Many-Body Invariants of

Electric Multipoles and More



Byungmin Kang (KIAS)

Gil Young Cho



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

Byungmin Kang, and GYC, in preparation

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

Proposal:

Generic Definitions of Electric Multipoles in Solids



...many-body invariants for various topological states

Contents

1. Introduction

: Why do you want to care about electric multipoles?

2. Multipoles in Crystals

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3. Conclusions & Outlooks

1. Introduction

: Why do you want to care about electric multipoles?

Warm-up: classical multipoles



Input: Charge Distribution $ho(ec{r})$

Output: Well-defined Multipoles

Ex:
$$\mathbf{p}(\mathbf{r}) = \int\limits_V
ho(\mathbf{r}_0) \, \left(\mathbf{r}_0 - \mathbf{r}
ight) \, d^3 \mathbf{r}_0$$

Electric Field Lines

Ex:
$$\mathbf{E}(\mathbf{R}) = rac{3\left(\mathbf{p}\cdot\hat{\mathbf{R}}
ight)\hat{\mathbf{R}} - \mathbf{p}}{4\pi\varepsilon_0R^3}$$

Warm-up: classical multipoles

Multipole expansion

From Wikipedia, the free encyclopedia

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

$$P_lpha \equiv \sum_{i=1}^N q_i r_{ilpha}$$

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



Classical Multipoles seem to be Done

: Why do I still care about Electric Multipoles?

Difficulties in Crystals [at low temperature]:

(1) Quantum-mechanical Electrons

[may well be highly-correlated]

(2) Lattice (Periodicity)

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[may well be highly-correlated]

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Bad: Non-trivial to define multipoles

Good: Links to Topological Band Insulators

Infinite Lattice (Crystal):



Unit translation

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

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Position \boldsymbol{x} of Electrons \bigcirc ?



Momentum Space:



Warm-up: Dipole/Polarization Remarks on $\exp(2\pi i \mathbf{P}_{\mathbf{x}}) = \exp\left[i \oint \operatorname{Tr} A_k dk\right]$

1. Polarization: $P_x = P_x \mod 1$ (symmetry-independent)



Warm-up: Dipole/Polarization Remarks on $\exp(2\pi i \mathbf{P}_{\mathbf{x}}) = \exp\left[i \oint \operatorname{Tr} A_k dk\right]$

1. Polarization: $P_x = P_x \mod 1$ (symmetry-independent)



2. Symmetry
$$R_x: x \to -x$$

: $P_x \to -P_x$ $P_x = 0, \frac{1}{2} \mod 1$ (discrete values only)

- 3. Not clear how to write in real space (later)
- 4. Not clear how to apply to interacting electrons (later)



Relevant for, e.g., Su-Schrieffer-Heeger model



6. Boundary Charge (Physical Consequence of Polarization)



...consistent with $Q_{\rm bdry} = \vec{P} \cdot \vec{n}$ (classical electromagnetism)

7. Many-body real-space formula (Resta's formula)

VOLUME 80, NUMBER 9PHYSICAL REVIEW LETTERS2 March 1998

Quantum-Mechanical Position Operator in Extended Systems

Raffaele Resta





Recent Progresses: Electric Multipoles

Quantized electric multipole insulators

Wladimir A. Benalcazar,¹ B. Andrei Bernevig,² Taylor L. Hughes¹*

Dipolar Insulators

Quadrupolar Insulators

Octupolar Insulators



Focus: Two Primary Higher-Order TIs:



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

 $P_{x} = P_{y} = 0$ $P_{x} = P_{y} = 0$ $Q_{xy} \neq 0 \mod 1$ $Q_{ab} = Q_{ba} = 0$ $Q_{xyz} \neq 0 \mod 1$

...which can be shown only when "discrete", e.g., $Q_{xy} = \frac{1}{2}$, 0 mod 1

Quantized electric multipole insulators

[Science 2017]

Wladimir A. Benalcazar,¹ B. Andrei Bernevig,² Taylor L. Hughes¹*

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

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

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

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

Not Generic Measure of Multipoles

E.g., for the quadrupoles: symmetry **[1.** C_4 **]** or **[2.** $M_x \times M_y$ two mirrors]



Tight-binding Model

(1) Gapped Spectrum

E.g., for the quadrupoles: symmetry [1. C_4] or [2. $M_x \times M_y$ two mirrors]



"Nested Wilson Loop Approach" = Capturing Boundary Polarization

Consider a Wilson line:

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

...and investigate its polarization

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



"Nested Wilson Loop Approach" = Capturing Boundary Polarization

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...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]

By definition, nested Wilson loop is not a generic measure!



For example, when the symmetries are relaxed...

Disagreement with the physical quadrupole moment





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

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

1. Generic momentum-space invariants (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 invariant for multipoles

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

3. Of course, no link is given for 1 & 2 (since they are absent)

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∎ 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)

2. 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 propose:

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

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

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

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

Essentially,

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

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

Data first and then Proof

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

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

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

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

...from computer?

Symmetry-Protected Quadrupoles 1.



Symmetry-Protected Quadrupoles 2.

An anomalous higher-order topological insulator

S. Franca,¹ J. van den Brink,^{1,2} and I. C. Fulga¹

¹Institute for Theoretical Solid State Physics, IFW Dresden, 01171 Dresden, Germany ²Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany (Dated: November 30, 2018)

despite having a trivial topological invariant. We introduce a concrete example of an anomalous HOTI, which has a <u>quantized bulk quadrupole moment and fractional corner charges</u>, <u>but a vanishing</u> <u>nested Wilson loop index</u>. 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]

So far, consistent with nested Wilson loop indices

So far, consistent with nested Wilson loop indices

Can I go beyond nested Wilson approaches?

I.E., regime where quantizing symmetries are relaxed

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



When this is uniformly stacked,



So we compare the following two:





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

Beyond nested Wilson loop



Seems working.

But why do they work?

Path-integral Interpretation of the overlap:

$$\langle \mathbf{GS} | \mathbf{U}_2 | \mathbf{GS} \rangle = \frac{1}{Z} \operatorname{Tr} e^{-\beta H} \mathbf{U}_2 \propto \exp\left(\frac{i \mathbf{S}_{\text{eff}} \left[A_{\mu}\right]\right)$$

Applying Dyson's formula:

Path-integral Interpretation of the overlap:

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Applying Dyson's formula:



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
$$S_{eff}[A_{\mu}]$$
?

Effective Responses of Multipoles:

1. Charge (monopole)

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

-q



$$S_{eff} = \iiint dtd^{2}x \ q \ V(x, y) - q \ V(x + d, y)$$
$$\approx \iiint dtd^{2}x \ qd \ \partial_{x}V(x, y) = \iiint dtd^{2}x \ P \cdot E_{x}$$

3. Quadrupole (2nd multipole)

$$\begin{array}{c} -\mathbf{q} \\ +\mathbf{q} \\ +\mathbf{q} \end{array} \qquad \mathbf{S}_{eff} = \iiint dtd^2 x \ [\mathbf{q} \ \mathbf{V}(\mathbf{x}, \mathbf{y}) - \mathbf{q} \ \mathbf{V}(\mathbf{x} + \mathbf{d}, \mathbf{y}) + \cdots] \\ \\ \end{array}$$

For the gauge fields: $A_{\mu} = \delta_{\mu 0} \delta(\tau) \frac{2\pi}{L_{\chi} L_{\gamma}} xy$

 $\langle \mathrm{GS}|\mathrm{U}_2|\mathrm{GS}\rangle \propto \exp\left(i\mathrm{S}_{\mathrm{eff}}\left[A_{\mu}\right]\right) \propto \exp\left(2\pi i Q_{xy}^{ph}\right) = \exp\left(2\pi i Q_{c}\right)$



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

Spins?

[1] B Kang, K Shiozaki, and GYC (2018)



[Each dot is spin-1/2]

$$H_p = \lambda \sum_{a=x,y} \left(\sigma_1^a \sigma_2^a + \sigma_2^a \sigma_3^a + \sigma_3^a \sigma_4^a + \sigma_4^a \sigma_1^a \right)$$

[Ref. Dubinkin-Hughes (2018)]

At the exactly-soluble limits:

(1) $\lambda \neq 0$ and t = 0: Topological

- Dangling spin- $\frac{1}{2}$'s at the corners

$$\langle U_2 \rangle = -1$$

(2) $\lambda = 0$ and $t \neq 0$: Trivial

 $\langle U_2 \rangle = +1$

Other models?

Reviewer 1's model:

To verify that the value of the order parameter proposed in this manuscript indeed describes the multipole moments in a more general setting, <u>I calculated the value of the order parameter for a model</u> which is a modification of the model in Eq 4 in that, instead of threading \pi flux per plaquette, only half of that flux is





Other models?

Review 1

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With Boundary Polarizations

$$Q_c = P_x^{bdry} + P_y^{bdry} - Q_{xy}$$



Other models?

Higher Order Topological Insulators in Amorphous Solids

Adhip Agarwala,^{1, 2, *} Vladimir Juričić,^{3, †} and Bitan Roy^{2, ‡}

[Amorphous, Disordered Fermionic (2019 Feb)]

Nonsymmorphic Topological Quadrupole Insulator in Sonic Crystals

Zhi-Kang Lin,
1 Hai-Xiao Wang,
2,1 Ming-Hui Lu,
3 and Jian-Hua Jiang
1, \ast

[Nonsymmorphic, Bosonic (2019 Mar)]

Higher-order topological insulator out of equilibrium: Floquet engineering and quench dynamics

Tanay Nag,^{1, 2, *} Vladimir Juričić,^{3, †} and Bitan Roy^{2, ‡}

[Nonequilibrium, Floquet-driven (2019 April)]

So far so good if there is a Wannier gap.

Cf. S Ono, L Trifunovic, and H Watanabe (2019)

In short,

We found working 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)

Beyond Multipoles:

Byungmin Kang, and GYC, in preparation

For U(1) symmetric states:

 $S_{top} = \text{Im} [S_{eff}]$ can be gradient expanded by A_{μ}

We find a unitary U with spatial geometry M:



Byungmin Kang (KIAS)

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For U(1) symmetric states:

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We find a unitary U with spatial geometry M:

1: Phase of $\langle GS(M)|U|GS(M)\rangle$ detects **the topology**

Ex: bulk dipole, bulk quadrupole, bulk octupole etc

Resta (1999); Kang, Shiozaki, and GYC (2018)

Ex: boundary polarizations, Chern numbers

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Byungmin Kang (KIAS)

2: $|\langle GS(M)|U|GS(M)\rangle|$ detects "metallicity/gap" of the excitation

Ex: Resta's conjecture, Wannier gap for multipoles

Resta (1999), Kang, Shiozaki, and GYC (2018); Dubinkin, May-mann, and Hughes (2019)

3. Conclusions & Outlooks

Conclusions

- 1. Proposed (definition of) many-body invariants for multipoles
- 2. Numerically confirmed the invariants
- **3. Analytic Supports from Effective QFT**
- 4. Generalization to other topological states

Outlooks

- **1. Momentum-Space Indices of Our Many-Body Invariants**
- 2. Cases without Wannier gap

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

Thanks for your attention!

Remarks on the modulus of Unitaries 1.

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

$$|\langle {m U}_1
angle| o {m 0}$$
 as $\Delta_{gap} o {m 0}$ ("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
$$U_2 = \exp\left(\frac{2\pi i}{L_x L_y} \sum xy \rho(x)\right)$$

 $|\langle U_2 \rangle| \rightarrow 0 \text{ as } \Delta_{W-gap} \rightarrow 0 \quad [\text{``dipolar metal''} but ``charge insulator''?]$

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

Remarks on the modulus of Unitaries 2.

We plot...



Remarks on the modulus of Unitaries 3.



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

In short,

We found generic definitions of electric multipoles in Crystals

[phase part of unitary]

+ many-body measure of Wannier gap closing

[modulus of unitary]

Higher-Order Topology = Non-Trivial at "Boundary of Boundary"

Ex: In **2D**,



Quadrupolar Insulators

Higher-Order Topology = Non-Trivial at "Boundary of Boundary"

Octupolar Insulators

Ex: In **3D**,

