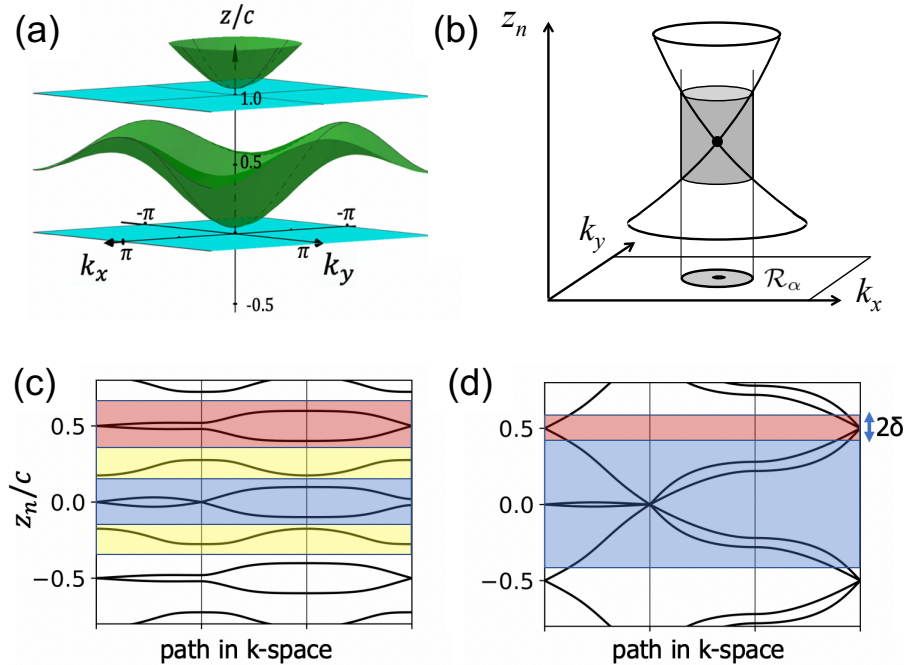


# Axion Magnetolectric Coupling in the Hybrid Wannier Representation

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(a) The hybrid Wannier representation works in reciprocal space in two dimensions (2D Brillouin zone is plotted horizontally), but in real space in the third (vertical) dimension. Vertical position indicates the charge center of the corresponding electron wave function, which repeats periodically with lattice constant  $c$ . (b) The hybrid Wannier structure sometimes contains the analog of Weyl points. (c) and (d), two possible arrangements of hybrid Wannier bands color-coded by the way they contribute to the axion coupling.

N. Varnava, I. Souza, and D. Vanderbilt, *Axion coupling in the hybrid Wannier representation*, arXiv:1912.11887.

## Scientific Achievement

A large class of topological insulators (TIs) is characterized by the presence of a quantized magneto-electric (ME) "axion" coupling. We have developed a detailed theory connecting this axion coupling to features of the hybrid Wannier (HW) representation, which has emerged as one of the most important theoretical tools for understanding TIs.

## Significance and Impact

Our work allows for a deeper understanding of an important but somewhat obscure concept in the theory of topological insulators, namely the ME axion coupling. In the presence of certain symmetries, this can take on only one of two values: zero (trivial), or  $e^2/2h$  (topological), where  $e$  = electron charge and  $h$  = Planck's constant. In the topological case, all insulating surfaces must display a half-integer quantized anomalous Hall effect.

## Research Details

We have applied a powerful theoretical tool, the HW (or "Wilson loop") representation, in which the electron occupation is described from a real-space point of view in one lattice direction while keeping a Bloch representation in the others. We clarified how the axion topology manifests itself in the HW representation, and conversely, how the axion topological index can often be determined directly from an inspection of the HW band structure.



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## What is axion magnetoelectric coupling?

- $\vec{E} \cdot \vec{B}$  term in effective energy inside material
- Its strength can be written as

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

- $\theta$  is known as the "axion angle"
- Some symmetries force  $\theta$  to be:

$\theta = 0$  : Trivial

$\theta = \pi$  : Topological

### Math details

Berry connection of Bloch states:

$$A_{a,nm} = i \langle u_{nk} | \partial_a | u_{mk} \rangle$$

Axion  $\theta$  as Brillouin zone integral:

$$\theta = -\frac{1}{4\pi} \int d^3k \epsilon_{abc} \text{tr} \left[ A_a \partial_b A_c - \frac{2i}{3} A_a A_b A_c \right]$$

Well defined only modulo  $2\pi$

<u>Symmetry</u>	<u>Known examples?</u>
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Time reversal	Bi <sub>2</sub> Se <sub>3</sub> etc.
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Inversion	Main target of our axion thrust
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Others*	Additional materials search space !
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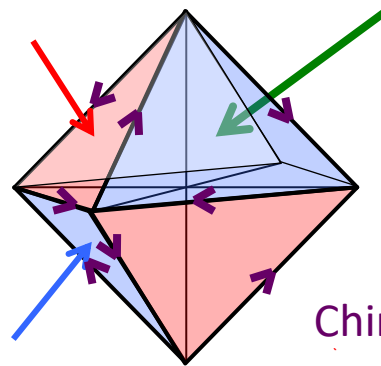
\* Mirrors, rotoinversions, time-reversed rotations, etc.

## Quantized surface anomalous Hall conductivity (AHC)

$$\sigma_{\text{AHC}} = \pm e^2/2h$$

Surface AHC  
 $+e^2/2h$

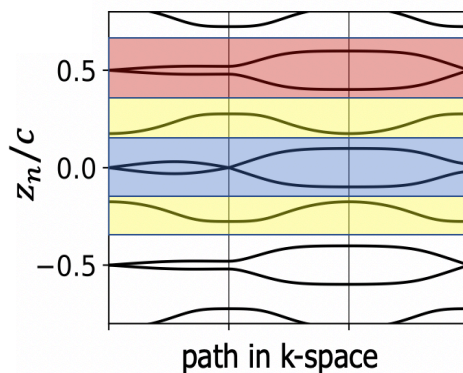
Surface AHC  
 $-e^2/2h$



Formal bulk  
magnetolectric  
coupling  $e^2/2h$   
protected by  
some symmetry

Chiral hinge modes

## Hybrid Wannier representation as a tool



- Investigate *all* symmetries that protect axion topology, not just TR and inversion
- Study "bulk-boundary correspondence"
- Facilitate widened search for topological materials