Title: Electric Multipole Insulators

Speakers: Taylor Hughes

Date: February 01, 2021 - 12:30 PM

URL: http://pirsa.org/21020001

Abstract: In this talk I will present a general framework to distinguish different classes of charge insulators based on whether or not they insulate or conduct higher multipole moments (dipole, quadrupole, etc.). This formalism applies to generic many-body systems that support multipolar conservation laws. Applications of this work provide a key link between recently discovered higher order topological phases and fracton phases of matter.

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## **Collaborators**



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Yizhi You



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## **Outline**

Part 1: Classical Multipole Moments

Part 2: Quantized Multipole Moments in Crystals

Part 3: Calculating Multipole Moments

Part 4: Many-body Multipole Insulators

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## **Classical Multipole Moments of Point Charges**



Monopole Moment (charge)

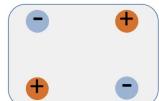
dim

$$P^i = \sum_{\alpha} q_{\alpha} x_{\alpha}^i$$

**Dipole Moment** 

1

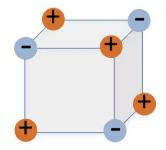
$$Q^{ij} = \sum_{\alpha} q_{\alpha} x_{\alpha}^{i} x_{\alpha}^{j}$$



Quadrupole Moment

2

$$O^{ijk} = \sum_{\alpha} q_{\alpha} x_{\alpha}^{i} x_{\alpha}^{j} x_{\alpha}^{k}$$

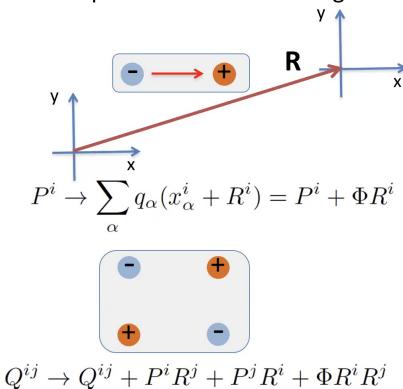


Octupole Moment

3

## **Classical Multipole Moments of Point Charges**

Constraints for Independence of Global Origin of Coordinates



For *n*-th moment to be well-defined all lower moments must vanish.

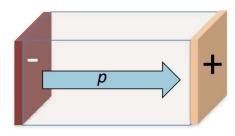
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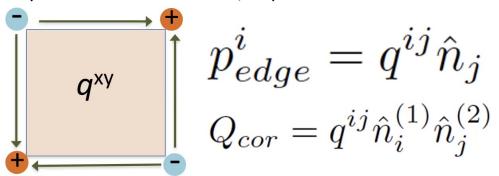


Polarization  $p^i$  (dipole moment per volume) is only well-defined in a neutral material



$$\sigma = \vec{p} \cdot \hat{n}$$

Quadrupole density  $oldsymbol{q}^{ij}$  is only well-defined in neutral, unpolarized materials

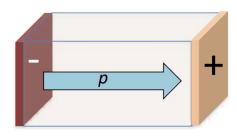


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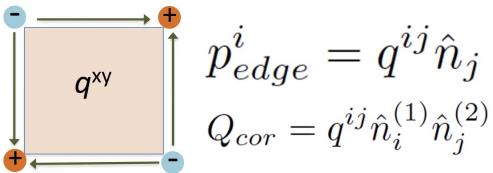


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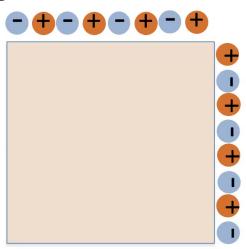
Quadrupole density  $oldsymbol{q}^{\mathsf{i}\mathsf{j}}$  is only well-defined in neutral, unpolarized materials



Note: In their intrinsic dimensions each multipole moment density has units of charge.

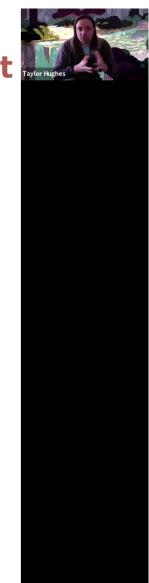
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Take an insulating sheet that is neutral in the bulk, and unpolarized.

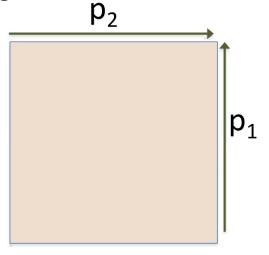


Attach polarization only on boundary.

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Take an insulating sheet that is neutral in the bulk, and unpolarized.

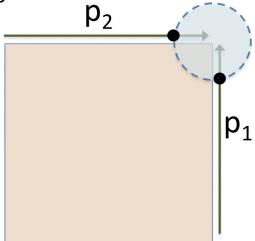


Attach polarization only on boundary.

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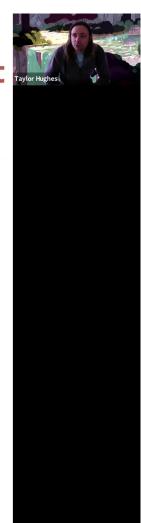


Take an insulating sheet that is neutral in the bulk, and unpolarized.



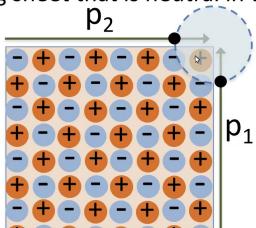
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$$Q_{cor} = p_1 + p_2$$





Take an insulating sheet that is neutral in the bulk, and unpolarized.



Attach polarization only on boundary.

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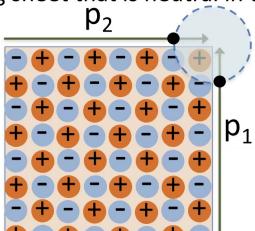
Bulk quadrupole moment captures the failure of this equation

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Take an insulating sheet that is neutral in the bulk, and unpolarized.



Attach polarization only on boundary.

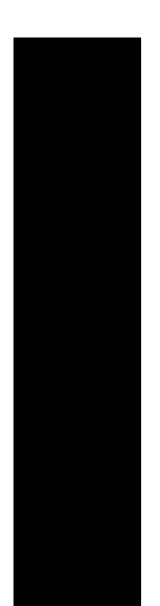
$$Q_{cor} = p_1 + p_2$$

Bulk quadrupole moment captures the failure of this equation

$$Q_{cor} - p_1 - p_2 = -q^{xy}$$

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# Part 2: Quantized Multipole Moments in Crystals

Wladimir Benalcazar, B. Andrei Bernevig, TLH (*Science* 2017)

Wladimir Benalcazar, B. Andrei Bernevig, TLH (PRB 2017)



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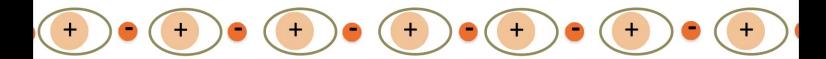






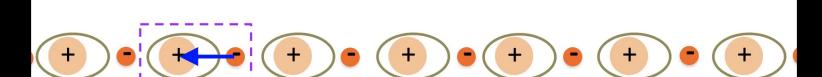


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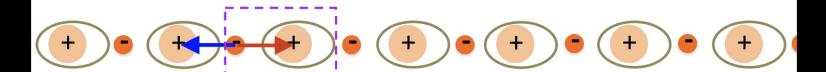
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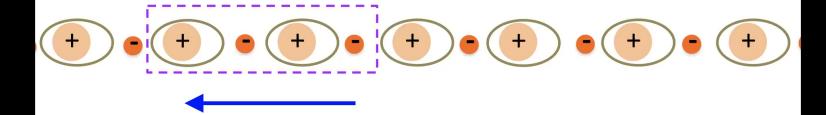








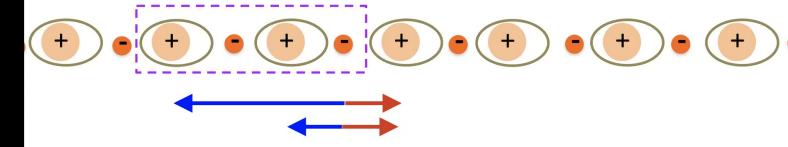
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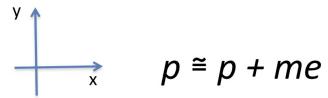
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In each case the 1D polarization differs by an integer multiple of the charge e.



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## **Quantization of Polarization in Crystals**















Pick a symmetry under which the polarization is odd and enforce it Ex: Inversion, Reflections, C2 rotations, Charge-conjugation

$$p = -p$$

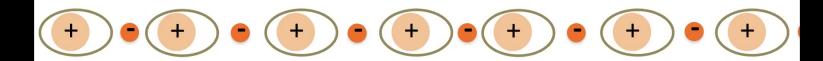
$$2p = 0 \mod e$$

$$p = 0 \text{ or } e/2$$

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## **Quantization of Polarization in Crystals**



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$$p = -p$$

$$2p = 0 \mod e$$

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## **Example: 1D Insulators with Reflection Symmetry**

$$p = 0$$





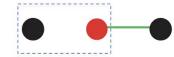


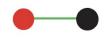






$$p = e/2$$













Calculation of polarization in momentum space (Vanderbilt, King-Smith 1993)

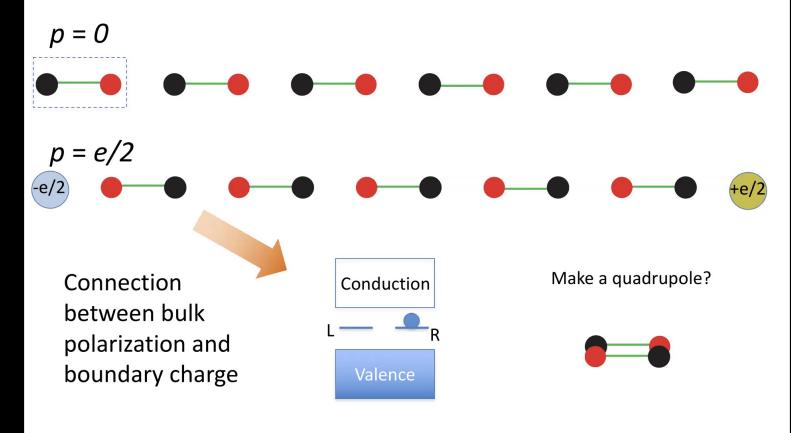
Given: H(k)

Construct:  $A^{mn}(k) = -i\langle u_m(k)|\partial_k|u_n(k)\rangle$ 

Calculate:  $p = \frac{e}{2\pi} \int_{BZ} \text{Tr} \left[ A(k) \right] dk$ 

 $\hat{x} \sim -i\partial_k$ 

## **Polarization and Boundary Charge**

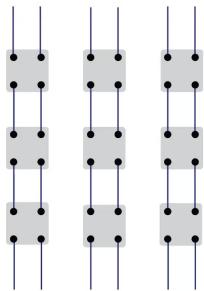


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#### **Expectations:**

- 1. Quadrupole is formed from two dipoles, expect we need at least two occupied bands. Want quantized, vanishing polarization.
- 2. Need to choose symmetries under which quadrupole and polarization are odd. We will impose reflection symmetries  $M_x$  and  $M_y$ .

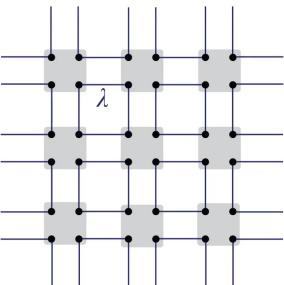


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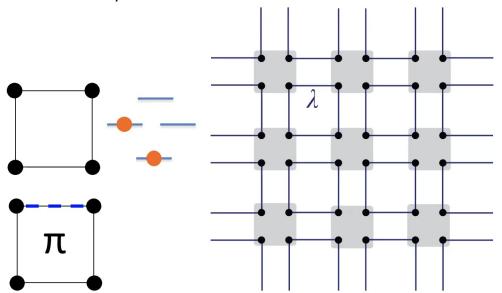


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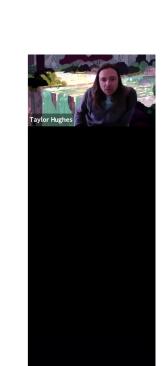


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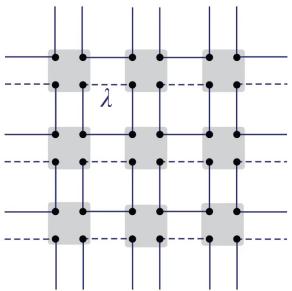


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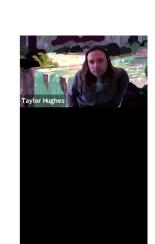


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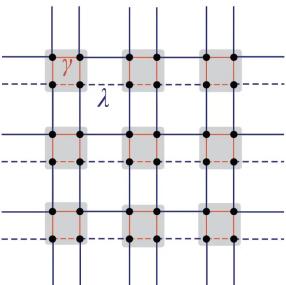


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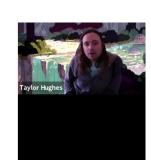


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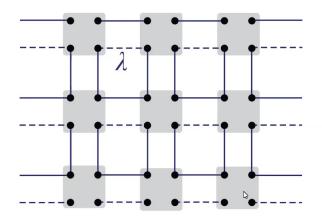


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#### **Expectations:**

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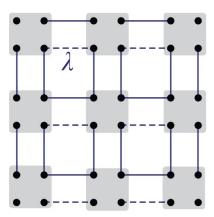


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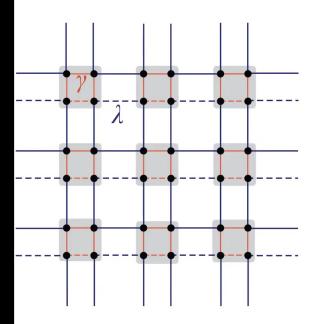
#### **Expectations:**

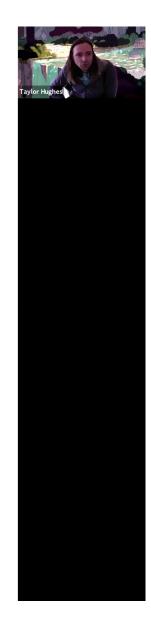
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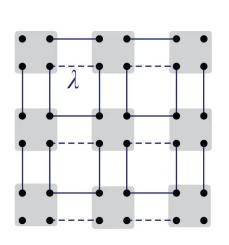
Bulk quadrupole density:  $q^{xy} = e/2$ 

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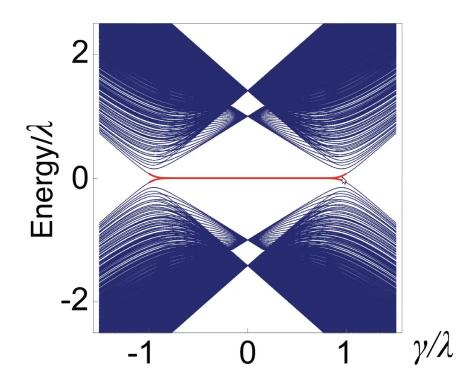




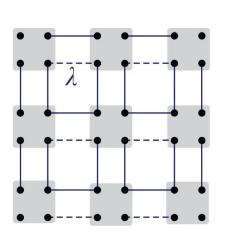
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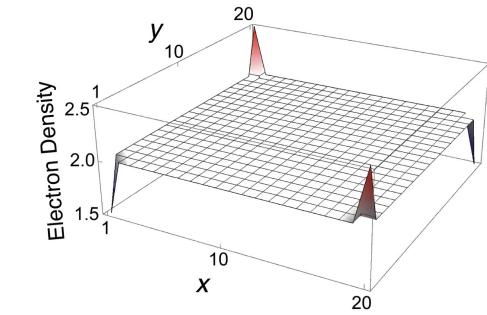


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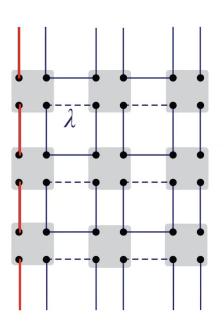


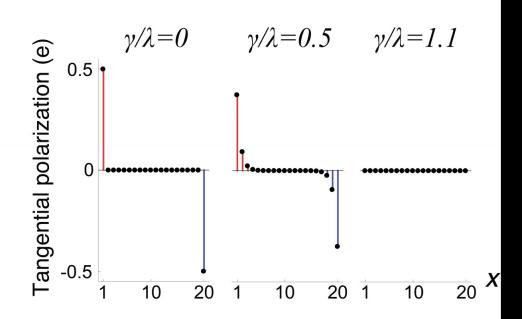


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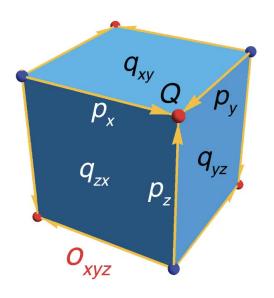


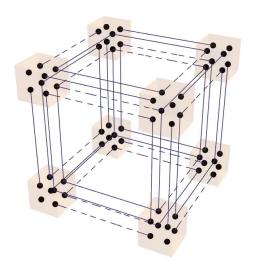


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### **Octupole Moment in 3D systems**

Simplest extension to 3D is with octupole moment  $o_{xyz}$ 





Need four occupied bands (two cancelling quadrupoles).

Quantized by keeping all three reflections m<sub>x</sub>, m<sub>y</sub>, m<sub>z</sub>

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# Part 3: Calculating Multipole Moments



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#### **Bulk Characterization of Quadrupole**

Quadrupole is just a product of two coordinates, e.g., X\*Y. The problem is that the effective electron position operators in the lattice do not commute with each other and cannot be measured simultaneously.

Can calculate corner charge and edge polarization:

$$Q_{cor} - p_1 - p_2 = -q^{xy}$$

Instead we want to be able to diagnose the multipole moments from the bulk. For the quantized cases we can look for topological invariants.

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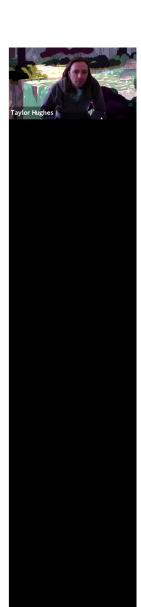
#### **Hidden Topology**

Sometimes when a topological invariant is zero, it can be non-zero in some subsector of the occupied states.

An example is the Quantum Spin Hall effect where the total Chern number is zero, but we can resolve the invariant further by looking at each spin component:

Chern Number = 0 = +1 (spin up) -1 (spin down)

However, in our case we do not have a nice quantum number like spin to resolve the topology.



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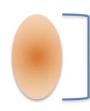
# **Resolving Topology in Real-Space**

Key idea: Resolve the electrons in real-space



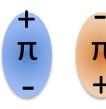
Resolve in x-direction:





Two separate clouds/sectors

If we look at each cloud individually is it topological?



Calculate Berry Phase

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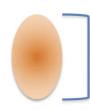


Key idea: Resolve the electrons in real-space



Resolve in x-direction:





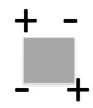
Two separate clouds/sectors

If we look at each cloud individually is it topological?





Calculate Berry Phase

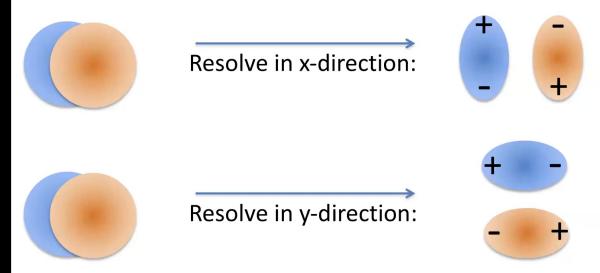


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# **Resolving Topology in Real-Space**

Key idea: Resolve the electrons in real-space

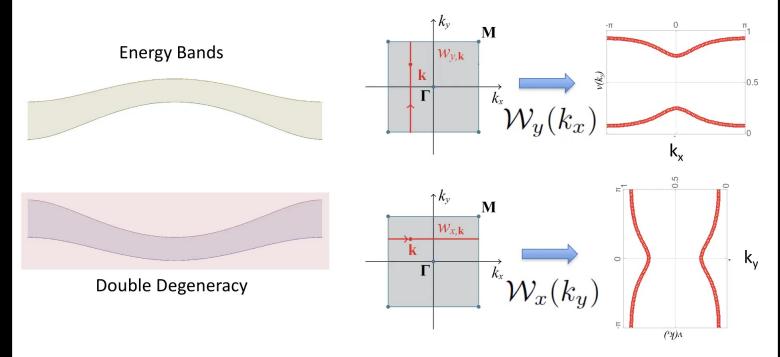


If both sets of Berry phases are non-trivial, then it has a topological quadrupole moment!

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# **Topological Characterization of Quadrupole**



Quadrupole phase characterized by  $\pi$  Berry phase of Wannier bands in both directions.

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# **Resolving Topology in Real-Space**

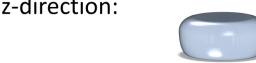
What else can we do? Let's look at 3D



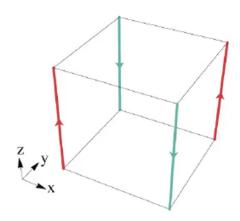
Resolve in z-direction:



Quasi-2D Electron Clouds



If the Chern number of each cloud is non-zero you find a chiral hinge insulator



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#### **Other Methods Needed**

Different symmetry classes?

- Can use other symmetry indicators.

Non-quantized quadrupole?

- Can go back to surface polarization and corner charge. Still need vanishing bulk dipole moment.

How can we generically diagnose from the bulk?

What about many-body systems?

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# Many-body calculation of electric polarization



Given:  $|\Psi_0
angle$  In 1D

Berry Phase: 
$$\Phi \qquad A_x = \frac{\Phi}{L_x}$$
 
$$P = \frac{1}{2\pi} {\rm Im} \int d\Phi \langle \Psi_0 | \partial_\Phi | \Psi_0 \rangle$$

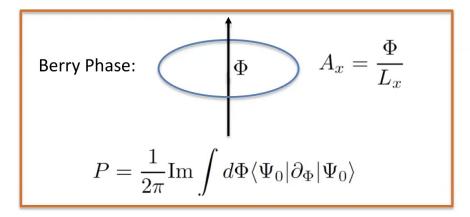
Ortiz, Martin (1994) Resta (1999)

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## Many-body calculation of electric polarization



Given:  $|\Psi_0\rangle$ In 1D



Many-body **Twist Operator:** 

$$U_X = \exp\left[\frac{2\pi i\hat{X}}{L_x}\right]$$
  $\hat{X} = \sum_{\alpha=1}^{N_e} \hat{x}_{\alpha}$ 

$$\hat{X} = \sum_{\alpha=1}^{N_e} \hat{x}_{\alpha}$$

$$U_X|\Psi_0\rangle = e^{2\pi i P} (|\Psi_0\rangle + O(1/L))$$

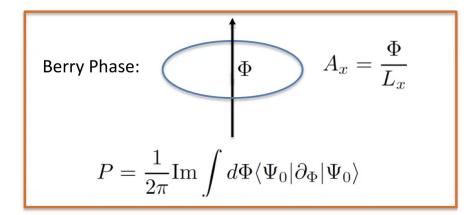
Ortiz, Martin (1994) Resta (1999)

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# Many-body calculation of electric polarization



Given: 
$$|\Psi_0
angle$$
 In 1D



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$$U_X|\Psi_0\rangle = e^{2\pi i P} (|\Psi_0\rangle + O(1/L))$$

$$z_X \equiv \langle \Psi_0 | U_X | \Psi_0 \rangle$$

$$P = \lim_{N_e \to \infty} \frac{1}{2\pi} \operatorname{Im} \log z_X$$

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#### Many-body calculation of electric quadrupole

Given:  $|\Psi_0\rangle$ 

In 2D

Nested

Berry Phase?

No obvious way to do this. Will come back to it later.

Many-body **Twist Operator:** 

$$U_{XY} = \exp\left[\frac{2\pi i \widehat{XY}}{L_x L_y}\right] \qquad \widehat{XY} = \sum_{\alpha=1}^{N_e} \hat{x}_{\alpha} \hat{y}_{\alpha}$$

$$\widehat{XY} = \sum_{\alpha=1}^{N_e} \hat{x}_{\alpha} \hat{y}_{\alpha}$$

$$z_{XY} \equiv \langle \Psi_0 | U_{XY} | \Psi_0 \rangle$$

$$q_{xy} = \lim_{N_e \to \infty} \frac{1}{2\pi} \operatorname{Im} \log z_{XY}$$

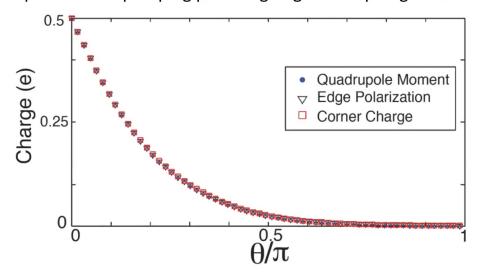
Wheeler, Wagner, TLH (2018) Kang, Shiozaki, Cho (2018)

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# **Many-Body Calculation of Quadrupole**

It works. Example here is a pumping process going from topological to trivial phase:

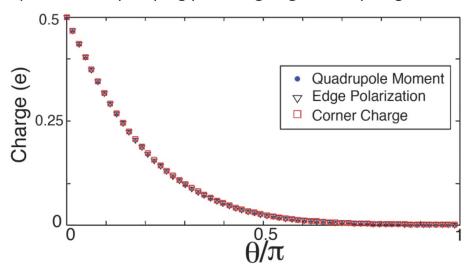


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# **Many-Body Calculation of Quadrupole**

It works. Example here is a pumping process going from topological to trivial phase:



But something unusual happens in thermodynamic limit

Insulator: 
$$U_X |\Psi_0\rangle = e^{2\pi i P} \left( |\Psi_0\rangle + O(1/L) \right) \longrightarrow \lim_{N\to\infty} |z_X| = 1$$

But we find:  $\lim_{N \to \infty} |z_{XY}| = 0$  So the is not v

So the phase, i.e., quadrupole moment is not well-defined in thermodynamic limit?

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#### Charge localization and dipole fluctuations

The approach of  $|z_X|$  to unity in the thermodynamic limit has a physical interpretation.

Charge localization length 
$$\xi^2=-\lim_{N\to\infty} \frac{L_x^2}{4\pi^2N}\log|z_X|^2$$
 For finite size  $|z_X|=1$  Only if  $\xi=0$ 

For finite size 
$$\left|z_X\right|=1$$

Only if 
$$\xi = 0$$

$$\xi^2 = \lim_{N o \infty} rac{1}{N} \left( \langle \hat{X}^2 
angle - \langle \hat{X} 
angle^2 
ight)$$
 — Dipole fluctuations

$$U_X|\Psi_0\rangle = e^{2\pi i P} \left(|\Psi_0\rangle + O(1/L)\right)$$

Leads to a criterion:

$$\xi 
ightarrow \infty$$
 Metal Resta, Sorella (1999)  
Aligia, Ortiz (2000)

$$\xi o const.$$
 Insulator Souza, Wilkens, Martin (2000)

Even if dipole moment vanishes on average, the fluctuations can seemingly cause issues with the calculation of the quadrupole moment.



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Taylor Hughes

Want to study systems having  $\,\xi=0\,$ 

- Free fermion insulators: Wannier functions must be delta-functions. Too restrictive.
- Many-body insulators: Just need U(1) charge and dipole conservation

Charge: 
$$e^{i\alpha}$$
  $e^{i\alpha}c_i^{\dagger}e^{-i\alpha}c_j=c_i^{\dagger}c_j$ 

Dipole: 
$$e^{i\alpha\hat{X}} \qquad e^{i\alpha x}c_{(x,y)}^{\dagger}e^{-i\alpha(x+1)}c_{(x+1,y)}e^{i\alpha(x+1)}c_{(x+1,y+1)}^{\dagger}e^{-i\alpha x}c_{(x,y+1)}$$
 
$$= c_{(x,y)}^{\dagger}c_{(x+1,y)}c_{(x+1,y+1)}^{\dagger}c_{(x,y+1)} \qquad \text{One example: ring exchange}$$

Pretko, PRB (2018)

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#### **Dipole Conserving Hamiltonians**

Taylor Hughes

Want to study systems having  $\,\xi=0\,$ 

#### Consequence 1:

$$U_X|\Psi_0\rangle = e^{2\pi i P_x}|\Psi_0\rangle$$
  $U_Y|\Psi_0\rangle = e^{2\pi i P_y}|\Psi_0\rangle$ 

#### Consequence 2:

Can couple the system to a rank-2 gauge field, e.g.,  $A_{xy}$  [Pretko, PRB (2018)]

$$c_{(x,y)}^{\dagger}c_{(x+1,y)}c_{(x+1,y+1)}^{\dagger}c_{(x,y+1)} \rightarrow e^{iA_{xy}}c_{(x,y)}^{\dagger}c_{(x+1,y)}c_{(x+1,y+1)}^{\dagger}c_{(x,y+1)}$$

Heuristically: 
$$A_{xy}=rac{1}{2}(\partial_x A_y+\partial_y A_x)$$

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#### **Dipole Insulator and Dipole Metal Criterion**



Generalize Kohn's Criterion (sensitivity to shifts in gauge field):  $A_{xy} o A_{xy} + \mathfrak{q}$ 

$$D_d=-rac{\pi}{V}\left.rac{\partial^2 E_0}{\partial \mathfrak{q}^2}
ight|_{\mathfrak{q}=0}$$
 Dipole stiffness (aka dipole Drude weight)

Dipole localization: 
$$\lambda_d^2 = -\lim_{N_d \to \infty} \frac{L_x^2 L_y^2}{4\pi^2 N_d} \log|z_{XY}|^2 \qquad \quad [\lambda_d] = Length^2$$

Quadrupole fluctuations: 
$$\lambda_d^2 = \lim_{N_d \to \infty} \frac{1}{N_d} \left( \langle \widehat{XY}^2 \rangle - \langle \widehat{XY} \rangle^2 \right)$$

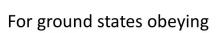
#### Leads to a criterion:

$$\lambda_d = const, \ D_d = 0$$
 Dipole Insulator

$$\lambda_d = \infty, \ D_d = const$$
 Dipole Metal

Dubinkin, May-Mann, TLH (2019)

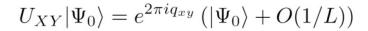
#### **Rank 2 Berry Phase**



$$U_X|\Psi_0\rangle = |\Psi_0\rangle$$

$$U_Y|\Psi_0\rangle = |\Psi_0\rangle$$

Polarization vanishes



Rank-2 Berry phase gives quadrupole moment!

$$A_{xy} \to A_{xy} + \frac{2\pi}{L_x L_y}$$

$$q_{xy} = \frac{1}{2\pi} \operatorname{Im} \int_{0}^{2\pi/L_x L_y} d\mathfrak{q} \langle \Psi_0 | \partial_{\mathfrak{q}} | \Psi_0 \rangle$$

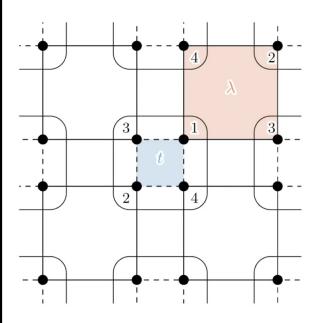
Connection to Araki, Mizoguchi, Hatsugai? (1906.00218)

Dubinkin, May-Mann, TLH (2019)

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#### **An Example Model:**



$$H = \lambda \sum_{\mathbf{p}} \left| \stackrel{\frown}{\bullet} \right\rangle \left\langle \stackrel{\bullet}{\bullet} \right| + t \sum_{\mathbf{s}} \left| \stackrel{\frown}{\bullet} \right\rangle \left\langle \stackrel{\bullet}{\bullet} \right| + h.c.$$

Let t=0

$$|\psi\rangle_{\mathbf{p}} = \frac{1}{\sqrt{2}} \left( \left| \mathbf{\hat{p}} \right\rangle_{\mathbf{p}} - \left| \mathbf{\hat{p}} \right\rangle_{\mathbf{p}} \right)$$

$$|GS\rangle = \bigotimes_{\mathbf{p}} |\psi\rangle_{\mathbf{p}}$$

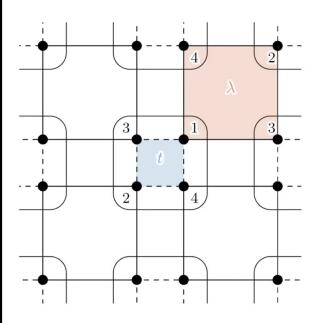
$$\lambda_d = a^2/2$$
 Dipole insulator

$$|\psi(\mathfrak{q})\rangle_{\mathbf{p}} = \frac{1}{\sqrt{2}} \left( e^{-i\frac{\mathfrak{q}}{2}} \left| \stackrel{\bullet}{\bullet} \stackrel{\bullet}{\bullet} \right\rangle_{\mathbf{p}} - e^{i\frac{\mathfrak{q}}{2}} \left| \stackrel{\bullet}{\bullet} \stackrel{\bullet}{\bullet} \right\rangle_{\mathbf{p}} \right) \longrightarrow \operatorname{Im} \sum_{\mathbf{p}=1}^{L_x L_y} \int_0^{2\pi/L_x L_y} d\mathfrak{q} \langle \psi(\mathfrak{q}) | \partial_{\mathfrak{q}} | \psi(\mathfrak{q}) \rangle_{\mathbf{p}} = \pi$$

Dubinkin, May-Mann, TLH (2019); You, Burnell, TLH (2019)



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Two dipole insulator phases, t=0 and  $\lambda$  = 0 differ by rank 2 Berry phase (quadrupole)

Dubinkin, May-Mann, TLH (2019); You, Burnell, TLH (2019)

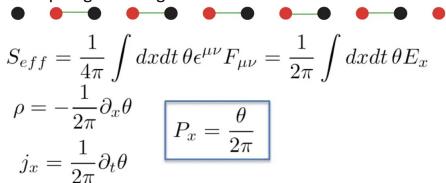


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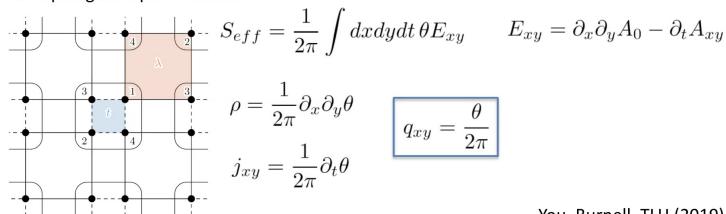




1D topological charge insulator



2D topological dipole insulator

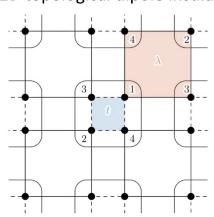


You, Burnell, TLH (2019)

#### 2D Topological "Dipole" Insulator



2D topological dipole insulator



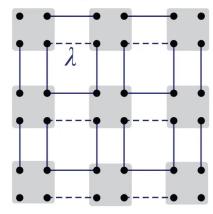
$$S_{eff} = \frac{1}{2\pi} \int dx dy dt \, \theta E_{xy}$$

Break dipole U(1), But keep total polarization zero

$$E_{xy} = \frac{1}{2}(\partial_x E_y + \partial_y E_x)$$



2D higher order TI



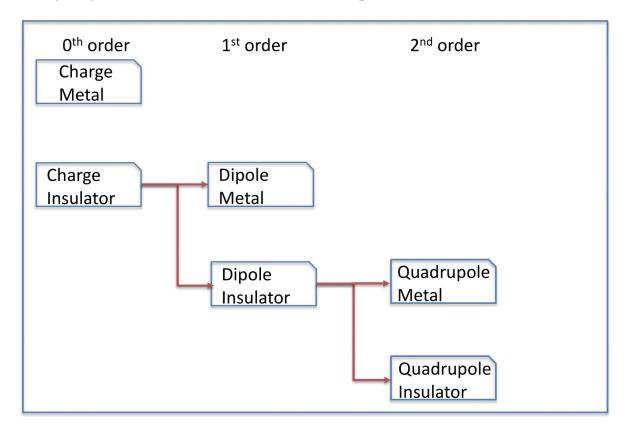
$$S_{eff} = \frac{1}{2} \int dx dy dt \, q_{ij} \partial_i E_j$$

You, Burnell, TLH (2019)

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## **Summary: Multipole Metals and Insulators**

We propose a refinement of charge insulators



Dubinkin, May-Mann, TLH (2019)

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