Title: Many-Body Invariants for Electric Multipoles in Higher-Order Topology

Date: Jan 18, 2019 02:00 PM

URL: http://pirsa.org/19010065

Abstract: <blockquote type="cite">
<p>In crystals, quantum electrons can be spatially distributed in a way that the bulk solid supports macroscopic electric multipole moments, which are deeply </p>

<p>related with emergence of topology insulators in condensed matter systems. However, unlike the classical electric multipoles in open space, </p>

<p>defining electric multipoles in crystals is a non-trivial task. So far, only the dipolar moment, namely polarization, has been successfully defined and served as a classic example of topological insulators. </p>

<p>In this talk, we propose the general definition, i.e., many-body invariants, for electric multipoles in crystals, which are related with recently-discovererd higher-order topological insulators. </p>

<p>Our invariants are designed to measure the distribution of electron charge in unit cells and thus can detect multipole moments purely from the bulk ground state wavefunctions. </p>

<p>We provide analytic as well as numerical proofs for our invariants. Application of our invariants to spin systems as well as various other aspects of the many-body invariants will be briefly discussed.</p>
</blockquote>

Many-Body Invariant of Electric Multipoles

In Condensed Matter Systems

Gil Young Cho

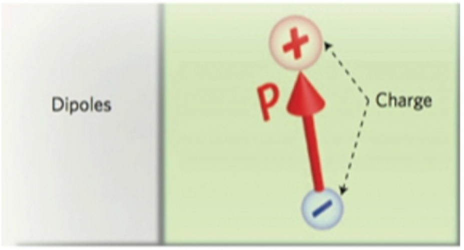
POSTECH

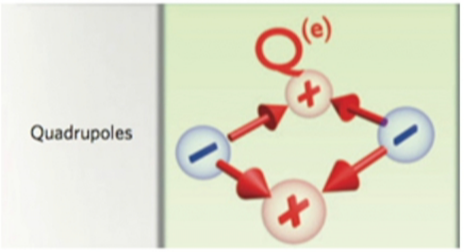
Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

See also: William Wheeler, Lucas Wagner, and Taylor Hughes, arxiv:1812.06990 (2018)

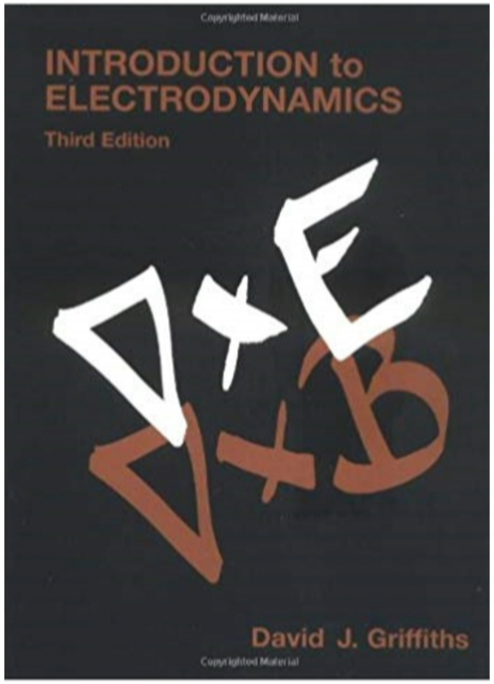
Goal:

Definitions of (bulk) Electric Multipoles in Solids





Warm-up: classical multipoles



Input: Charge Distribution $\rho(\vec{r})$

Output: Well-defined Multipoles

Ex: $$\mathbf{p}(\mathbf{r}) = \int_V \rho(\mathbf{r}_0)\ (\mathbf{r}_0 - \mathbf{r})\ d^3\mathbf{r}_0$$

Electric Field Lines

Ex: $$\mathbf{E}(\mathbf{R}) = \frac{3\left(\mathbf{p}\cdot\hat{\mathbf{R}}\right)\hat{\mathbf{R}} - \mathbf{p}}{4\pi\varepsilon_0 R^3}$$

Warm-up: classical multipoles

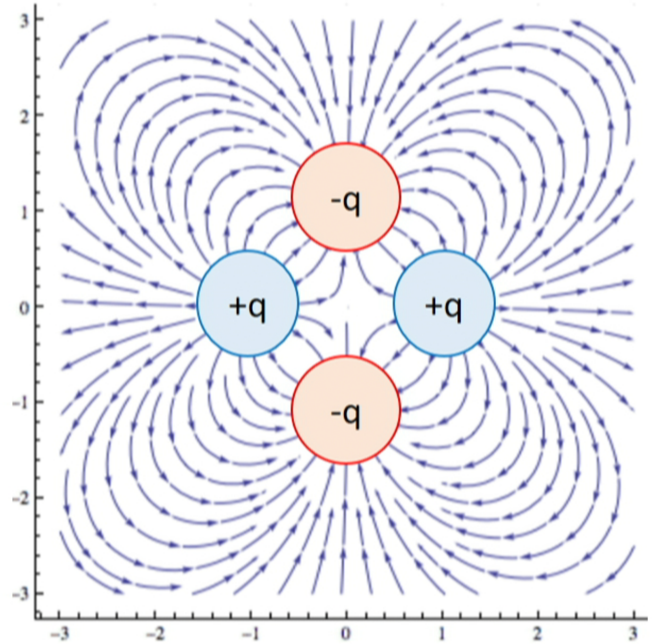
Multipole expansion

From Wikipedia, the free encyclopedia

$$q_{\text{tot}} \equiv \sum_{i=1}^{N} q_i$$

$$P_\alpha \equiv \sum_{i=1}^{N} q_i r_{i\alpha}$$

$$Q_{\alpha\beta} \equiv \sum_{i=1}^{N} q_i (3 r_{i\alpha} r_{i\beta} - \delta_{\alpha\beta} r_i^2)$$



$$4\pi\varepsilon_0 V(\mathbf{R}) = \frac{q_{\text{tot}}}{R} + \frac{1}{R^3} \sum_{\alpha=x,y,z} P_\alpha R_\alpha + \frac{1}{2R^5} \sum_{\alpha,\beta=x,y,z} Q_{\alpha\beta} R_\alpha R_\beta + \cdots$$

Difficulties in Crystals [at low temperature]:

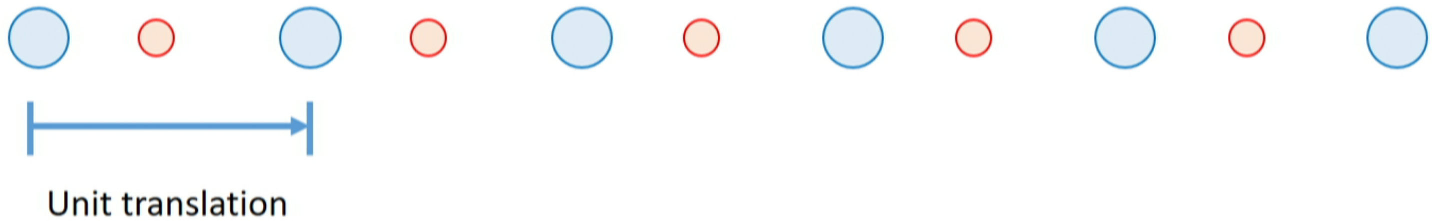
(1) Quantum-mechanical Electrons

[may well be highly-correlated]

(2) Lattice (Periodicity)

Warm-up: Dipole/Polarization

Infinite Lattice (Crystal):

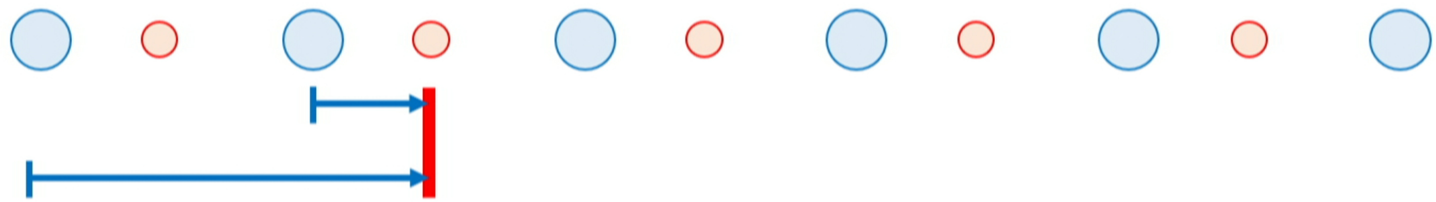


Dipole moment: $P_x = \sum x q_x \rightarrow \sum \langle \psi | x | \psi \rangle q_x\,?$

Warm-up: Dipole/Polarization

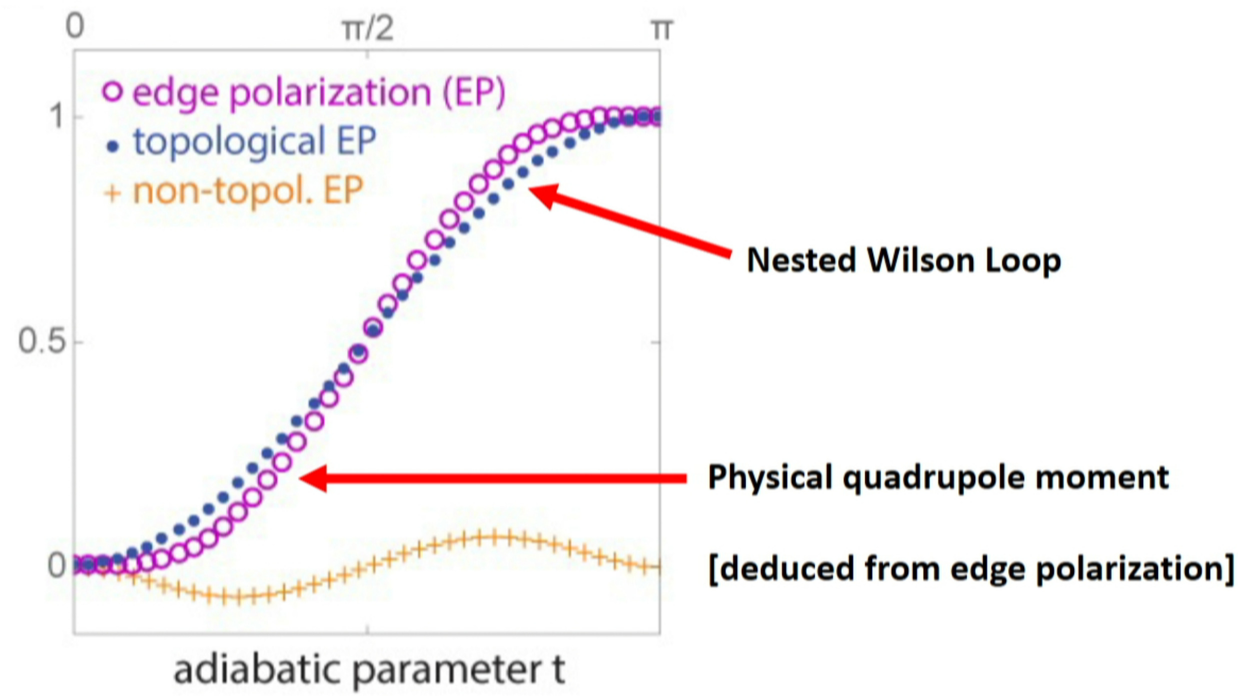
Remarks on $\exp(2\pi i \boldsymbol{P_x}) = \exp\left[i \oint \mathrm{Tr}\, A_k \, dk\right]$

1. Polarization: $\boldsymbol{P_x} = \boldsymbol{P_x}\ \mathbf{mod\ 1}$ (symmetry-independent)



E.g., when the symmetries are relaxed...

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



"Nested Wilson Loop Approach" =

A (successful) "topological band index" but not a physical measure.

Quantized electric multipole insulators

[Science 2017]

Wladimir A. Benalcazar,[1] B. Andrei Bernevig,[2] Taylor L. Hughes[1*]

...found insulators with quantized (discrete) electric multipoles

$$Q_{xy} = \frac{1}{2} \bmod 1 \quad \& \quad O_{xyz} = \frac{1}{2} \bmod 1$$

+ "Symmetry-Protected" Band Indices ["Nested Wilson Loops"]

Successful Band Index

But not generic measure of multipoles

So, what is missing? [Ref. Benalcazar-Bernevig-Hughes, Science, 2017]

1. Generic momentum-space measures (for free fermion!) for multipoles

[i.e., Nested Wilson loop seems fundamentally different from $P_x = \frac{1}{2\pi}\oint A_k$ in 1d]

2. Generic many-body & real-space measure for multipoles

[i.e., No analogue of $\boldsymbol{U_1} = \mathbf{exp}\left(\frac{\boldsymbol{2\pi i}}{\boldsymbol{L}}\sum \boldsymbol{x}\,\widehat{\boldsymbol{N}}(\boldsymbol{x})\right)$ for multipoles]

3. No link is given for 1 & 2 (since they are absent)

What is done? [Ref. Benalcazar-Bernevig-Hughes, Science, 2017]

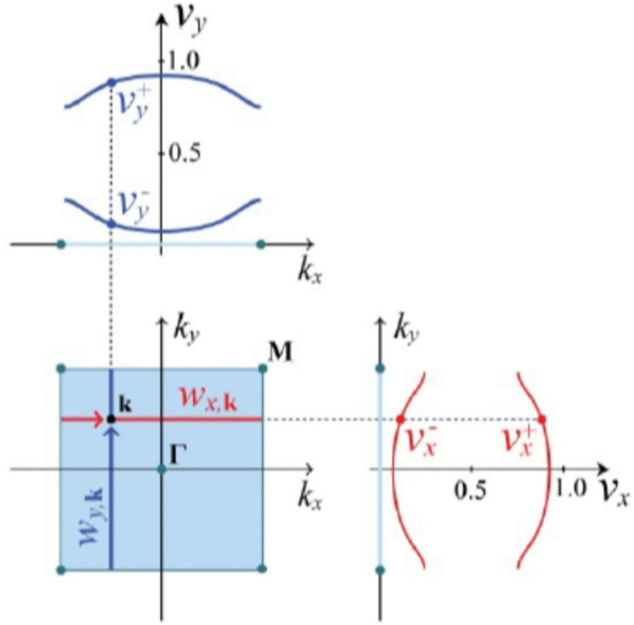
"Nested Wilson Loop Approach" = Capturing Boundary Polarization

Consider a Wilson line:

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

...and investigate its polarization

[i.e., Wilson of Wilson = Nested Wilson]



Reasoning:

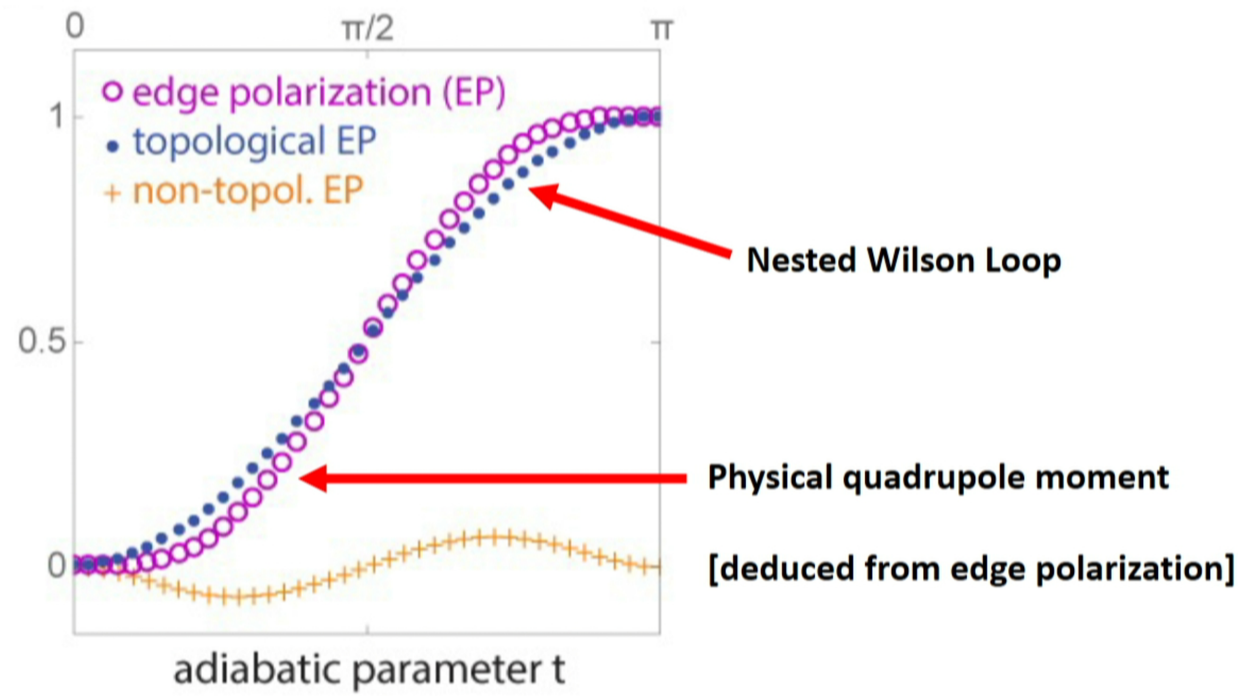
$H_{W_c}(k) \approx H_{edge}(k)$ **[adiabatic equivalence]**

➡ **Polarization of** $H_{W_c}(k)$ = **Polarization of** $H_{edge}(k)$ **[when** C_4 **or mirrors present]**

I.E., nested Wilson loop is not a generic measure!

E.g., when the symmetries are relaxed…

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



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2. Generic many-body & real-space measure for multipoles

[i.e., No analogue of $\boldsymbol{U_1} = \mathbf{exp}\left(\frac{2\pi i}{L}\sum \boldsymbol{x}\,\widehat{\boldsymbol{N}}(\boldsymbol{x})\right)$ for multipoles]

3. No link is given for 1 & 2 (since they are absent)

Our progress

In short,

We look for Generic Definitions of Electric Multipoles in Crystals

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

See also: William Wheeler, Lucas Wagner, and Taylor Hughes, arxiv:1812.06990 (2018)

We define:

[1] **Quadrupole** in **a crystal** is defined by:

$$Q_{xy} = \frac{1}{2\pi} \mathrm{Im} \log \langle GS | U_2 | GS \rangle \quad \text{with } U_2 = \exp\left(\frac{2\pi i}{L_x L_y} \sum xy\, \rho(x) \right)$$

[2] **Octupole** in **a crystal** is defined by:

$$O_{xyz} = \frac{1}{2\pi} \mathrm{Im} \log \langle GS | U_3 | GS \rangle \quad \text{with } U_3 = \exp\left(\frac{2\pi i}{L_x L_y L_z} \sum xyz\, \rho(x) \right)$$

Here: $|GS\rangle$ = many-body states on Torus (we will generalize later)

Essentially,

$$\langle U_2 \rangle = |\langle U_2 \rangle| \ \mathrm{Exp}\left(2\pi i Q_{xy}\right)$$

$$\langle U_3 \rangle = |\langle U_3 \rangle| \ \mathrm{Exp}\left(2\pi i O_{xyz}\right)$$

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Data first and then Proof

Q. If I perform the explicit computation on my computer:

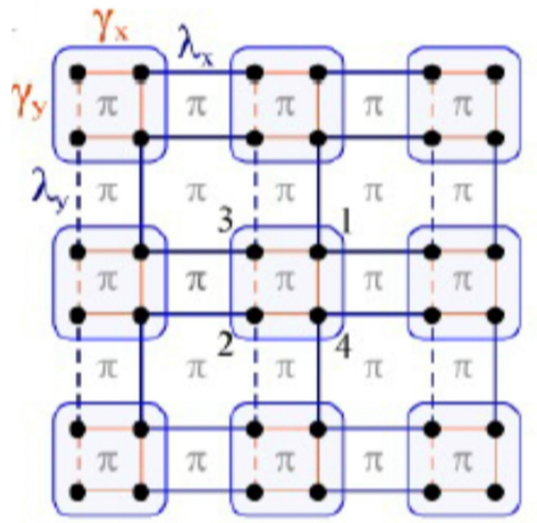
$$Q_{xy} = \frac{1}{2\pi} \mathrm{Im} \log \langle GS| U_2 |GS\rangle \quad \text{with} \quad U_2 = \exp\left(\frac{2\pi i}{L_x L_y} \sum xy\, \rho(x)\right)$$

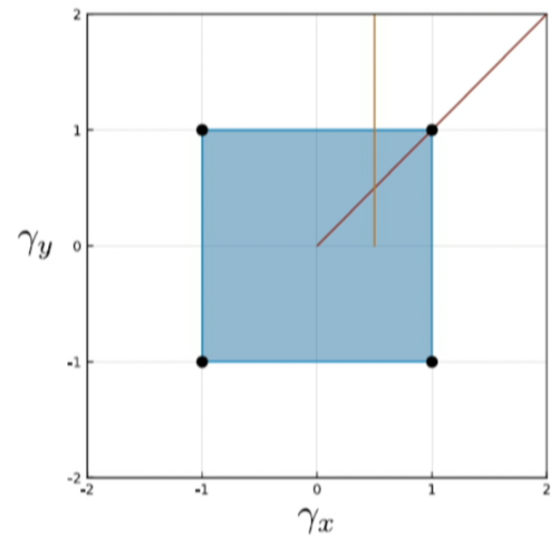
...on the models in literature, do I find:

Topological state: $Q_{xy} = \frac{1}{2} \bmod 1$
Trivial state: $Q_{xy} = 0 \bmod 1$

...from computer?

Symmetry-Protected Quadrupoles 1.

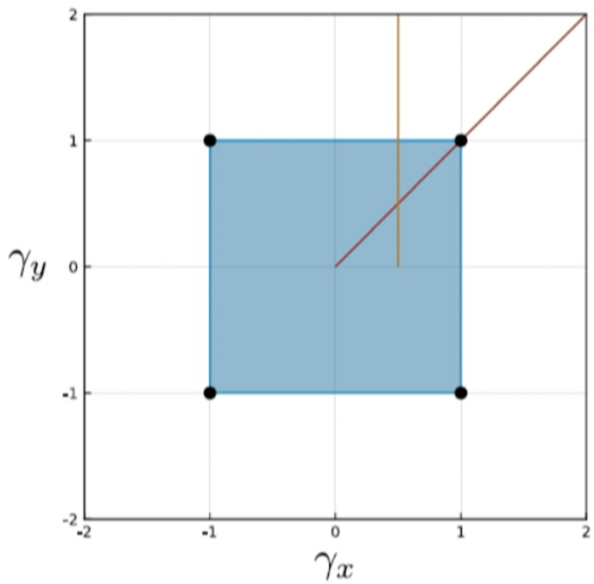


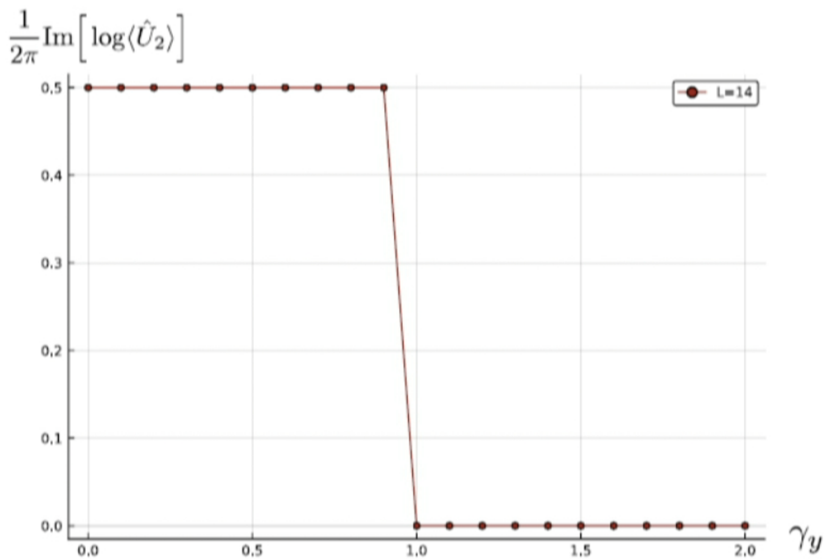


[Phase Diagram of $\lambda_x = \lambda_y = 1$]

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Symmetry-Protected Quadrupoles 1.





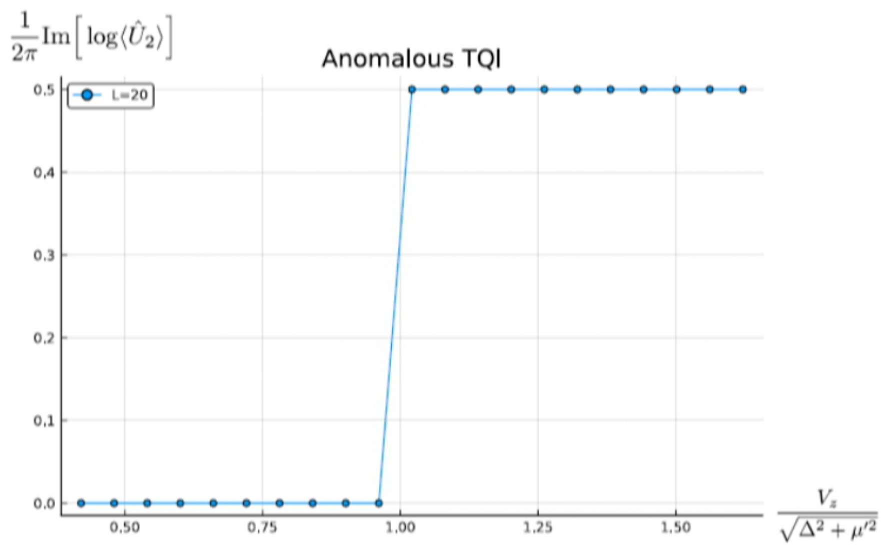
Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Symmetry-Protected Quadrupoles 2.

An anomalous higher-order topological insulator

S. Franca,[1] J. van den Brink,[1,2] and I. C. Fulga[1]

despite having a trivial topological invariant. We introduce a concrete example of an anomalous HOTI, which has a quantized bulk quadrupole moment and fractional corner charges, but a vanishing nested Wilson loop index. A new invariant able to capture the topology of this phase is then constructed. Our work shows that anomalous topological phases, previously thought to be unique to periodically driven systems, can occur and be used to understand purely time-independent HOTIs.



[Note: there is a modified index from nested Wilson loops]

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

So far, consistent with nested Wilson loop indices

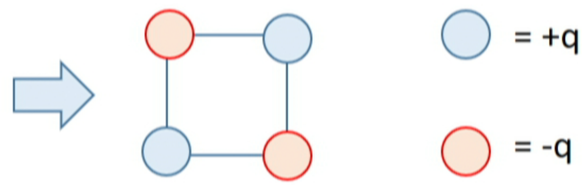
Can I go beyond nested Wilson approaches?

I.E., regime where quantizing symmetries are relaxed

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

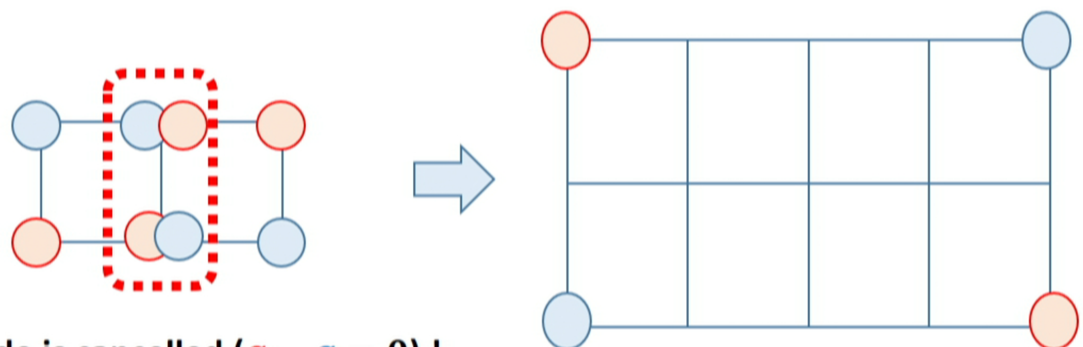
Remind: Corner charge $Q_c = Q_{xy}^{ph}$ physical Quadrupole moments

$$Q_{xy}^{ph} = q$$



When this is uniformly stacked,

Ex:

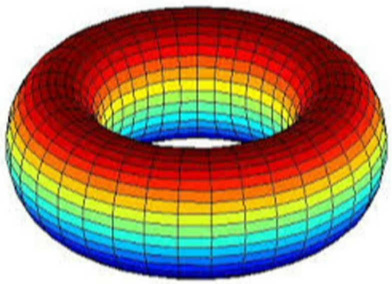


Inside is cancelled ($q - q = 0$) !

Only the boundary is left

So we compare the following two:

1. Periodic BC on Torus

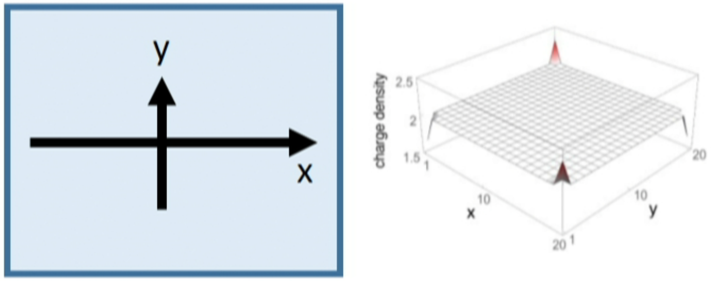


Many-body Calculation

$$Q_{xy} = \frac{1}{2\pi} \mathrm{Im}\log \langle \mathrm{GS}|\, U_2 |\mathrm{GS}\rangle$$

with $U_2 = \exp\left(\frac{2\pi i}{L_x L_y} \sum xy\, \hat{\rho}(x)\right)$

2. Open BC



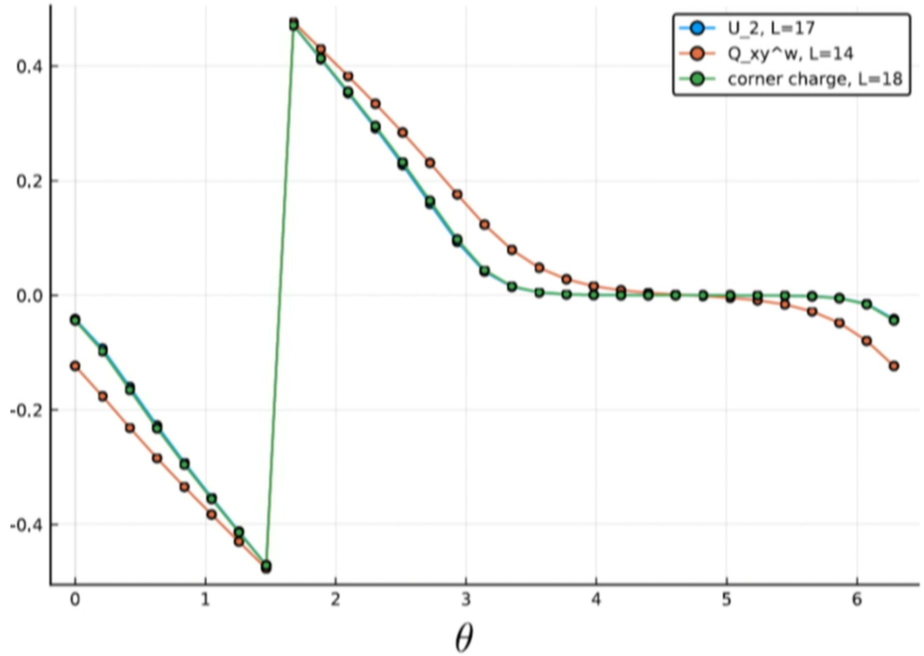
Single-particle Observable

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

$$= \sum \langle \hat{\rho}(x) - \bar{\rho} \rangle_{\text{single particle}}$$

Do I find $Q_{xy} = Q_c \left(= Q_{xy}^{ph}\right)$?

Beyond nested Wilson loop



Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Seems working.

But why do they work?

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Path-integral Interpretation of the overlap:

$$\langle \mathbf{GS}|\mathbf{U_2}|\mathbf{GS}\rangle = \frac{1}{Z}\,\mathbf{Tr}\,\mathbf{e}^{-\beta H}\mathbf{U_2} \propto \;\mathbf{exp}\left(i\mathbf{S_{eff}}\left[A_\mu\right]\right)$$

It's simple application of Dyson's formula:

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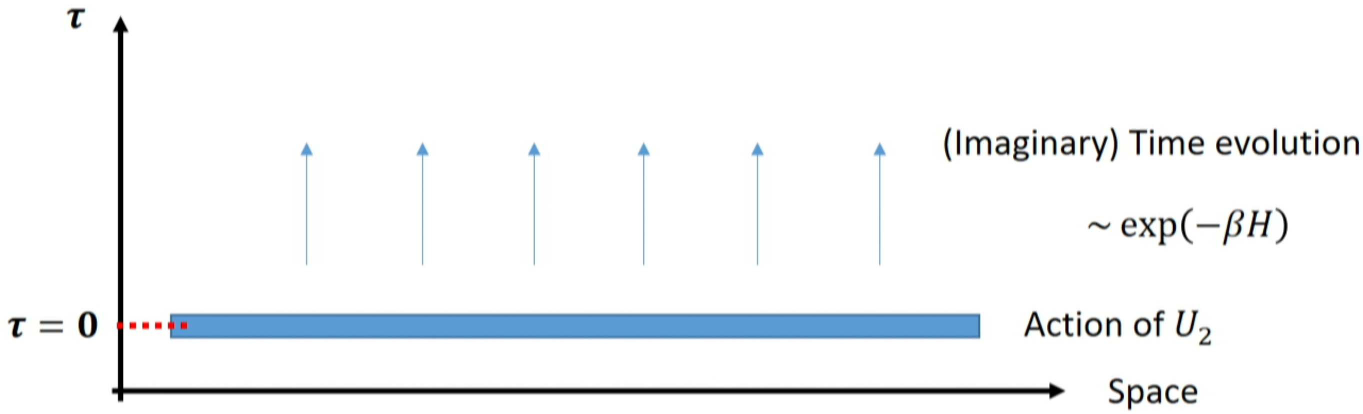


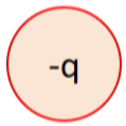
Here A_μ is generated by U_2, i.e., $A_\mu = \delta_{\mu 0}\delta(\tau)\frac{2\pi}{L_x L_y}xy$

So, what is $S_{eff}[A_\mu]$?

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

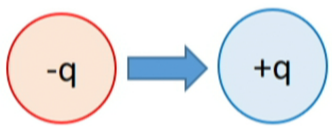
Effective Responses of Multipoles:

1. Charge (monopole)



$$\mathbf{S_{eff}} = \iiint \mathbf{dtd^2x\ q\ V(x,y)}$$

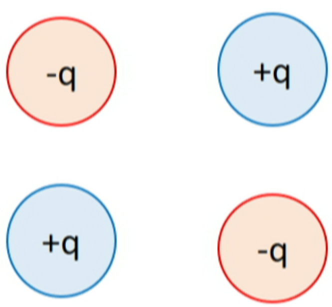
2. Dipole (1^{st} multipole)



$$\mathbf{S_{eff}} = \iiint \mathbf{dtd^2x\ q\ V(x,y) - q\ V(x+d,y)}$$

$$\approx \iiint \mathbf{dtd^2x\ qd\ \partial_x V(x,y)} = \iiint \mathbf{dtd^2x\ P \cdot E_x}$$

3. Quadrupole (2^{nd} multipole)



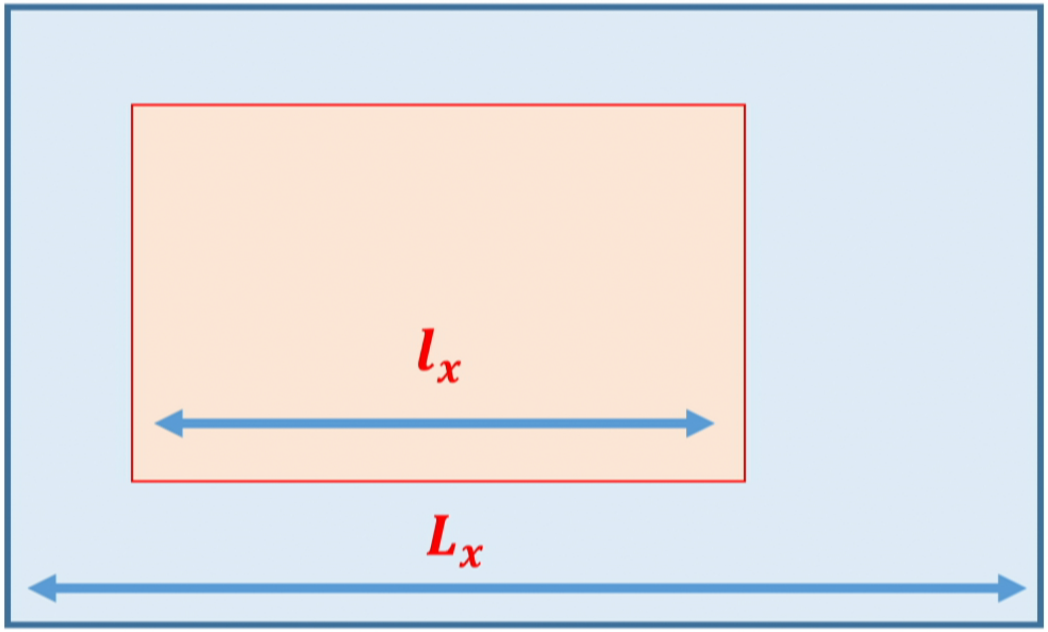
$$\mathbf{S_{eff}} = \iiint \mathbf{dtd^2x\ [q\ V(x,y) - q\ V(x+d,y) + \cdots]}$$

$$= \iiint \mathbf{dtd^2x\ Q_{xy}^{ph} \frac{[\partial_x E_y + \partial_y E_x]}{2}}$$

In fact,

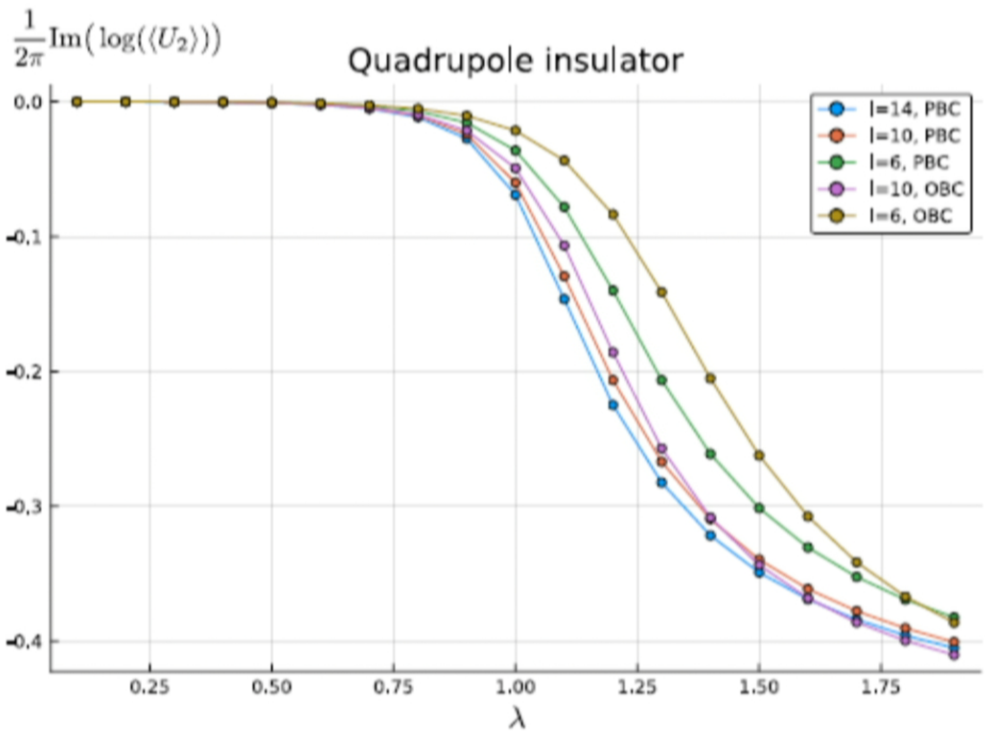
U_2 can be any unitary which saturates $S_{eff}\left[A; Q_{xy}^{ph}\right] = 2\pi Q_{xy}^{ph}$

E.g. $U_2 = \exp\left(\frac{2\pi}{l_x l_y}\sum xy\,\hat{n}\right)$ with $l_x < L_x$ and $l_y < L_y$ in Open BCs



Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

E.g., PBC/OBC are taken:



They tend to collapse to the corner charge in bigger systems.

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

In short,

We found generic definitions of electric multipoles in Crystals

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

See also: William Wheeler, Lucas Wagner, and Taylor Hughes, arxiv:1812.06990 (2018)

Remarks on the modulus of Unitaries 1.

1. Resta's conjecture on $U_1 = \exp\left(\frac{2\pi i}{L_x} \sum x\, \rho(x)\right)$

$$|\langle U_1 \rangle| \to 0 \text{ as } \Delta_{gap} \to 0 \text{ ("metal")}$$

...so that P_x as the phase of $\langle U_1 \rangle$ **ill-defined**.

[Ref. Resta (1998); **more precise statement in** Kobayashi-Nakagawa-Fukusumi-Oshikawa (2018)]

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2. Our conjecture on $U_2 = \exp\left(\frac{2\pi i}{L_x L_y} \sum xy\, \rho(x)\right)$

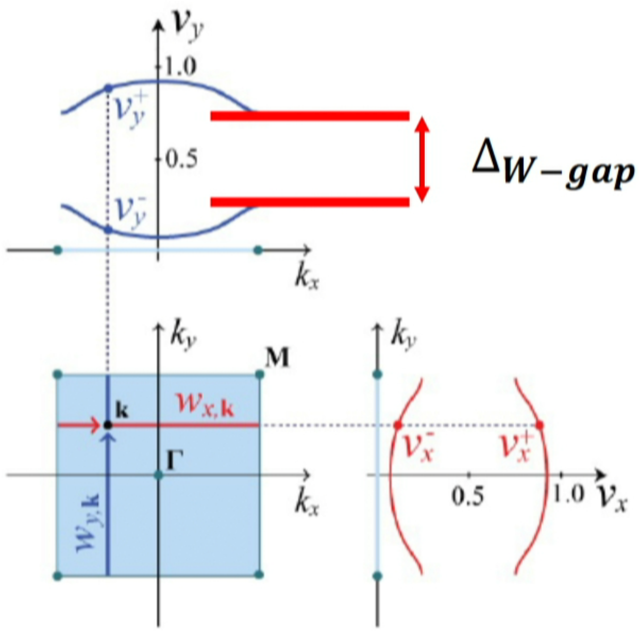
$$|\langle U_2 \rangle| \to 0 \text{ as } \Delta_{W-gap} \to 0$$ ["dipolar metal" but "charge insulator"?]

Note: $\Delta_{W-gap} \neq 0$ is necessary to define quadrupoles in nested Wilson loops

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Remarks on the modulus of Unitaries 2.

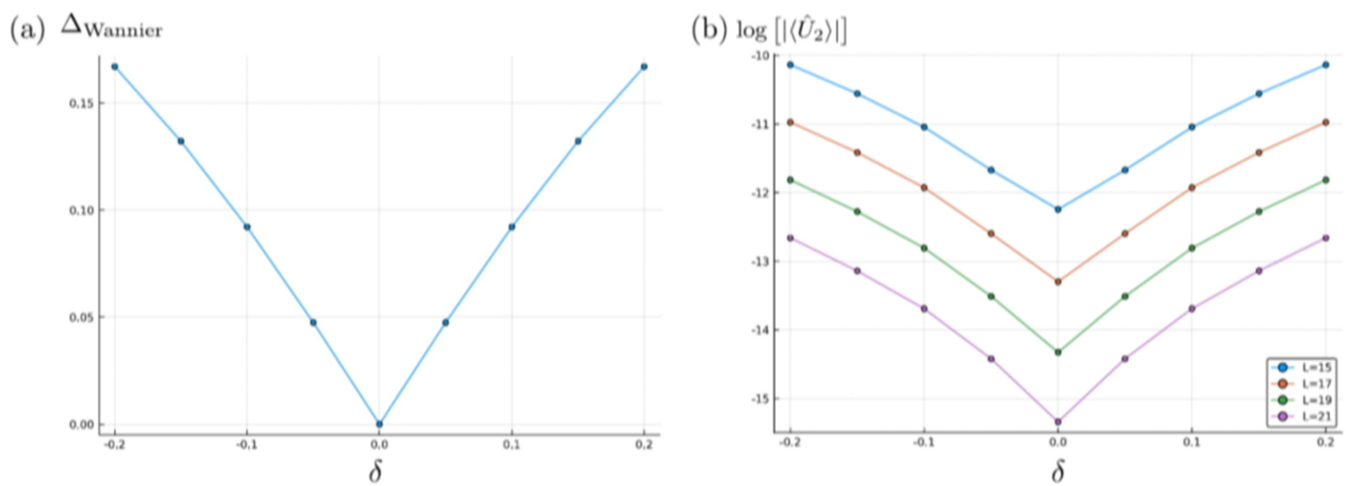
We plot…



v.s.

$$|\langle U_2 \rangle|$$

Remarks on the modulus of Unitaries 3.



$$|\langle U_2 \rangle| \rightarrow 0 \text{ as } \Delta_{W-gap} \rightarrow 0 \text{ (“Dipole Metal”)}$$

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

In short,

We found **generic definitions of electric multipoles** in Crystals

[phase part of unitary]

+ many-body measure of **Wilson loop spectrum gap closing**

[modulus of unitary]

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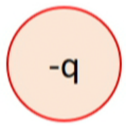

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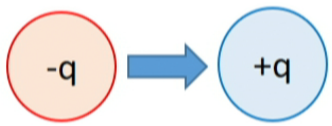
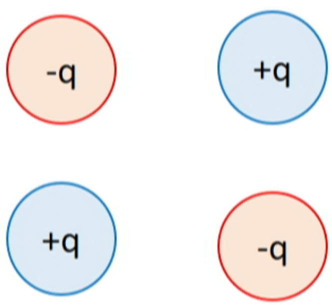


$$\mathbf{S_{eff}} = \iiint \mathbf{dtd^2x\ \ q\,V(x,y) - q\,V(x+d,y)}$$

$$\approx \iiint \mathbf{dtd^2x\ \ qd\ } \boldsymbol{\partial_x} \mathbf{V(x,y)} = \iiint \mathbf{dtd^2x\ \ P \cdot E_x}$$

3. Quadrupole (2nd multipole)



$$\mathbf{S_{eff}} = \iiint \mathbf{dtd^2x\ \ [q\,V(x,y) - q\,V(x+d,y) + \cdots]}$$

$$= \iiint \mathbf{dtd^2x\ \ Q_{xy}^{\boldsymbol{ph}}} \frac{[\boldsymbol{\partial_x E_y + \partial_y E_x}]}{\mathbf{2}}$$

Conclusions

1. Proposed (definition of) many-body invariants for multipoles

2. Numerically confirmed the invariants

3. Analytic Supports from Effective QFT

Outlooks

1. Application to Bosonic HOTIs + Interacting HOTIs

2. Momentum-Space Expressions of Our Many-Body Invariants

3. Novel Lieb-Schultz-Mattis-like theorem?

Ref. Byungmin Kang, Ken Shiozaki, and GYC, arxiv:1812.06999 (2018)

Thank you for your attention!