpha \equiv \frac{\epsilon_s - \epsilon_p}{4(t_s + t_p)}$$

$$\beta \equiv \frac{t'_p - t'_s}{2(t_s + t_p)} = -\frac{t'_s}{2t_s}.$$

$(k_x, k_y) = (0, \pi) \rightarrow k_z = \pm(\pi - k_0)$

$(k_x, k_y) = (\pi, \pi) \rightarrow k_z = \pm k_1$

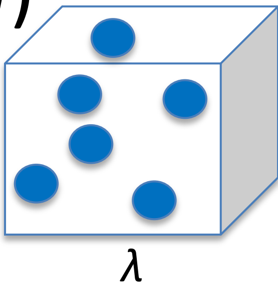
$$k_0 \equiv \cos^{-1}[\frac{\alpha}{\beta}],$$

$$k_1 \equiv \cos^{-1}[-\frac{1+\alpha}{\beta}].$$

Why is Weyl semimetal robust against randomness?

(by Syzranov et al., PHYSICAL REVIEW B **91**, 035133 (2015))

- effective fluctuation $\Delta W = W/(\lambda/a)^{d/2} = W(ka)^{d/2}$

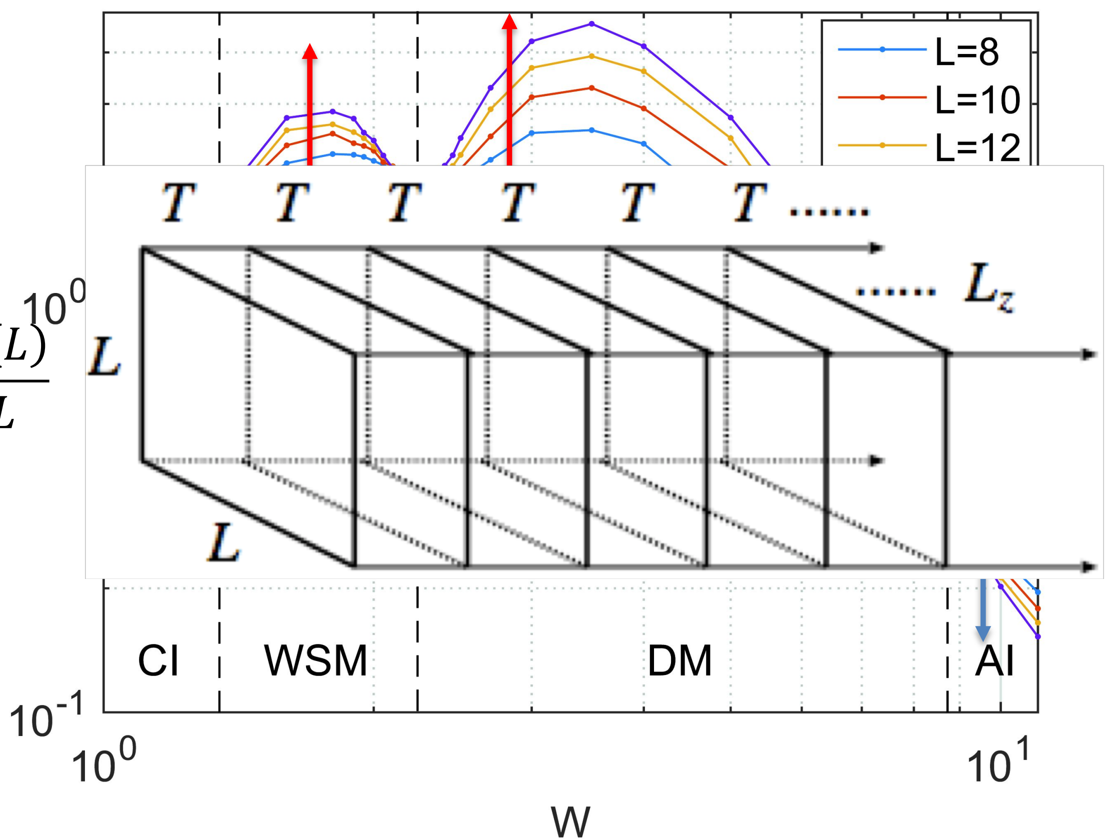


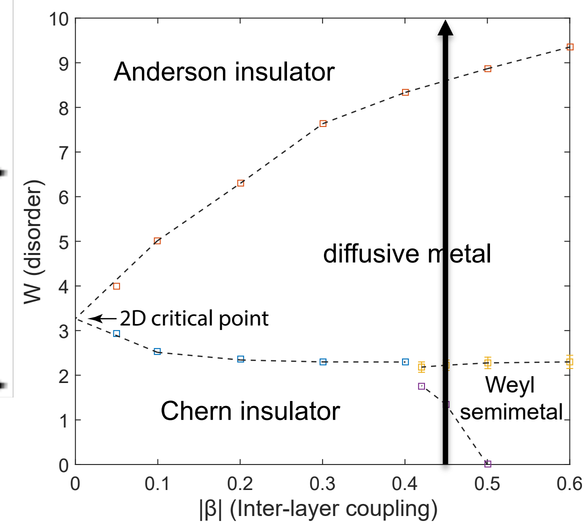
- Kinetic Energy $E = bk^{\alpha}$
- At band edge, $k \rightarrow 0$, $E >> \Delta W$ for $d\text{-}2\alpha > 0$
- In case of Schrodinger Eq. ($\alpha=2$), randomness becomes relevant at band edge when $d<4$.
- In case of Dirac/Weyl semimetal ($\alpha=1$), randomness becomes irrelevant at band edges when $d>2$.
- RG analysis, Goswami et al. '11, Syzranov et al. '16

How did we determine the phase diagram?

- Localization length calculation by transfer matrix method along z-direction.

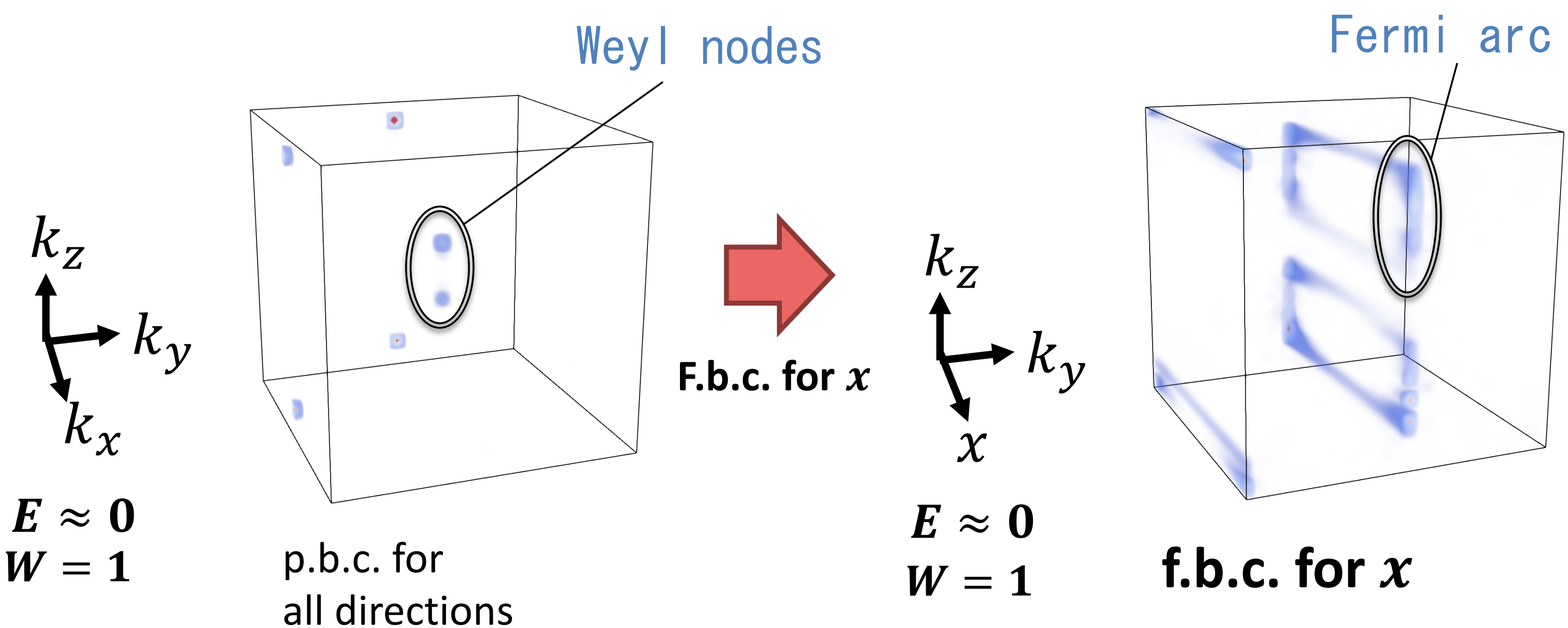
$$\Lambda = \frac{\xi(L)}{L}$$



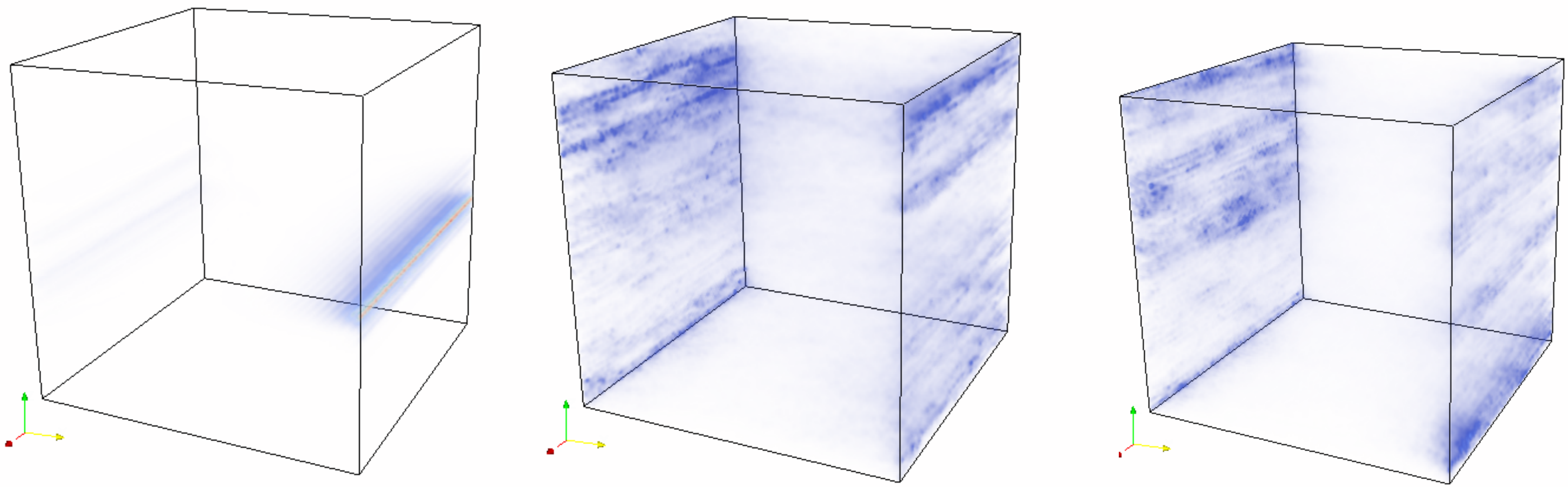


3D Weyl semimetal（3DWSM）

- semimetal ⟺ Existence of Dirac/Weyl nodes
- Pairs of Weyl nodes move as a function of mass and disorder
- Fermi arcs appear on specific surfaces



$|\psi(\vec{x})|^2$
diagonalization for 80 x 80 x 80 system



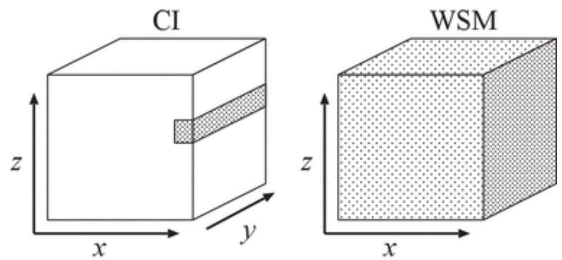
β=0.45
W=0.8

β=0.45
W=1.7

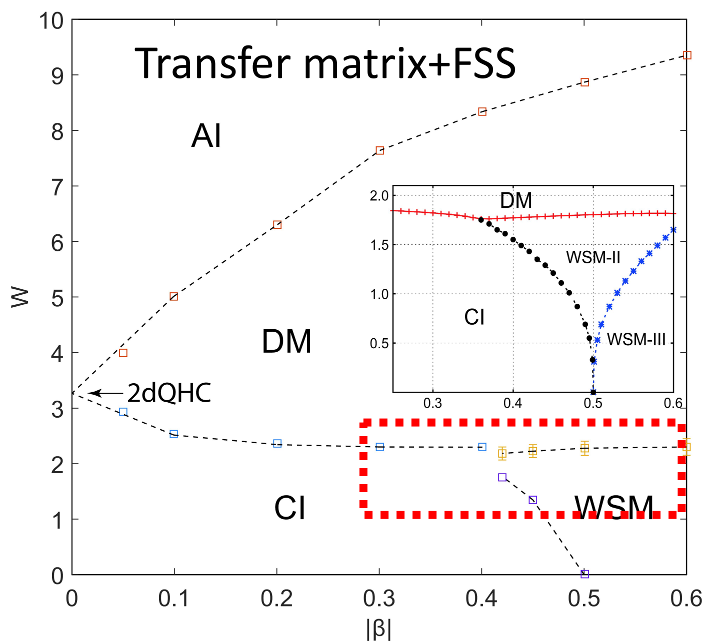
β=0.6
W=1.5

Phase diagram for 3DWSM : real space analysis

T. Ohtsuki, T. Ohtsuki, JPSJ ‘16, ‘17



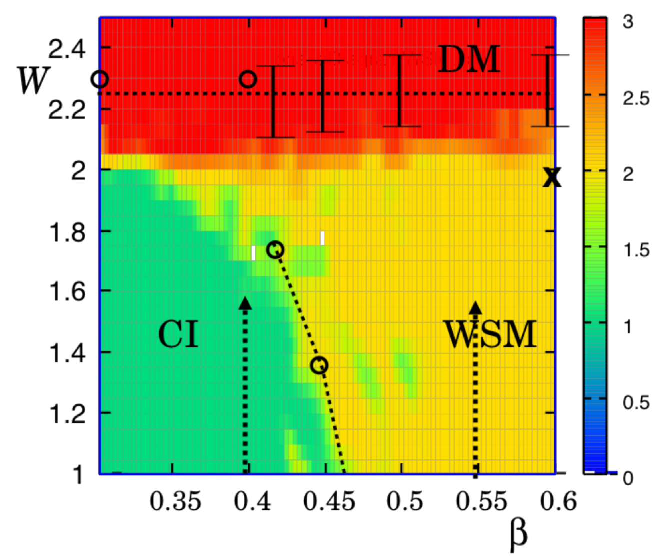
Integrate along ***y***



E **≈ 0, fbc for** ***x*** **direction**

S.Liu, T.Ohtsuki, R.Shindou, PRL’16

$1 \times P_{\mathrm{CI}} + 2 \times P_{\mathrm{WSM}} + 3 \times P_{\mathrm{DM}}$



・Can we distinguish WSMⅡ/WSMⅢ?

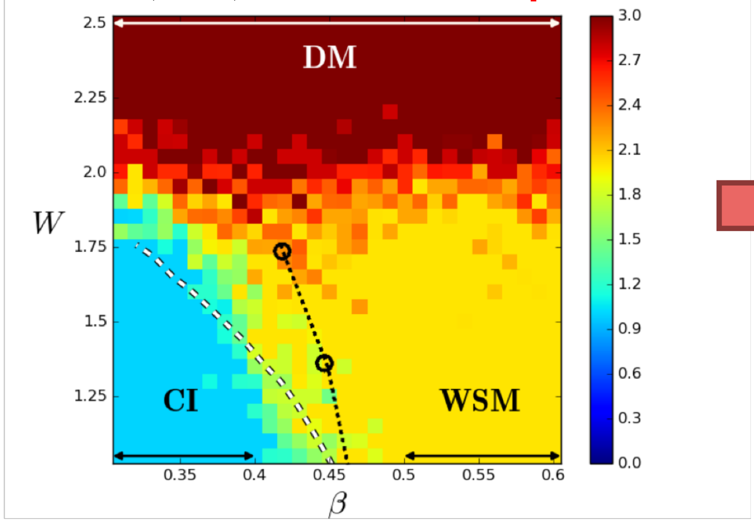
2 pairs　　3 pairs

Application to Weyl semimetals

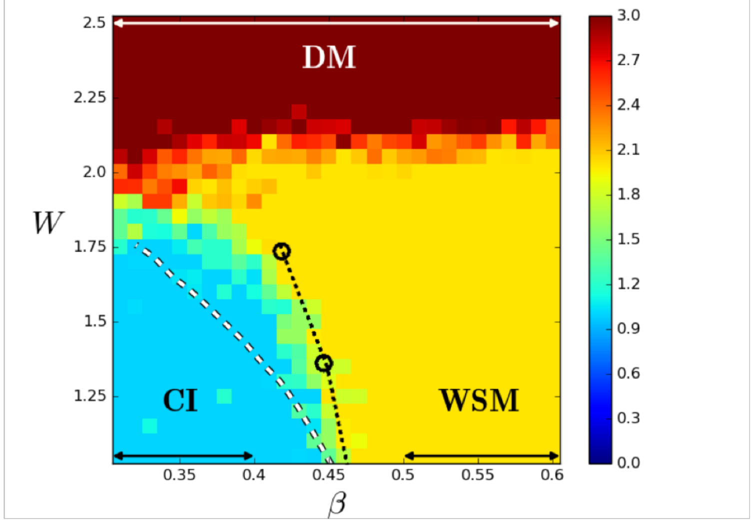
$32 \times 32 \times 32$, Conv-Pool-Conv-Pool (Mano et al., unpublished) $|\psi(\vec{x})|^2$ vs. $|\psi(\vec{k})|^2$

PRELIMINARY

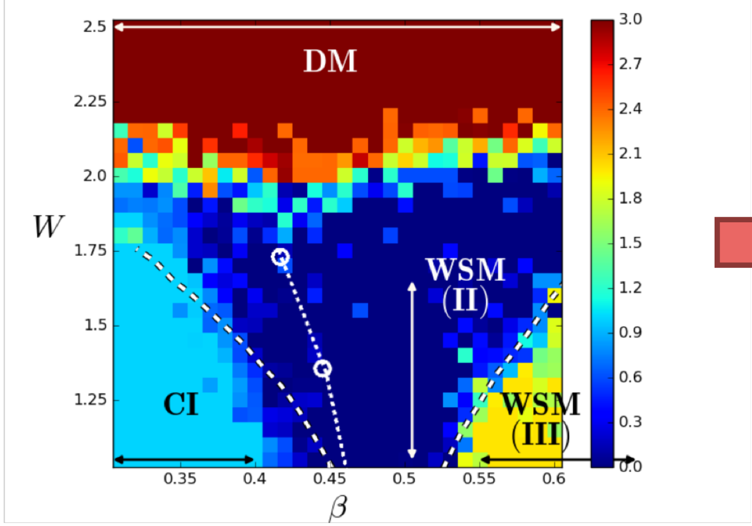
DM/CI/WSM, real space



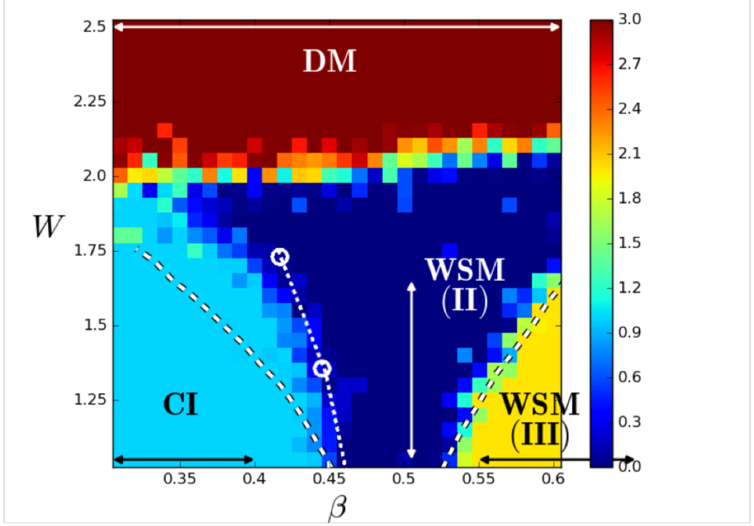
DM/CI/WSM, k-space



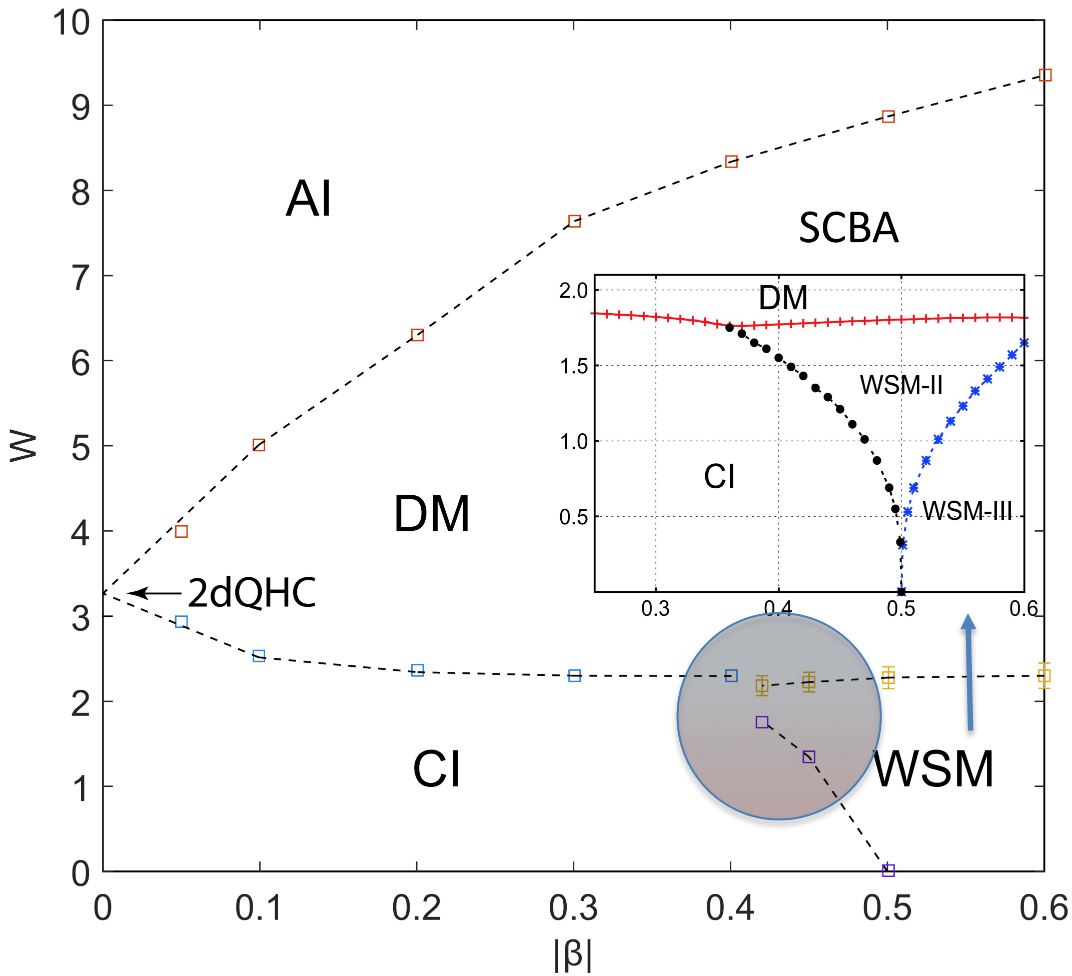
DM/CI/WSM(II, III), real space



DM/CI/WSM(II, III), k-space



phase diagram



W: strength of disorder

Scaling behavior from WSM to Metal

$$\beta \equiv \frac{t'_p - t'_s}{2(t_s + t_p)}$$

Density of state scaling for WSM to Metal

(Kobayashi et al., PRL14, Dirac semimetal in 3D TI)

Number of states below ε $$N(\epsilon, L) = F\left(L/\xi, \epsilon/\epsilon_0\right) \;;$$

Relate energy scale to length scale via *z* $$\epsilon_0 \propto \xi^{-z} \, .$$

In thermodynamic limit, $$N(\epsilon, L) = (L/\xi)^d f\left(\epsilon \xi^z\right) \, .$$

DOS per volume is derived as $$\rho(\epsilon) = \frac{1}{L^d} \frac{dN(\epsilon, L)}{d\epsilon} \, ,$$

$$\rho(\epsilon) = \rho(-\epsilon) = \xi^{z-d} f'(|\epsilon|\xi^z) \, .$$

Distance from the critical point $\delta = |W - W_{\rm c}|/W_{\rm c}$

$$\xi \sim \delta^{-\nu} \, , \qquad \rho(\epsilon) \sim \delta^{(d-z)\nu} f'(|\epsilon|\delta^{-z\nu}) \, .$$

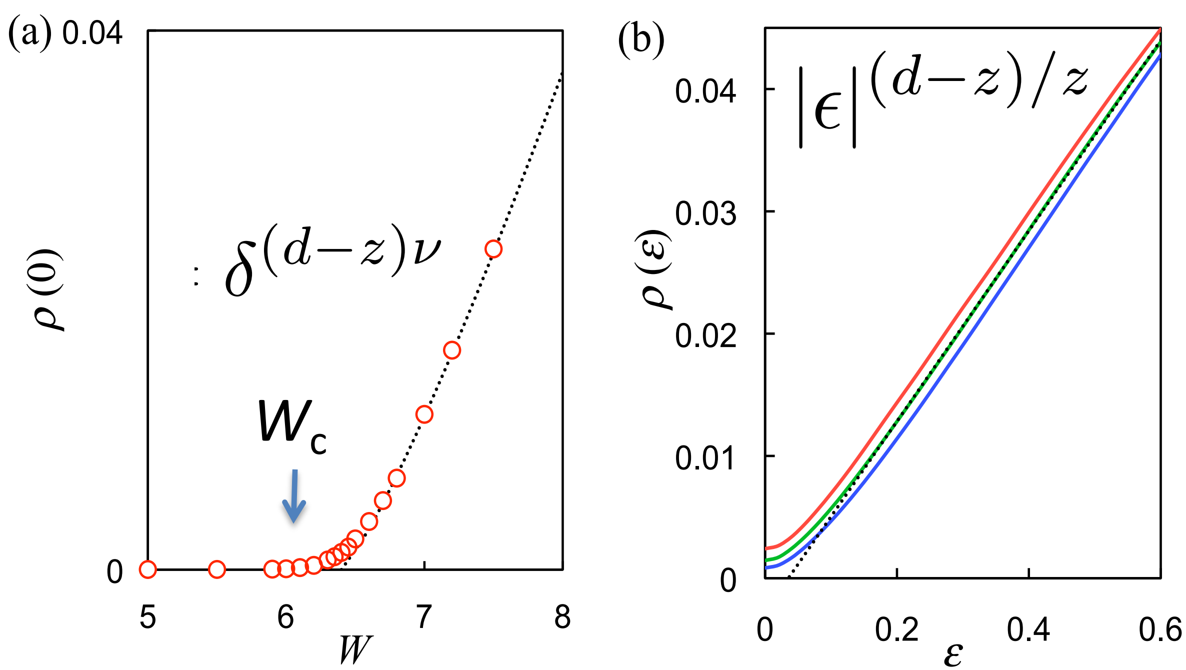
cf. McMillan-Shklovskii scaling for Anderson Mott transition, Kravtsov et al, NJP ‘14

From $\rho(\epsilon) \sim \delta^{(d-z)\nu} f'(|\epsilon|\delta^{-z\nu})$.

Weyl/Dirac SM $\rho(\epsilon) \sim \delta^{(d-z)\nu}(|\epsilon|\delta^{-z\nu})^{d-1} = |\epsilon|^{d-1}\delta^{-(z-1)d\nu}$.

metallic $\rho(0) \sim \delta^{(d-z)\nu}(|\epsilon|\delta^{-z\nu})^{0} = \delta^{(d-z)\nu}$. Fradkin, '86

Critical point $\rho(\epsilon) \sim \delta^{(d-z)\nu}(|\epsilon|\delta^{-z\nu})^{(d-z)/z} = |\epsilon|^{(d-z)/z}$.



$$(3-z)/z = 1.00 \pm 0.15\,,$$
$$z = 1.5 \pm 0.1\,.$$

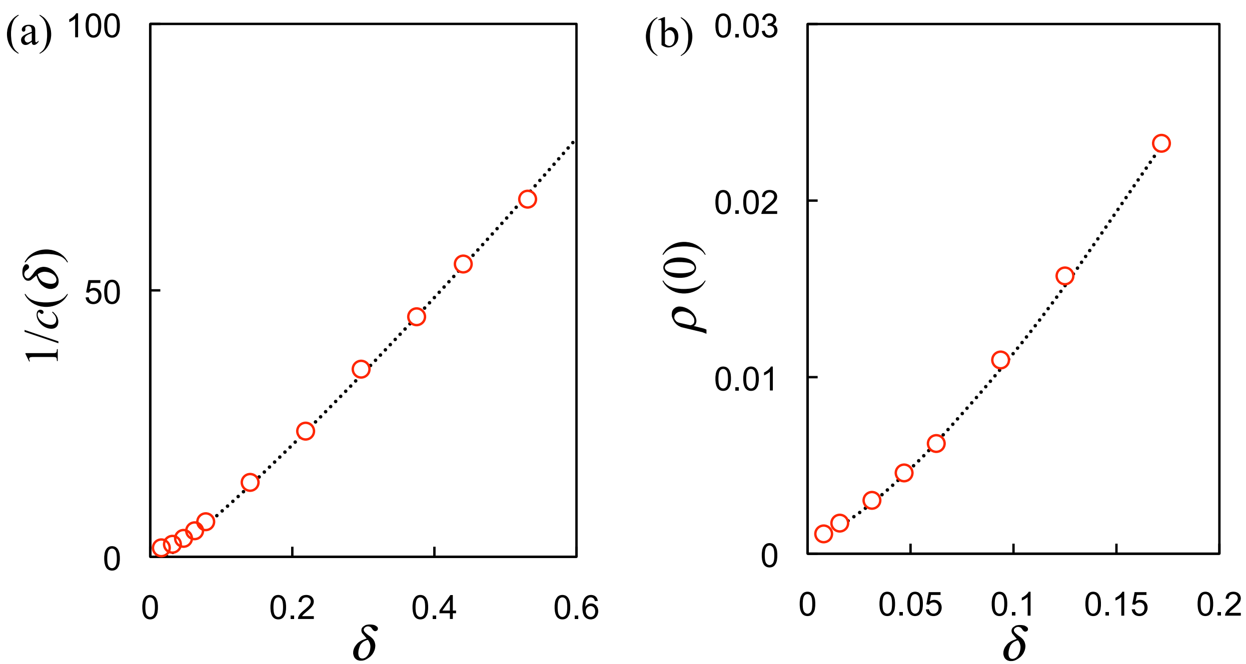
Estimates of exponents

For DSM

$$\rho(\epsilon) \sim c(\delta)|\epsilon|^2 \,,$$
$$c(\delta)^{-1} \sim \delta^{3(z-1)\nu_{\rm DSM}} \,,$$
$$v \sim \delta^{(z-1)\nu} \approx \delta^{0.4} \,.$$

For metal

$$\rho(0) \sim \delta^{(d-z)\nu}$$

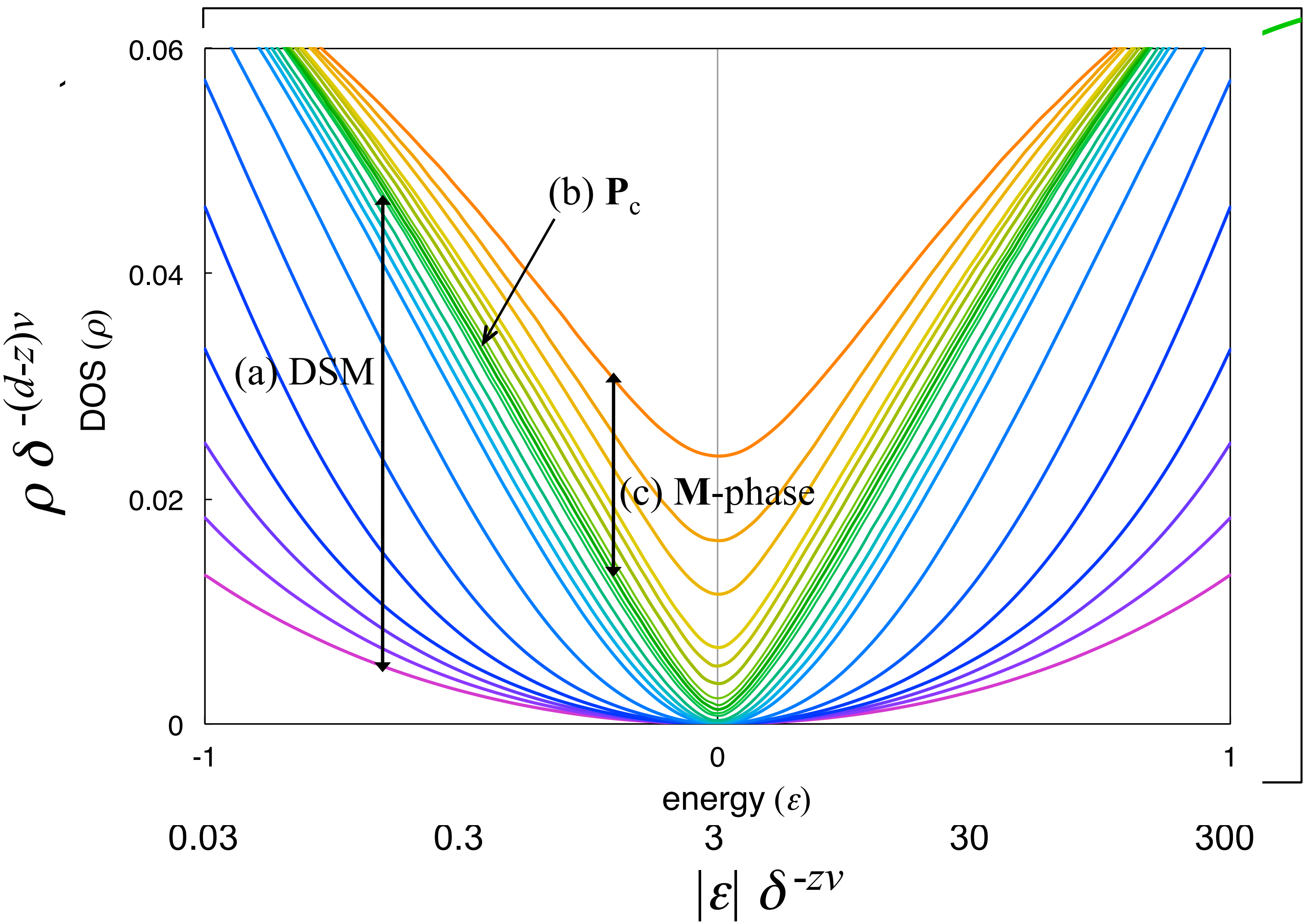


$$3(z-1)\nu_{\rm DSM} \simeq 1.16 \pm 0.05 \,,$$
$$\therefore \;\; \nu_{\rm DSM} \simeq 0.81 \pm 0.21 \,.$$

$$(3-z)\nu_{\rm M} \simeq 1.36 \pm 0.09 \,,$$
$$\therefore \;\; \nu_{\rm M} \simeq 0.92 \pm 0.13 \,.$$

single parameter scaling plot

$$\rho(\epsilon) \sim \delta^{(d-z)\nu} f'(|\epsilon|\delta^{-z\nu})\,.$$



Scaling laws

Distance from the critical point: $\delta = |W - W_c|/W_c$

Diverging length scale: $\xi \sim \delta^{-\nu}$,

Vanishing energy scale: $\epsilon_0 \propto \xi^{-z}$.

	Weyl semimetal	Diffusive Metal
DoS @ ε=0	0	$\delta^{(d-z)\nu}$
Effective velocity	$\delta^{(z-1)\nu}$	-
Diffusion Constant @ ε=0	∞	$\delta^{(z-2)\nu}$
Conductivity σ @ ε=0	$\delta^{(d-2)\nu}$	$\delta^{(d-2)\nu}$

The same scaling law as the Anderson transition.

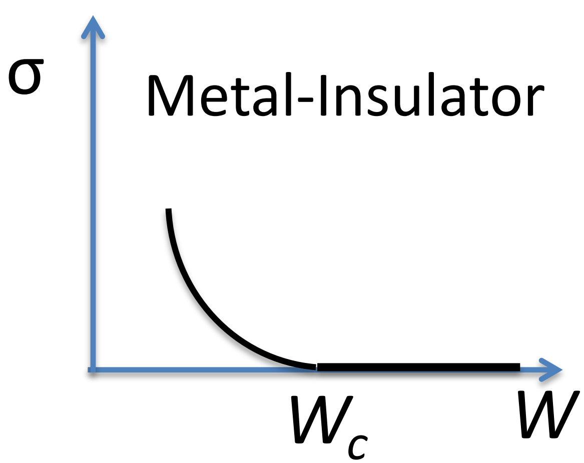
DoS @ Critical point: $\rho(\varepsilon) \sim |\varepsilon|^{(d-z)/z}$

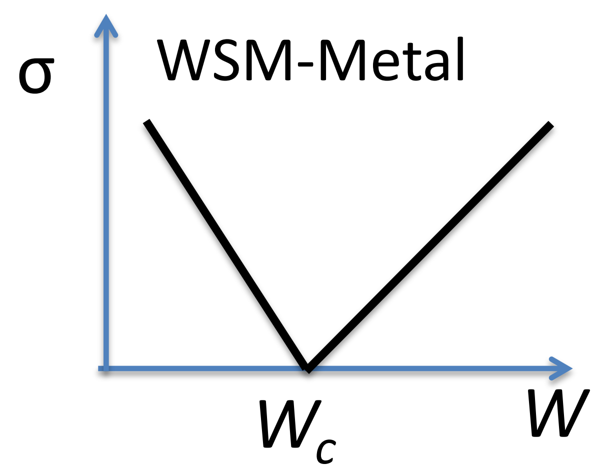
Conductivity scaling: from WSM side

Weyl semimetal to W_c: $D = v^2 \tau / d$, $\rho \propto 1/\tau \rightarrow$

$$\sigma(E=0) \propto \overline{v}^2 \text{ with } \overline{v} \propto \delta^{(z-1)\nu}$$

assuming $z=d/2$, we recover $\sigma(0) \sim \delta^{(d-2)\nu}$,



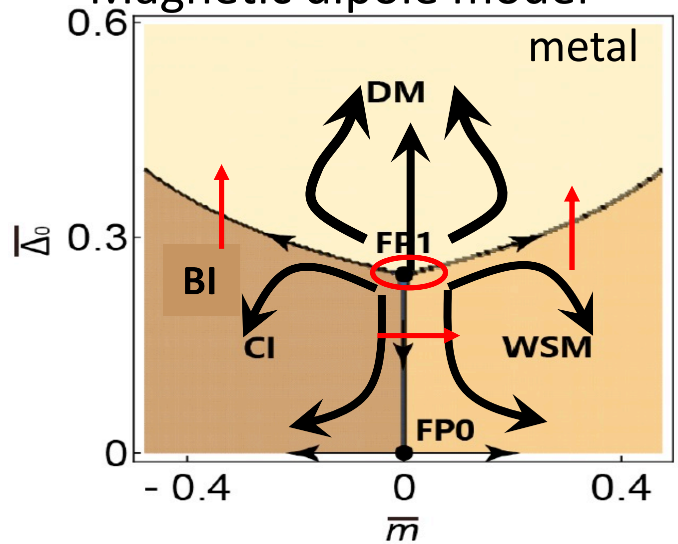


Scaling behaviors in other parts of the phase diagram

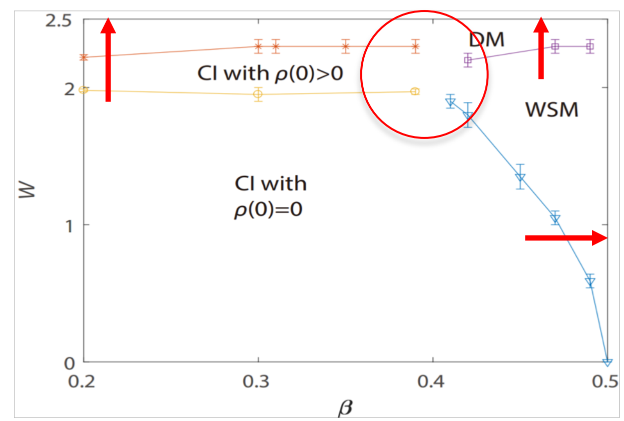
- ◆ Quantum Multicritical point (QMCP) is encompassed by three phases: band insulator , renormalized Weyl semimetal and diffusive metal phases

✓BI-WSM phase transition is controlled by FP0 in the clean limit;
unconventional scaling
X. Luo, *et. al. Phys. Rev. B* 98, 020201(R) (2018)

Magnetic dipole model



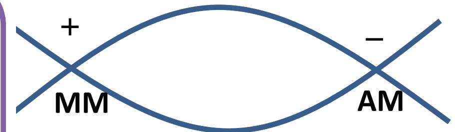
Layered Chern insulator



Magnetic dipole model for BI-WSM transition

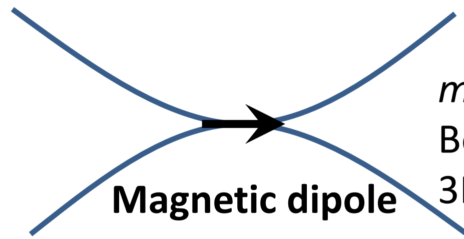
$$\mathcal{H}_{\rm eff} = \int d^2\boldsymbol{x}_\perp dx_3\, \psi^\dagger(\boldsymbol{x})\Big\{ -iv(\partial_1\boldsymbol{\sigma}_1 + \partial_2\boldsymbol{\sigma}_2) + ((-i)^2 b_2\partial_3^2 - m)\boldsymbol{\sigma}_3 \Big\}\psi(\boldsymbol{x}),$$

Yang, Moon, Isobe, Nagaosa, Nat. Phys. '14

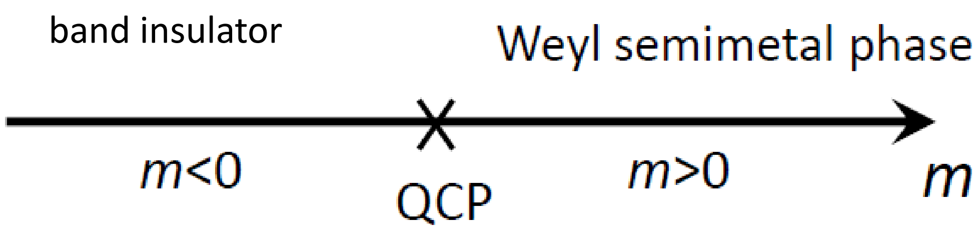


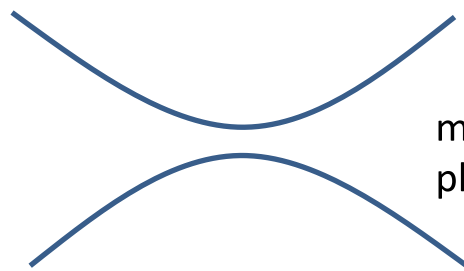
m>0 : WSM phase

MM and AM locate at $(p_1, p_2, p_3) = (0, 0, \pm\sqrt{m/b_2})$.



m=0 : a critical point Between WSM phase and 3D band insulator





m<0 : 3D band Insulator phase

B. Roy, *et.al.* arXiv:1610.08973 (2016)
X. Luo, *et. al. Phys. Rev. B* 97, 045129 (2018)

Effect of Disorders on Magnetic dipole model

$$\mathcal{H}_{\rm eff} = \int d^2\boldsymbol{x}_\perp dx_3\, \psi^\dagger(\boldsymbol{x})\Big\{ -iv\big(\partial_1\boldsymbol{\sigma}_1 + \partial_2\boldsymbol{\sigma}_2\big) + \big((-i)^2 b_2\partial_3^2 - m\big)\boldsymbol{\sigma}_3 \Big\}\psi(\boldsymbol{x}),$$

the model has a quadratic dispersion along the dipole direction, and a linear dispersion along the in-plane direction in the clean limit

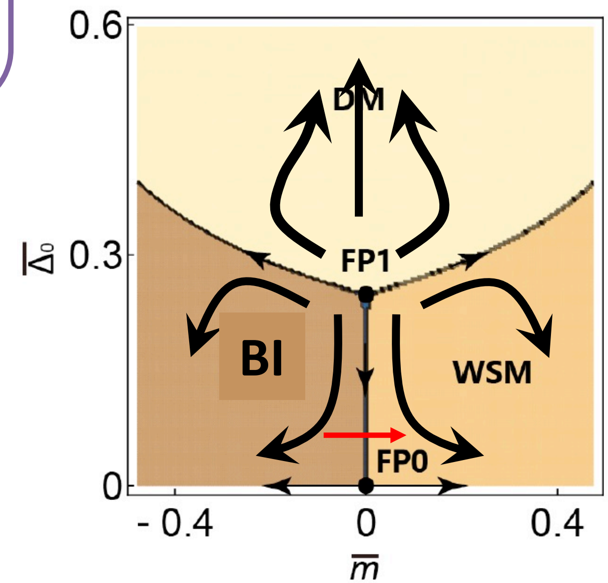
$$x_z' = b^{1/2}\, x_z$$

$$\boldsymbol{x}_\perp' = b\, \boldsymbol{x}_\perp$$

unconventional scaling forms →

- conductance
- localization length
- density of states

b: block size in k-space



B. Roy, *et.al.* arXiv:1610.08973 (2016)
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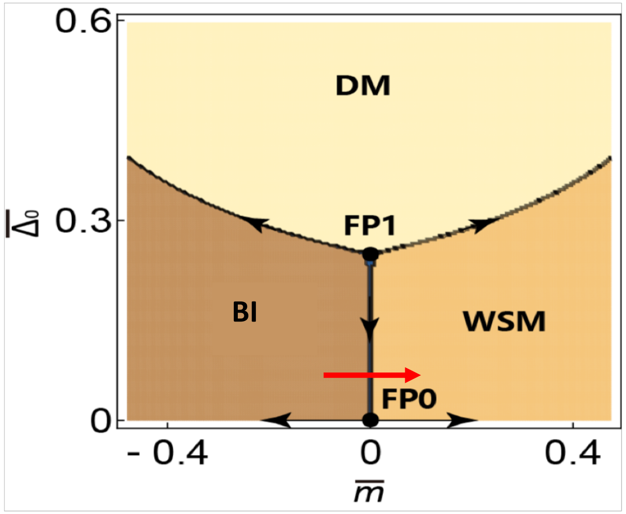
unconventional scaling form of conductance along BI-WSM transition

$x'_z = b^{1/2}\, x_z$

$\boldsymbol{x}'_\perp = b\, \boldsymbol{x}_\perp$

$$\begin{cases} \rho' = b^{-(d-\frac{1}{2}-z)}\rho \quad (\, V' = b^{d-\frac{1}{2}}V\,) \\ D'_\perp = b^{-(z-2)}D_\perp,\; D'_z = b^{-(z-1)}D_z. \end{cases}$$



With Einstein relation: $\sigma_\mu = e^2 D_\mu \rho$, we obtain:

$$\sigma'_\perp = b^{-d+\frac{5}{2}}\,\sigma_\perp,\; \sigma'_z = b^{-d+\frac{3}{2}}\,\sigma_z.$$

$\mu = z, \perp$

$$\left.\begin{aligned} G'_\perp(L'_z, L'_\perp, \Delta', m') &= G_\perp(L_z, L_\perp, \Delta, m), \\ G'_z(L'_z, L'_\perp, \Delta', m') &= G_z(L_z, L_\perp, \Delta, m), \end{aligned}\right\}$$

set m to be tiny, $m' = b^{-1}m = 1$

$$G_\mu(L_z, L_\perp, m) = \Phi_\mu(m^{1/2}L_z, mL_\perp).$$

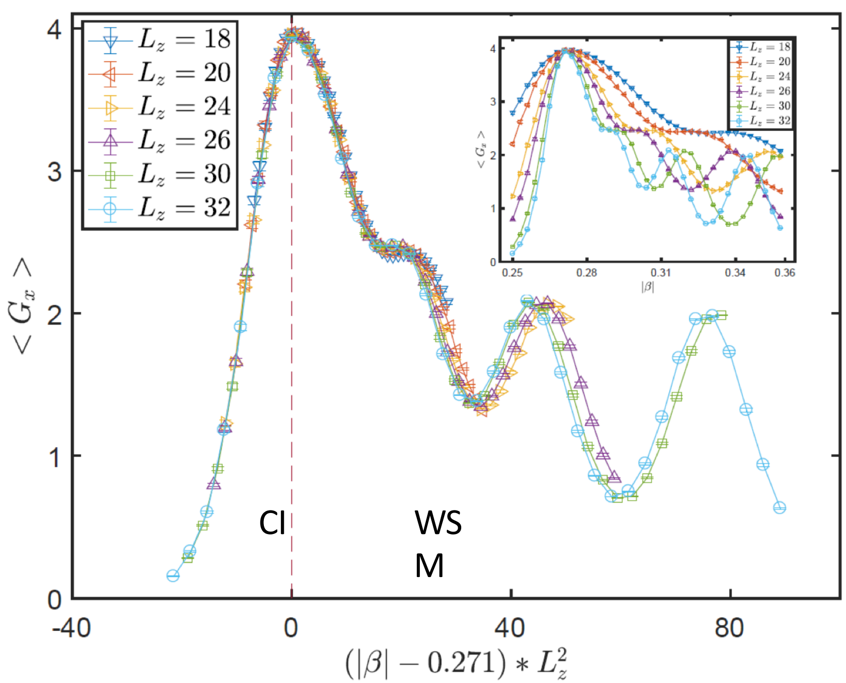
$L_\perp = \eta L_z^2$

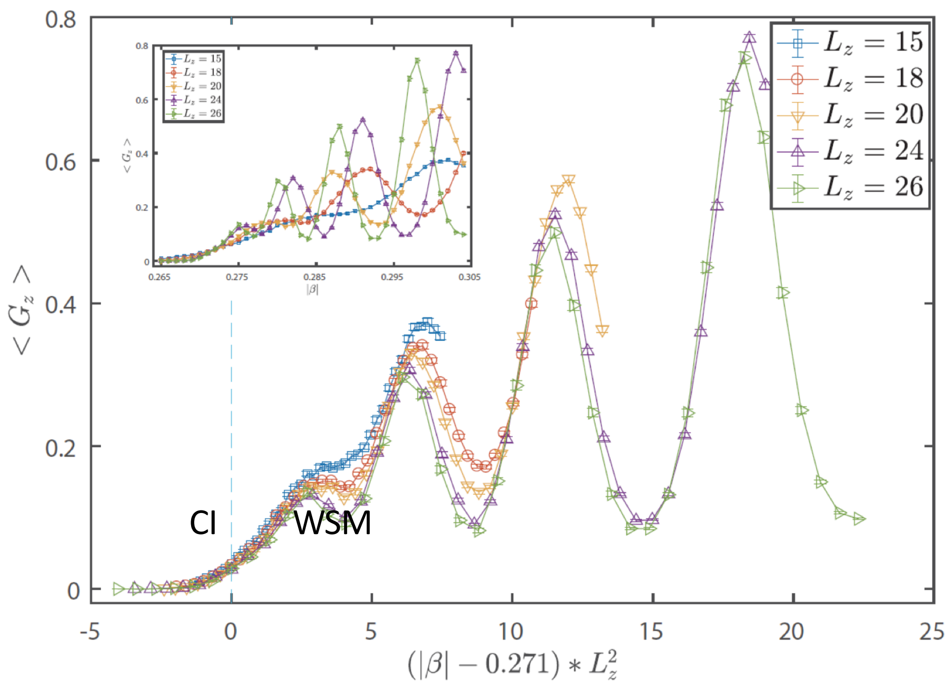
$$\begin{aligned} L'_z &= b^{\frac{1}{2}}L_z \\ L'_\perp &= bL_\perp \\ \Delta' &= b^{-y_\Delta}\Delta \\ m' &= b^{-1}m \end{aligned}$$

$y_\Delta = -d + \frac{5}{2} < 0$

$$G_\mu(L_z, L_\perp, m) = \Phi_\mu(m^{1/2}L_z, \eta\, mL_z^2) = f(m^{1/2}L_z).$$

numerical test for unconventional scaling form of conductance



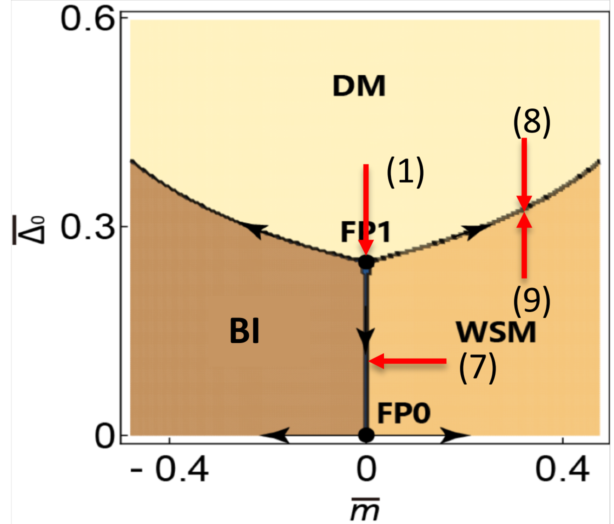


anisotropic system size:
$L_\perp = \eta L_z^2$

$$G_\mu(L_z, L_\perp, m) = f(mL_z^2) \qquad \mu = z, \perp \qquad m = \beta - \beta_c$$

CI-WSM transition:
(unconventional scaling)

- Density of states
- conductance



	$\rho(0)$ or $\rho(\mathcal{E})$	$\sigma_3(0)$ or $\sigma_3(\mathcal{E})$	$\sigma_\perp(0)$ or $\sigma_\perp(\mathcal{E})$
(1)	$\delta\overline{\Delta}_0^{\frac{2d-1-2z}{2y_\Delta}}$	$\delta\overline{\Delta}_0^{\frac{2d-3}{2y_\Delta}}$	$\delta\overline{\Delta}_0^{\frac{2d-5}{2y_\Delta}}$
(2)	$\lvert\mathcal{E}\rvert^{d-\frac{3}{2}}$	$\lvert\mathcal{E}\rvert^{d-\frac{3}{2}}$	$\lvert\mathcal{E}\rvert^{d-\frac{5}{2}}$
(3)	$\lvert\delta\overline{\Delta}_0\rvert^{\frac{2d-1}{2}\frac{1-z}{y_\Delta}}\lvert\mathcal{E}\rvert^{d-\frac{3}{2}}$	$\lvert\delta\overline{\Delta}_0\rvert^{\frac{2d-3}{2}\frac{1-z}{y_\Delta}}\lvert\mathcal{E}\rvert^{d-\frac{3}{2}}$	$\lvert\delta\overline{\Delta}_0\rvert^{\frac{2d-5}{2}\frac{1-z}{y_\Delta}}\lvert\mathcal{E}\rvert^{d-\frac{5}{2}}$
(4)	$\lvert\mathcal{E}\rvert^{\frac{d-z'}{z'}}$	$\lvert\mathcal{E}\rvert^{\frac{d-2}{z'}}$	same as σ_3
(5)	$m^{\frac{2d(z'-z)-z'}{2z'y_m}}\lvert\mathcal{E}\rvert^{\frac{d-z'}{z'}}$	$m^{\frac{2d(z'-z)+4z-3z'}{2z'y_m}}\lvert\mathcal{E}\rvert^{\frac{d-2}{z'}}$	$m^{\frac{2d(z'-z)+4z-5z'}{2z'y_m}}\lvert\mathcal{E}\rvert^{\frac{d-2}{z'}}$
(6)	$\lvert\mathcal{E}\rvert^{\frac{2d-1-2z}{2z}}$	$\lvert\mathcal{E}\rvert^{\frac{2d-3}{2z}}$	$\lvert\mathcal{E}\rvert^{\frac{2d-5}{2z}}$
(7)	$m^{-\frac{1}{2}}\lvert\mathcal{E}\rvert^{d-1}$	$m^{d-\frac{3}{2}}$	$m^{d-\frac{5}{2}}$
(8)	$\delta\overline{\Delta}_0^{\frac{d-z'}{y'_\Delta}}$	$\delta\overline{\Delta}_0^{\frac{d-2}{y'_\Delta}}$	same as σ_3
(9)	$\lvert\delta\overline{\Delta}_0\rvert^{-\frac{dz'-d}{y'_\Delta}}\lvert\mathcal{E}\rvert^{d-1}$	$\lvert\delta\overline{\Delta}_0\rvert^{\frac{d-2}{y'_\Delta}}$	same as σ_3

Phys. Rev. B 97, 045129 (2018).
Phys. Rev. B 98, 020201(R) (2018).

Summary

- Rich phase diagram: Chern insulator, Anderson insulator, Weyl semimetal, diffusive metal
- Phase diagram: machine learning in real and k-space
- Scaling behaviors: nontrivial behaviors of
  - Density of states scaling for WSM/Metal, similar to Coulomb glass/metal transition.
  - Conductivity scaling.
- 3D Topological insulator?