

Many-Body Invariants of

Multipolar Higher-order Topological Insulators

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(POSTECH)



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Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and **GYC**, in progress

Main Research Themes:

1. Developing Novel Theories

for Topological States/Strongly-Correlated States

Ex: new types of quantum field theory (geometric deg. of. freedom)

anomalies, topological field theory, and so on

Today, but no equation/no field theory

2. Designing Models for Topological States

Ex: Topological superconductors [Majorana fermions]

Anyons in fractional quantum Hall states, and/or heterostructures

Contents:

1. Introductions

2. Conjectures & Numerical Results

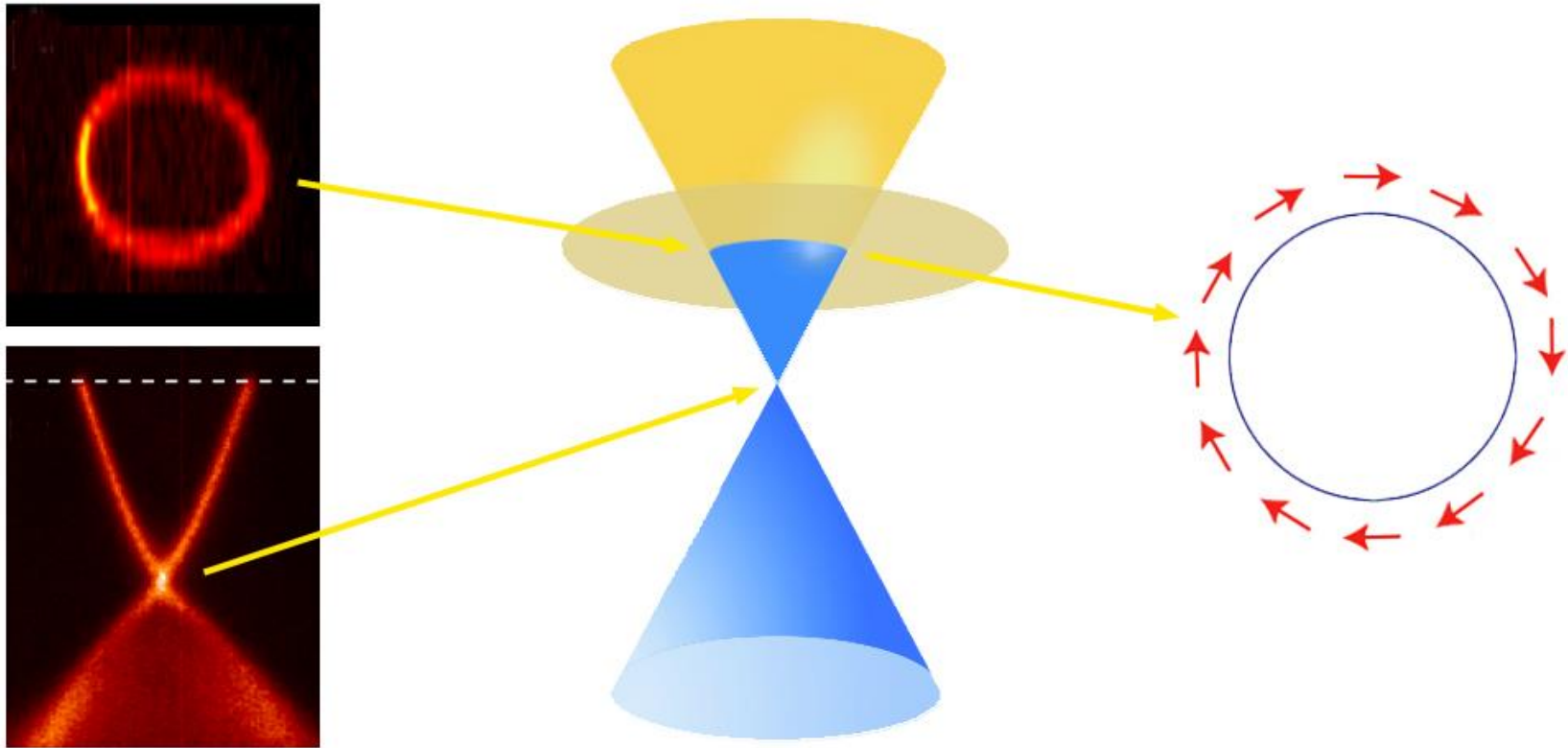
3. Conclusions

1. Introductions

Topological Insulators

:Topological properties often manifested by “Surface States”

EX: 3D Topological Insulator



Surface: Symmetry-protected Dirac cone

New Generation of Topological Insulators:

“Higher-Order Topological Insulators”

RESEARCH

TOPOLOGICAL MATTER

Quantized electric multipole insulators

Wladimir A. Benalcazar,¹ B. Andrei Bernevig,² Taylor L. Hughes^{1*}

[Science, 2017]

Reflection-Symmetric Second-Order Topological Insulators and Superconductors

Josias Langbehn, Yang Peng, Luka Trifunovic, Felix von Oppen, and Piet W. Brouwer
Phys. Rev. Lett. **119**, 246401 – Published 11 December 2017

[PRL, 2017]

Higher-Order Topology in Bismuth

Frank Schindler,¹ Zhijun Wang,² Maia G. Vergniory,^{3,4,5} Ashley M. Cook,¹ Anil Murani,⁶
Shamashis Sengupta,⁷ Alik Yu. Kasumov,^{6,8} Richard Deblock,⁶ Sangjun Jeon,⁹ Ilya Drozdov,¹⁰
Hélène Bouchiat,⁶ Sophie Guéron,⁶ Ali Yazdani,⁹ B. Andrei Bernevig,⁹ and Titus Neupert¹

[Nat. Phys., 2018]

SCIENCE ADVANCES | RESEARCH ARTICLE


MATERIALS SCIENCE

Higher-order topological insulators

Frank Schindler,¹ Ashley M. Cook,¹ Maia G. Vergniory,^{2,3*} Zhijun Wang,⁴ Stuart S. P. Parkin,⁵
B. Andrei Bernevig,^{4,2,6†} Titus Neupert^{1†}

[Science, 2018]

Observation of a phononic quadrupole topological insulator

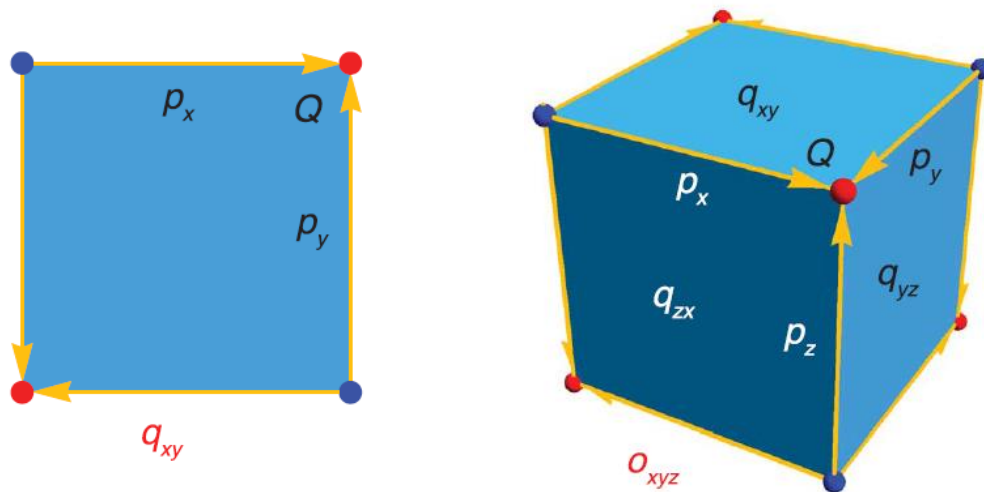
Marc Serra-Garcia, Valerio Peri, Roman Süssstrunk, Osama R. Bilal, Tom Larsen, Luis Guillermo Villanueva & Sebastian D. Huber 

[Nature, 2018]

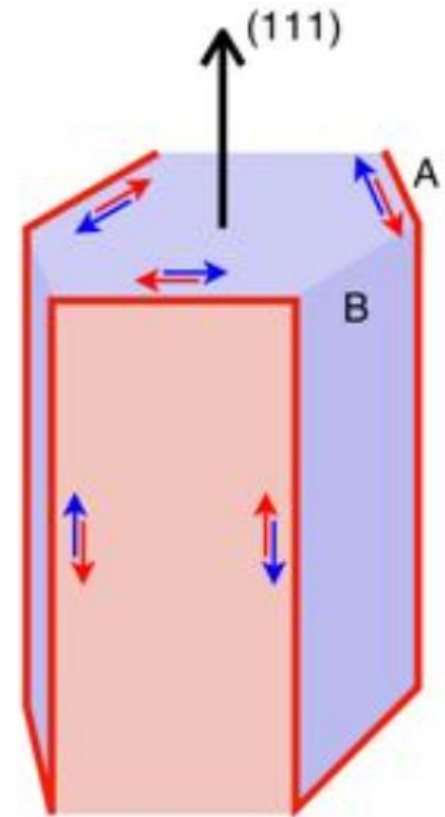
...and so on.

Higher-Order Topological Insulators (HOTI):

“Topology” = Non-trivial Edge of Edge states



Dangling states at “Corner” [Science 2017]

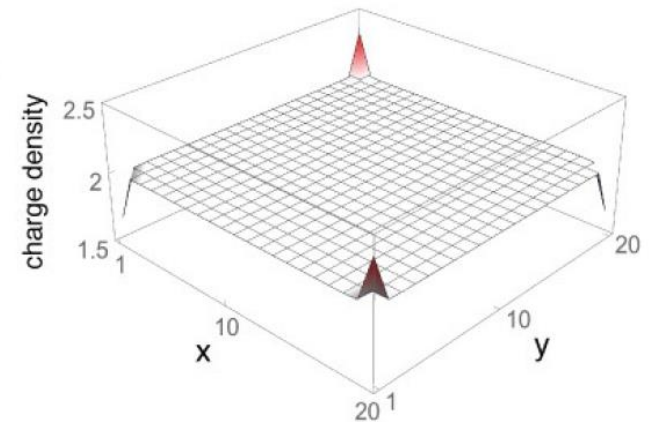
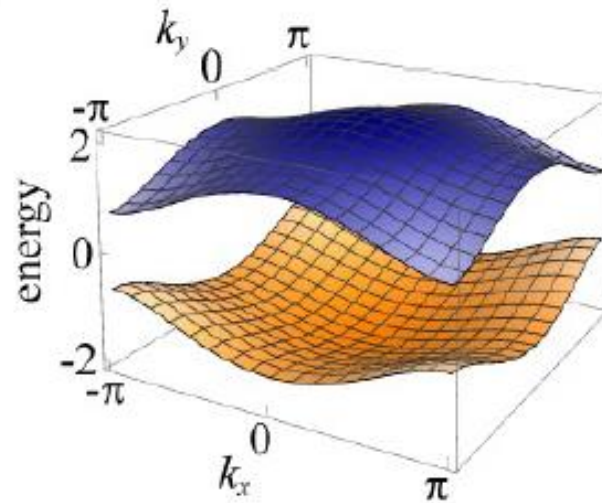
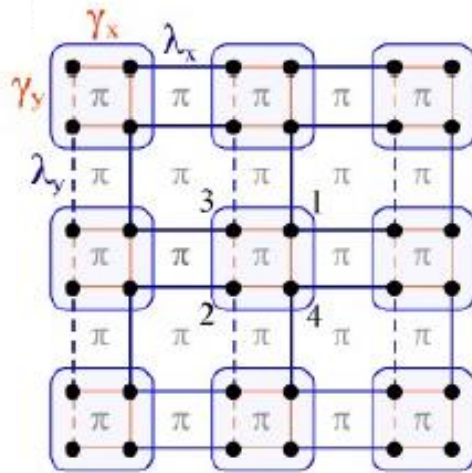


Bismuth [Nat. Phys. 2018]

Many variants, but we consider today only **prototypical HOTI**

“Multipolar Charge Distribution” from Corner States

[Ref. Benalcazar-Bernevig-Hughes, Science, 2017]



Topological if $|\lambda_a| > |\gamma_a|$ for $a = x, y$

Quadrupolar Corner Charges

Using **semi-classical** arguments, it has been shown that:

[Ref. Benalcazar-Bernevig-Hughes, Science, 2017]

This state has “**quantized quadrupolar moments** $Q_{xy} = \frac{1}{2} \bmod 1$ ”

Key claims: [Ref. Benalcazar-Bernevig-Hughes, Science, 2017]

1. Multipoles can be quantized.

1. With proper symmetries: mirrors $\{M_x, M_y\}$ and/or C_{4z}

2. When lower poles are vanishing:

E.g., Translation by \vec{d} : $Q_{xy} = \sum xy q \rightarrow Q_{xy} + d_x P_y + d_y P_x + d_x d_y Q_{tot}$

[Invariance (well-defined): P_x, P_y vanish (no polarization)]

2. Topologically Trivial/non-trivial Multipoles

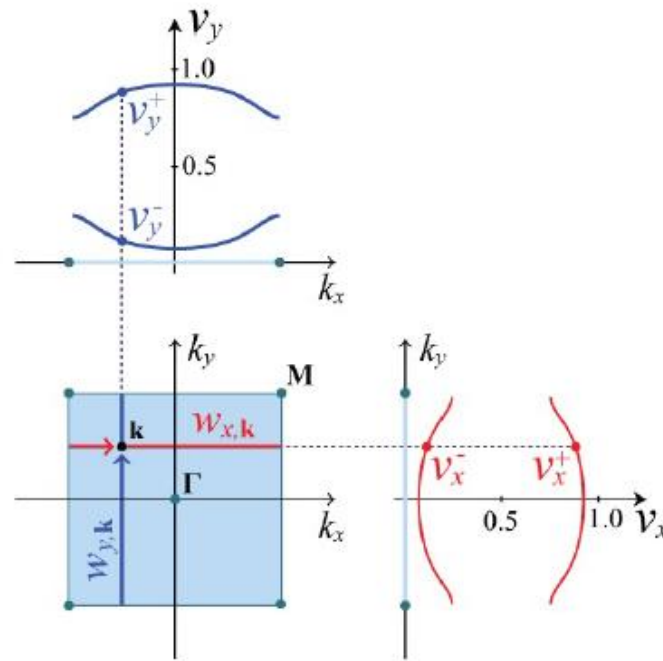
Ex: quadrupole in 2d with C_{4z} and no polarization

$Q_{xy} = \frac{1}{2} \bmod 1$ for higher-order topological states

$Q_{xy} = 0 \bmod 1$ for trivial states

Topological Band Indices:

“Polarizations” of “Wilson Loop Operators”



$$\mathcal{W}_{C,\mathbf{k}} \equiv e^{iH\mathcal{W}_C(\mathbf{k})}.$$

Not clear enough for me...

Can we diagnose “**Multipoles**” in Condensed Matter Systems?

[Generically “Quantum” + “Many Body”

I.E., Beyond “*free fermion + momentum space*” definitions]

(Simpler) ***Definitions of Multipoles?***

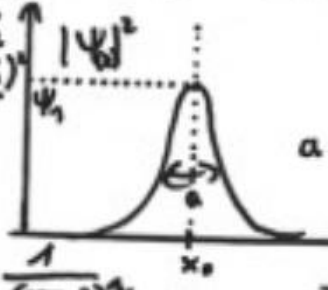
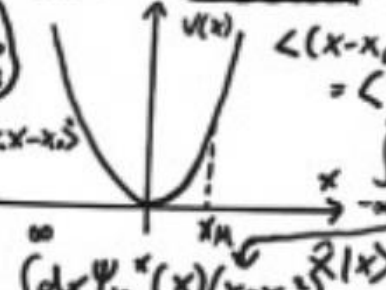
In a fully-quantum, interacting set-up

Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and **GYC**, in progress

2. Conjectures & Numerical Results

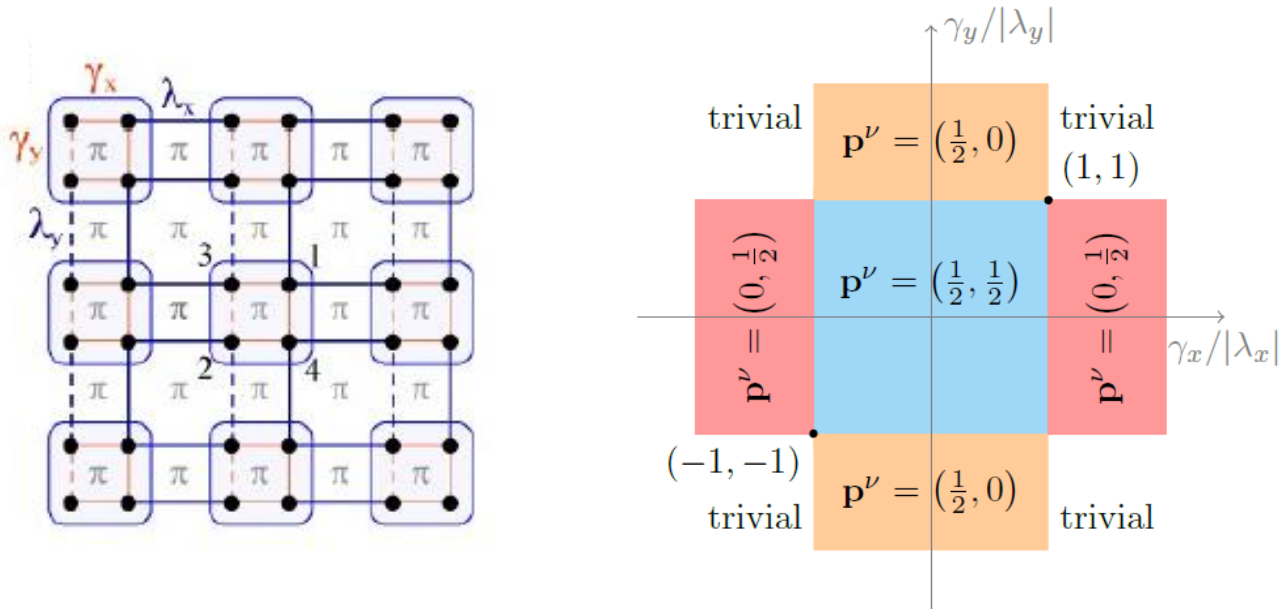
Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and **GYC**, in progress

Instead of *showing you lengthy arguments* for this

$$\begin{aligned}
 \langle \phi_n | \phi_{n'} \rangle &= \langle \phi_n | \int dx |x\rangle \langle x| \phi_{n'} \rangle \Rightarrow \left(\sum_n n + \frac{1}{2} \right) \frac{\pi}{2} = \frac{\pi}{2} (2n-1), \quad n=1,2,\dots \Rightarrow K_0 = -\frac{\pi}{2} \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
 \langle \phi_n | \phi_{n'} \rangle &= \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \phi_n^*(x) \cdot \phi_{n'}(x) \quad \psi_n(x) = \sqrt{\frac{2}{L}} \cos \left[\frac{\pi}{L} (2n-1)x \right]; \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin \left[\frac{2\pi}{L} nx \right] \\
 \langle \phi_n | \phi_{n'} \rangle &= \frac{1}{L} \int dx e^{-ikx} e^{ik'x} \stackrel{!}{=} 0; \quad k \neq k' \\
 |\psi(x)|^2 &= |\psi_0|^2 e^{-\frac{(x-x_0)^2}{2a^2}} \quad \int_{-\infty}^{\infty} dx e^{-Ax^2} = \sqrt{\frac{\pi}{A}} \\
 A &= \frac{1}{2a^2} \Rightarrow |\psi_0| = \frac{1}{(\pi a^2)^{1/4}} \\
 \hat{H} \psi_n &= -\frac{\hbar^2}{2m} \partial_x^2 \psi_n(x) = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} [2n-1] \right)^2 \psi_n(x) \\
 E_{ns} &= \frac{\hbar^2}{2m} \frac{\pi^2}{L^2} (2n-1)^2, \quad n=1,2,\dots; \quad \hat{H} \psi_{ns}(x) = \frac{\hbar^2}{2m} \left(\frac{2\pi n}{L} \right)^2 \psi_{ns}(x) \\
 \hat{H} \psi_a &= -\frac{\hbar^2}{2m} \partial_x^2 \psi_a(x) = \frac{\hbar^2}{2m} \frac{1}{2a^2} \psi_a(x) - \frac{\hbar^2}{2m} \frac{1}{4a^4} (x-x_0)^2 \psi_a(x) \\
 &= -\frac{\hbar^2}{2m} \left(-\frac{1}{2a^2} + \left(\frac{1}{2a^2} (x-x_0) \right) e^{-\frac{(x-x_0)^2}{4a^2}} \right) \psi; \quad V(x) = \frac{\hbar^2}{2m a^4} (x-x_0)^2 \\
 \hat{H} &\rightarrow \hat{H} = -\frac{\hbar^2}{2m} \partial_x^2 + V(x); \quad \hat{H} \psi_a = \frac{\hbar^2}{2m} \frac{1}{2a^2} \psi_a = E_a \psi_a \\
 V(x) &= \frac{1}{2} m \omega^2 (x-x_0)^2 \rightarrow m \omega^2 = \frac{\hbar^2}{m a^4} \Rightarrow \omega = \frac{\hbar}{2ma} \quad E_0 = \frac{\hbar^2}{2m} \frac{1}{2a^2} \\
 [\hat{p}, \hat{x}] &= \frac{\hbar}{i}; \quad \hat{p} = \frac{\hbar}{i} \partial_x / \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \\
 1. \quad a^2 + b^2 &= (a+ib)(a-ib); \quad a, b \in \mathbb{R}; \quad 2. \quad (a\hat{p} + ib\hat{x})(a\hat{p} - ib\hat{x}), \quad a, b \in \mathbb{R} \\
 &= a^2 \hat{p}^2 + ib a \hat{x} \hat{p} - i a b \hat{p} \hat{x} + b^2 \hat{x}^2 = a^2 \hat{p}^2 + b^2 \hat{x}^2 - b a \hbar \\
 \hat{H} &= (a\hat{p} + ib\hat{x})(a\hat{p} - ib\hat{x}) = b a \hbar; \quad a^2 = \frac{1}{2m}; \quad b^2 = \frac{1}{2} m \omega^2 \\
 \text{Def: } C^+ &= \frac{1}{\sqrt{\hbar m \omega}} (a\hat{p} + ib\hat{x}); \quad C^- = \frac{1}{\sqrt{\hbar m \omega}} (a\hat{p} - ib\hat{x}) \Rightarrow \hat{H} = \hbar \omega C^+ C^- + \frac{1}{2} \hbar \omega \\
 (\omega \pm \epsilon) & \dots \dots \dots \quad A \rightarrow \omega \bar{A} \omega^{-1} + \frac{1}{2} \hbar \omega
 \end{aligned}$$



...which you probably don't care

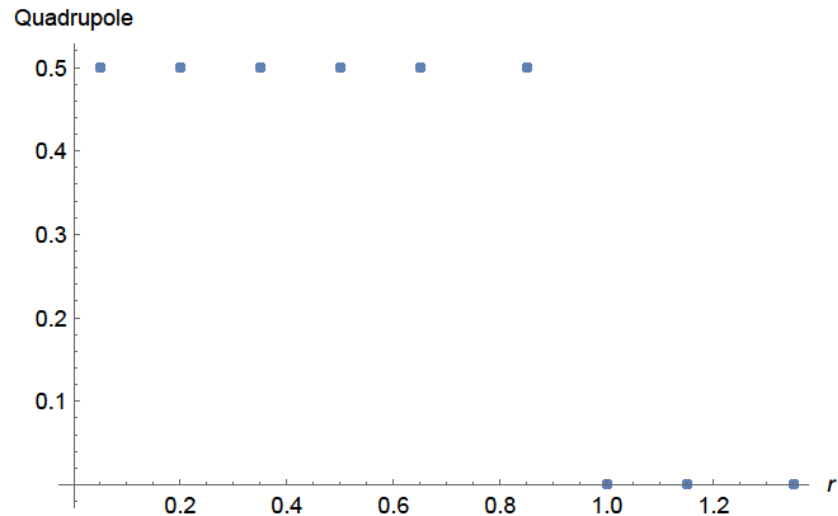
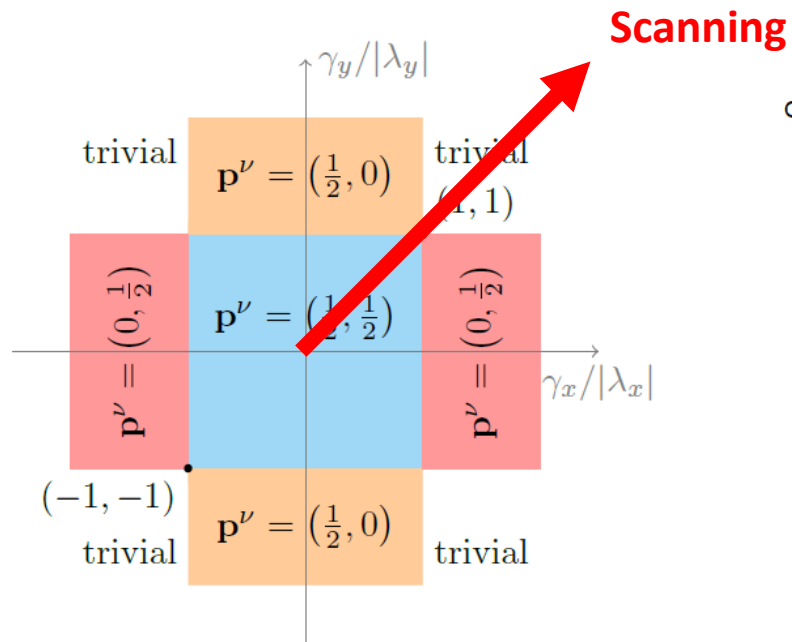
“seeing” is “believing”



Blue Region: $Q_{xy} = \frac{1}{2} \bmod 1$ (topological)

Others: $Q_{xy} = 0 \bmod 1$ (trivial)

“seeing” is “believing”



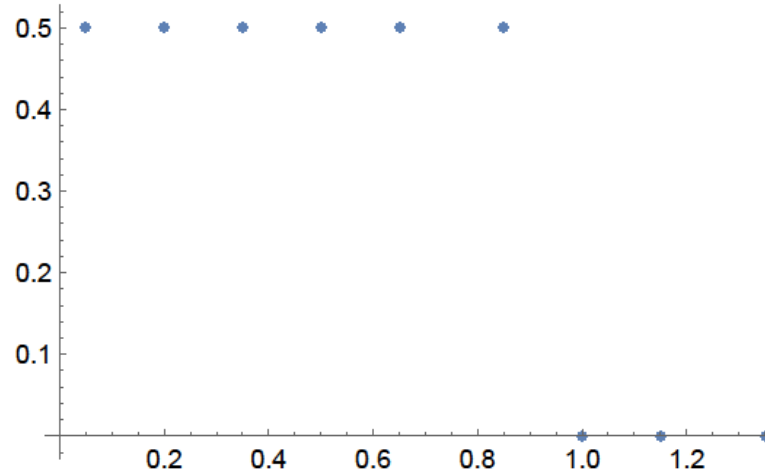
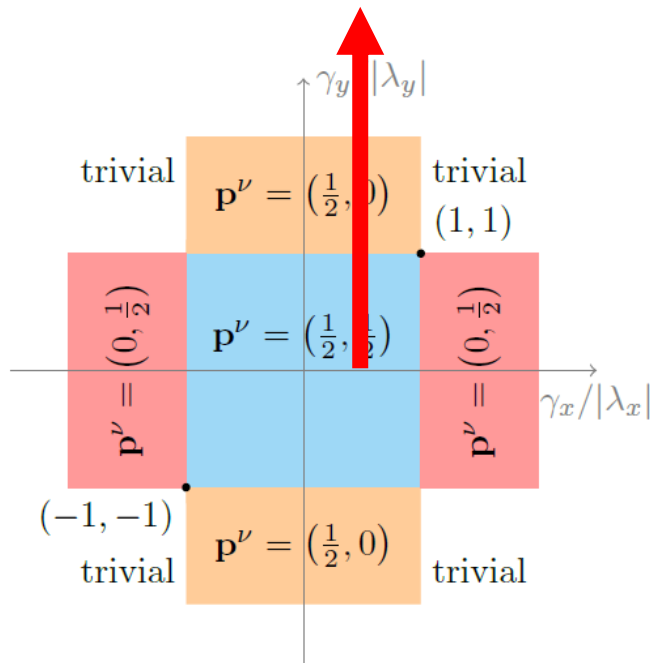
$$Q_{xy} = \frac{1}{2\pi} \text{Im} \log \langle GS | \mathbf{U}_2 | GS \rangle$$

Reproduces (i) quantization, (ii) phase transition, (iii) topological/non-topological dichotomy

Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and **GYC**, in progress

“seeing” is “believing”

Scanning [No gap closing in energy spectrum]

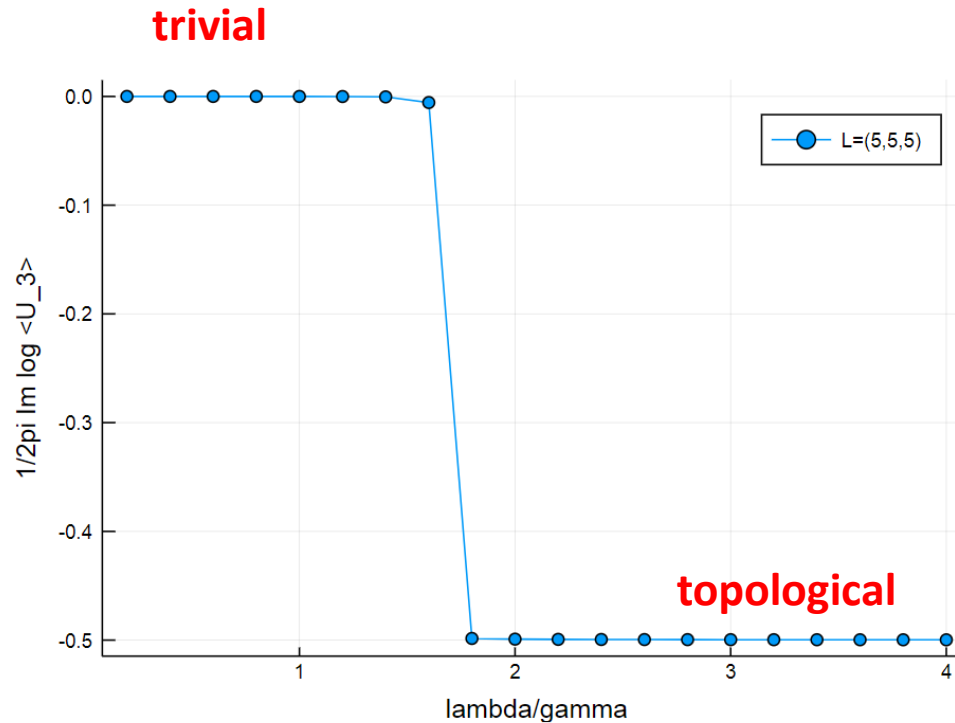


$$Q_{xy} = \frac{1}{2\pi} \text{Im} \log \langle GS | \mathbf{U}_2 | GS \rangle$$

Reproduces (i) quantization, (ii) phase transition, (iii) topological/non-topological dichotomy

Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and **GYC**, in progress

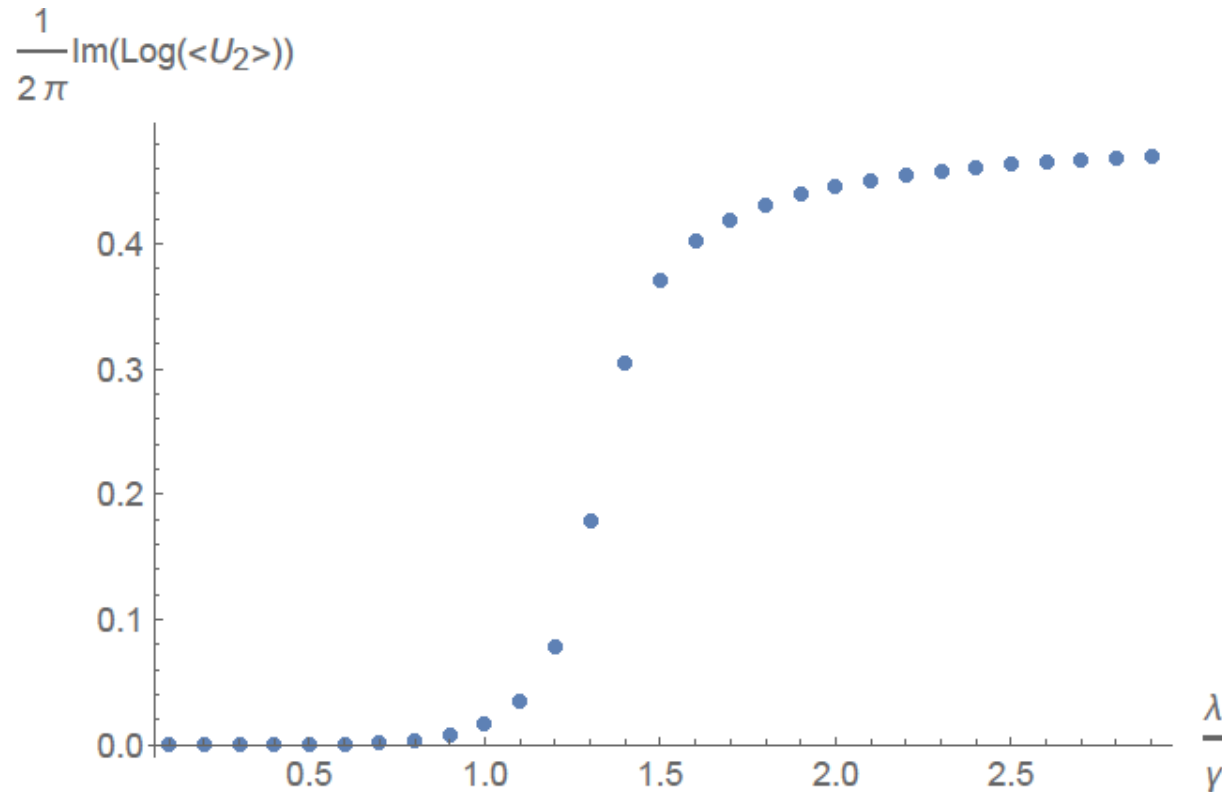
“seeing” is “believing”



$$O_{xyz} = \frac{1}{2\pi} \text{Im log } \langle GS | U_3 | GS \rangle$$

Reproduces: (i) quantization, (ii) phase transition (with finite size effect)
(iii) topological/non-topological dichotomy

Note: with (weak) symmetry breaking terms

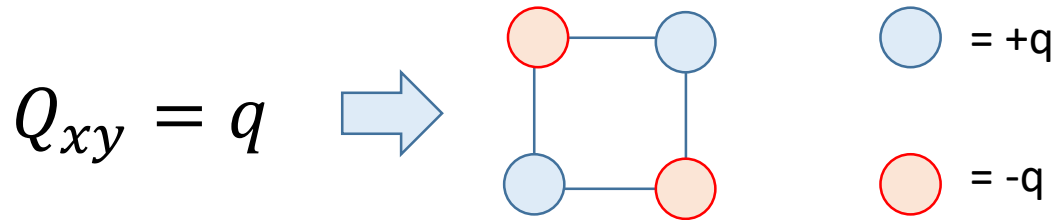


Smooth phase boundary + non-quantization (as expected).

Physically, what can we learn from this?

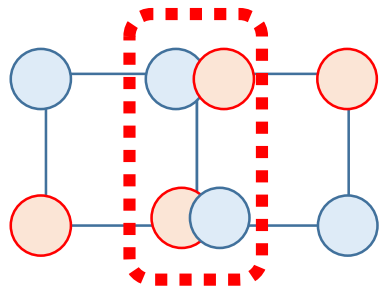
If $Q_{xy} = q$ is **the quadrupolar density**, then...

q is **the charge localized at the boundary**

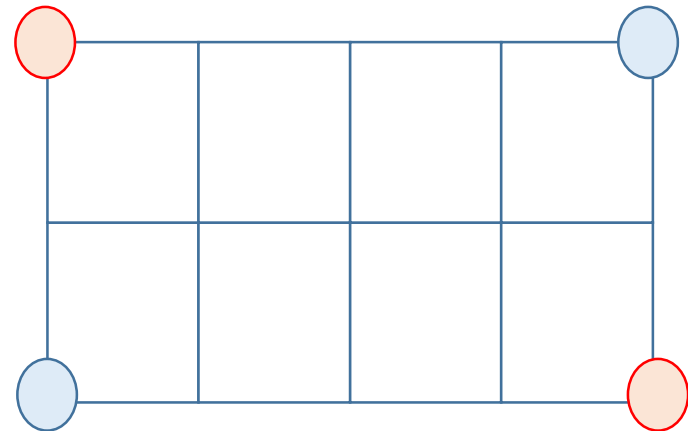
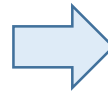


When the quadrupolar density is uniformly stacked,

Ex:



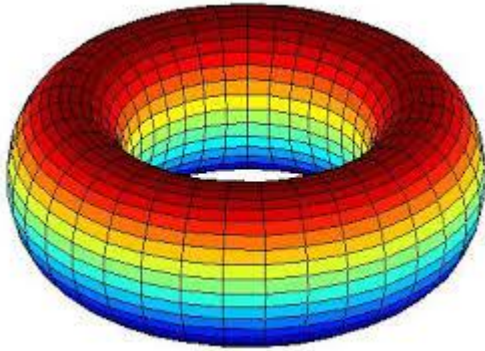
Inside is cancelled ($q - q = 0$) !



Only the boundary is left

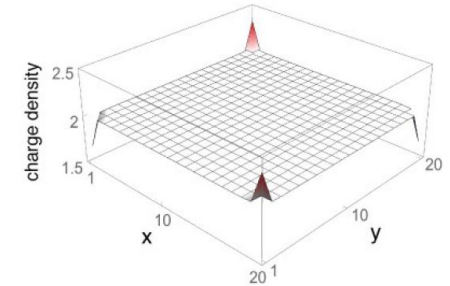
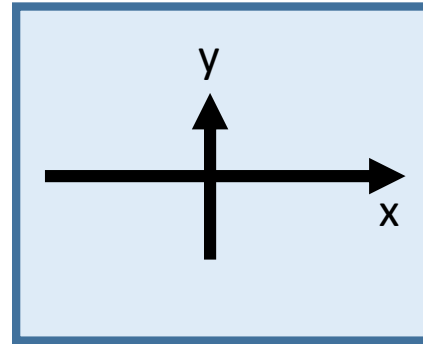
So we compare the following two quantities:

1. Periodic BC on Torus



Many-body Invariants

2. Open BC

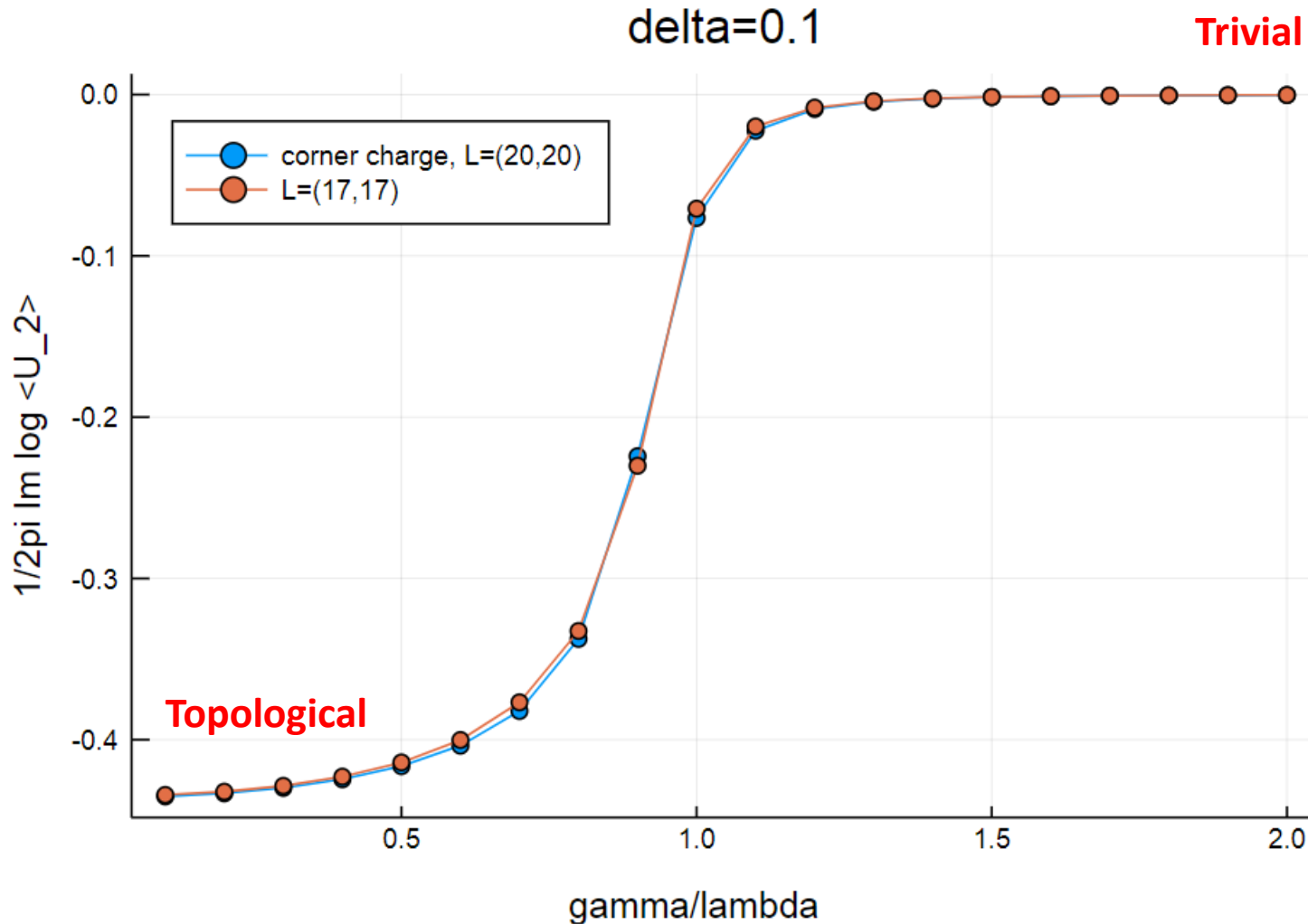


Single-particle Observable

$$\mathbf{q} = \int d^2x \langle GS | \hat{\rho}(x) - \bar{\rho} | GS \rangle$$

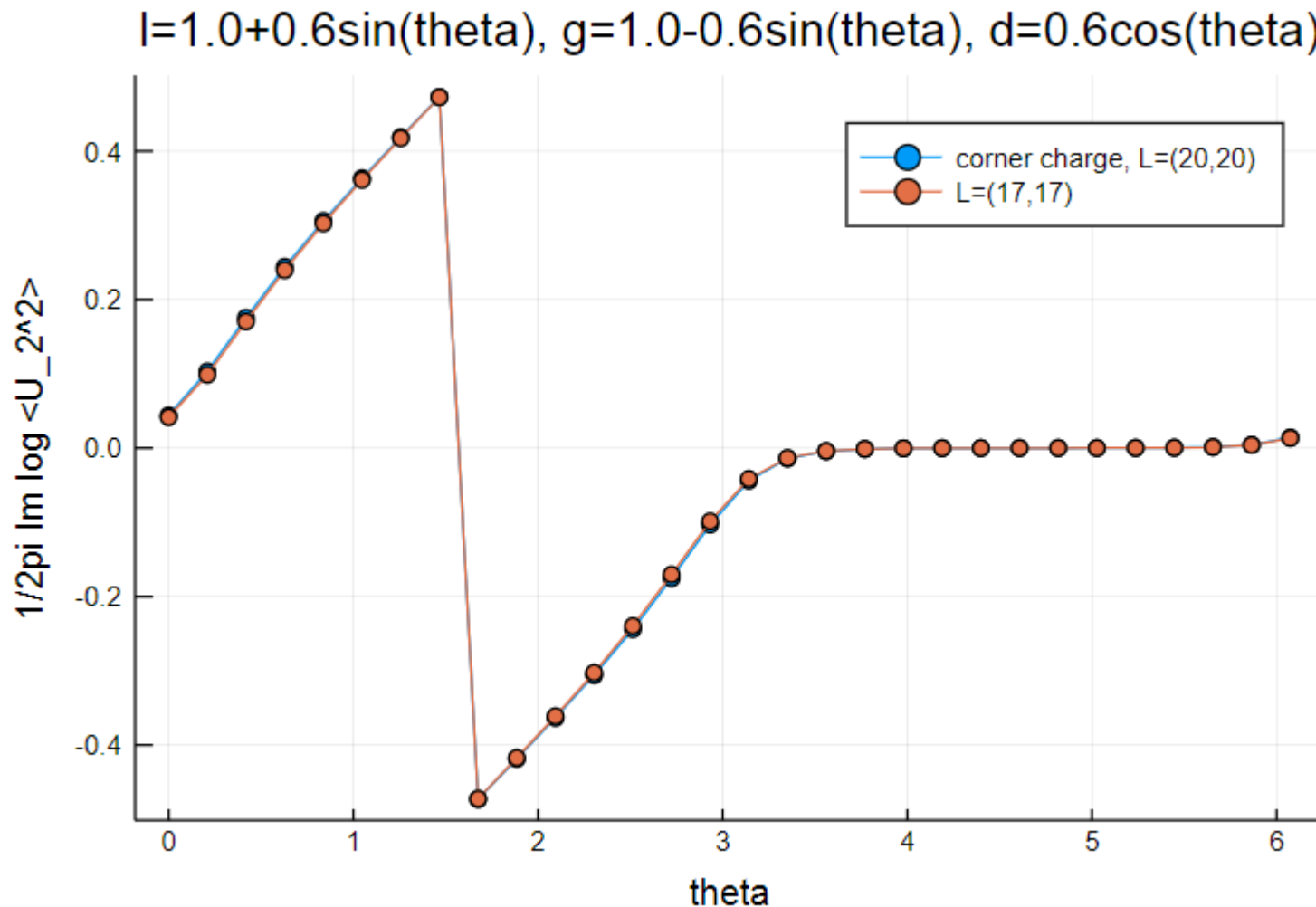
Do I find $Q_{xy} = \mathbf{q}$?

From bulk invariant to boundary charge



Many-body invariant exactly matches localized boundary charge!

Even for more complicated processes, e.g., Thouless pumping

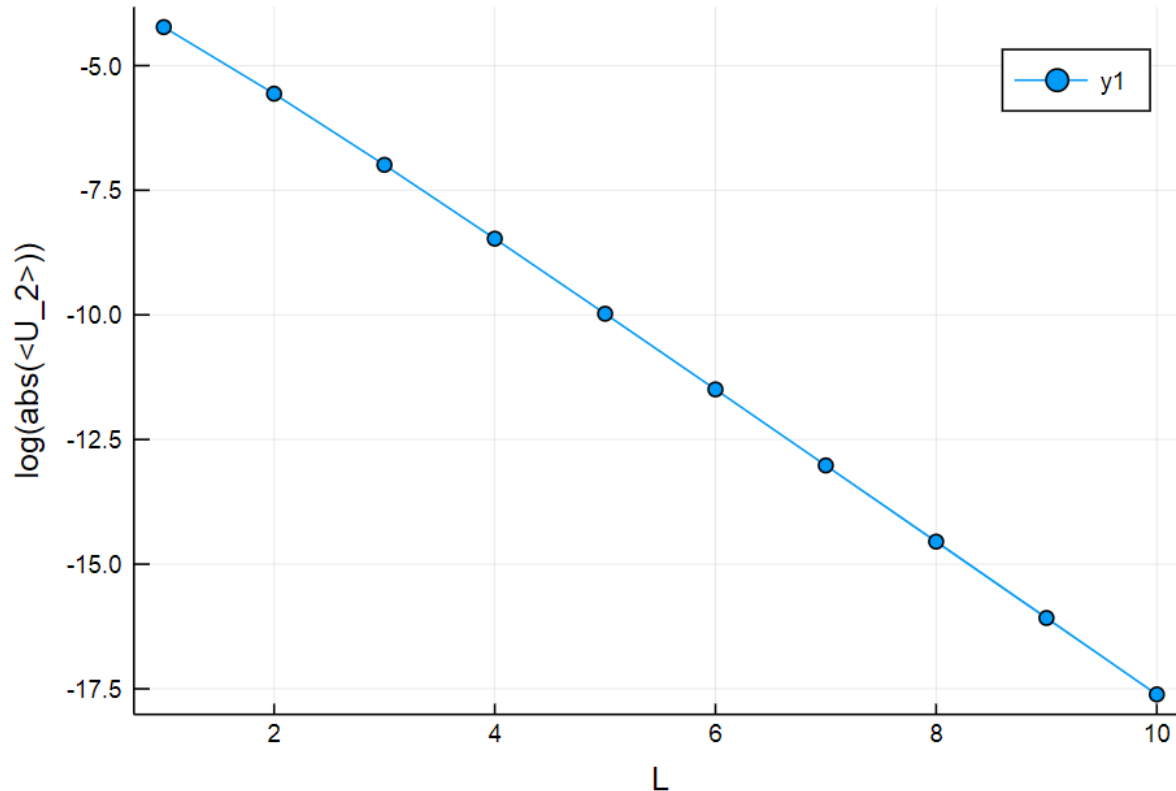


Q_{xy} tracks well of the charge over the full parameter space !

Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and GYC, in progress

New Order parameter for Metals & Insulators

At the critical point: $|\langle U_2 \rangle| \rightarrow 0$ as $L_x \rightarrow \infty$



2d critical: $|\langle U_2 \rangle| \sim c_1 \exp(-aL_x) \rightarrow 0$

[2d insulator: $|\langle U_2 \rangle| \sim \text{const.}$]

This is analogous with the original Resta's conjecture.

In Summary:

$\langle U_2 \rangle = |\langle U_2 \rangle| \text{Exp} (2\pi i Q_{xy})$ is an **order parameter**

(1) Phase = (Detail-free) Topology = Multipoles

(2) Amplitude = Spectral Property, i.e. Metal/Insulator

3. Conclusions

Conclusions:

- 1. Conjectured (definition of) many-body invariants for multipoles**
- 2. Numerically confirmed the invariants**
- 3. Novel order parameter for “metal” & “insulator”**

Ref. Byungmin Kang, Hyun Woong Kwon, Kwon Park, and **GYC**, in progress

- 4. Several future directions**

Thank you for your attention !