Topological Electromagnetic and Thermal Responses of Time-Reversal Invariant Superconductors and Chiral-Symmetric band insulators

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Topological insulator/superconductor

characterized by topological invariant in k-space (BZ) ⟷ Electromagnetic properties
Transport properties

e.g.

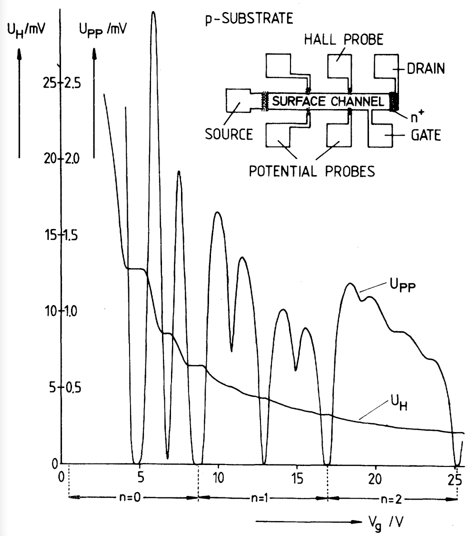
Quantum Hall effect in 2D DEG

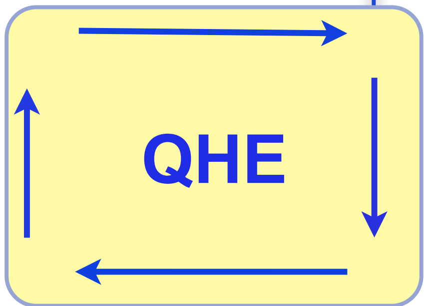
(Thouless, Kohmoto et al.)

first Chern number

$\mathbb{Z}$ ***invariant*** (any integer)

$$\sigma_{xy} = \frac{e^2}{h} \underline{n_c}$$





3D time-reversal invariant topological insulator

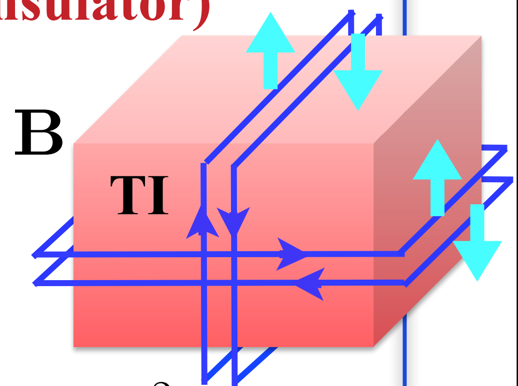
(Kane, Zhang, Qi et al.)

$\mathbb{Z}_2$ ***invariant*** (only two values)

$\theta = 0$ **(trivial insulator)**

or $\theta = \pi$ **(topological insulator)**

$$\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h} \mathbf{E} \cdot \mathbf{B}$$



$$J_x = \frac{e^2}{2\pi h} \theta E_y$$

$$\boldsymbol{M} = -\frac{e^2}{2\pi h} \theta \boldsymbol{E} \quad \boldsymbol{P} = -\frac{e^2}{2\pi h} \theta \boldsymbol{B}$$

• For most classes of TI and TSC, relations between topological invariants characterizing bulk topological features and physically observable quantities have been well clarified.

• However, case of ***Z topological insulators/superconductors in odd spatial dimensions*** has not yet been well understood !

e.g.

✦ **3D TRI topological SC** **(class DIII)**

^{3}He (B phase) **$Cu_xBi_2Se_3$?** *(Fu-Berg, Sasaki et al.)*

Li_2Pt_3B ? (NCS P+s-wave SC)

✦ **1D or 3D topological insulators with chiral symmetry (sub-lattice symmetry)** **(class AIII)**

✦ **Kitaev's Majorana chain (1D spinless p-wave SC)** **(class BDI)**

also, modified Su-Schrieffer-Heeger model

• In this case, ***the topological invariant takes any integer values N***. However, it has not yet been well clarified in what physical quantities this topological invariant can be detected !

$\mathbb{Z}$ Topological insulator/superconductor in odd dimensions

Periodic table of TI and TSC

AZ	Θ	Ξ	Π	1	2	3	e.g.
	Symmetry			spatial dimension			
A	0	0	0	0	$\mathbb{Z}$	0	
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	
AI	1	0	0	0	0	0	
BDI	1	1	1	$\mathbb{Z}$	0	0	**Kitaev model**
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	**^3He Li_2Pt_3B $Cu_xBi_2Se_3$**
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	
C	0	-1	0	0	$\mathbb{Z}$	0	
CI	1	-1	1	0	0	$\mathbb{Z}$	

(Schnyder et al., Kitaev)

Θ Time-reversal sym.

Ξ Charge conjugation (particle-hole sym.) [superconductivity]

$\Pi = \Theta\Xi$ Chiral sym. (sublattice sym.)

Z invariant in odd dimensions:

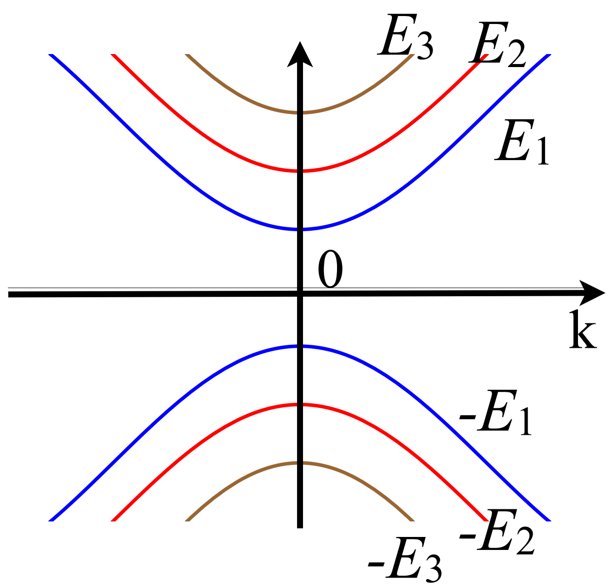
winding number

arises from *chiral symmetry*

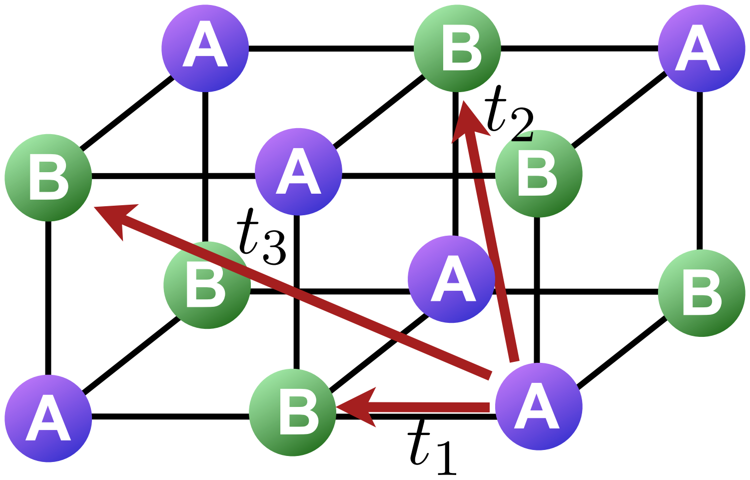
$$\mathcal{H}\Pi = -\Pi\mathcal{H}$$

$$\mathcal{H}\psi = E\psi$$

$$\mathcal{H}\Pi\psi = -E\Pi\psi$$



An example of 3D class AIII topological insulator



- Band insulator on cubic lattice with AB sublattice
- Electron hopping is only between A- and B-sublattices
- Energy levels at A (E_A) and B (E_B) sites are equal (put 0)

$$
\begin{array}{cc}
 & \begin{array}{cc} |\mathrm{A}\rangle & |\mathrm{B}\rangle \end{array} \\
\mathcal{H} = & \begin{pmatrix} 0 & q(\boldsymbol{k}) \\ q^\dagger(\boldsymbol{k}) & 0 \end{pmatrix} \begin{array}{c} |\mathrm{A}\rangle \\ |\mathrm{B}\rangle \end{array}
\end{array}
$$

$$q(\boldsymbol{k}) = A(\boldsymbol{k}) + \boldsymbol{\sigma} \cdot \boldsymbol{B}(\boldsymbol{k})$$

$$
\begin{aligned}
A(\boldsymbol{k}) = &-8t_2 \cos k_x \cos k_y \cos k_z \\
&-4t_3[\cos k_x(\cos 2k_y + \cos 2k_z) \\
&+\cos k_y(\cos 2k_z + \cos 2k_x) \\
&+\cos k_z(\cos 2k_x + \cos 2k_y)]
\end{aligned}
$$

$$\boldsymbol{B}(\boldsymbol{k}) = it_1(\sin k_x, \sin k_y, \sin k_z)$$

(arise from SO int.+ magnetic order)

chiral symmetry $\mathcal{H}\Pi = -\Pi\mathcal{H}$ ⟷ *There is no diagonal element of* $\mathcal{H}$ *in AB sub-lattice space (sub-lattice symmetry)*

$$\Pi = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

3D TRI (class DIII) topological superconductor

^3He $Cu_xBi_2Se_3$ Li_2Pt_3B (NCS P+s-wave SC)

There is no explicit sub-lattice structure

chiral symmetry ⟷ *combination of time-reversal symmetry and particle-hole symmetry*

$$E \longleftrightarrow -E \qquad E \xleftrightarrow{\text{TRS}} E \xleftrightarrow{\text{PHS}} -E$$

$$\boldsymbol{k} \longleftrightarrow \boldsymbol{k} \qquad \boldsymbol{k} \longleftrightarrow -\boldsymbol{k} \longleftrightarrow \boldsymbol{k}$$

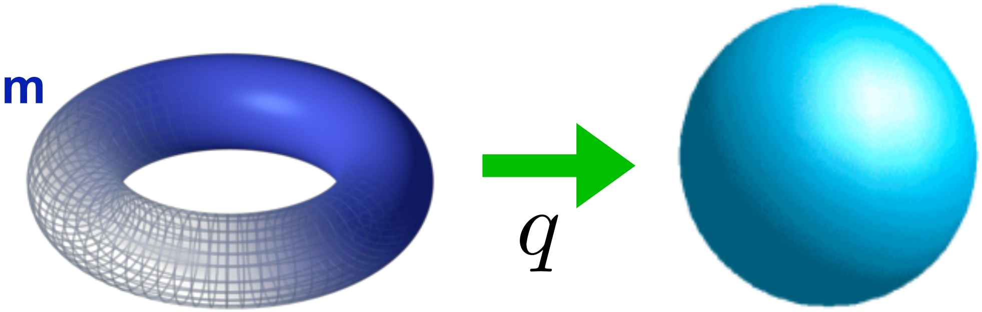
Z invariant in odd dimensional TI / TSC: winding number *N*

3D case $$N = \frac{\epsilon_{\mu\nu\lambda}}{24\pi^2}\int d\boldsymbol{k}\,\mathrm{tr}[q\partial_{k_\mu}q^\dagger q\partial_{k_\nu}q^\dagger q\partial_{k_\lambda}q^\dagger]$$ **e.g. He^3, Li_2Pt_3B etc.**

for ^{3}He (B phase) $$q = \frac{\varepsilon_{\boldsymbol{k}} + i\boldsymbol{d}(\boldsymbol{k})\cdot\boldsymbol{\sigma}}{\sqrt{\varepsilon_{\boldsymbol{k}}^2 + |\boldsymbol{d}(\boldsymbol{k})|^2}}$$

$\boldsymbol{d}(\boldsymbol{k}) = (d_x, d_y, d_z)$ **: d-vector of SC**

3D momentum space (Brillouin zone)



3D sphere

$\boldsymbol{n}_{\boldsymbol{k}}/|\boldsymbol{n}_{\boldsymbol{k}}|$

$\boldsymbol{n}_{\boldsymbol{k}} = (\varepsilon_{\boldsymbol{k}}, d_x, d_y, d_z)$

- ***N*** **is the winding of the mapping from 3D BZ to 3D sphere homeomorphic to the Hilbert space of class AIII TI and class DIII TSC**

- ***N*** **is the total number of gapless surface Dirac (Majorana) fermions**

- **How does the winding number *N* appear in electromagnetic or thermal responses and transport phenomena ?**

Effective low energy theory for Z topological insulator in 3 D

Ryu et al., Qi et al.

3D class AIII top. insulator

$$\mathcal{L}_{\text{eff}} = \frac{\theta e^2}{2\pi h} \boldsymbol{E} \cdot \boldsymbol{B}$$

$$\theta = 0 \text{ or } \pi \pmod{2\pi}$$

because of chiral symmetry

e.g. Quantum anomalous Hall effect

$$J_x = \frac{e^2}{2\pi h} \theta E_y$$

Magnetoelectric effect

$$\boldsymbol{M} = -\frac{e^2}{2\pi h} \theta \boldsymbol{E} \quad \boldsymbol{P} = -\frac{e^2}{2\pi h} \theta \boldsymbol{B}$$

in analogy with Axion electrodynamics of 3D TRI Z_2 top. insulators

✦ **However, only Z_2 part ($\theta = 0$ or π) is captured.**

✦ **The Z invariant *N* (winding number taking any integer) is actually the number of topologically protected gapless surface modes. However, it is hidden in the above electromagnetic responses.**

✦ **Is it possible to detect the Z invariant *N* in any electromagnetic responses ?**

Effective low energy theory for Z topological superconductor in 3D

Ryu et al., Qi et al.

3D TRI (class DIII) top. superconductor ***basically, spin-triplet SC***

Since charge and spin are not conserved, topological characters (quantization of physical quantities) do not appear in electromagnetic responses

$\longleftrightarrow$ **surface gapless states are Majorana fermions**

However, instead, topological characters appear in *thermal responses*, because of energy conservation

Thermal responses $\longrightarrow$ ***gravitational field theory***

$\frac{E}{c^2}$ **couples to gravity potential** ϕ_g *(Luttinger (1964))*

$\boldsymbol{E}_g = \nabla \phi_g$ **gravitoelectric field** $\sim -\frac{\nabla T}{T}$

$\boldsymbol{B}_g$ **gravitomagnetic field** **associated with circulating heat (energy) current**

Effective low energy theory for Z topological superconductor in 3D

Ryu et al., Qi et al., Nomura et al.

gravitational field theory for low-energy effective theory of TRI TSC in 3D

$$\mathcal{L} = \frac{\pi k_B^2 T^2}{12h} \theta \boldsymbol{B}_g \cdot \boldsymbol{E}_g$$

$$\theta = 0 \text{ or } \pi \quad (\text{mod } 2\pi)$$

Thermal responses !

$\boldsymbol{E}_g$ **gravitoelectric field** $\sim -\frac{\nabla T}{T}$

$\boldsymbol{B}_g$ **gravitomagnetic field**

e.g. Quantum anomalous thermal Hall effect

$$J_x^{\mathrm{H}} = -\frac{\pi k_B^2 T}{12h} \theta \frac{\partial T}{\partial y}$$

Thermal-analogue of ME effect

$$\boldsymbol{M}^{\mathrm{H}} = -\frac{\pi k_B^2 T^2}{12h} \theta \boldsymbol{E}_g$$

$$\boldsymbol{P}^{\mathrm{H}} = -\frac{\pi k_B^2 T^2}{12h} \theta \boldsymbol{B}_g$$

in analogy with Axion electrodynamics of 3D TRI Z_2 top. insulators

✦ **However, only Z_2 part ($\theta = 0$ or π) is captured.
Incomplete description for Z topological features !**

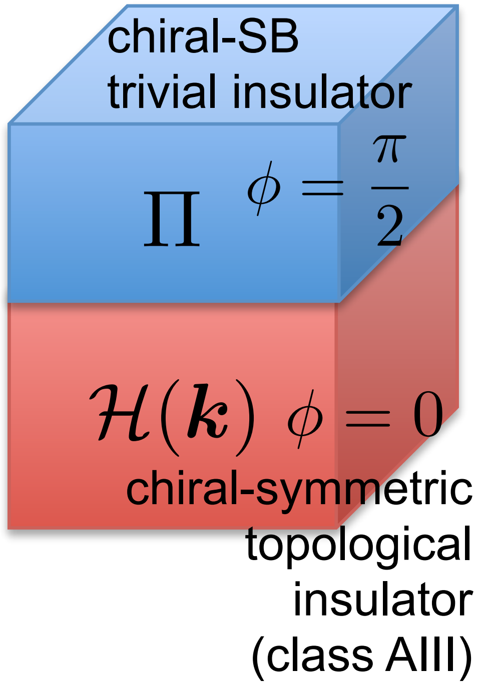
✦ **Is it possible to detect the Z invariant *N* in any thermal responses ?**

Electromagnetic and thermal responses which characterize Z topological non-triviality of class AIII TIs and class DIII TSCs : An idea using heterostructure systems

Basic Key Idea:

in 3D cases, we can make a connection between the winding number *N* and θ of the axion field theory by considering ***spatially (temporally) varying systems*** (e.g. heterostructure systems), which consist of ***chiral-symmetric topological insulators (or superconductors)*** and ***chiral-symmetry-broken trivial insulators (or superconductors)***.

$$\int_0^{\frac{\pi}{2}} \frac{d\phi}{2\pi} \frac{d\theta(\phi)}{d\phi} = \frac{N}{2}$$



Hamiltonian for heterostructure systems

$$\tilde{\mathcal{H}}(\phi) = \mathcal{H}\cos\phi + \Pi\sin\phi$$

$$\phi = \phi(\boldsymbol{r}, t) \qquad 0 \leq \phi \leq \frac{\pi}{2}$$

$\mathcal{H}(\boldsymbol{k})$: Hamiltonian of class AIII topological insulator in 3D

$$\mathcal{H}\Pi = -\Pi\mathcal{H}$$

$$\Pi = \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}$$ itself is the chiral-symmetry breaking field.

Quantum anomalous Hall effect

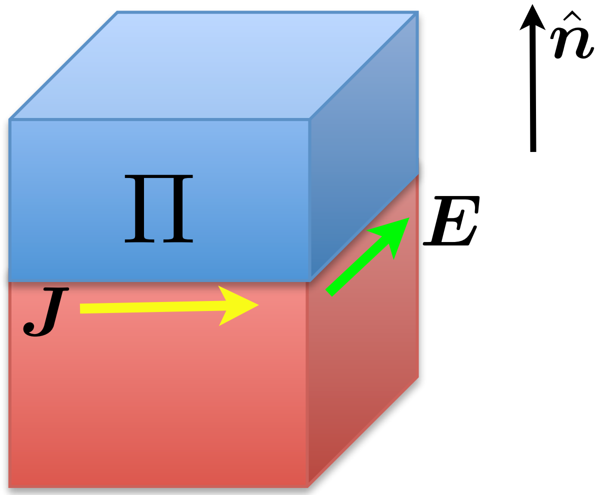
$$\boldsymbol{J}_{\rm total} = \int_0^{\frac{\pi}{2}} d\phi \frac{d\boldsymbol{J}(\phi)}{d\phi} = \frac{e^2}{2h} N \hat{\boldsymbol{n}} \times \boldsymbol{E}$$

(from axion EM)

$$\boldsymbol{J} = \frac{e^2}{2\pi h} \int dz \nabla_z \theta \times \boldsymbol{E}$$

$$\int_0^{\frac{\pi}{2}} \frac{d\phi}{2\pi} \frac{d\theta(\phi)}{d\phi} = \frac{N}{2}$$

$\phi = \frac{\pi}{2}$ chiral-SB trivial insulator



$\phi = 0$ class AIII topological insulator

Hall current carried by surface states

surface mode gives quantized conductivity

$$\Pi = \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}$$

energy level difference between A-B sublattices

Topological magnetoelectric effect

$$\boldsymbol{M}_{\text{total}} = \int_0^{\frac{\pi}{2}} d\phi \frac{d\boldsymbol{M}(\phi)}{d\phi} = -\frac{e^2}{2h} \underline{N} \boldsymbol{E}$$

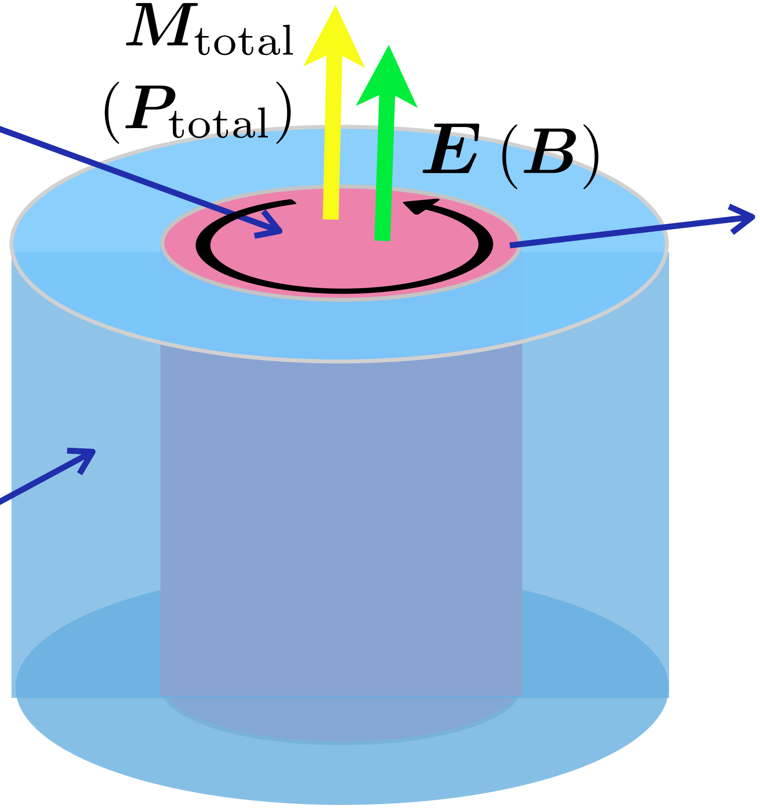
$$\boldsymbol{P}_{\text{total}} = \int_0^{\frac{\pi}{2}} d\phi \frac{d\boldsymbol{P}(\phi)}{d\phi} = -\frac{e^2}{2h} \underline{N} \boldsymbol{B}$$

axion EM

$$\boldsymbol{M} = -\frac{e^2}{2\pi h} \theta \boldsymbol{E}$$

$$\boldsymbol{P} = -\frac{e^2}{2\pi h} \theta \boldsymbol{B}$$

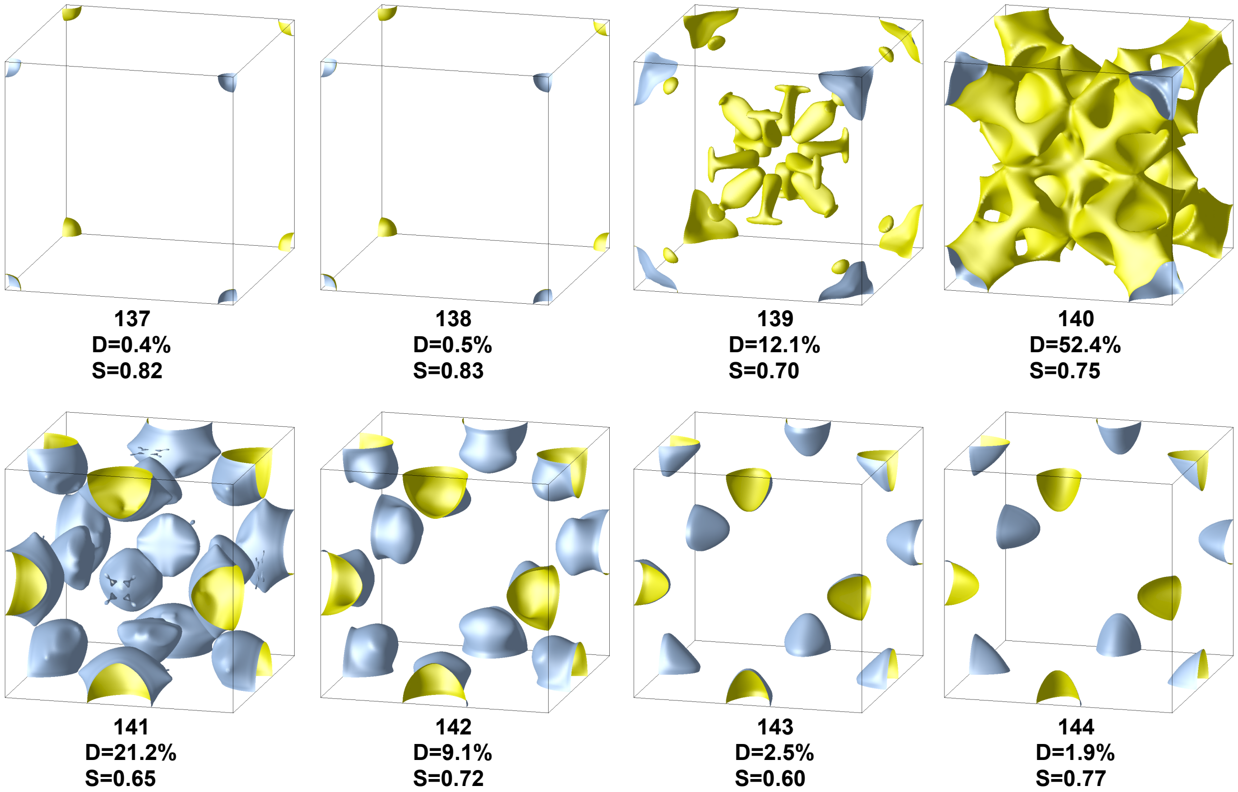
$$\int_0^{\frac{\pi}{2}} \frac{d\phi}{2\pi} \frac{d\theta(\phi)}{d\phi} = \frac{N}{2}$$



Case of class DIII (TRI) topological superconductor

- ^3He (BW phase) 1-band with spins spherical Fermi surface → winding number N=1
- $Cu_xBi_2Se_3$ (p-wave SC) 1-band with spins → winding number N=1 ?
- Li_2Pt_3B (noncentrosymmetric P+s-wave SC)

  4 band systems with SO split pairs → winding number N>1 (or < -1)



(Shishidou and Oguchi)

Case of class DIII (TRI) topological superconductor

What is chiral-symmetry-breaking perturbation ?

3D p-wave SC (BW-phase)

$$\mathcal{H} = \begin{pmatrix} \varepsilon_{\boldsymbol{k}} & \boldsymbol{d}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma} i\sigma_y \\ -i\sigma_y \boldsymbol{d}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma} & -\varepsilon_{\boldsymbol{k}} \end{pmatrix} \xrightarrow{\text{change basis}} \mathcal{H} = \begin{pmatrix} 0 & q(\boldsymbol{k}) \\ q^\dagger(\boldsymbol{k}) & 0 \end{pmatrix}$$

$$\boldsymbol{d}_{\boldsymbol{k}} \propto \boldsymbol{k}$$

s-wave gap

$$\mathcal{H}' = \begin{pmatrix} 0 & \Delta_s i\sigma_y \\ -\Delta_s^* i\sigma_y & 0 \end{pmatrix} \longrightarrow \mathcal{H}' = i\frac{\Delta_s - \Delta_s^*}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Delta_s \neq \Delta_s^*$$

chiral-symmetry breaking field is

Time reversal symmetry breaking s-wave SC gap !

Quantum anomalous thermal Hall effect

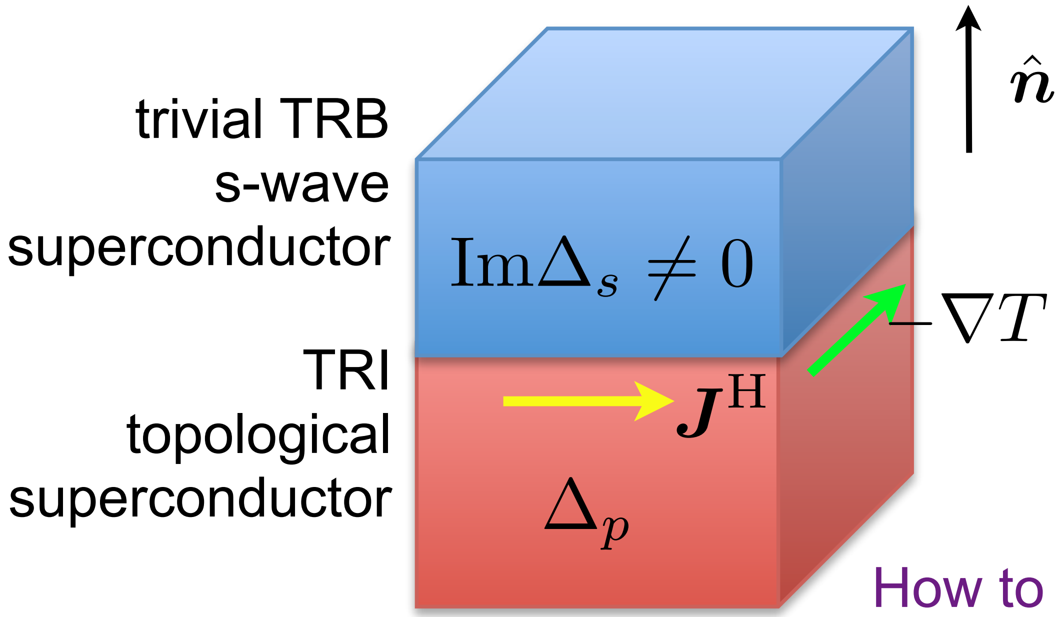
$$\boldsymbol{J}^{\mathrm{H}}_{\mathrm{total}} = \frac{\pi^2 k_{\mathrm{B}}^2 T^2}{12h} \underline{N} \hat{\boldsymbol{n}} \times \boldsymbol{E}_g$$
$$= -\frac{\pi^2 k_{\mathrm{B}}^2 T}{12h} \underline{N} \hat{\boldsymbol{n}} \times \nabla T$$

N: winding number

$$\int_0^{\frac{\pi}{2}} \frac{d\phi}{2\pi} \frac{d\theta(\phi)}{d\phi} = \frac{N}{2}$$

c.f. axion gravitational field theory

$$J^{\mathrm{H}}_x = -\frac{\pi k_{\mathrm{B}}^2 T}{12h} \theta \frac{\partial T}{\partial y}$$



Heat Hall current carried by surface states

How to realize phase difference ?

- bias between s-wave SC and TSC
- dynamical effect, $\mathrm{Im}\Delta_s(\omega) \neq 0$ for $\omega \neq 0$ due to inelastic scattering

c.f. *Wang, Qi, Zhang*, similar result based on argument of surface Majorana fermions.

Topological gravitomagnetoelectric effect
(Thermal analogue of topological magnetoelectric effect)

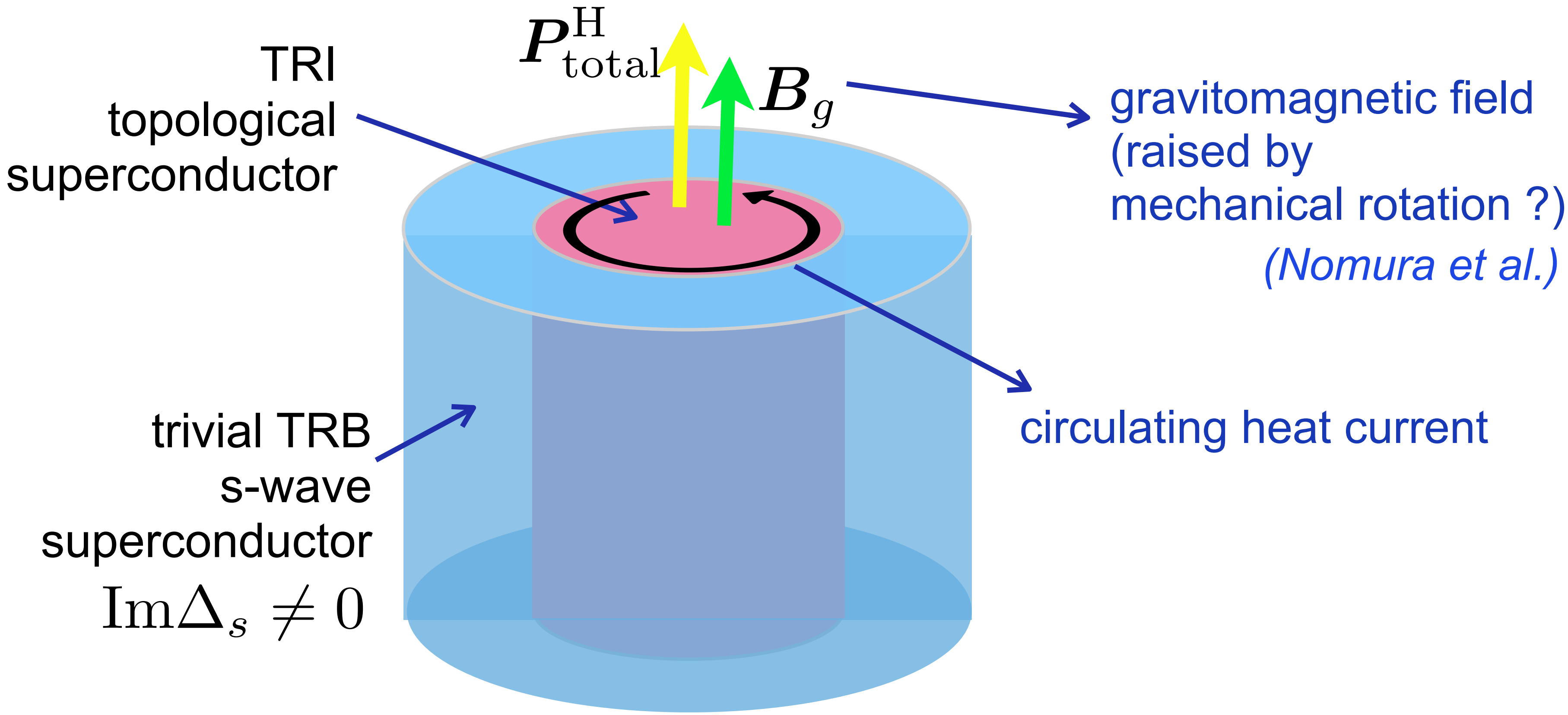
$$\boldsymbol{P}^{\mathrm{H}}_{\mathrm{total}} = -\frac{\pi^2 k_{\mathrm{B}}^2 T^2}{12h} \underline{N} \boldsymbol{B}_g$$

N: winding number

c.f. axion gravitational field theory

$$\boldsymbol{P}^{\mathrm{H}} = -\frac{\pi k_{\mathrm{B}}^2 T^2}{12h} \theta \boldsymbol{B}_g$$

$\boldsymbol{P}^{\mathrm{H}}$: heat polarization which induces temperature gradient ∇T



Implications for dynamical axion

K. Shiozaki, S.F.,
poster presentation on 13 June

TRI topological insulator — magnetic fluctuations → dynamical axion

(Li,Wang,Qi,Zhang) *break quantization of* θ

TRI topological SC — fluctuations of TRSB s-wave OP → dynamical axion

Case of non-centrosymmetric SC

admixture of p-wave gap $\Delta_p e^{i\phi_p}$ and s-wave gap $\Delta_s e^{i\phi_s}$

relative phase fluctuation a la Leggett mode $\delta\phi_p - \delta\phi_s$
is dynamical axion !!

Bulk electromagnetic responses characterizing Z topological non-triviality : Chiral charge polarization

Chiral charge polarization: bulk quantity related to the winding number

$$\boldsymbol{P}^5 = -e \sum_{n \in occ} \langle w_{n\boldsymbol{R}} | \Pi \hat{\boldsymbol{r}} | w_{n\boldsymbol{R}} \rangle$$

c.f. charge polarization:

$$\boldsymbol{P} = -e \sum_{n \in occ} \langle w_{n\boldsymbol{R}} | \hat{\boldsymbol{r}} | w_{n\boldsymbol{R}} \rangle$$

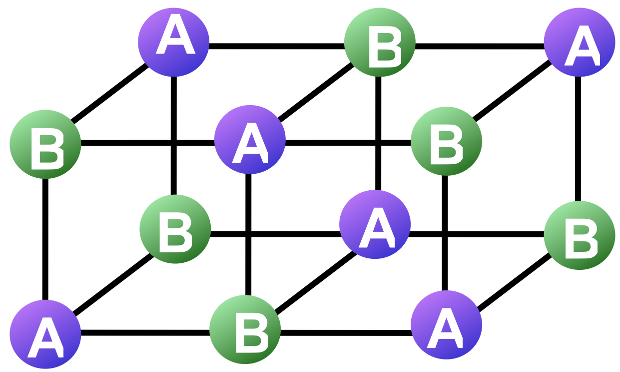
$|w_{n\boldsymbol{R}}\rangle$: Wannier func.

Π : operator for chiral symmetry

For class AIII systems, $\boldsymbol{P}^5$ is the difference of the charge polarization between A-sublattice and B-sublattice

$$\begin{array}{cc} & \begin{array}{cc} |\mathrm{A}\rangle & |\mathrm{B}\rangle \end{array} \\ \mathcal{H} = & \begin{pmatrix} 0 & q(\boldsymbol{k}) \\ q^\dagger(\boldsymbol{k}) & 0 \end{pmatrix} \begin{array}{c} |\mathrm{A}\rangle \\ |\mathrm{B}\rangle \end{array} \end{array}$$

$$\Pi = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



$\boldsymbol{P}^5$ ***is gauge-invariant even for periodic B.C. !***

$\longleftrightarrow$ polarization is gauge-dependent

Chiral charge polarization: bulk quantity related to the winding number

1D case **(class AIII, class BDI)**

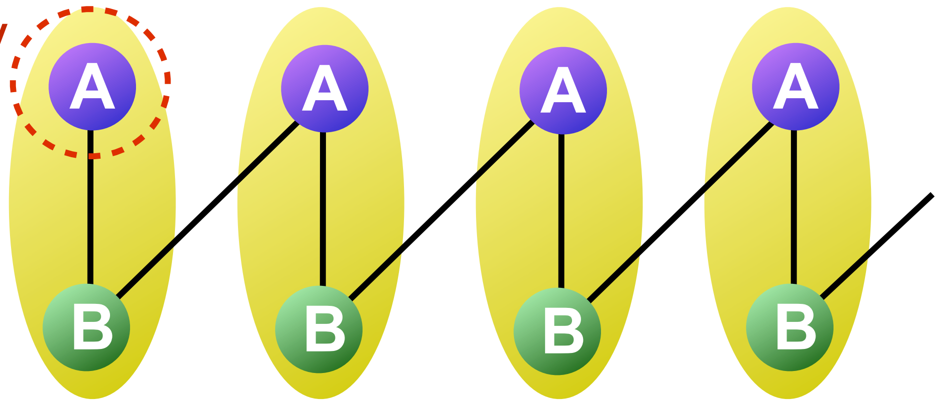
chiral polarization is indeed equivalent to the winding number !

$$P^5 = -e \sum_{n \in occ} \langle w_{n\boldsymbol{R}} | \Pi \hat{x} | w_{n\boldsymbol{R}} \rangle = -e \frac{N}{2}$$

$$N = \frac{1}{2\pi i} \int d\boldsymbol{k} \mathrm{tr}[q \partial_k q^\dagger]$$ winding number in 1D

$\boldsymbol{P}^5$ corresponds to fractional charge (or # of Majorana fermions) emergent at open edges

zero-energy edge state



modified SSH model

Kitaev's Majorana chain model

Chiral charge polarization: bulk quantity related to the winding number

3D class AIII

$\boldsymbol{P}^5$ is induced by an applied magnetic field, and, remarkably, related to the bulk winding number !!

$$\boldsymbol{P}^5 = -\frac{e^2}{2h} N \boldsymbol{B}$$

N : winding number

Topological magnetoelectric effect

- This relation is obtained by first-order perturbative calculation
- $\boldsymbol{P}^5$ is gauge-invariant. (uniquely defined without heterostructure!)

$\Updownarrow$

Topological ME effect from axion field theory (only Z_2 part)

$$\boldsymbol{P} = -\frac{e^2}{2\pi h} \theta \boldsymbol{B} \qquad \theta = \pi \pmod{2\pi}$$ (gauge-dependent)

Summary

(i) The Z topological invariant in 3D can be observed in the quantum anomalous (thermal) Hall effect and topological (gravito-) magnetoelectric effects in heterostructure systems which consist of the chiral-symmetric TI (TRI TSC) and chiral-symmetry-broken trivial insulators (superconductors).

(ii) In 3D class AIII TI, the winding number appears in chiral charge polarization induced by an applied magnetic field.

$$\boldsymbol{P}^5 = -\frac{e^2}{2h} N \boldsymbol{B}$$