# Disordered topological insulators with time-reversal symmetry: $Z_2$ invariants

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- HK & T. Koma, *J. Math. Phys*. **57**, 021903 (2016); arXiv:1611.01928.

# Outline

## 1. Topological insulators (TI)

- Classification & characterization
- What about disordered systems?

## 2. Topological invariants of 2D & 3D class AII TI

- Time-reversal symmetry & Kramers' theorem
- $Z_2$ index (Noncommutative ver.)

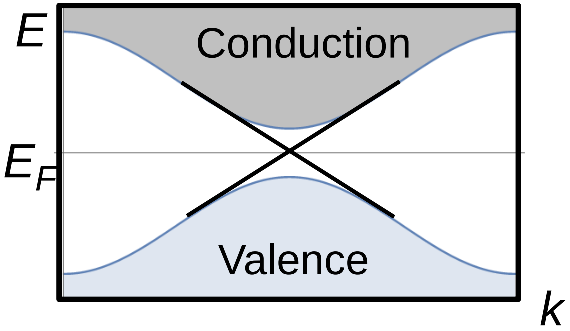
## 3. Application

- 3D Wilson-Dirac model, phase diagram
- Numerical results

## 4. Summary

# What are topological insulators (TI)?

- Band insulators (free-fermions)
- Characterized by **topological invariants**
  TKNN invariant = Chern #
- Robust gapless **edge/surface states**




Reviews and textbooks:
M.Z. Hasan and C.L. Kane, *RMP*. **82**, 3045 (2010).
X-L. Qi and S-C. Zhang, *RMP*. **83**, 1057 (2010), …

## ■ Examples

- Integer quantum Hall effect ('80s) Magnetic field
  von Klitzing *et al*., TKNN
- **2D** Quantum spin Hall effect Spin-orbit
  Kane-Mele ('05), Molenkamp's group, …
- **3D** TI ($Bi_{1-x}Sb_x$, $Bi_2Se_3$, $Bi_2Te_3$)
  Fu-Kane-Mele, Hasan's group, …

# Periodic Table -- Classification of TI & SC --

Symmetries: Time-reversal(T), particle-hole(C) & Chiral(S).

Topo. Num. : $\mathbf{Z}_2 = \{0,1\}$, $\mathbf{Z}=\{0, \pm 1, \pm 2, \ldots\}$, $2\mathbf{Z}=\{0, \pm 2, \pm 4, \ldots\}$

Schnyder *et al*., *PRB* **78** (2008); Kitaev, AIP Conf. Proc. **1134** (2008).

| Symmetry | | | | Spatial dimension $d$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CAZ | TRS | PHS | CHS | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| A | 0 | 0 | 0 | | $\boxed{\mathbb{Z}}$ | | $\mathbb{Z}$ | | $\mathbb{Z}$ | | $\mathbb{Z}$ |
| AIII | 0 | 0 | 1 | $\mathbb{Z}$ | | | | $\mathbb{Z}$ | | $\mathbb{Z}$ | |
| AI | $+1$ | 0 | 0 | | | | $2\,\mathbb{Z}$ | | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ |
| BDI | $+1$ | $+1$ | 1 | $\mathbb{Z}$ | | | | $2\,\mathbb{Z}$ | | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ |
| D | 0 | $+1$ | 0 | $\mathbb{Z}_2$ | $\boxed{\mathbb{Z}}$ | | | | $2\,\mathbb{Z}$ | | $\mathbb{Z}_2$ |
| DIII | $-1$ | $+1$ | 1 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | | | | $2\,\mathbb{Z}$ | |
| AII | $-1$ | 0 | 0 | | $\boxed{\mathbb{Z}_2}$ | $\boxed{\mathbb{Z}_2}$ | $\mathbb{Z}$ | | | | $2\,\mathbb{Z}$ |
| CII | $-1$ | $-1$ | 1 | | | $\mathbb{Z}$ | | $\mathbb{Z}$ | | | |
| C | 0 | $-1$ | 0 | | $2\,\mathbb{Z}$ | | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | | |
| CI | $+1$ | $-1$ | 1 | | | $2\,\mathbb{Z}$ | | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | |

IQHE

p+ip SC

QSHE

3D TI

Bott Periodicity

Derivation based on Random matrix, *K*-theory, …

Can be refined with additional symmetry, e.g., inversion.

*What are topo. invariants that can distinguish different phases?*

# What about disordered systems?

## ■ Characterization

A **disordered TI** is an insulator with edge/surface states that do not ***Anderson localize***.

Physics of $d$-dim TI → ($d$-1)-dim Anderson loc.

## ■ Topological invariant

Momentum $k$ is not a good quantum num. Can we define topo. num?

- Niu-Thouless-Wu formula (IQHE)
  Niu-Thouless-Wu, *PRB* **31** (1985).
  $(k_x, k_y) \rightarrow (\theta_x, \theta_y)$: boundary twists

$$\frac{d}{dk} \rightarrow [iX, \ldots]$$

- Noncommutative Geometry
  Avron, Seiler & Simon, *CMP* **159** (1994).
  $k$-derivative → Commutator in real space

An extension gives a precise definition of topo. Invariant for each element in periodic table!

HK and T. Koma, arXiv:1611.01928. 95 pages, no figures…
Today, I will focus on ***killer apps***. 2D & 3D class AII TI.

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## 2. Topological invariants of 2D & 3D class AII TI

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# Time-reversal operation

## ■ Preliminaries

- Wavefunction: $\varphi_{a,\sigma}(x)$ ( *a*: orbital, *σ*: spin, *x*: position)
- Complex conjugation: $K$ $K\varphi_{a,\sigma}(x) = \varphi^*_{a,\sigma}(x)$
- Unitary operation: $U$ $U\varphi_{a,\sigma}(x) = \sum_{b,\tau} U_{a\sigma,b\tau}\,\varphi_{b,\tau}(x)$
- Time reversal: $\Theta = UK$

Antiunitary operation!

$\Theta^2 = +1$ : even time reversal, $\Theta^2 = -1$ : odd time reversal

Standard choice: $\Theta = I \otimes (-i\sigma_y)$ with $\Theta^2 = -1$.

## ■ Important property

$$\langle \Theta\psi, \Theta\varphi\rangle = \langle \varphi, \psi\rangle$$

*Consequence of anti-unitarity.*
*Frequently used later.*

Proof)

$$\langle \Theta\psi, \Theta\varphi\rangle = \langle U\psi^*, U\varphi^*\rangle = \langle \psi^*, \varphi^*\rangle = \langle \varphi, \psi\rangle$$

# Kramers' theorem

## ■ Time-reversal symmetry (TRS)

Hamiltonian $H$ commutes with Θ, $[H,\Theta]=0$.

$$UH^*U^\dagger = H$$

*H* is real modulo unitary.

- $H$ has even-TRS if $\Theta^2=+1$.
- $H$ has odd-TRS if $\Theta^2=-1$.

## ■ Theorem

Consider a Hamiltonian $H$ with odd-TRS. The multiplicity of any energy eigenvalue of $H$ must be even.

Proof)

If $\varphi_1$ is an eigenstate of $H$ with energy $E$ ($H\varphi_1=E\varphi_1$), then $\varphi_2=\Theta\varphi_1$ is also an eigenstate of $H$ with energy $E$.

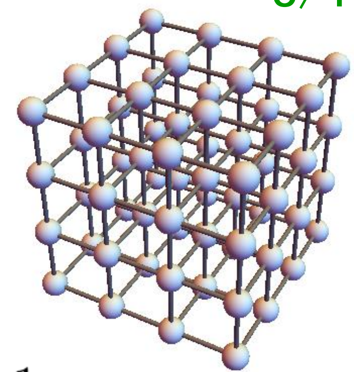
The states $\varphi_1$ and $\varphi_2$ are orthogonal, because

$$\langle\varphi_1,\varphi_2\rangle=\langle\Theta\varphi_2,\Theta\varphi_1\rangle=\langle\Theta^2\varphi_1,\Theta\varphi_1\rangle=-\langle\varphi_1,\Theta\varphi_1\rangle=-\langle\varphi_1,\varphi_2\rangle$$

Property $\langle\Theta\psi,\Theta\varphi\rangle=\langle\varphi,\psi\rangle$

$\Theta^2=-1$

# Lattice model



## ■ Setting

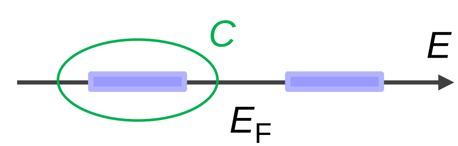
- Lattice $\mathbf{Z}^3$ (infinite cubic lattice)
- Wavefunction $\varphi_{a,\sigma}(x)$ ($a$=1,…,$r$, $\sigma$=↑, ↓, $x\in$ $\mathbf{Z}^3$)
- Tight-binding Hamiltonian $H$ with odd-TRS: $\Theta^2 = -1$
  Short-ranged, may be inhomogeneous
- Dirac operator $D_a(x) := \frac{1}{|x-a|}(x-a)\cdot\gamma$

$a = (1/2, 1/2, 1/2)$ is the origin of the dual lattice $(\mathbf{Z}^3)^*$
$\gamma = (\sigma_1, \sigma_2, \sigma_3)$ acts on the auxiliary space ($\mathbb{C}^2$).

$$(D_a)^\dagger = D_A$$
$$(D_a)^2 = 1$$

## ■ Fermi projection

Assumption: Fermi level $E_F$ lies in the gap.
Projection to the states below $E_F$




$$P_F = \frac{1}{2\pi i}\oint_C (z-H)^{-1} dz$$

$$(P_F)^2 = P_F$$

# Index of a pair of projections

## ■ *A* and *B* operators

$$A := P - Q, \quad B := 1 - P - Q$$

*P* and *Q* : projections
$P^2 = P, \quad Q^2 = Q$

i) $A^2 + B^2 = 1$ (Kato, 1955)

ii) $\{A,\, B\} = AB + BA = 0$ (Avron-Seiler-Simon, 1993)

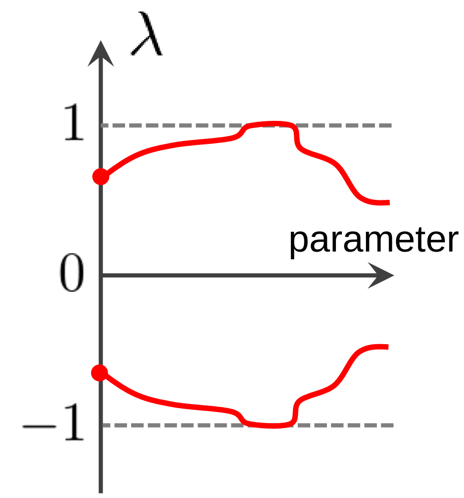
Proof) Almost trivial! Just use $P^2 = P, \quad Q^2 = Q$.

## ■ Relative index

$$\mathrm{Ind} = \dim\ker\,(A-1) - \dim\ker\,(A+1)$$

- SUSY structure
  Suppose $A\varphi_1 = \lambda\varphi_1$. Then $\varphi_2 := B\varphi_1$ satisfies $A\varphi_2 = -\lambda\varphi_2$ and $\varphi_2 \neq 0$ when $\lambda \neq \pm 1$.

$$\langle\varphi_2, \varphi_2\rangle = \langle\varphi_1, B^2\varphi_1\rangle = (1-\lambda^2)\,\langle\varphi_1, \varphi_1\rangle$$




- Eigenvalues $\pm\lambda$ come in pairs! $(|\lambda| \neq 1)$
  Index (Ind) is a topological Invariant.

# What does time-reversal symmetry imply?

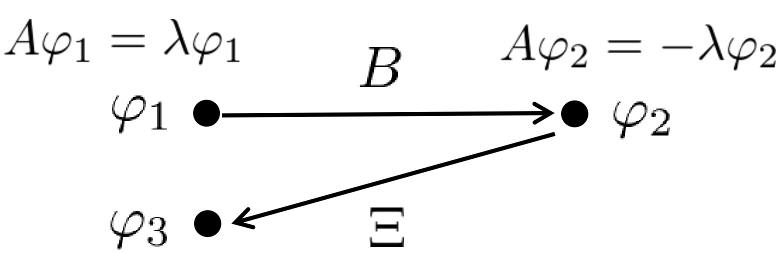
- Anti-unitary operator $\Xi$

$$\{\Xi, A\} = [\Xi, B] = 0, \quad \Xi^2 = -1.$$

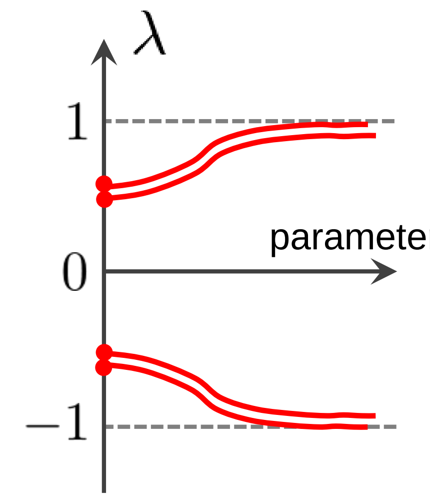
Suppose we have such $\Xi$ and $A\varphi_1 = \lambda\varphi_1$.
Then $\varphi_2' := \Xi\varphi_1$ is nonzero and satisfies $A\varphi_2' = -\lambda\varphi_2'$.

Eigenvalues $\pm\lambda$ come in pairs! Also applies to $\lambda = \pm 1$.
$\dim\ker(A-1) - \dim\ker(A+1)$ vanishes identically…

- Doublet structure




*λ=±1 is always pair-created or annihilated!*




- $\varphi_1$ and $\varphi_3$ are degenerate eigenstates of *A*.
- Orthogonality: $\langle\varphi_1, \varphi_3\rangle = \langle\Xi\varphi_3, \Xi\varphi_1\rangle = -\langle B\varphi_1, \Xi\varphi_1\rangle = -\langle\varphi_1, \varphi_3\rangle$
- The dimension of the eigenspace of λ is even unless λ=±1.
  ⇒ dim ker (*A*-1) is invariant modulo 2.

# $Z_2$ index for 3D class AII models

## Identification

Let's take $P = P_{\mathrm{F}}, \quad Q = D_a P_{\mathrm{F}} D_a, \quad \Xi = D_a \sigma_2 \Theta$

They satisfy all the desired algebraic relations.

$A = P_{\mathrm{F}} - D_a P_{\mathrm{F}} D_a$ can be used to define topo. invariant!

## $Z_2$ index

$$\mathrm{Ind}(P_{\mathrm{F}}, D_a P_{\mathrm{F}} D_a) := \dim\ker(\underbrace{P_{\mathrm{F}} - D_a P_{\mathrm{F}} D_a}_{A} - 1) \mod 2$$

Index = #(eigenstates of *A* with eigenvalue $\lambda = 1$) mod 2.

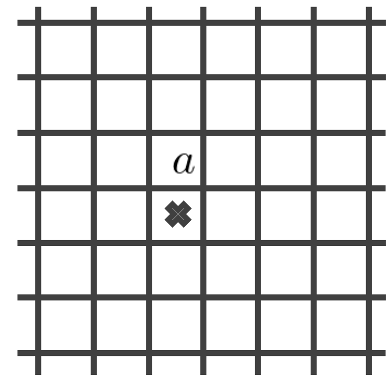
**The index is 0 (trivial) or 1 (topological), and**

- Quantized without ensemble average
- Robust against any odd-TRS perturbations (min-max thm.)
- But meaningful only in the infinite-volume limit
- A truncated version is very useful in numerics

# $\mathbf{Z}_2$ index for 2D class AII models

## ■ Setting

- Lattice $\mathbf{Z}^2$ (infinite square lattice), dual lattice $(\mathbf{Z}^2)^*$
- Tight-binding Hamiltonian *H* with odd-TRS:
  Short-ranged, may be inhomogeneous $\Theta^2 = -1$
- Dirac operator $$D_a(x) := \frac{1}{|x-a|}(x-a)\cdot\gamma$$




$\gamma = (\sigma_1, \sigma_2)$ acts on the auxiliary space ($\mathbb{C}^2$).

## ■ $\mathbf{Z}_2$ index

$$\mathrm{Ind} = \frac{1}{2}\dim\ker\left[\sigma_3(P_{\mathrm{F}} - D_a P_{\mathrm{F}} D_a) - 1\right] \mod 2$$

$$= \dim\ker\left(P_{\mathrm{F}} - \mathcal{D}_a^* P_{\mathrm{F}} \mathcal{D}_a - 1\right) \mod 2$$

$$D_a = \begin{pmatrix} 0 & \mathcal{D}_a^* \\ \mathcal{D}_a & 0 \end{pmatrix}$$

$$\mathcal{D}_a^*\mathcal{D}_a = \mathcal{D}_a\mathcal{D}_a^* = 1$$

**The index is 0 or 1, and**

- Quantized without ensemble average
- Robust against any odd-TRS perturbations

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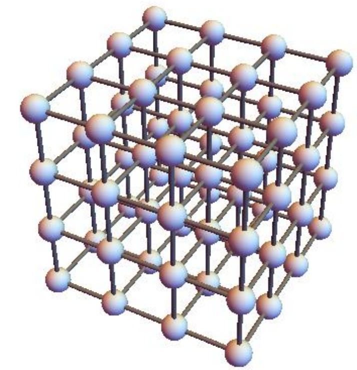
# 3D Wilson-Dirac model

## ■ Hamiltonian

A prototypical model of 3D class AII TI.
X-L. Qi *et al*., *PRB* **78** (2008); K.G. Wilson, *PRD* **10** (1974).



$$H = H_0 + H_{\rm hop} + H_{\rm dis},$$

$$H_0 = \sum_{\boldsymbol{x}} \sum_{\mu=1,2,3} \left[ c^\dagger_{\boldsymbol{x}+\boldsymbol{e}_\mu} \left( \frac{it}{2}\alpha_\mu - \frac{m_2}{2}\beta \right) c_{\boldsymbol{x}} + \text{h.c.} \right] + (m_0 + 3m_2) \sum_{\boldsymbol{x}} c^\dagger_{\boldsymbol{x}} \beta c_{\boldsymbol{x}},$$

$$H_{\rm hop} = t_0 \sum_{\boldsymbol{x}} \sum_{\mu=1,2,3} (c^\dagger_{\boldsymbol{x}+\boldsymbol{e}_\mu} c_{\boldsymbol{x}} + \text{h.c.}),$$

$$H_{\rm dis} = \sum_{\boldsymbol{x}} v_{\boldsymbol{x}}\, c^\dagger_{\boldsymbol{x}} c_{\boldsymbol{x}}. \qquad v_{\boldsymbol{x}} \in \left[ -\frac{W}{2}, \frac{W}{2} \right]$$

Spin and orbital (in total 4) degrees of freedom at each site.

$$c^\dagger_{\boldsymbol{x}} = (c^\dagger_{\boldsymbol{x}1\uparrow}, c^\dagger_{\boldsymbol{x}1\downarrow}, c^\dagger_{\boldsymbol{x}2\uparrow}, c^\dagger_{\boldsymbol{x}2\downarrow})$$

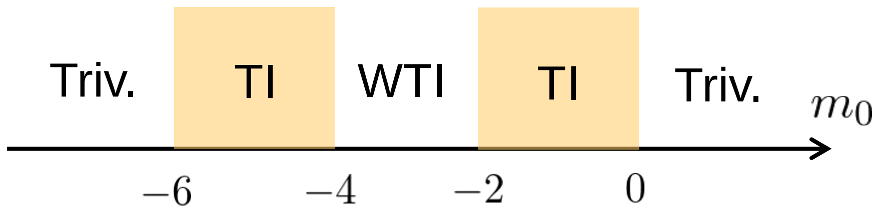
Gamma matrices: $\alpha_\mu = \sigma_1 \otimes \sigma_\mu \quad (\mu = 1, 2, 3), \quad \beta = \sigma_3 \otimes \sigma_0$
($\sigma_0$: 2x2 identity)

NOTE) In the continuum limit, $H_0$ reduces to $\mathcal{H}_0 = -i\, \partial_k\, \alpha_k + m\beta$

# Phase diagram

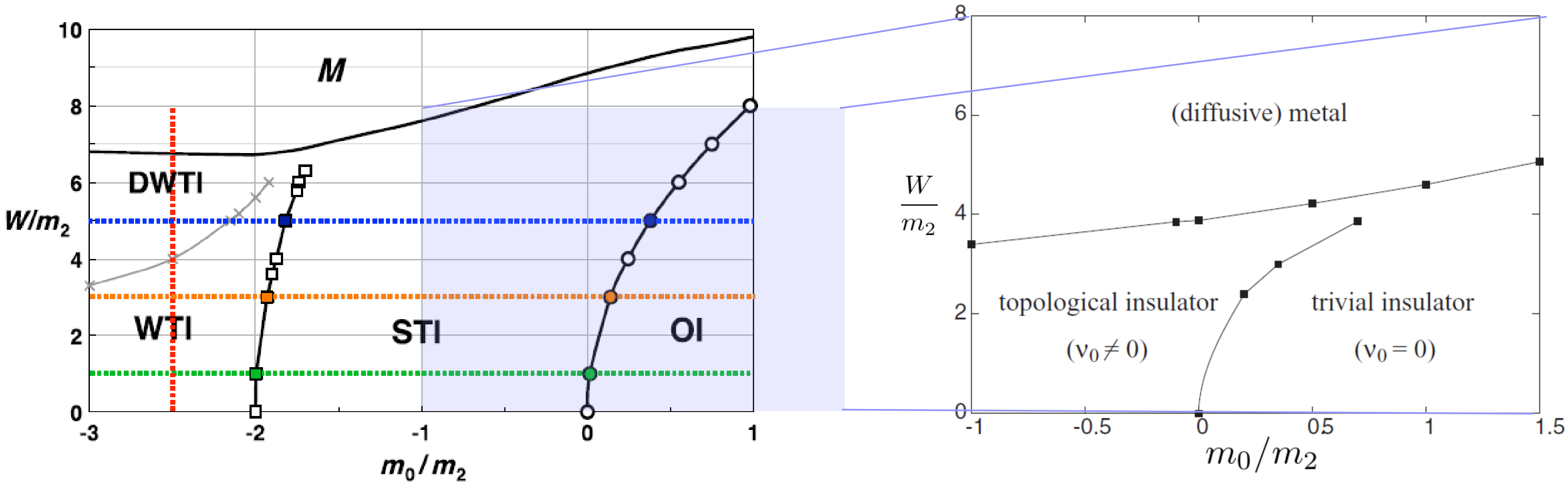
■ Uniform case

$m_2$ =1, $t$ =2, $t_0$=0 ($E_F$=0)



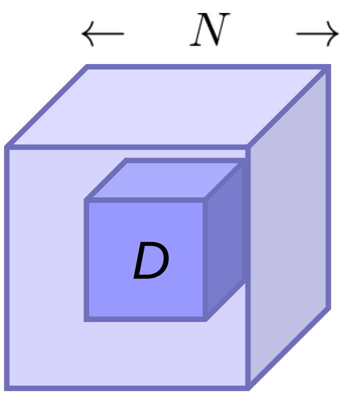

■ Disordered case

Transfer matrix studies:
Kobayashi, Ohtsuki, Imura, *PRL* **110**, 236803 (2013).
Ryu and Nomura, *PRB* **85**, 155138 (2012).



# Numerical result (1)

■ Finite-size approximation of $\mathbf{Z}_2$ index




- 3D lattice torus with PBC, $N^3$ sites
- Fermi projection $$P_{\mathrm{F}} = \sum_{E_n < E_{\mathrm{F}}} |\psi_n\rangle\langle\psi_n|$$
- Calculate projection $$A = P_{\mathrm{F}} - D_a P_{\mathrm{F}} D_a$$
- Truncated $A$ supported in domain $D$

$$A \to A_D$$ *D* is chosen, e.g. a cube with linear size $N/2$.

- Compute eigenvalues of $A_D$

■ Uniform case (Warm-up)

***Desired result!***

**dim ker (A-1) mod 2 = 1**

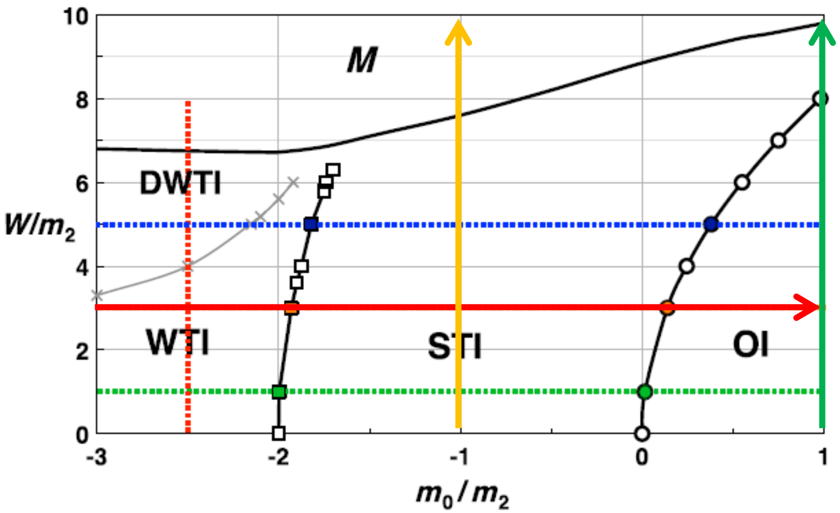
Linear size: $N$ = 12 (1728 sites)

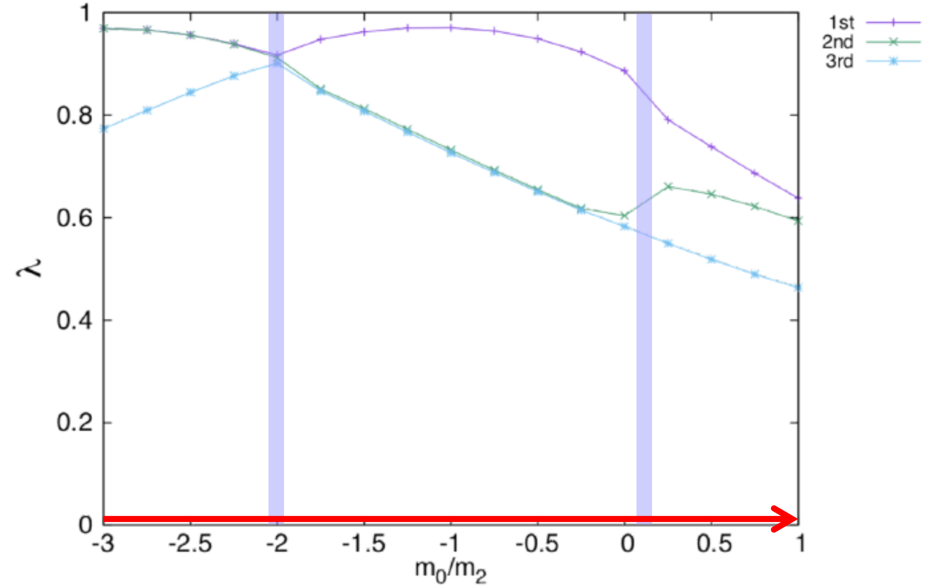
Parameters: $m_2$ =1.0, $t$ =2.0, $m_0$=-1, $t_0$=0.01 ($E_{\mathrm{F}}$=0)

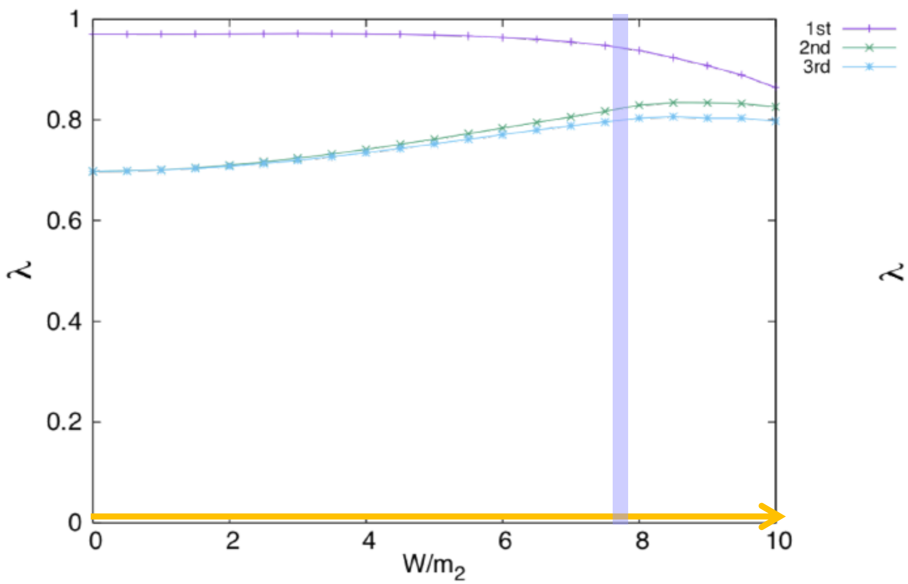
(First few) largest eigenvalues of $A_D$

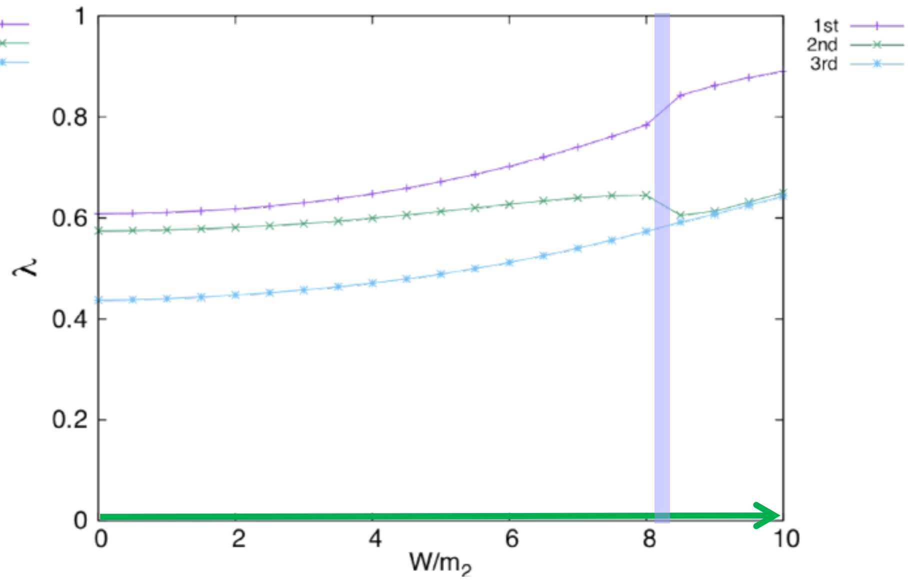
$\{\mathbf{0.99}084, 0.70443, 0.70443, 0.68628, 0.68628, \ldots\}$

# Numerical result (2)



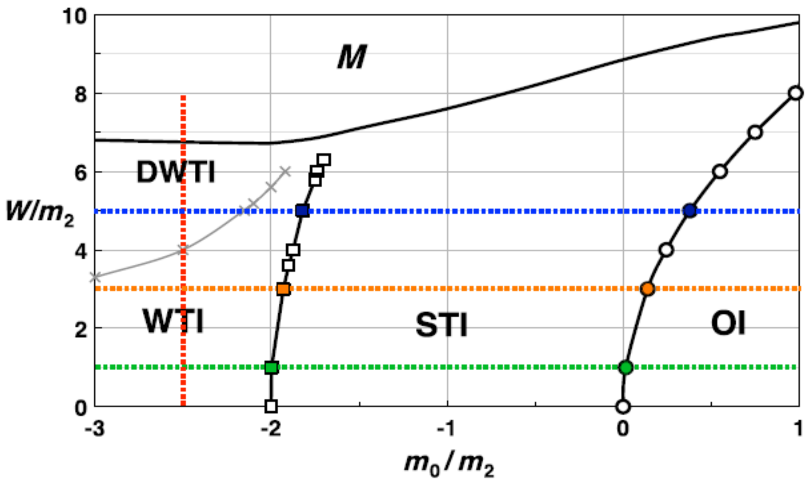



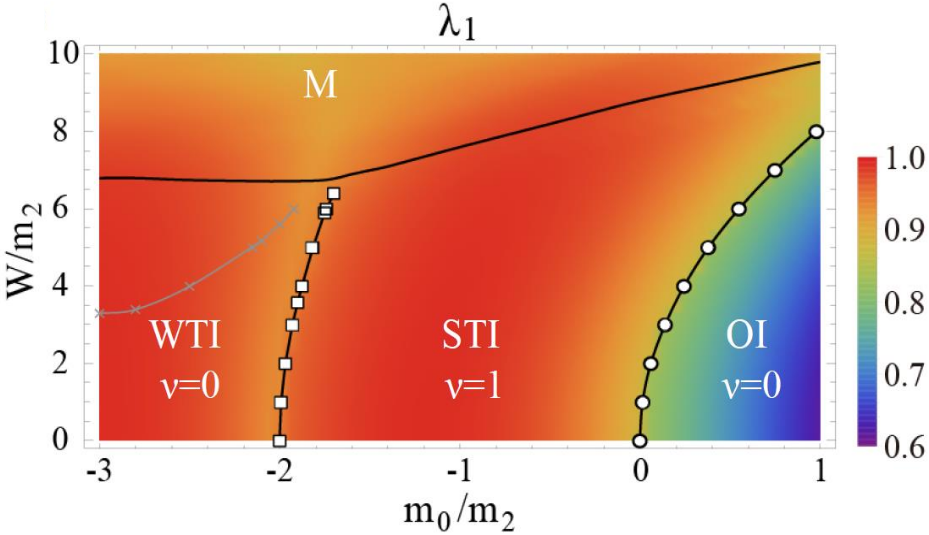



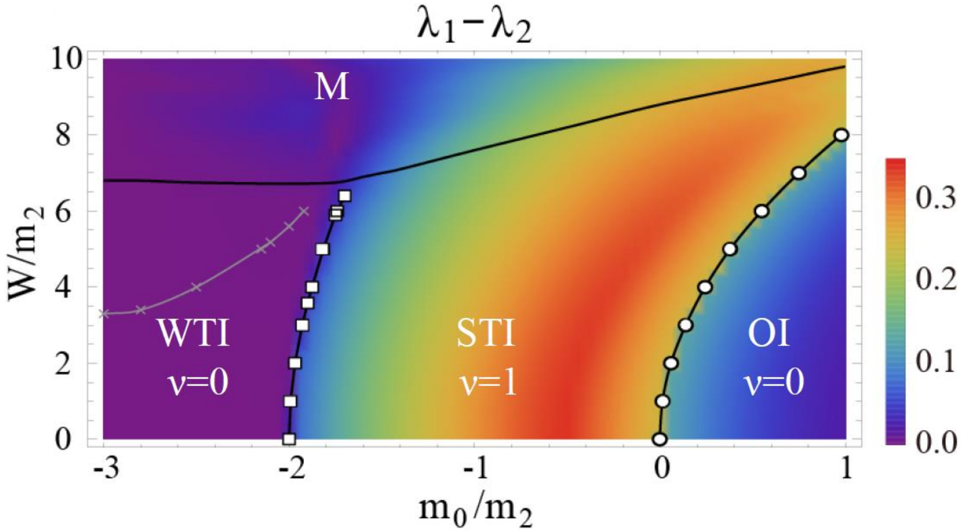



# Phase diagram

$m_2$ =1, $t$ =2, $t_0$=0, $N^3$ =1000 sites.




***Reproduces the phase diagram by Kobayashi et al.!***

# Summary

- Studied 3D disordered insulators with time-reversal symmetry
- Operator theoretic definition of $\mathbf{Z}_2$ index

$$\mathrm{Ind}(P_{\mathrm{F}},\, D_a P_{\mathrm{F}} D_a) := \dim\ker\left(P_{\mathrm{F}} - D_a P_{\mathrm{F}} D_a - 1\right) \mod 2$$

- Proved quantization and robustness
- Application to 3D Wilson-Dirac model

  Reproduced the phase diagram
  obtained by Kobayashi *et al*., *PRB* **85** (2012).

# Future directions

- Characterization of weak TI

  In a WTI phase, numerical result shows dim ker ($A$-1) = 2.
  Why? Can we always distinguish WTI from OI?
  Metallic surface v.s. dark side?

- Other applications

  1D and 2D Wilson-Dirac models. More realistic applications…