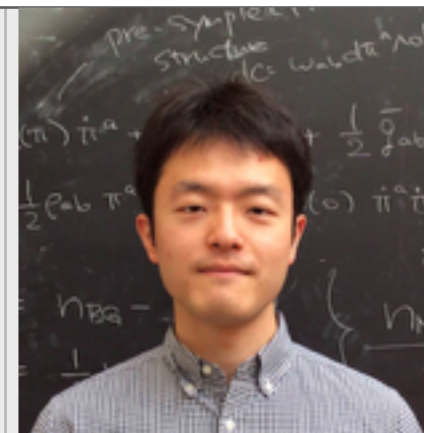
# Filling enforced topological phases in spin-orbit coupled crystals

Ashvin Vishwanath
UC Berkeley

# Acknowledgements


|  |  |  |
|---|---|---|
| Adrian Po | Haruki Watanabe | Mike Zaletel |
| UC Berkeley | Berkeley/MIT | UCSB |

EARLIER COLLABORATION

Parameswaran, Turner, Arovas, AV
- Nature Physics (2013).

& Arun Paramekanti

# Introduction

- Quantum ground state of Electrons in a crystal:
  - periodic potential + electron-electron interactions
  - spin orbit coupling (no spin rotation symmetry, time reversal)

Robust predictions from theory?

# Introduction

- Robust predictions from theory?
  - Topological properties
    - PART 1: A `topological insulator' diagnosed by e- filling. *(filling enforced quantum band insulator)*
  - Non-perturbative constraints (eg. Luttinger theorem)
    - PART 2: Identifying exotic phases eg. quantum spin liquids from electron filling (+ L.S)

# PART 1:

A `topological insulator' diagnosed by e$^-$ filling.

Adrian Po, Haruki Watanabe, Mike Zaletel, AV
arXiv:1506.03816

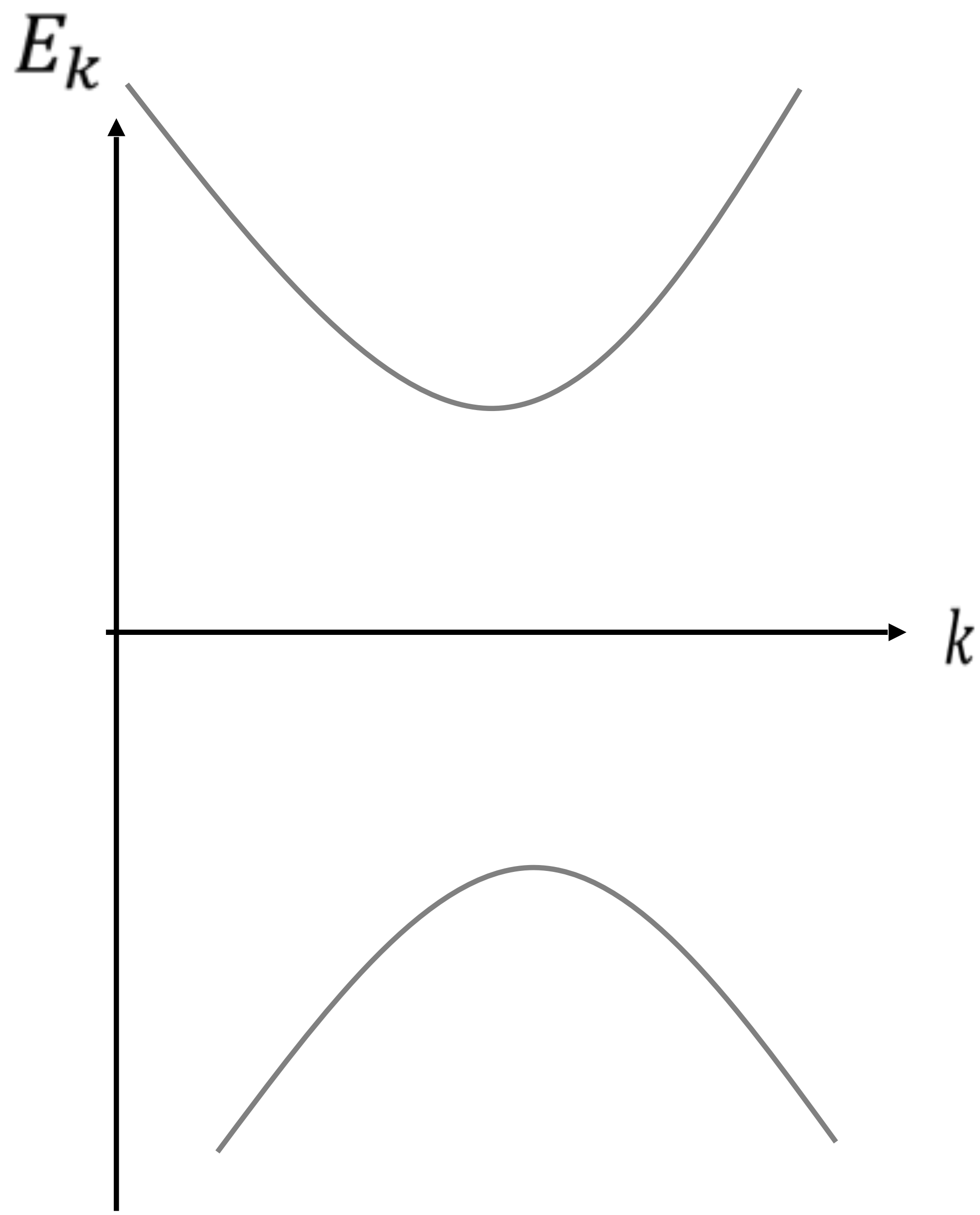
# A fundamental dichotomy

| Local Hamiltonian | | Momentum Eigenstates |
|---|---|---|
| $x$-space | | $k$-space |
| 'Particle' | | 'Wave' |
| Insulator | $\neq$ | Insulator |

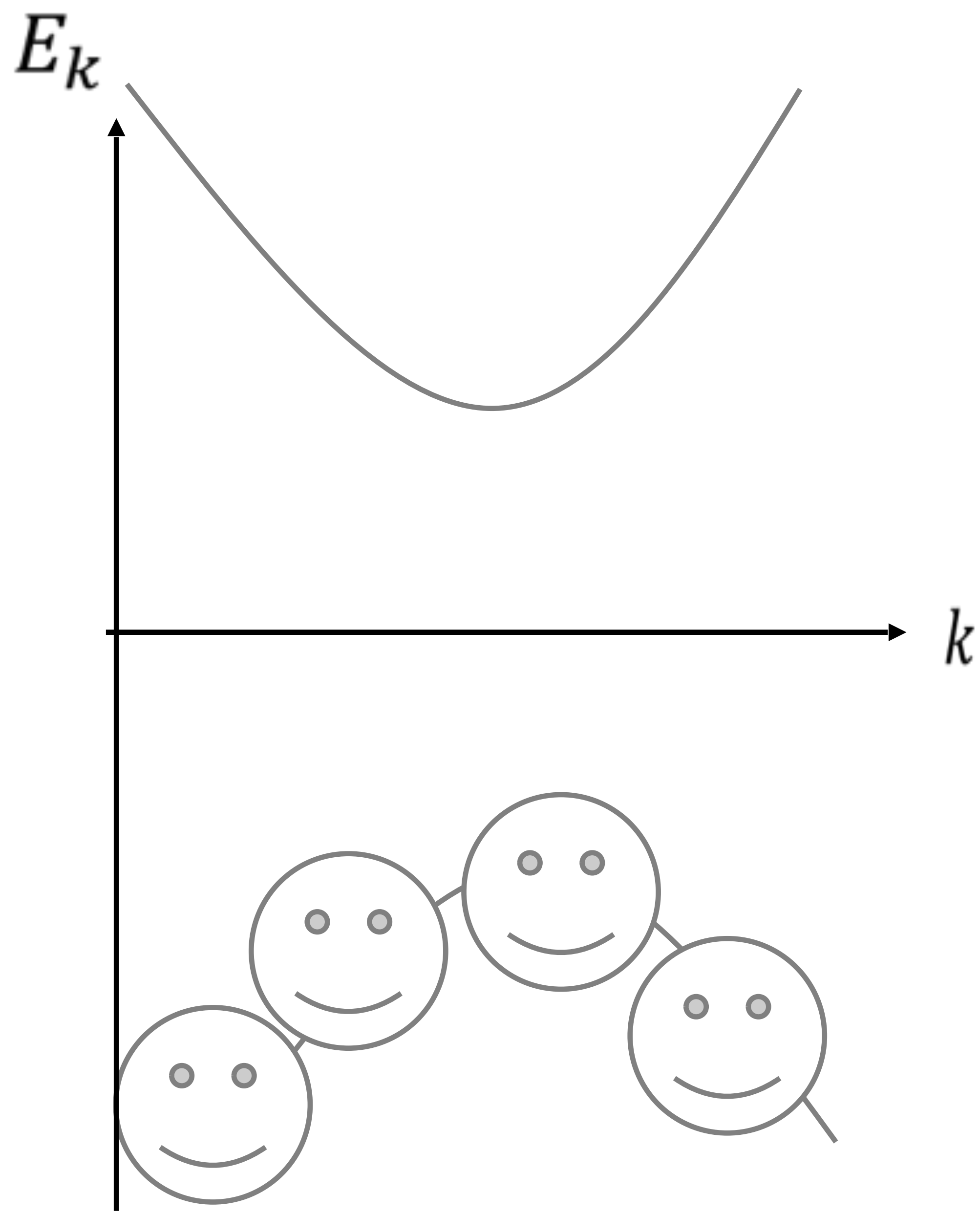
Real Space

Momentum Space

# Band Insulators

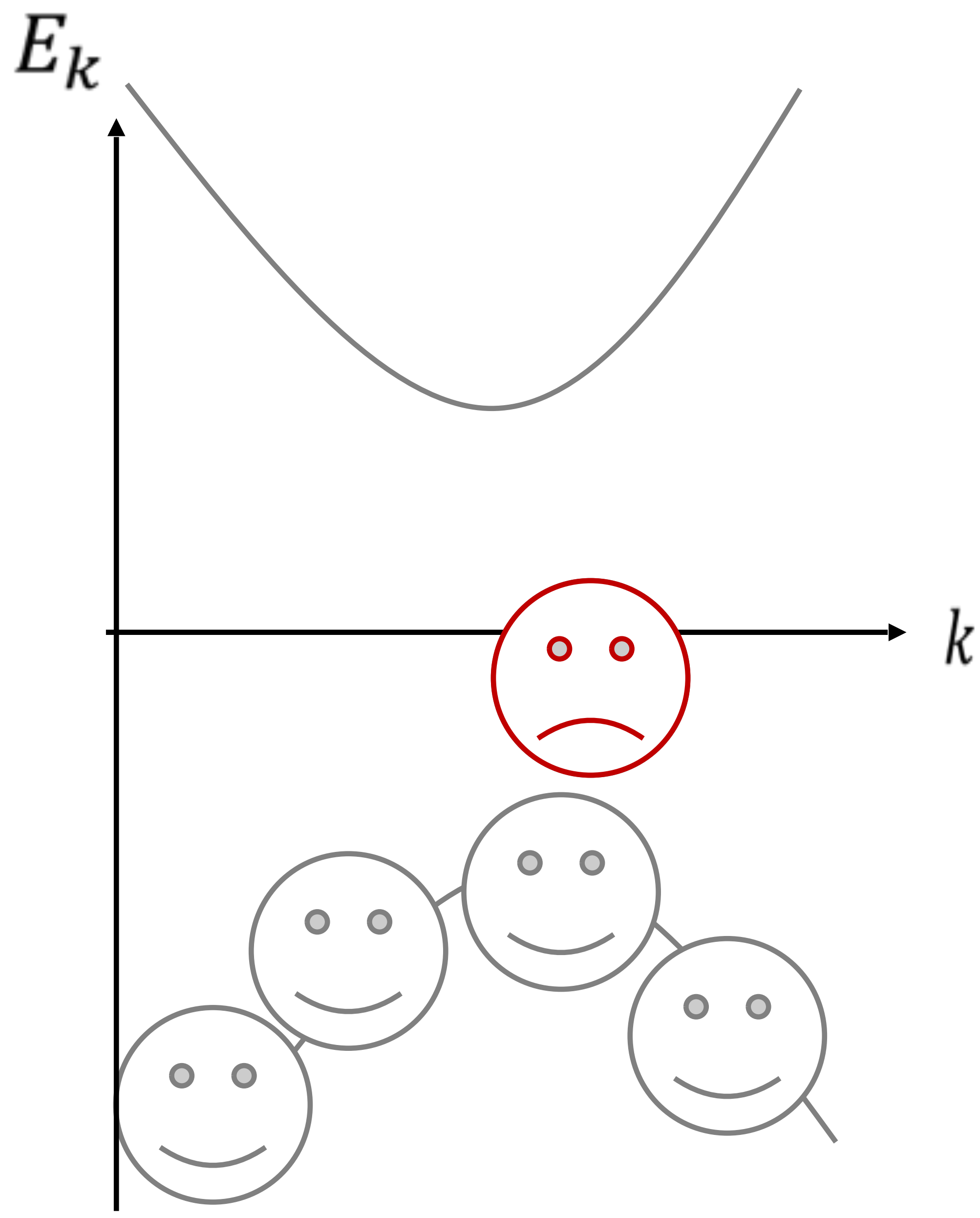


# Band Insulators



# Band Insulators

**Insulator = ‘Filled Bands’**



Real Space

Momentum Space

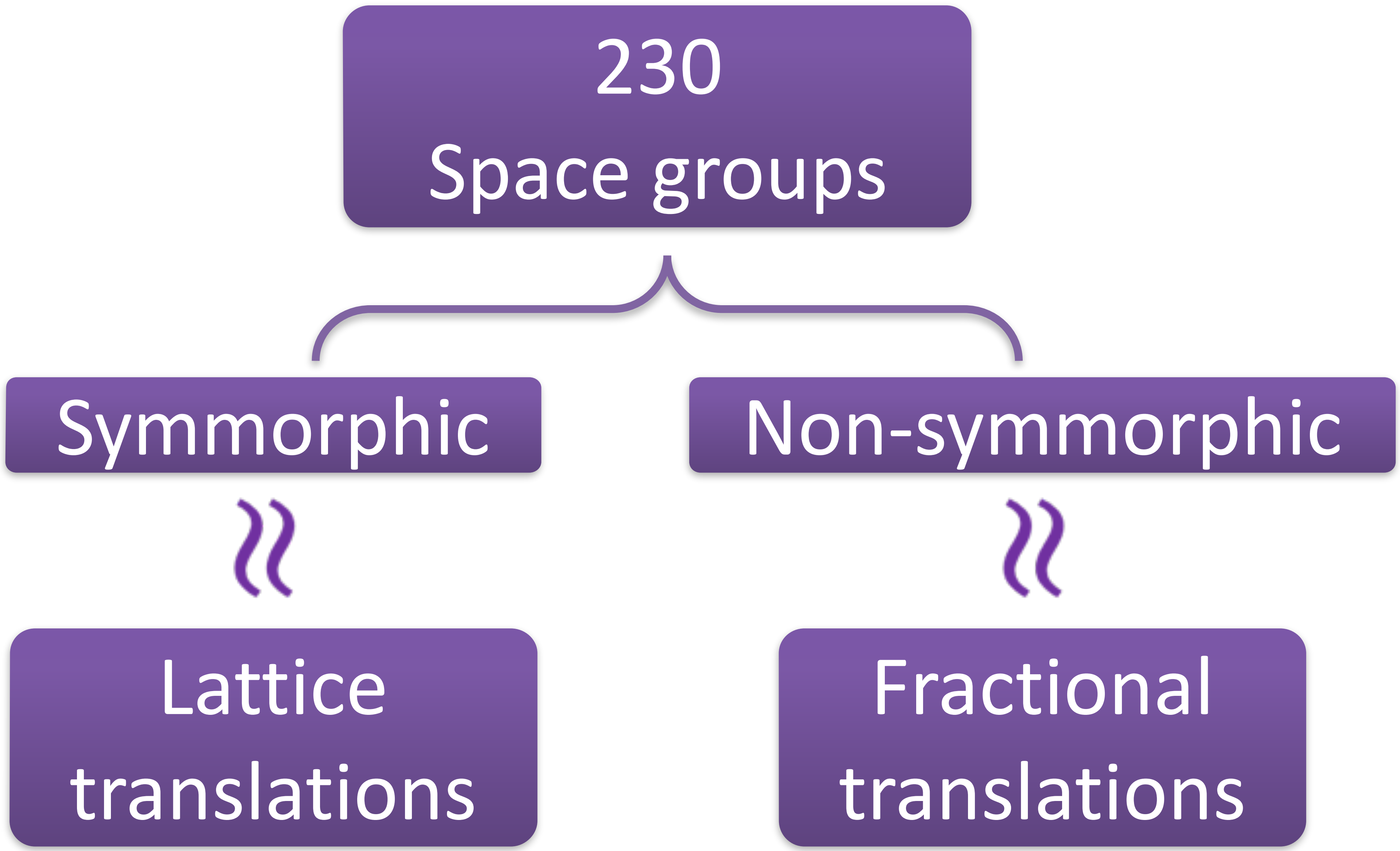
# Atomic Insulators

- A real-space product state has all e⁻ localized to sites (a ***strict*** atomic insulator)

**Time-reversal symmetry**

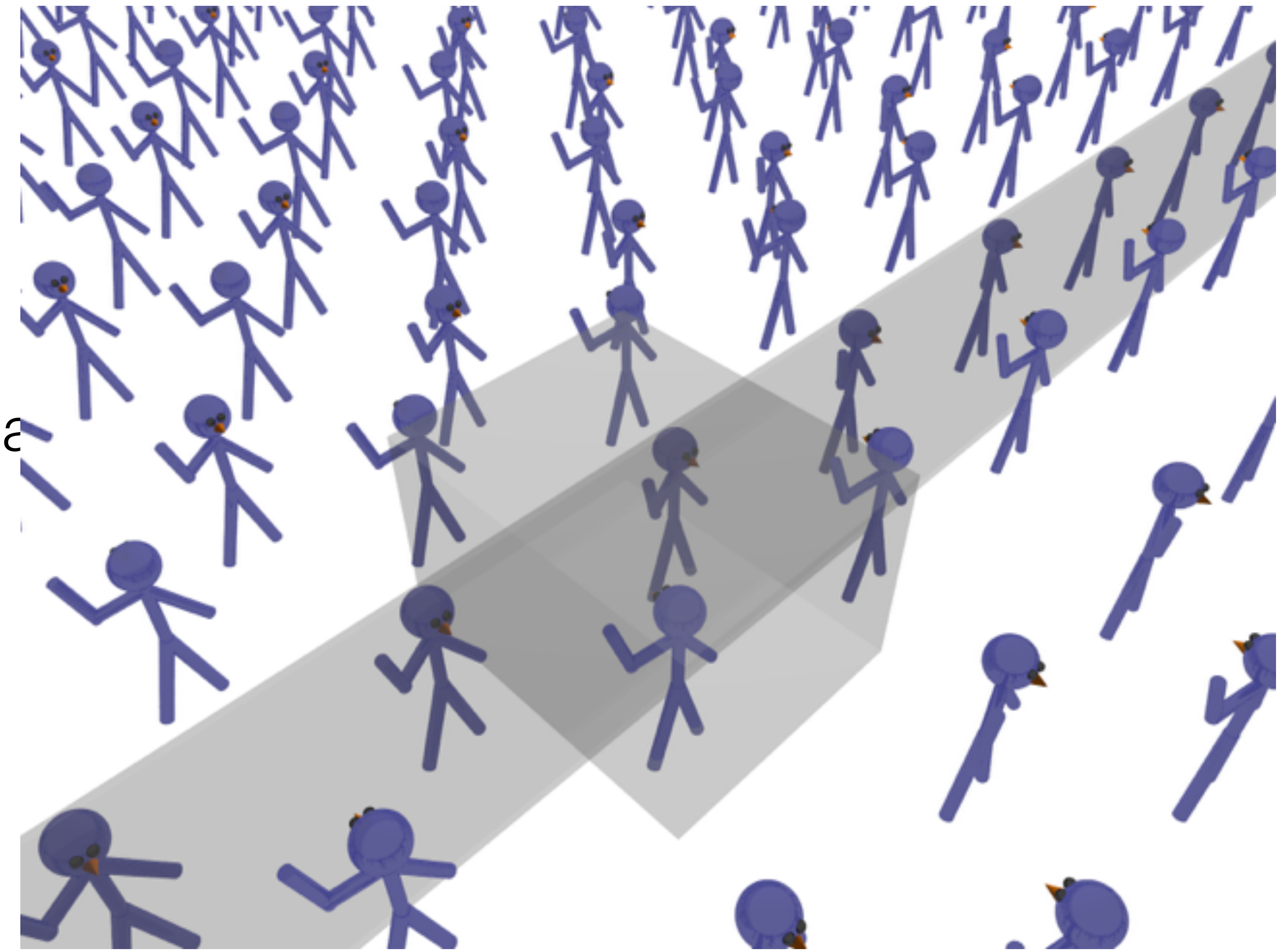
$$\nu^{\mathrm{AI}} = 2n$$

# Spatial symmetries

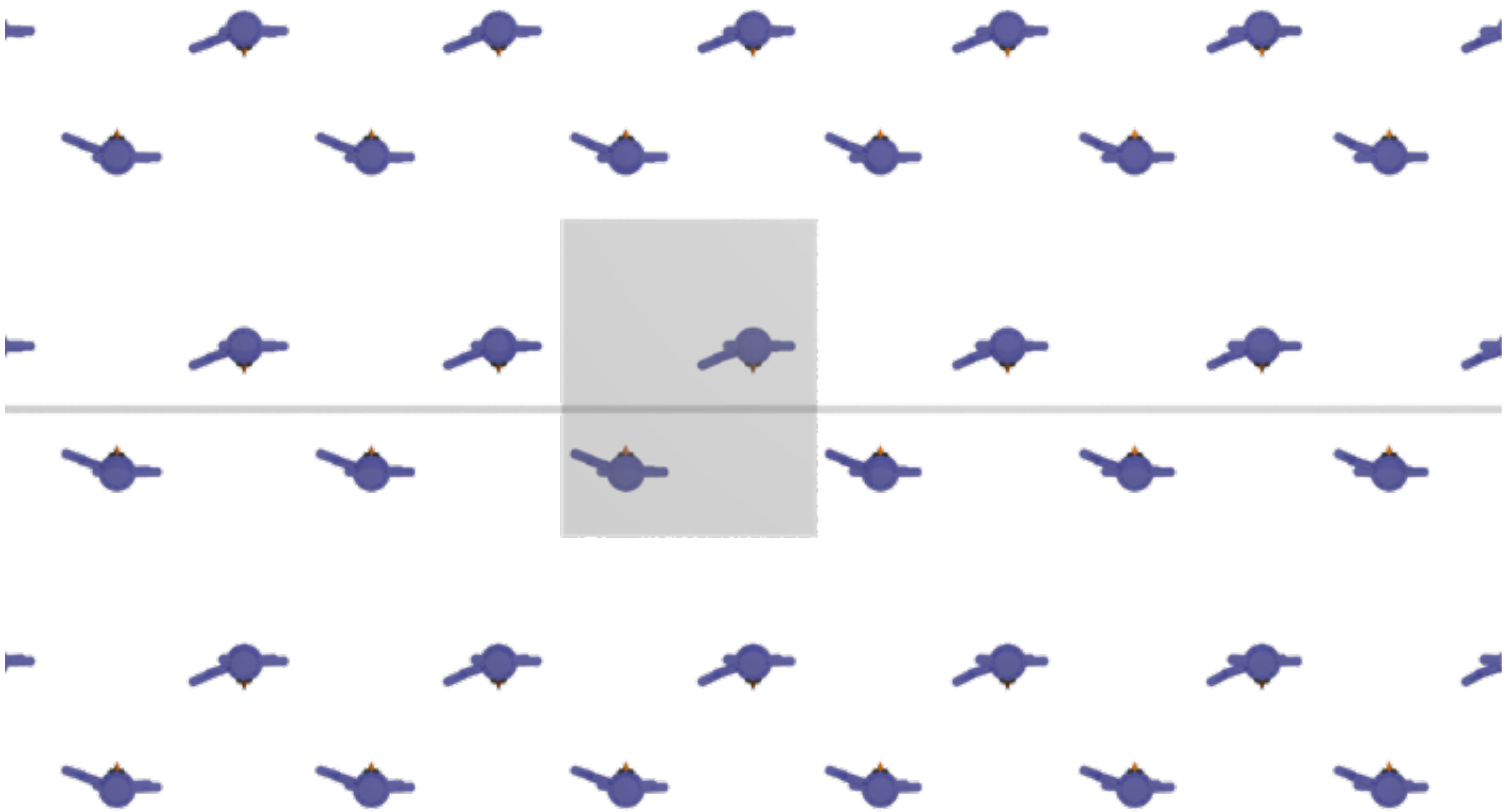


# Non-symmorphic symmetries

- e.g. a



# Bird's eye …



Glide: reflect and then translate by 1/2 a unit cell

Non-symmorphic

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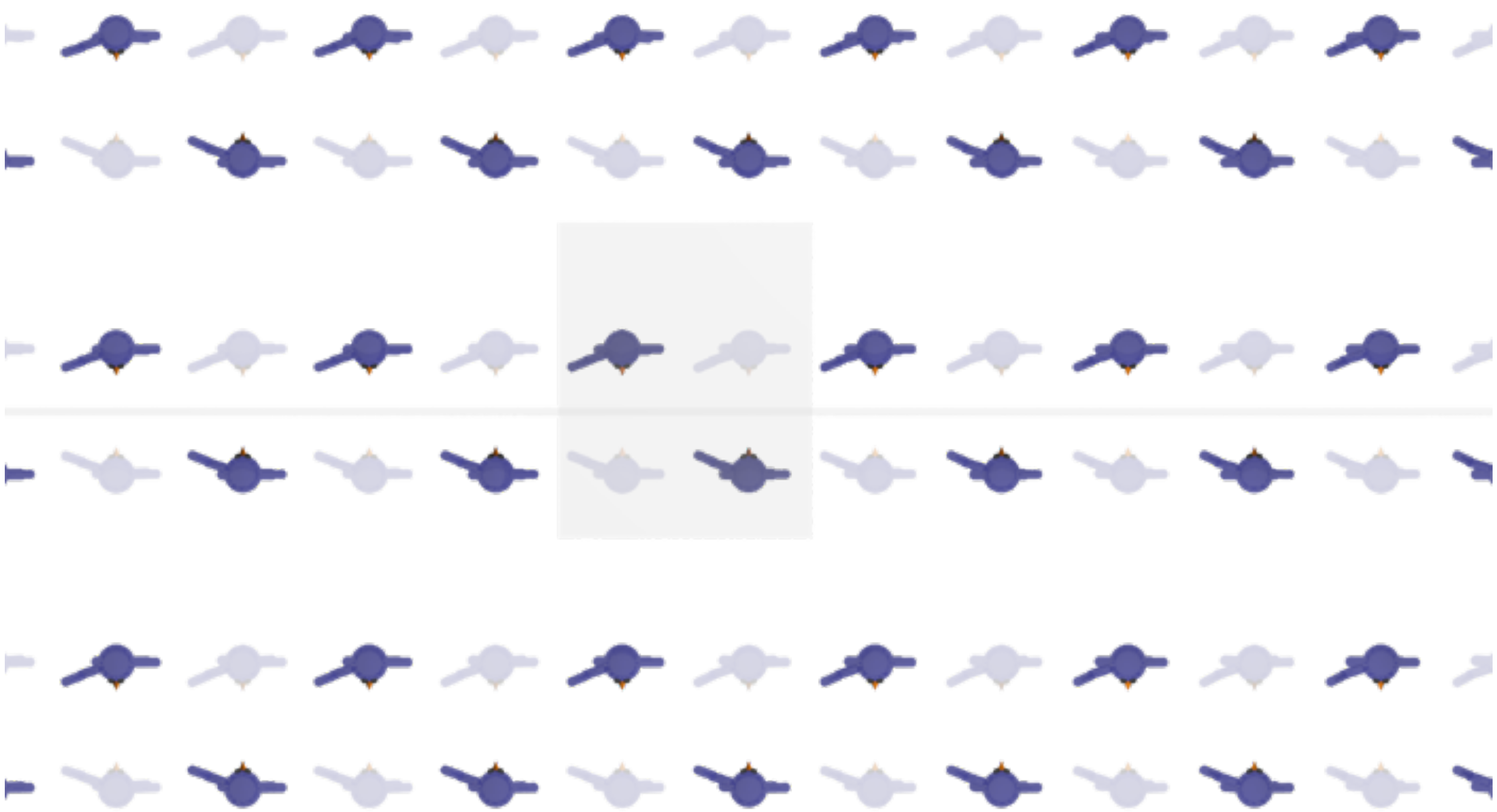

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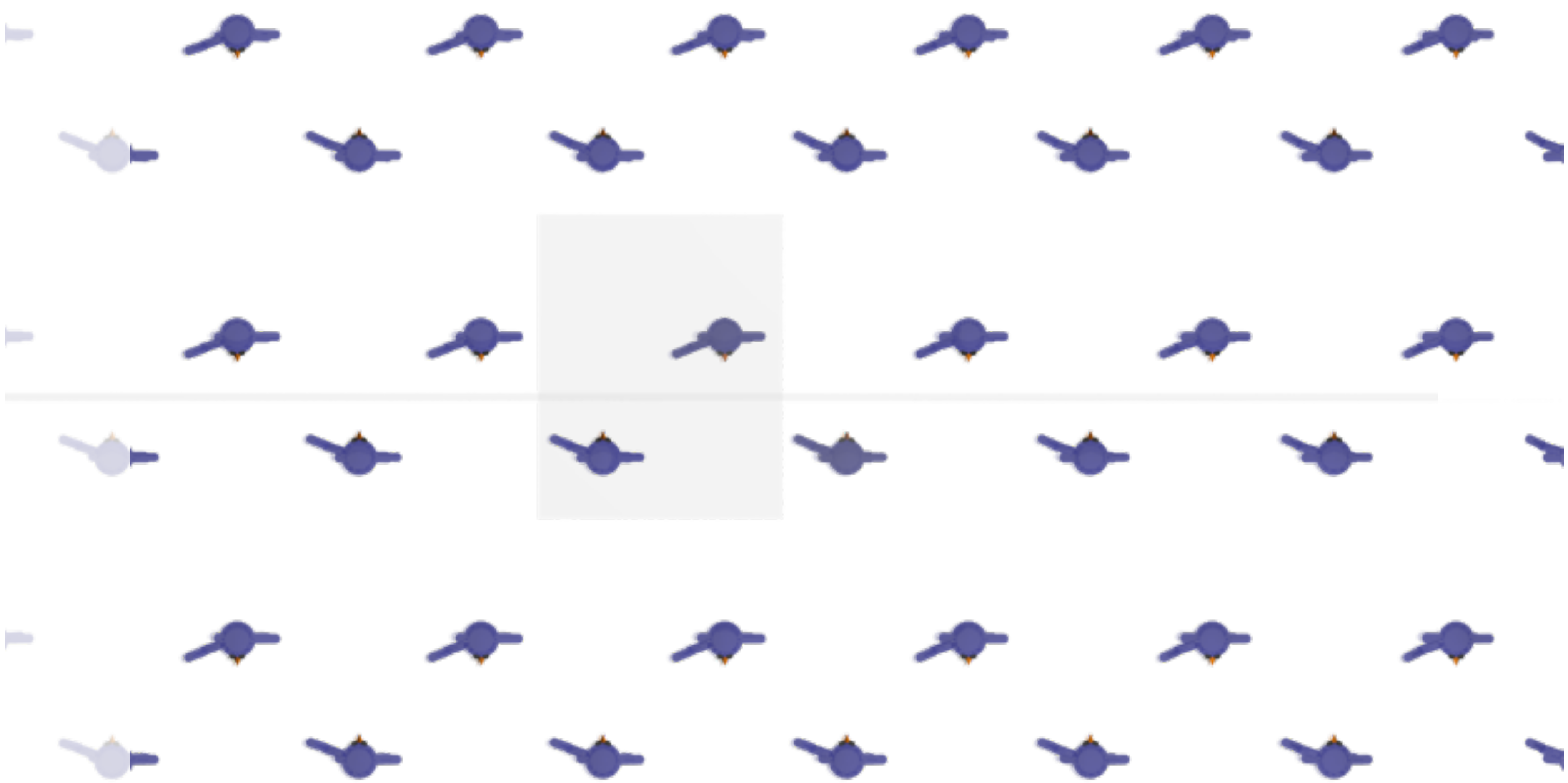

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Non-symmorphic

# Atomic 'Crystalline' insulators

$\nu = 2$

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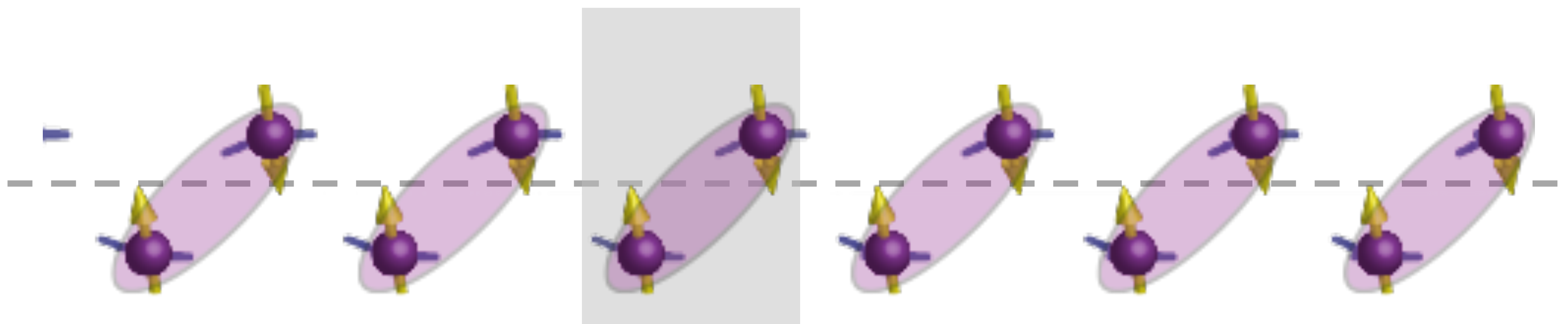

$\nu = 2$

e.g. glide:

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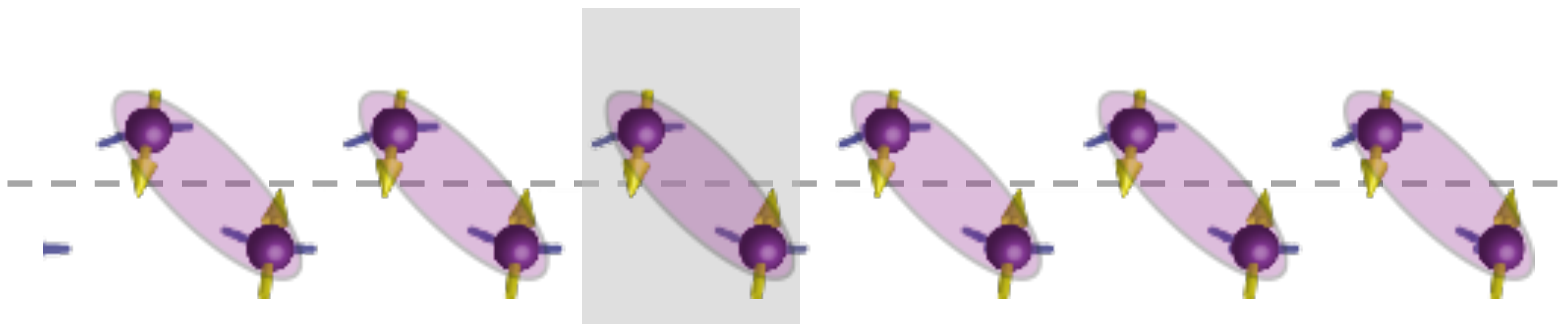
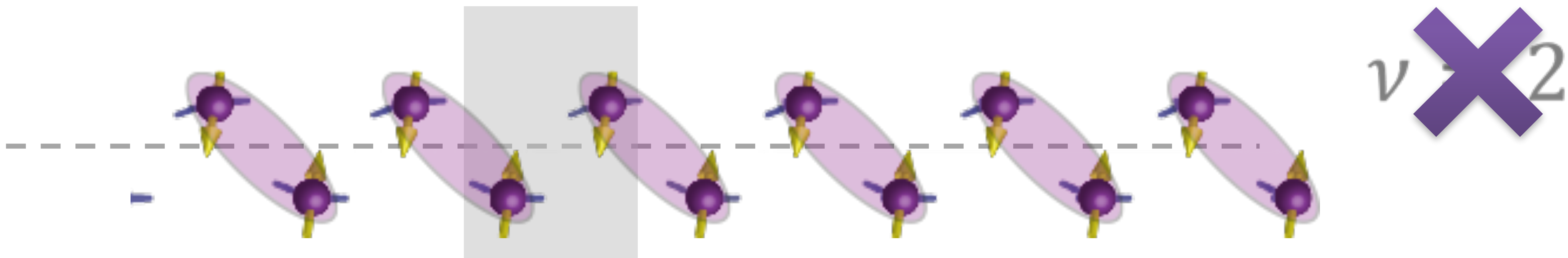


$\nu = 2$

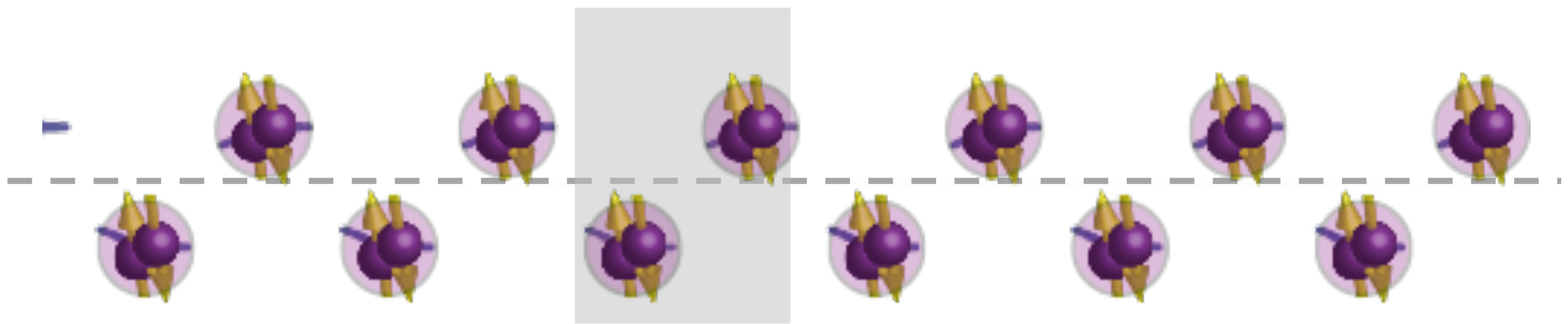
e.g. glide:

# Atomic ‘Crystalline’ insulators




e.g. glide: $\nu_{\mathrm{min}}^{\mathrm{AI}} \neq 2$

# Atomic 'Crystalline' insulators



$\nu = 4$

e.g. glide: $\nu_{\min}^{\mathrm{AI}} \neq 2$

$$\nu_{\min}^{\mathrm{AI}} = 2 \times 2 = 4$$

# Space Group constraints on AI

To form any Atomic Insulator (AI) respecting space group (SG) symmetries:

$$\nu_{\mathrm{SG}}^{\mathrm{AI}} = 2n \times m_{\mathrm{SG}}^{\mathrm{AI}}$$

Real Space

vs

Momentum Space

# AI vs BI

Atomic Insulator

vs

Band Insulator

# AI vs BI

'Wannier' representable

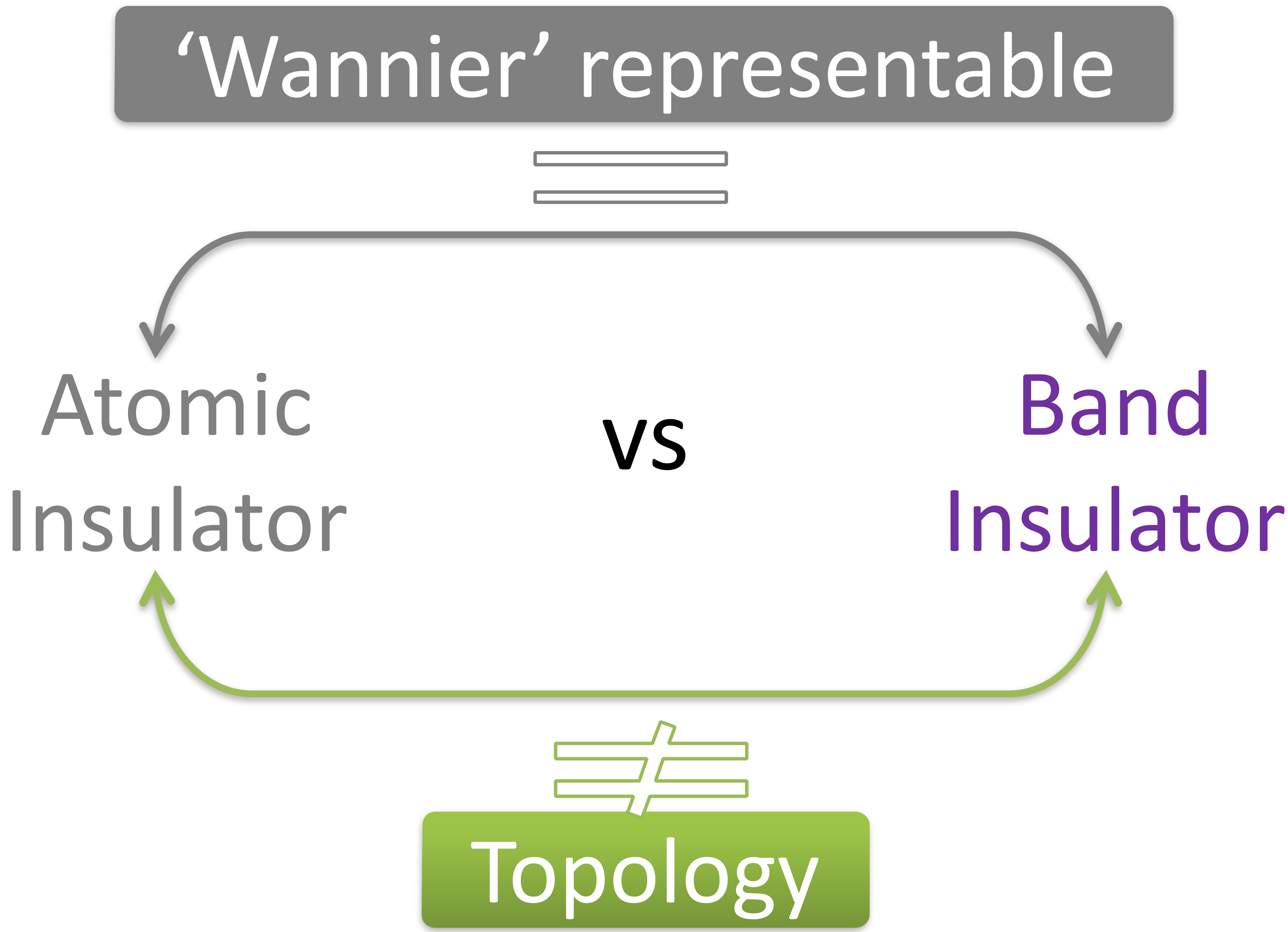
=

Atomic Insulator

vs

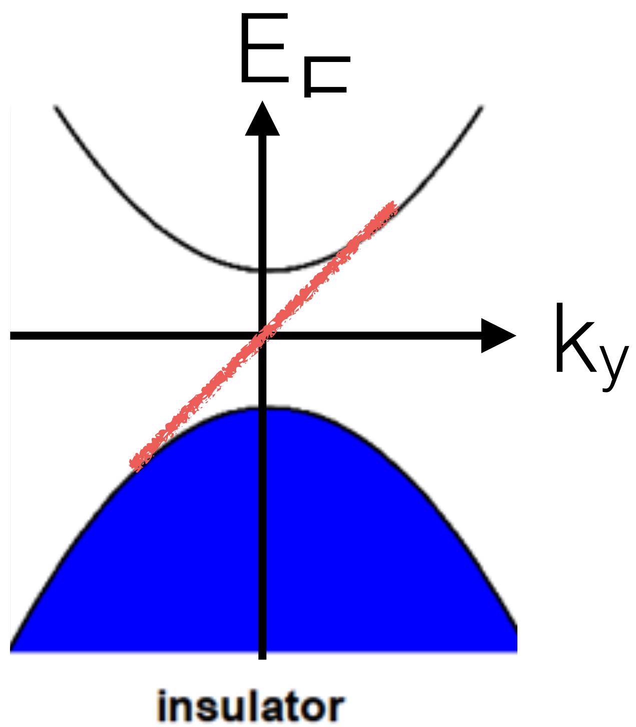
Band Insulator

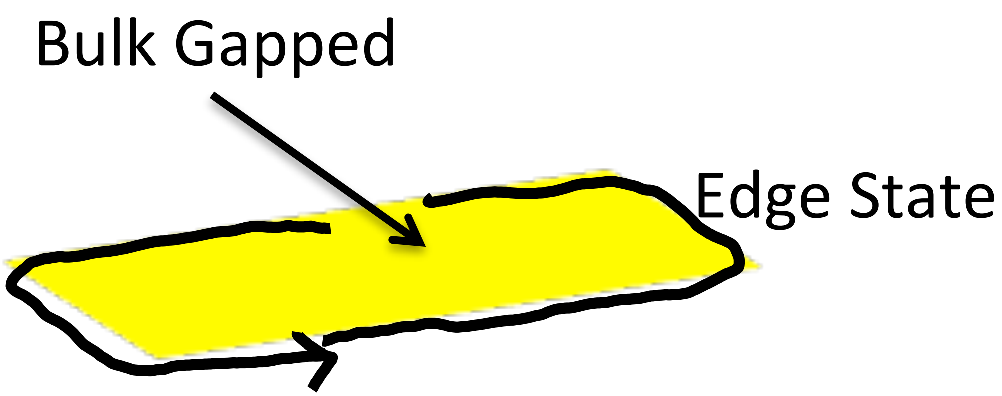
# AI vs BI

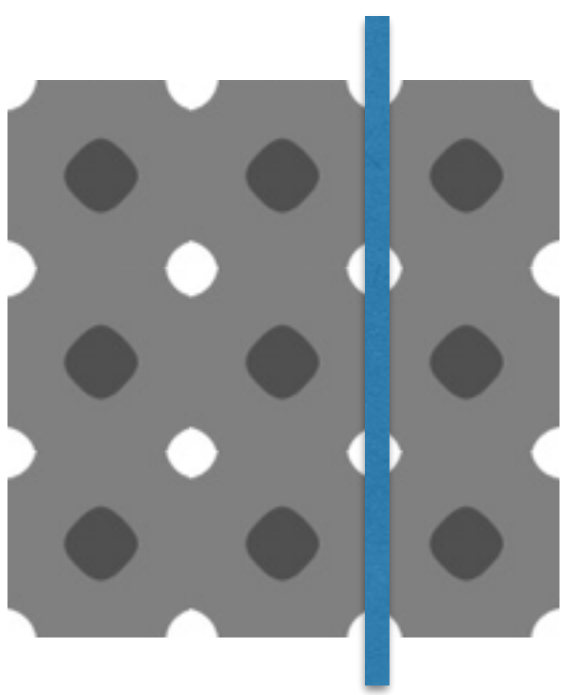


'Wannier' representable
Atomic Insulator
vs
Band Insulator
Topology

# Chern insulator

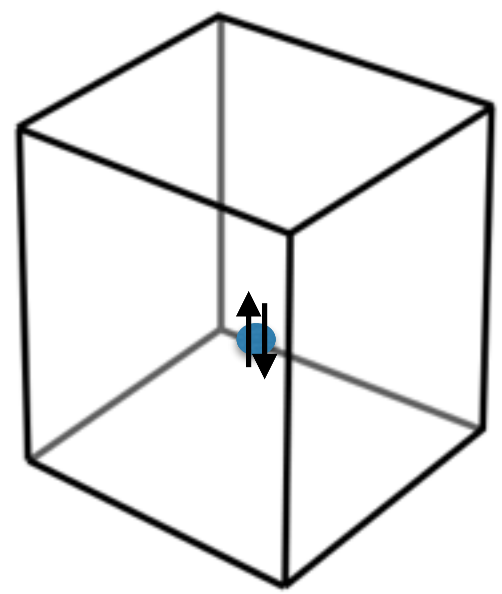


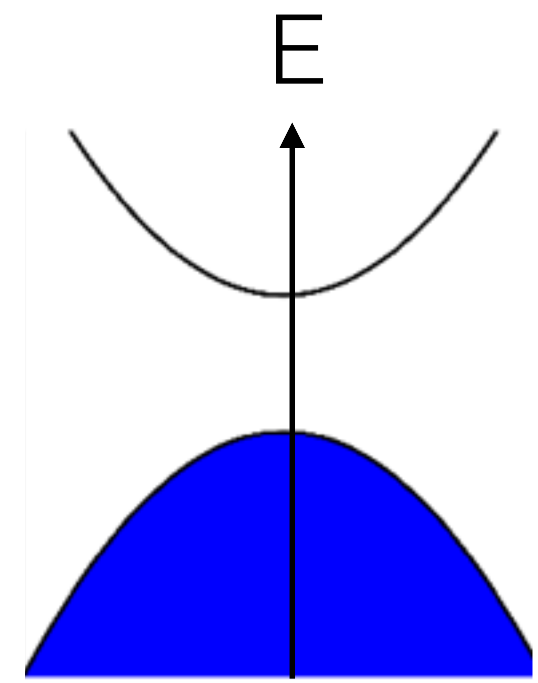



No exponentially localized Wannier functions.
No atomic insulator - only band picture.

# Filling Enforced Quantum Band Insulators



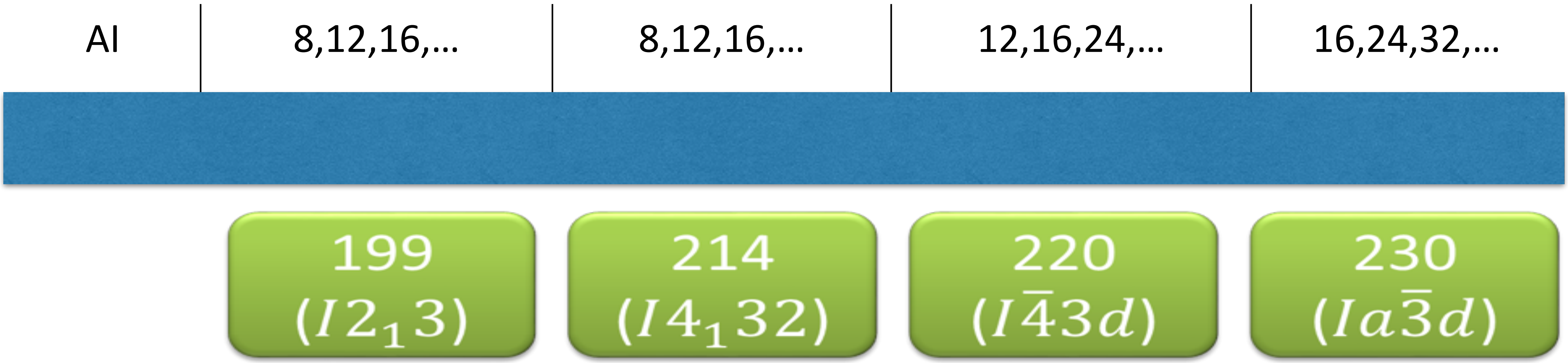
Atomic Picture




insulator

- Atomic limit of insulator - electrons localized on atomic site.
    - Atomic sites - Wyckoff positions.
- An example where the atomic picture is forbidden by the band *filling* itself? Eg. can $\nu < \nu_{\mathrm{AI}}$? YES.
- No atomic limit. No local Wannier representation

# Filling Enforced Quantum Band Insulators




- Out of *230* space groups, *4* are special. Allowed atomic insulator fillings contain gaps (from Wyckoff multiplicity).

- Band insulators can achieve `missing' fillings *if* spin orbit coupling present.

# Filling Enforced Quantum Band Insulators

| | | | | |
|---|---|---|---|---|
| AI | 8,12,16,… | 8,12,16,… | 12,16,24,… | 16,24,32,… |
| BI | 4,8,12,… | 4,8,12,… | 8,12,16,20,… | 8,16,24,… |
| | 199 ($I2_13$) | 214 ($I4_132$) | 220 ($I\bar{4}3d$) | 230 ($Ia\bar{3}d$) |

- Out of *230* space groups, *4* are special. Allowed atomic insulator fillings contain gaps (from Wyckoff multiplicity).
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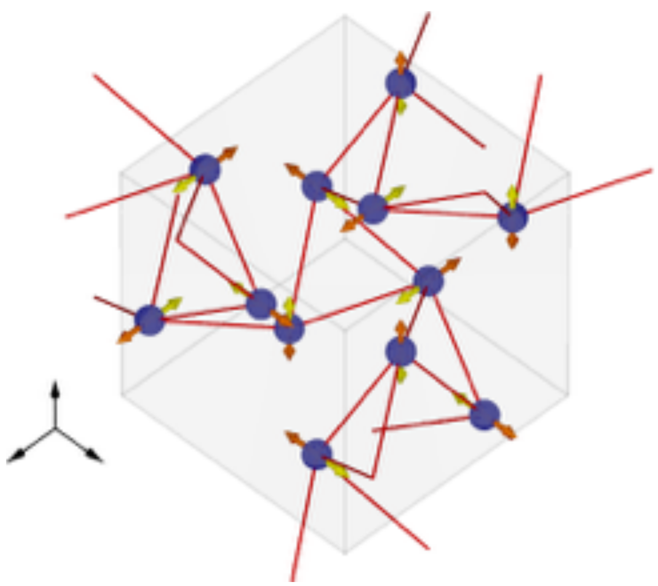
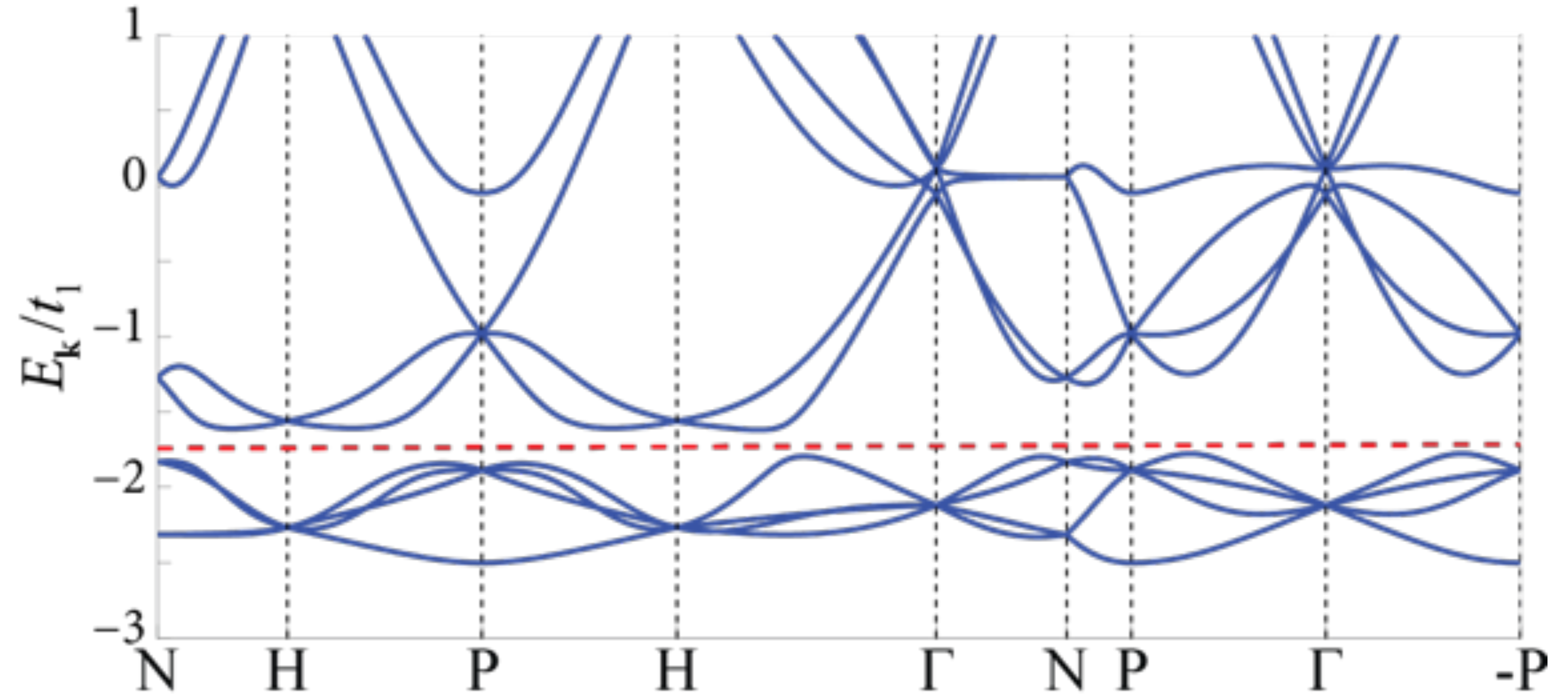
# Example of a Filling Enforced Quantum Band Insulator





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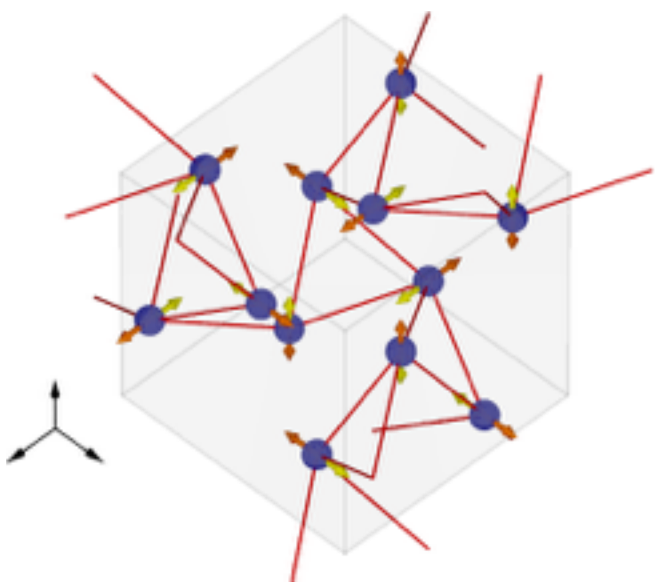

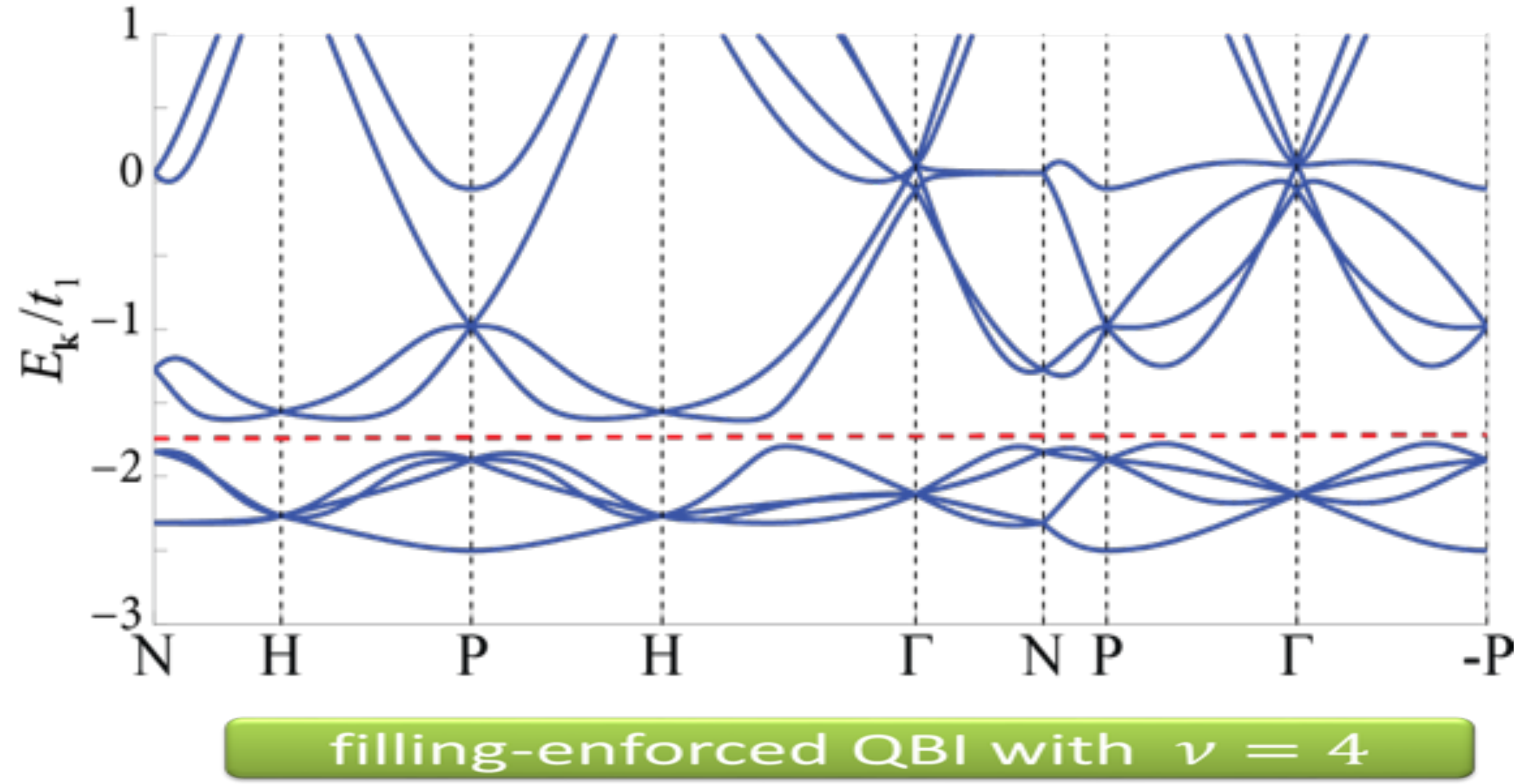

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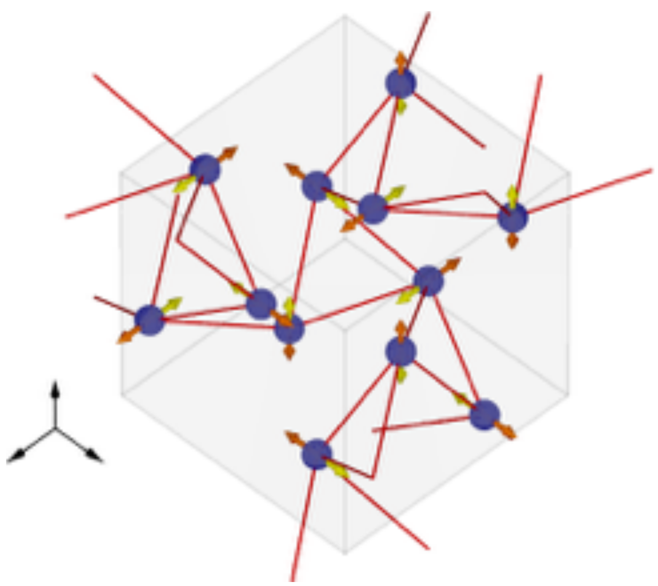
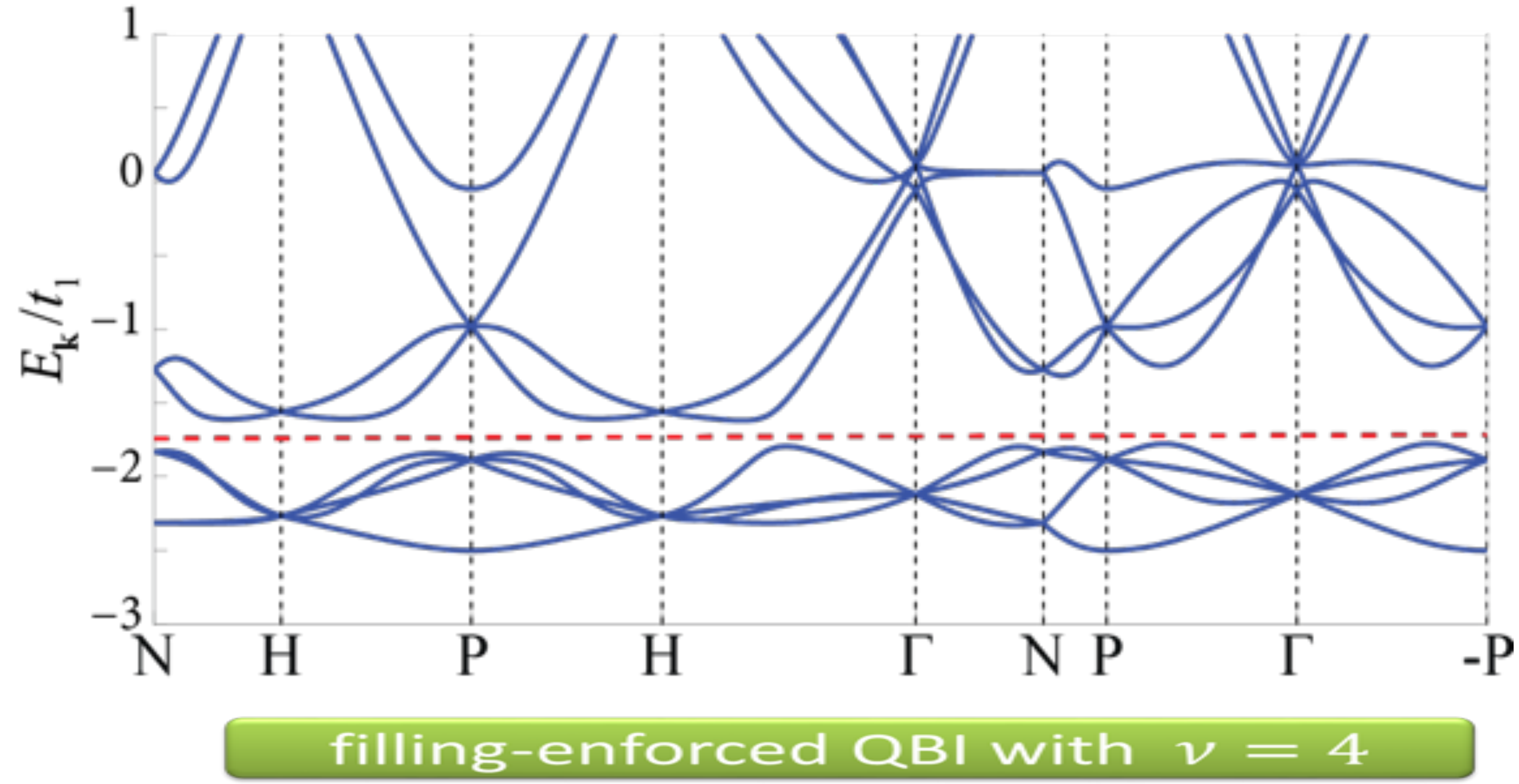


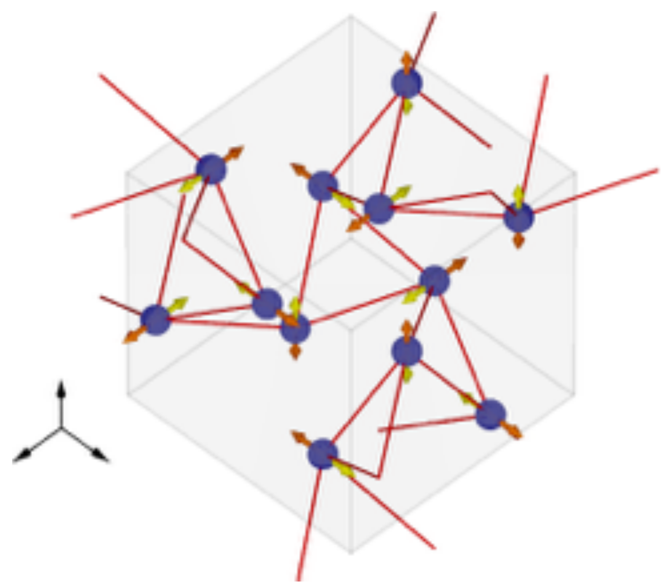


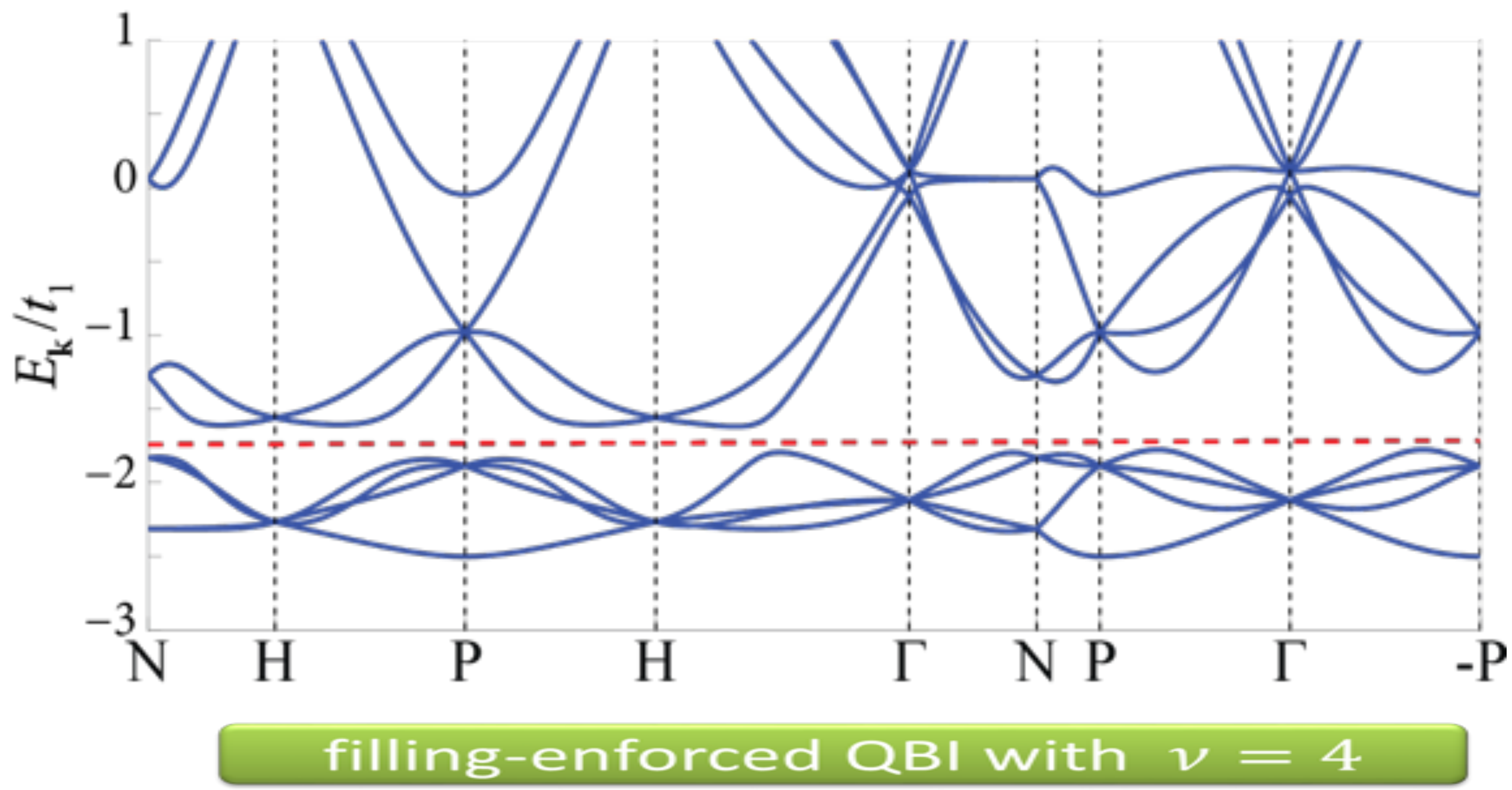

- Space Group -199 (non-symmorphic, *cubic* lattice)

- Minimum of 4 atomic sites in the unit cell - BUT - band structure with filling of 4 electrons. No atomic picture (Time reversal and crystal symmetry - needs 8e).

- Requires spin-orbit coupling.

# Example of a Filling Enforced Quantum Band Insulator



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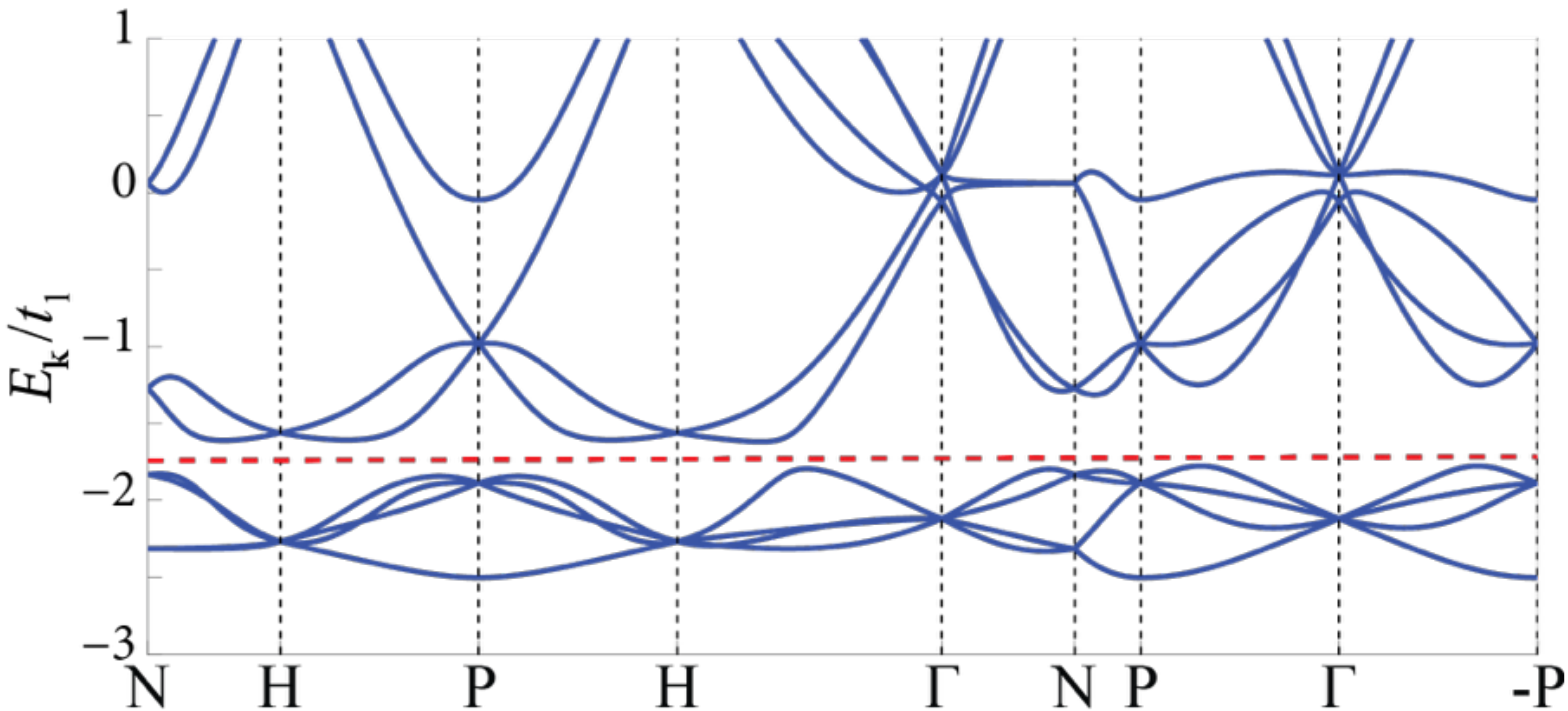
- Requires spin-orbit coupling.
- Surface states? surface breaks cubic symmetry. But entanglement signature

# SOC and feQBI

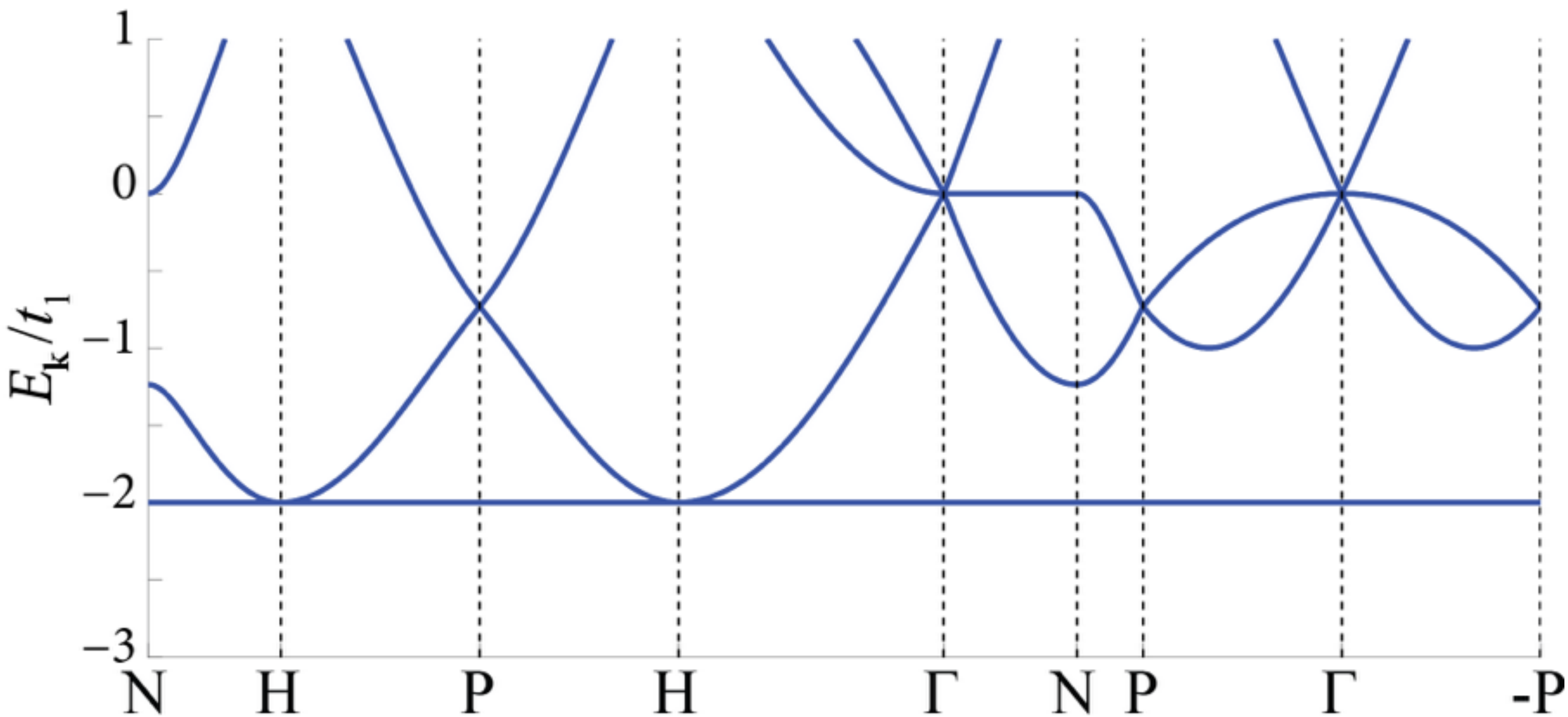
✗ Spin-rotation | ✓ Free | ✓ TR | Space Group



# SOC and feQBI

✓ Spin-rotation | ✓ Free | ✓ TR | Space Group

i.e. SOC-free



# Filling enforced quantum band insulator - Material?

- *Material*? Right crystal, filling & band structure.
  - **Ir** in hyperkagome lattice structure $Na_4Ir_3O_8$
  - but wrong filling (6e) - however $Na_3Ir_3O_8$

$Na_3Ir_3O_8$ [1/3 hole doped hyperkagome - Takagi et al. Sci. Rep. 4, 6818 (2014)]

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214
$(I4_132)$

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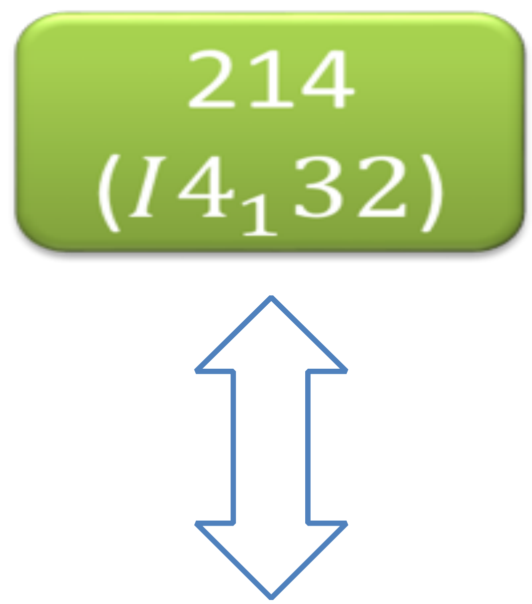


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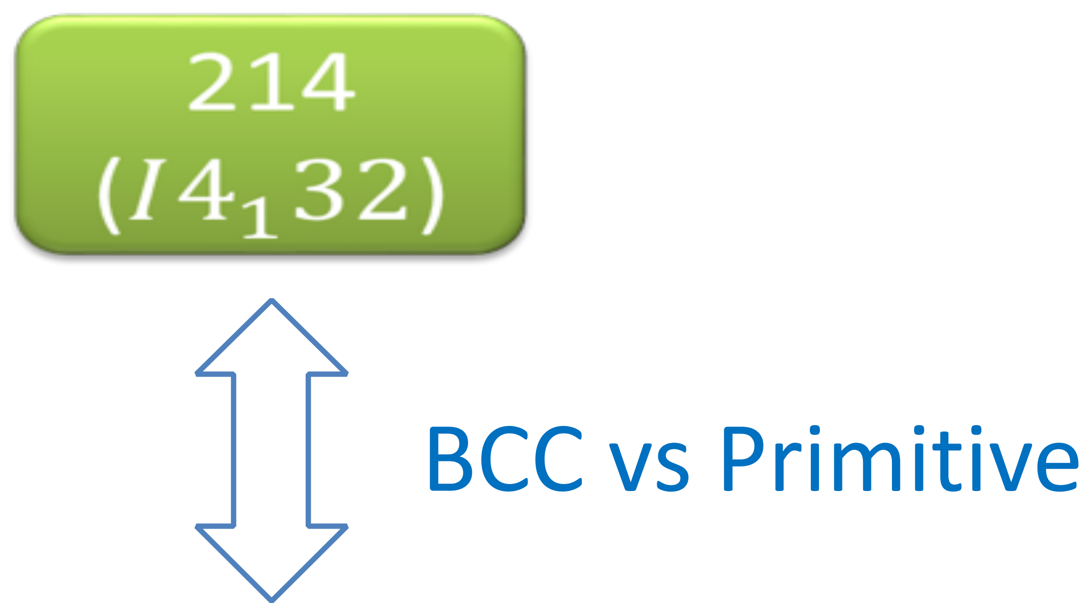


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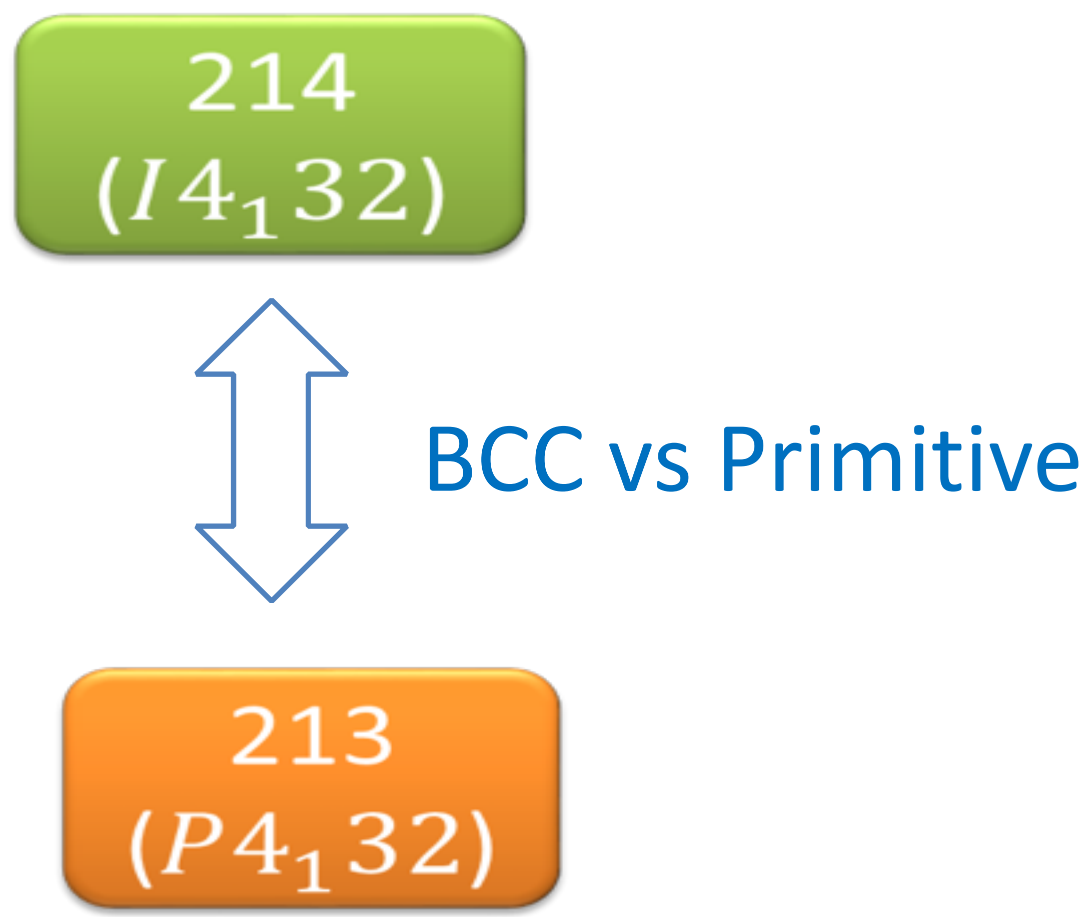


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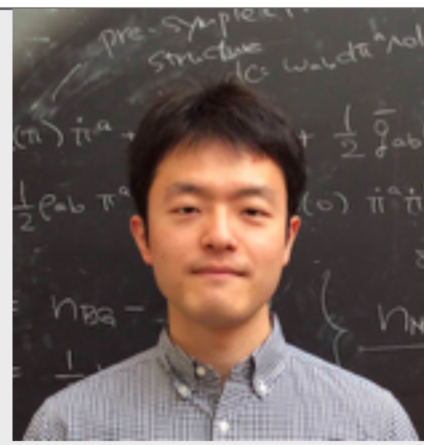
# PART 2:

Quantum spin liquids diagnosed by e$^{-}$ filling.

| | | |
|---|---|---|
|  |  |  |
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H. Watanabe, Adrian Po, AV, Mike Zaletel
arXiv:1505.04193

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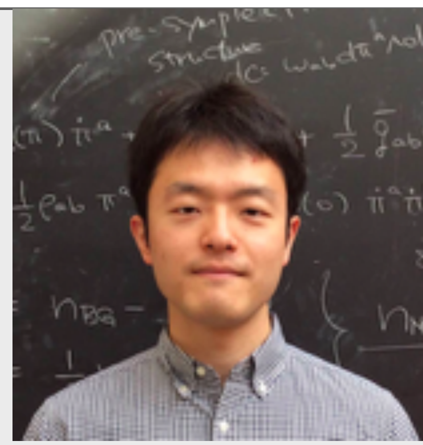
|  |  |  |
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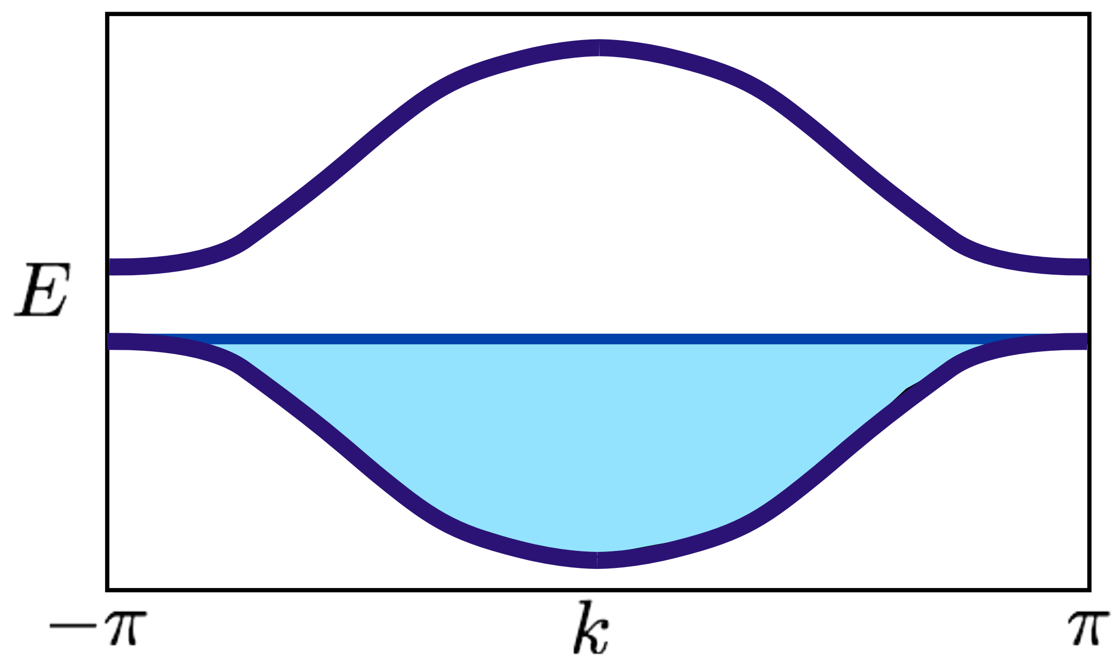
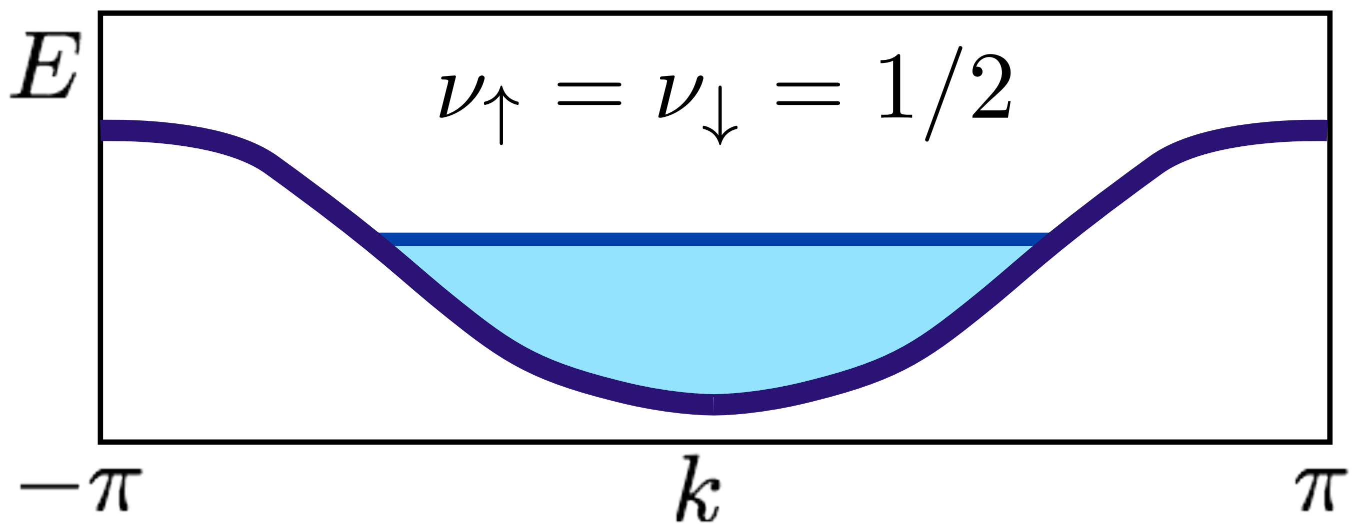
# Band Insulators in Interacting systems

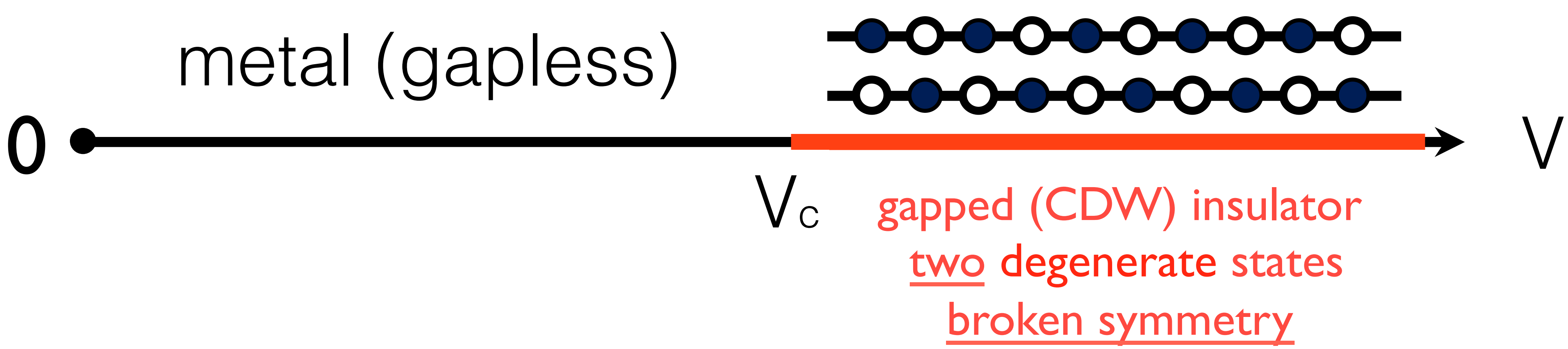



- Non-interacting electrons fill a band.
    - Filling ($\nu$=electrons/unit cell)?
    - Integer number of electrons per spin. $\nu_\uparrow = \nu_\downarrow = 1$
- Interacting definition: Featureless Insulator
    - Gapped & unique ground state.( No symmetry breaking. No topological order - unique ground state on torus. Short range entangled .).

# Half Filled Band




- No `featureless' insulator
  - Gapless OR Ground state degeneracy.
  - Nearest neighbor V.



# A d=1 Example

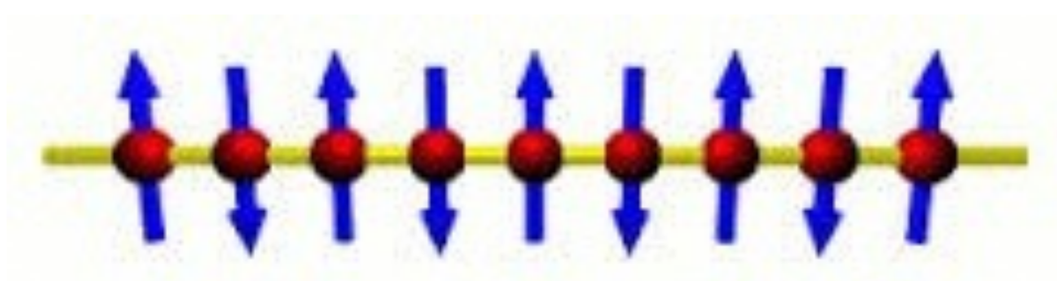
- If $\nu_\uparrow = \nu_\downarrow = 1/2$ - Mott Insulator?
  - S=1/2 Heisenberg model. No unique ground state.

ANNALS OF PHYSICS: **16,** 407–466 (1961)

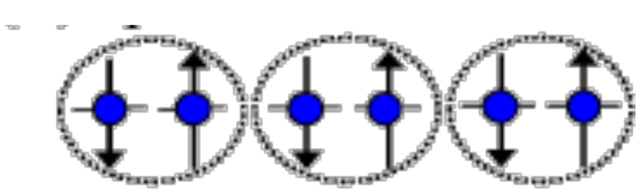
**Two Soluble Models of an Antiferromagnetic Chain**

ELLIOTT LIEB, THEODORE SCHULTZ, AND DANIEL MATTIS
*Thomas J. Watson Research Center, Yorktown, New York*

It is also shown that for spin ½ systems having rather general isotropic Heisenberg interactions favoring an antiferromagnetic ordering, the ground state is nondegenerate and there is no energy gap above the ground state in the energy spectrum of the total system.



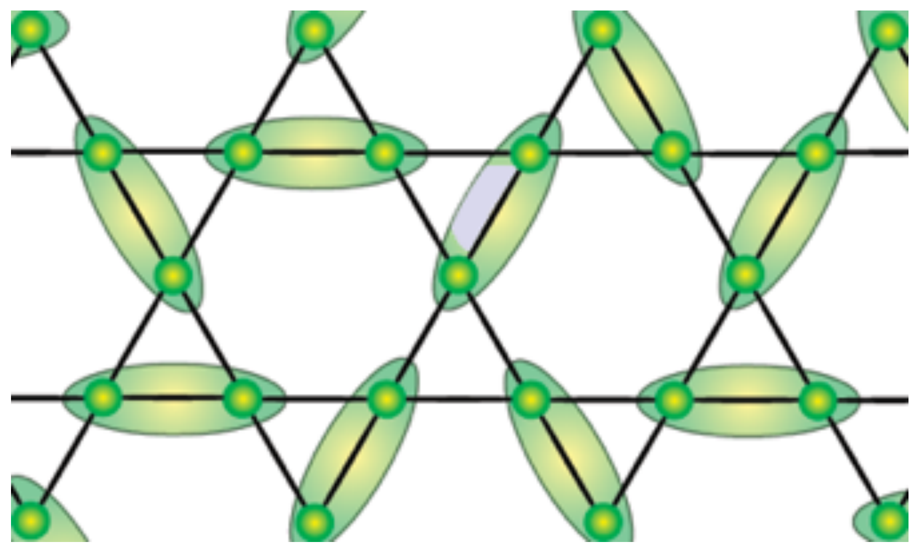
Luttinger liquid (gapless)



Spin Pierels (broken symmetry)

# In d>1, new possibility

- D=2 Mott Insulator ( $\nu_\uparrow = \nu_\downarrow = 1/2$ ). No trivial gapped phase. New possibility:



- Quantum spin liquid - gapped, respects symmetry BUT not short range entangled - eg. ground state degeneracy on torus.

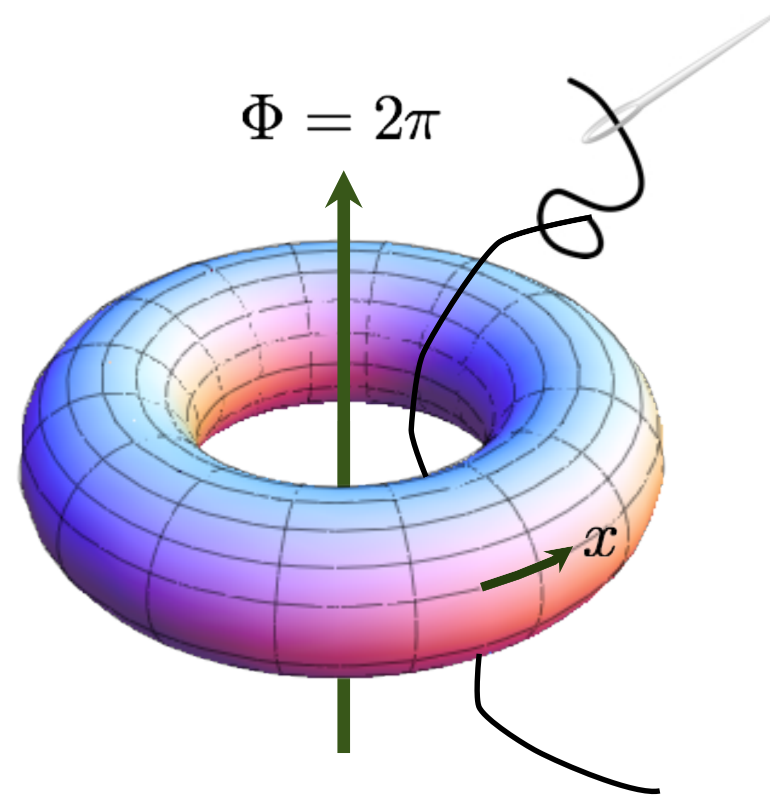
- Spinon excitations (S=1/2) etc.

# d>1; Oshikawa Hastings Argument

I. Thread $2\pi$ flux through 'handle'

$$|\Psi_0\rangle \longrightarrow |\Psi_0'\rangle$$

spectrum returns to itself




2. Gauge away inserted flux

$$\hat{H}(0) = \hat{U}\hat{H}(2\pi)\hat{U}^{-1}$$

$$|\Psi_0'\rangle \longrightarrow \hat{U}|\Psi_0'\rangle$$

If insulating phase, $|\Psi_0\rangle$ , $\hat{U}|\Psi_0'\rangle$ degenerate* eigenstates of $\hat{H}(0)$

[Hastings, PRB **69**, 104431 (2004); EPL **70,** 824 (2005)] [Oshikawa, PRL **84**, 1535 (2000)]

Arun Paramekanti and AV, PRB (2004)
Parmeswaran et al. Nature Physics 2012)

Extend to spin-orbit coupled systems?

# Allowed filling for spin orbit coupled `band insulators'

230
Space groups

Symmorphic

Non-symmorphic (155)

$\nu = 2n$

$\nu > 2n$

# Allowed filling for spin orbit coupled `band insulators’

| No.* | | No. | | No. | | No. | | No. | | No. | | No. | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | $4n$ | 39 | $4n$ | 66 | $4n$ | 100 | $4n$ | 129 | $4n$ | 165 | $4n$ | 201 | $4n$ |
| 7 | $4n$ | 40 | $4n$ | 67 | $4n$ | 101 | $4n$ | 130 | $8n$ | 167 | $4n$ | 203 | $4n$ |
| 9 | $4n$ | 41 | $4n$ | 68 | $4n$ | 102 | $4n$ | 131 | $4n$ | 169 | $12n$ | 205 | $8n$ |
| 11 | $4n$ | 43 | $4n$ | 70 | $4n$ | 103 | $4n$ | 132 | $4n$ | 170 | $12n$ | 206 | $4n$ |
| 13 | $4n$ | 45 | $4n$ | 72 | $4n$ | 104 | $4n$ | 133 | $4n^\dagger$ | 171 | $6n$ | 208 | $4n$ |
| 14 | $4n$ | 46 | $4n$ | 73 | $4n^\dagger$ | 105 | $4n$ | 134 | $4n$ | 172 | $6n$ | 210 | $4n^\dagger$ |
| 15 | $4n$ | 48 | $4n$ | 74 | $4n$ | 106 | $4n^\dagger$ | 135 | $4n^\dagger$ | 173 | $4n$ | 212 | $8n$ |
| 17 | $4n$ | 49 | $4n$ | 76 | $8n$ | 108 | $4n$ | 136 | $4n$ | 176 | $4n$ | 213 | $8n$ |
| 18 | $4n$ | 50 | $4n$ | 77 | $4n$ | 109 | $4n$ | 137 | $4n$ | 178 | $12n$ | 214 | $4n$ |
| 19 | $8n$ | 51 | $4n$ | 78 | $8n$ | 110 | $4n^\dagger$ | 138 | $8n$ | 179 | $12n$ | 218 | $4n$ |
| 20 | $4n$ | 52 | $8n$ | 80 | $4n$ | 112 | $4n$ | 140 | $4n$ | 180 | $6n$ | 219 | $4n$ |
| 24 | $4n$ | 53 | $4n$ | 84 | $4n$ | 113 | $4n$ | 141 | $4n$ | 181 | $6n$ | 220 | $4n^\ddagger$ |
| 26 | $4n$ | 54 | $8n$ | 85 | $4n$ | 114 | $4n$ | 142 | $4n^\dagger$ | 182 | $4n$ | 222 | $4n$ |
| 27 | $4n$ | 55 | $4n$ | 86 | $4n$ | 116 | $4n$ | 144 | $6n$ | 184 | $4n$ | 223 | $4n$ |
| 28 | $4n$ | 56 | $8n$ | 88 | $4n$ | 117 | $4n$ | 145 | $6n$ | 185 | $4n$ | 224 | $4n$ |
| 29 | $8n$ | 57 | $8n$ | 90 | $4n$ | 118 | $4n$ | 151 | $6n$ | 186 | $4n$ | 226 | $4n$ |
| 30 | $4n$ | 58 | $4n$ | 91 | $8n$ | 120 | $4n$ | 152 | $6n$ | 188 | $4n$ | 227 | $4n$ |
| 31 | $4n$ | 59 | $4n$ | 92 | $8n$ | 122 | $4n$ | 153 | $6n$ | 190 | $4n$ | 228 | $4n^\dagger$ |
| 32 | $4n$ | 60 | $8n$ | 93 | $4n$ | 124 | $4n$ | 154 | $6n$ | 192 | $4n$ | 230 | $4n^\dagger$ |
| 33 | $8n$ | 61 | $8n$ | 94 | $4n$ | 125 | $4n$ | 158 | $4n$ | 193 | $4n$ | | |
| 34 | $4n$ | 62 | $8n$ | 95 | $8n$ | 126 | $4n$ | 159 | $4n$ | 194 | $4n$ | | |
| 36 | $4n$ | 63 | $4n$ | 96 | $8n$ | 127 | $4n$ | 161 | $4n$ | 198 | $8n$ | | |
| 37 | $4n$ | 64 | $4n$ | 98 | $4n$ | 128 | $4n$ | 163 | $4n$ | 199 | $4n$ | | |

*Those space groups not listed here are symmorphic and hence $\nu = 2n$; $n$ in this table is a positive integer $1, 2, 3, \cdots$.

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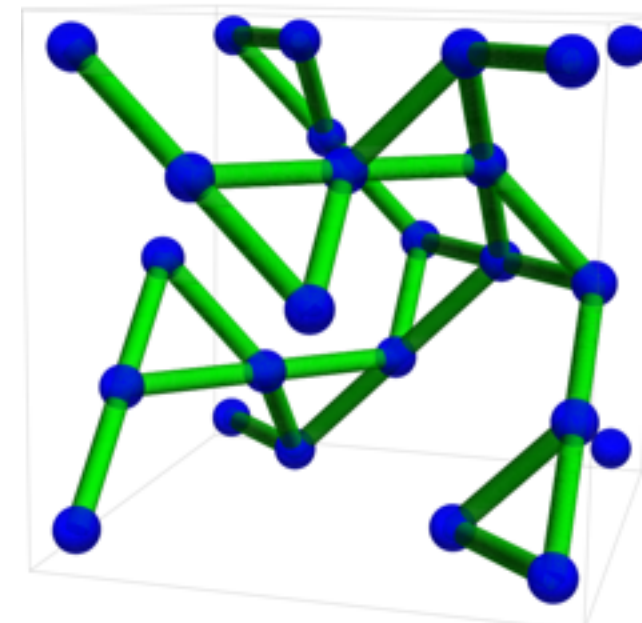
  (Okamoto,.. Takagi 2007)

- insulator with no symmetry breaking down to low temperatures.

- 12 electrons in the unit cell - not a classic `Mott' insulator (odd number of electrons per unit cell).

- spin orbit coupling is strong - could the low temperature state be a interacting `band insulator'?



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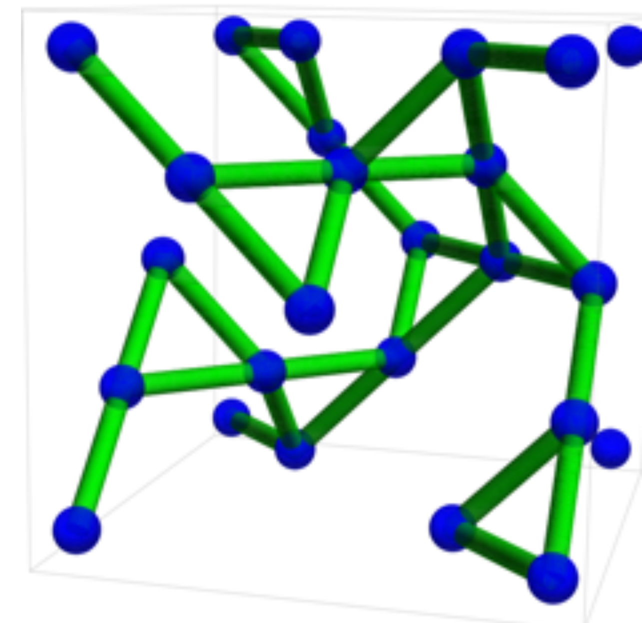

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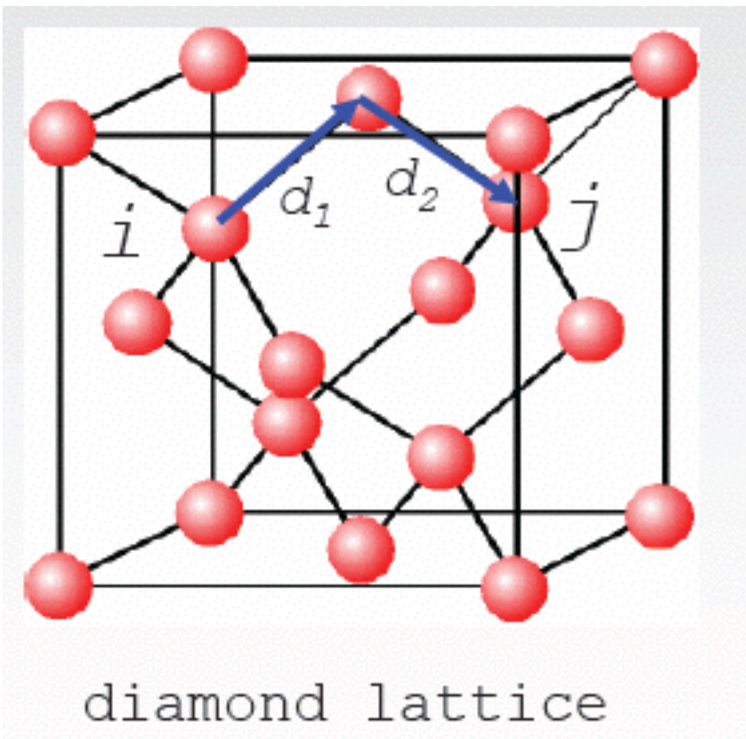
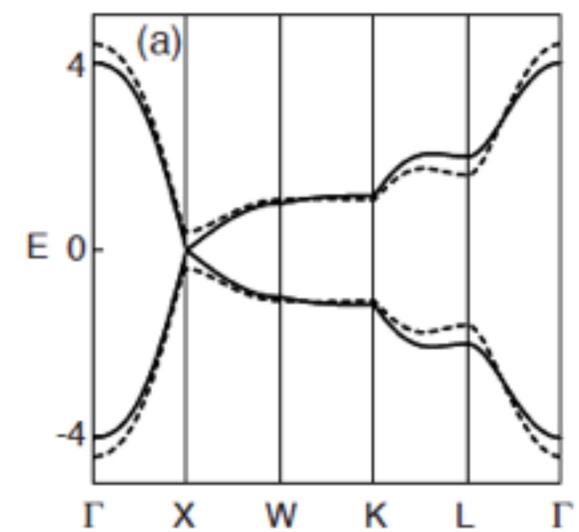
# Application II
# Dirac semimetal in Fu-Kane-Mele Model

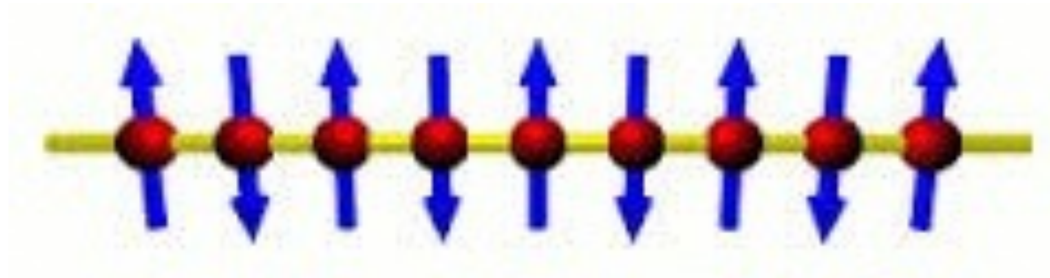



$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i\lambda \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger \vec{\sigma} \cdot (\vec{d}_1 \times \vec{d}_2) c_j$$




- Diamond lattice (#227) at half filling (2 electrons/unit cell)
- No `band insulator' allowed except at 4n. Minimal solution Dirac semimetal.
- Design principle for achieving semimetals?

# Lieb-Schultz-Mattis - Simple argument



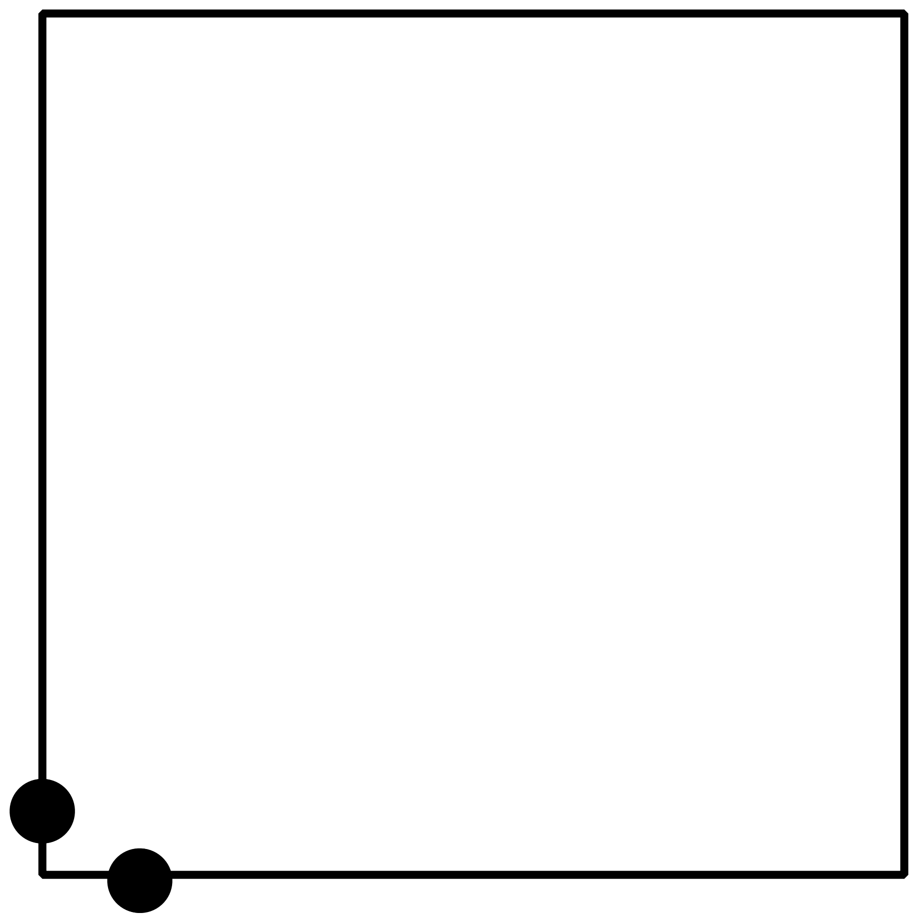
- Unique ground state? Periodic boundary condition with an ***odd*** number of sites

**Contradiction**

- A single spin-1/2 state has to 'point' somewhere
- Not compatible with a symmetric, gapped state with short range entanglement

# Extension to non-Symmorphic space groups

Translations



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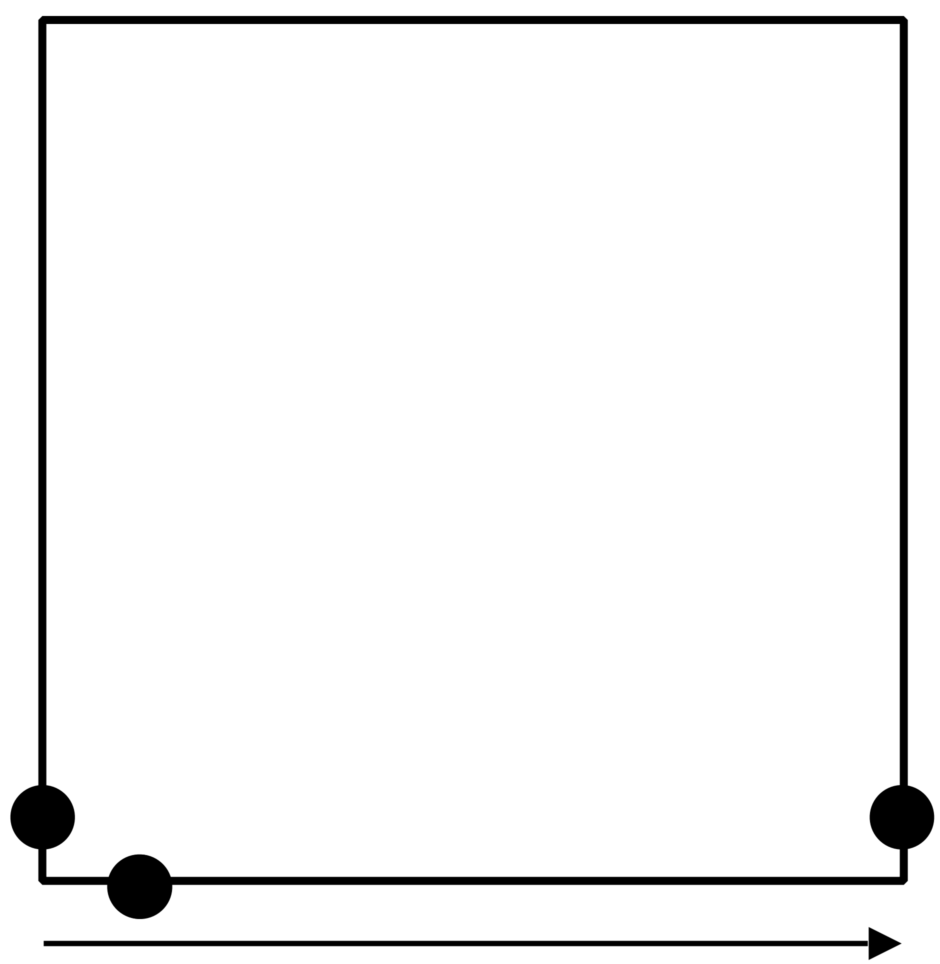

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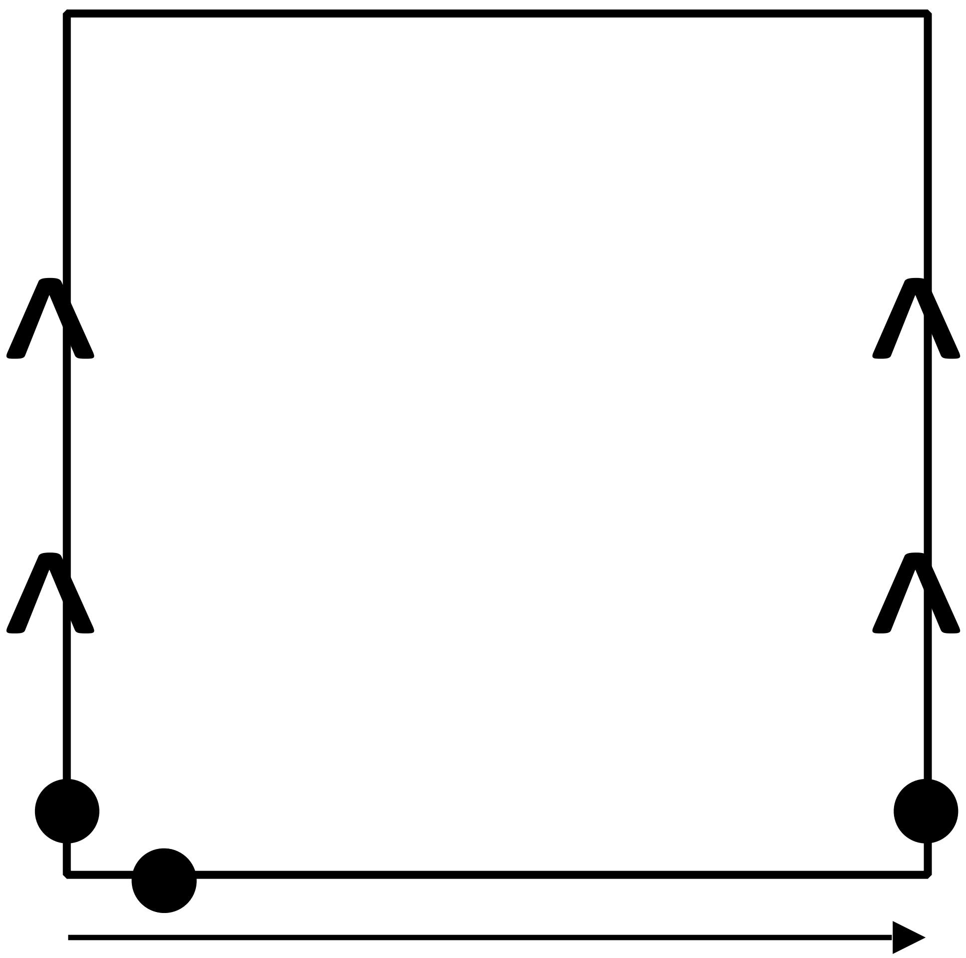

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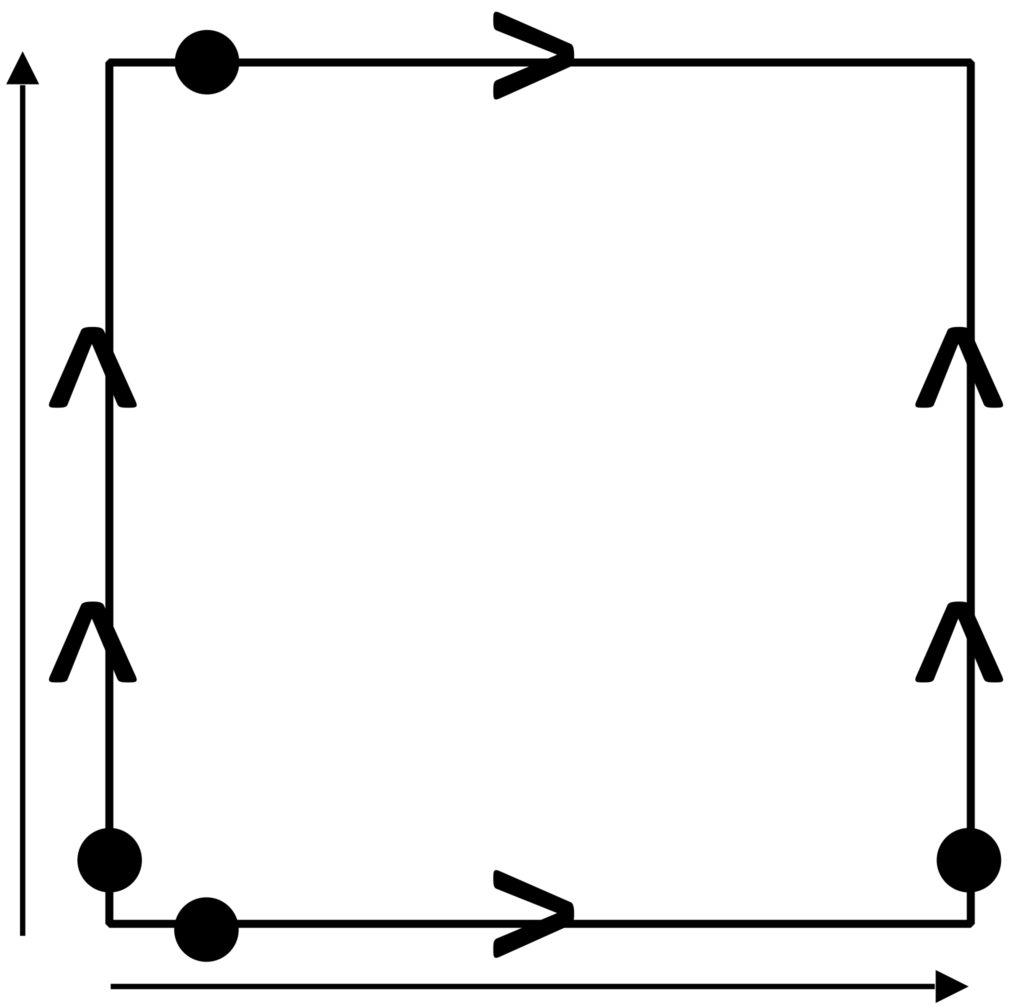

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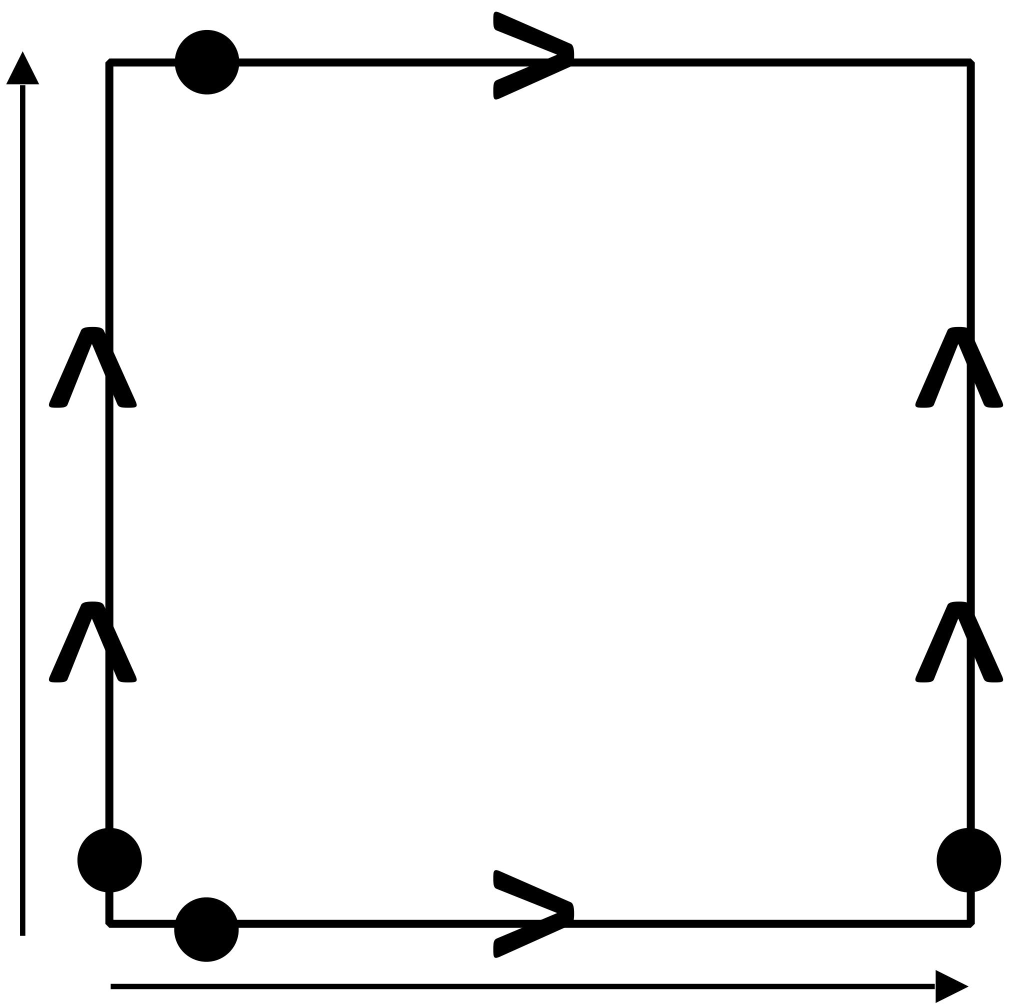

Torus

PBC; integer # of unit cells

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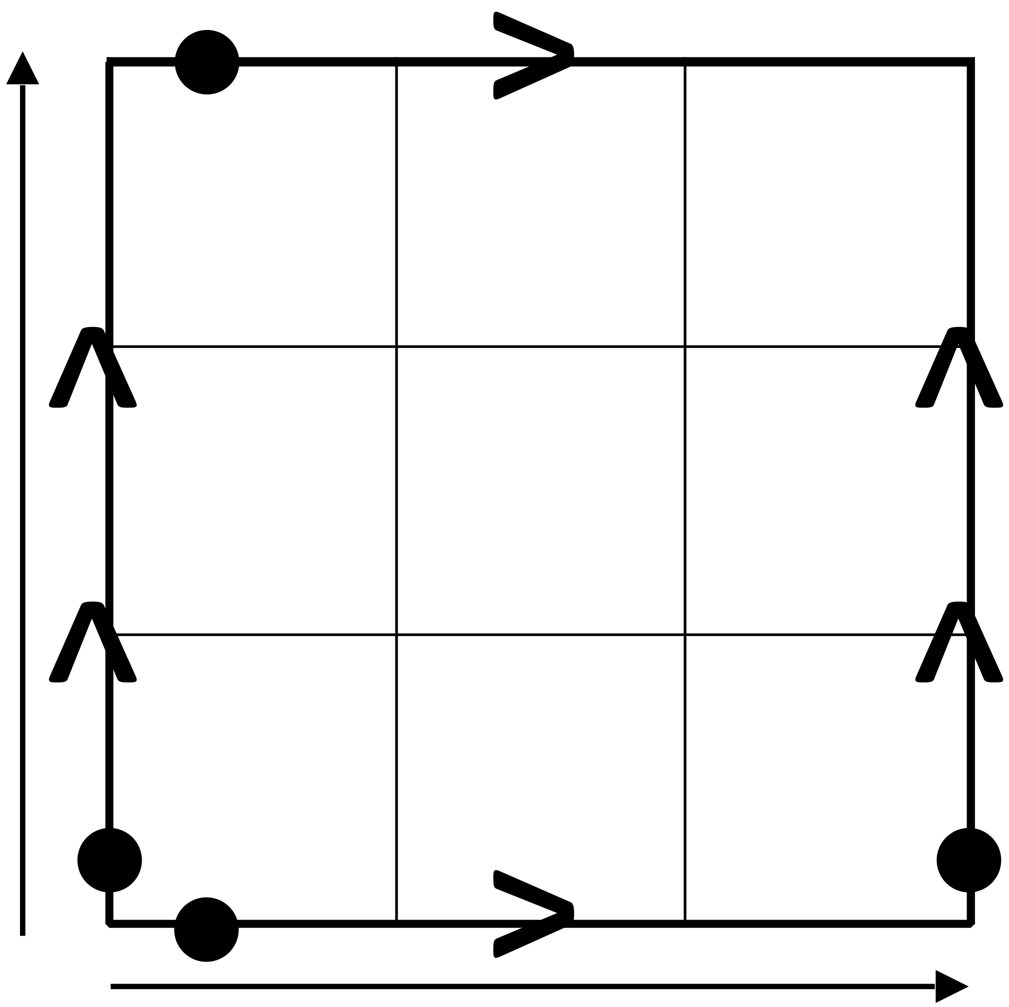

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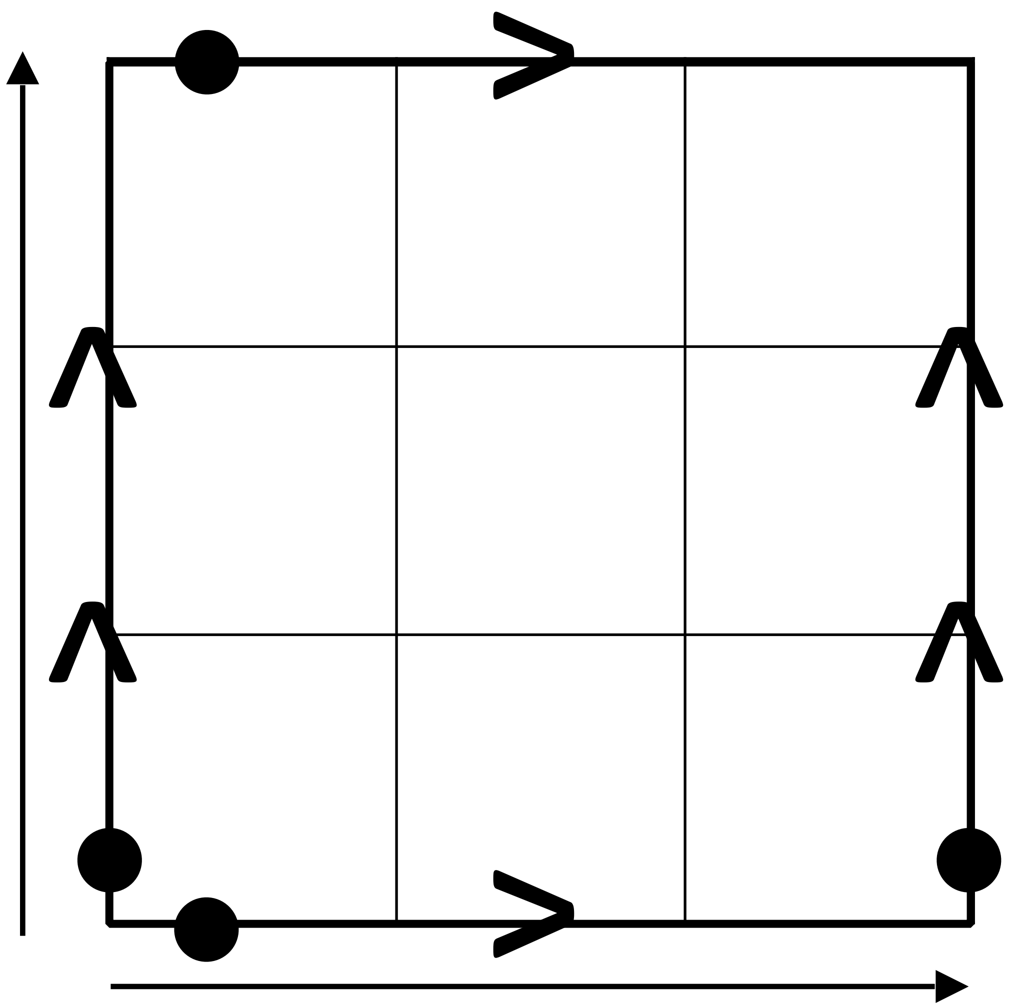

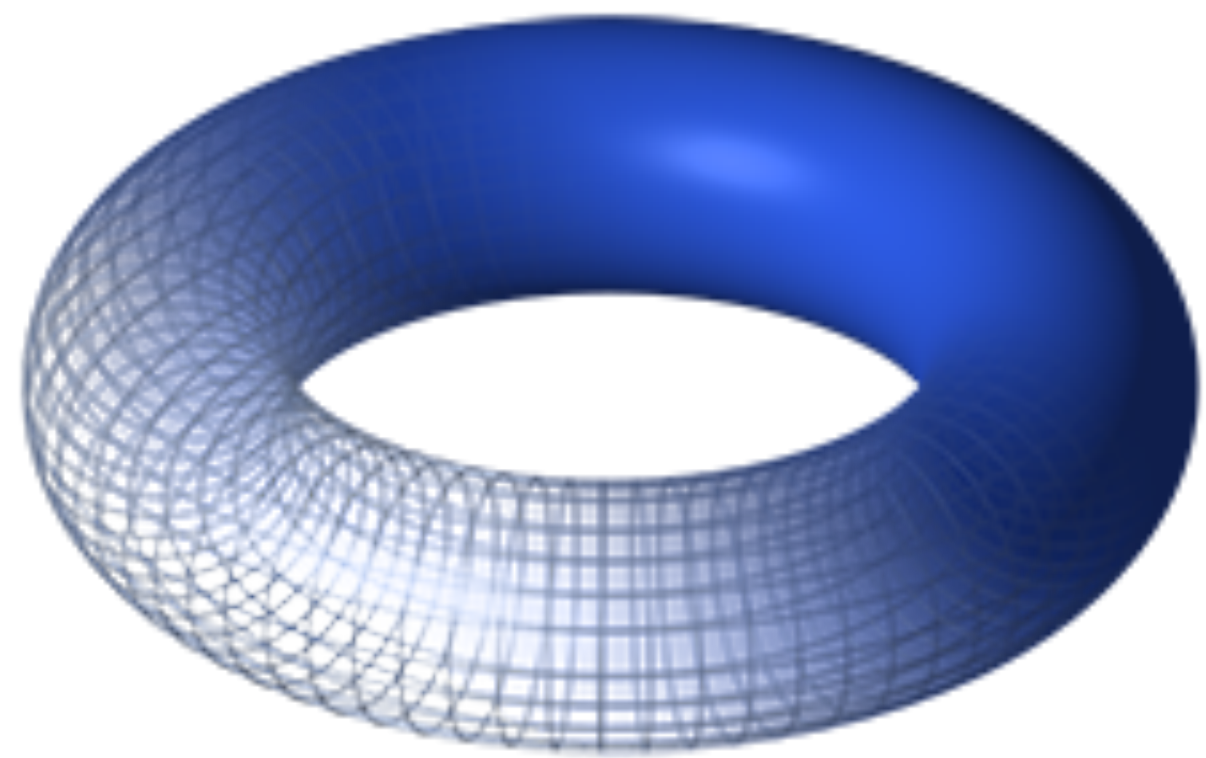

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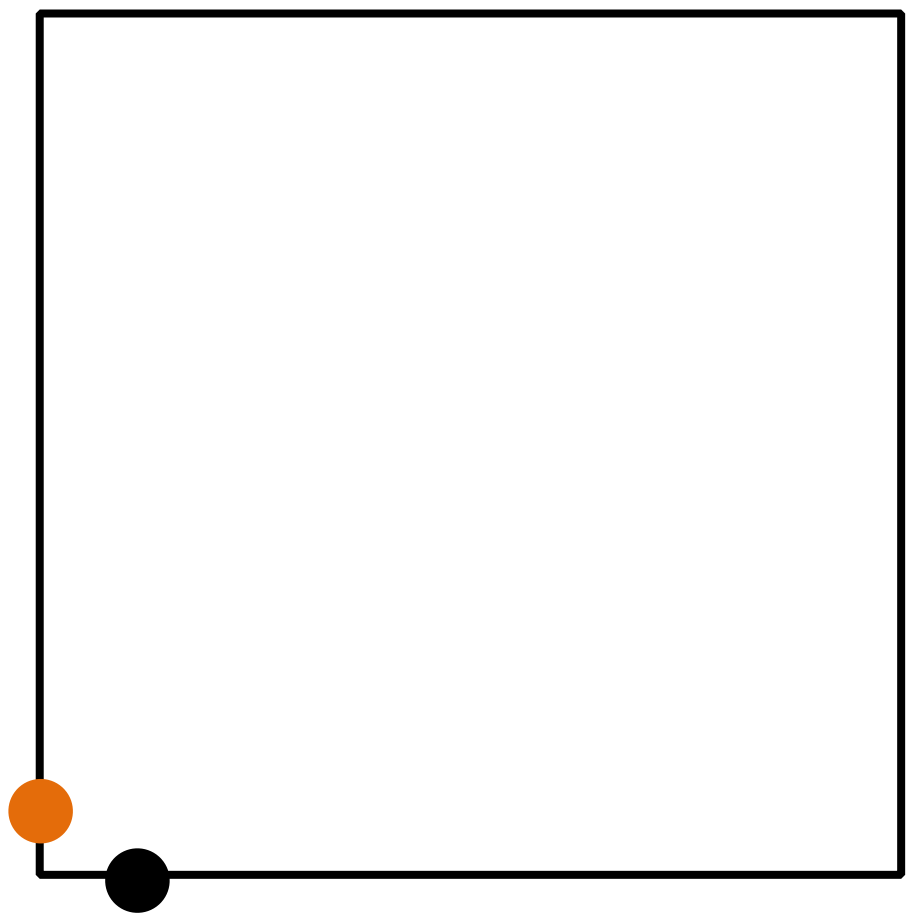

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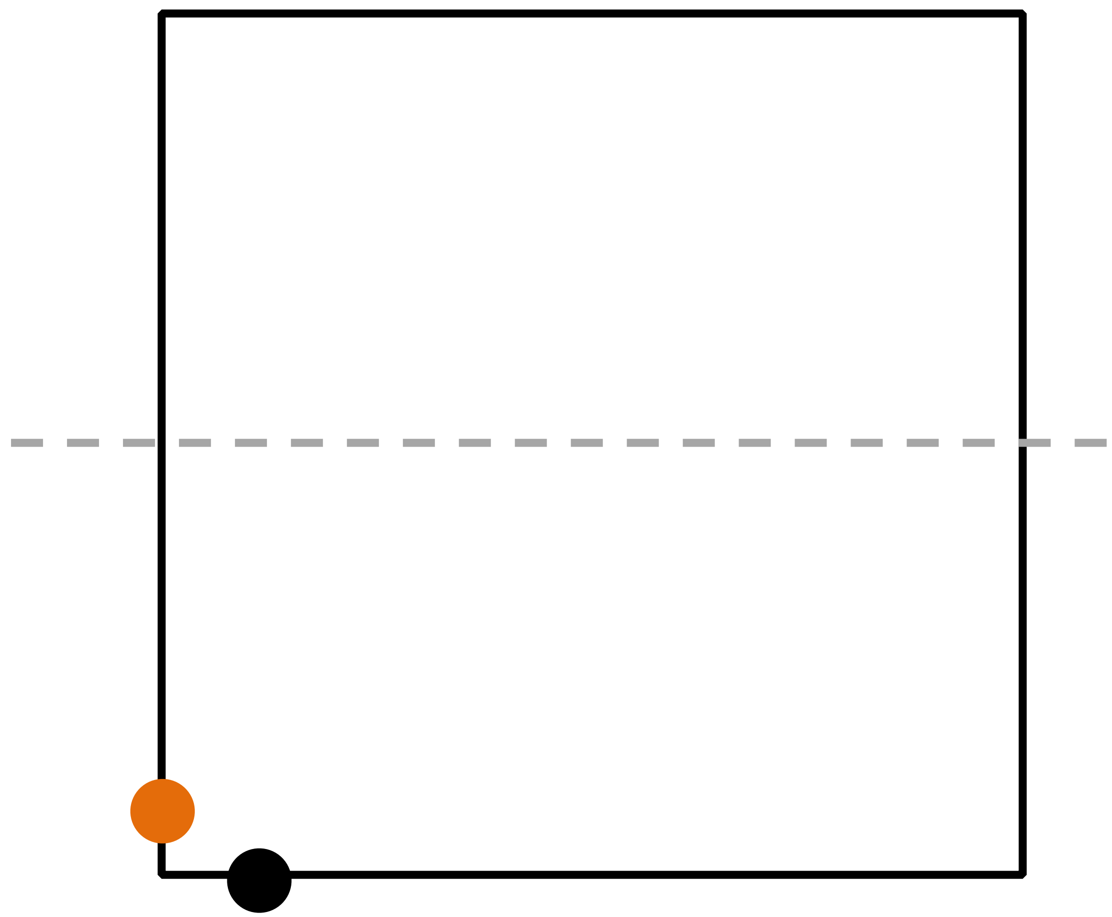

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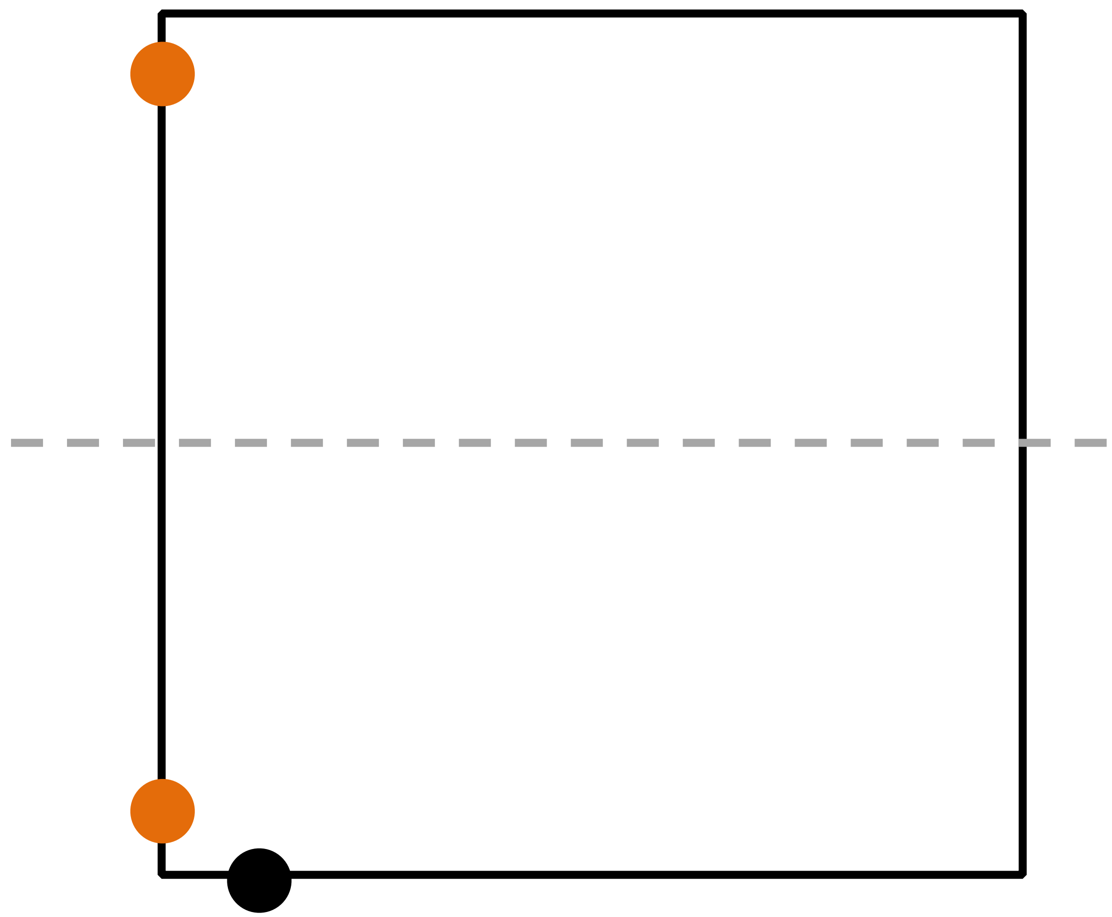

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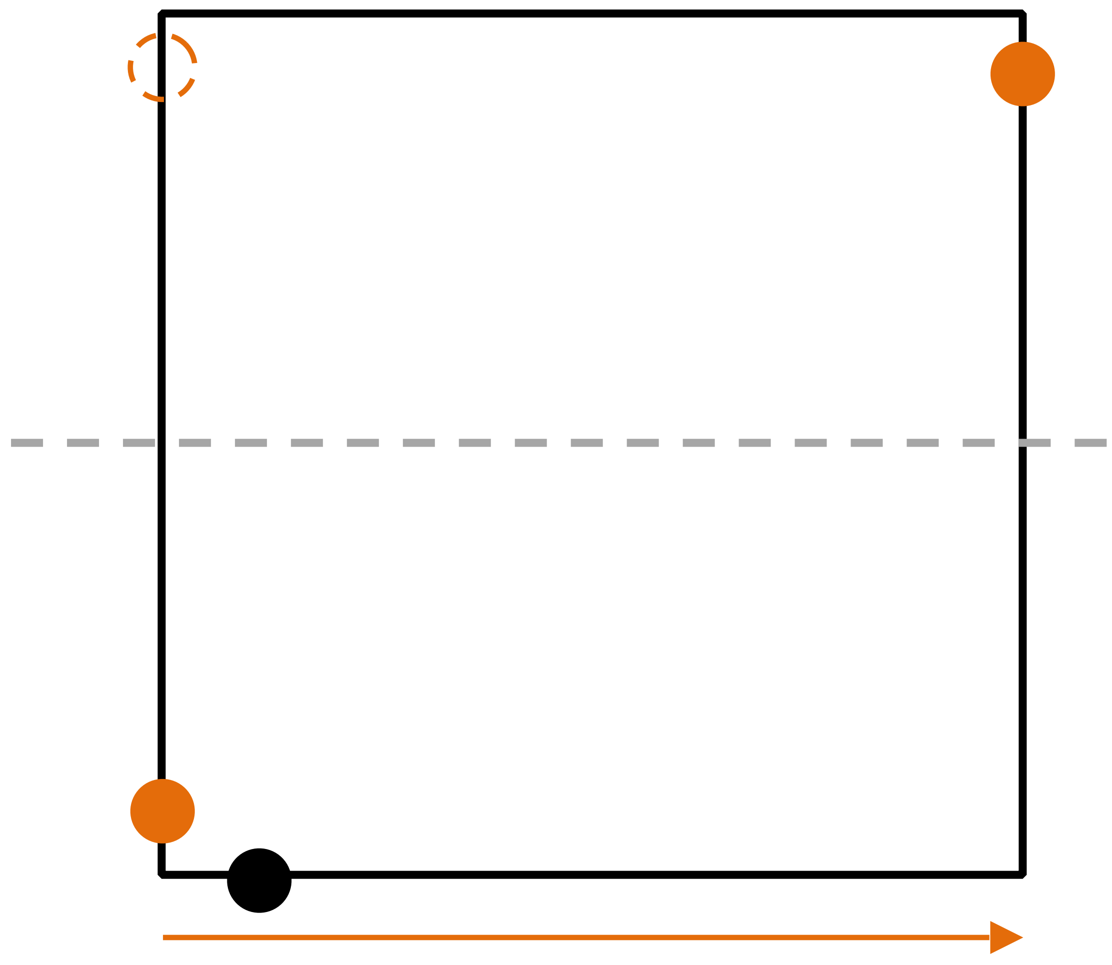

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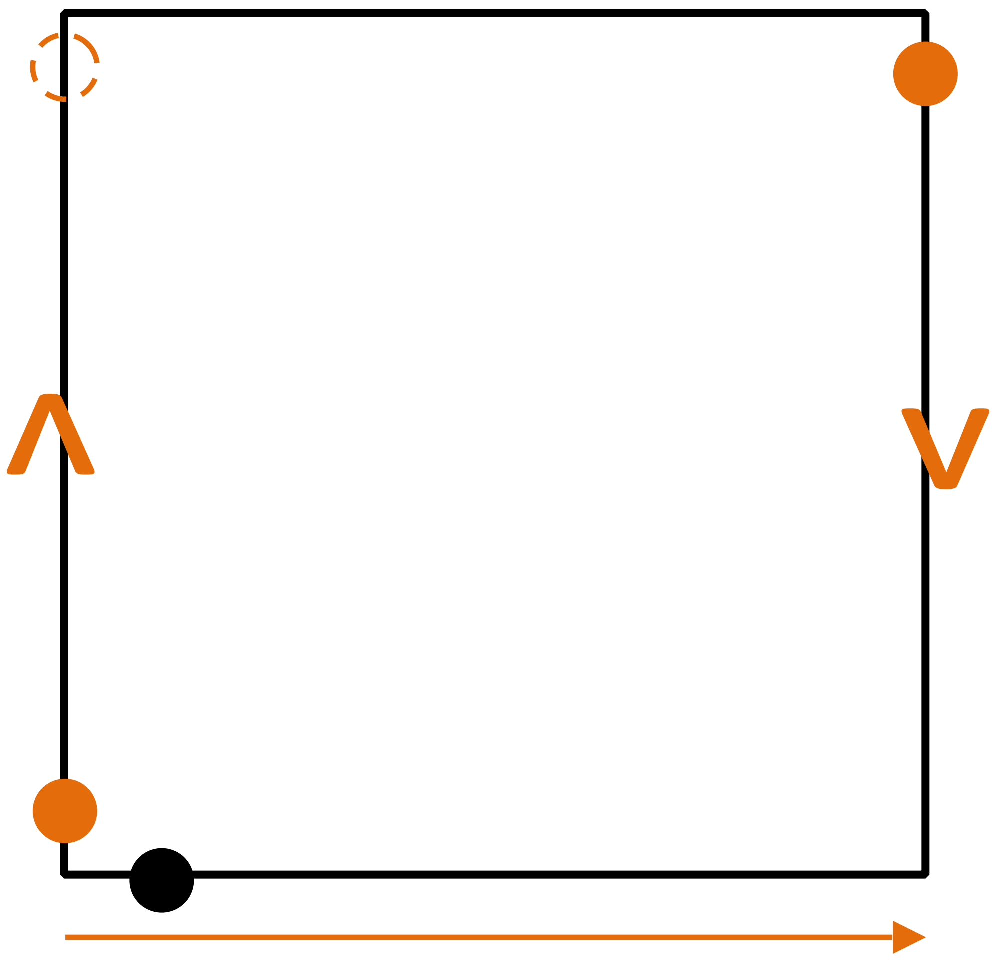

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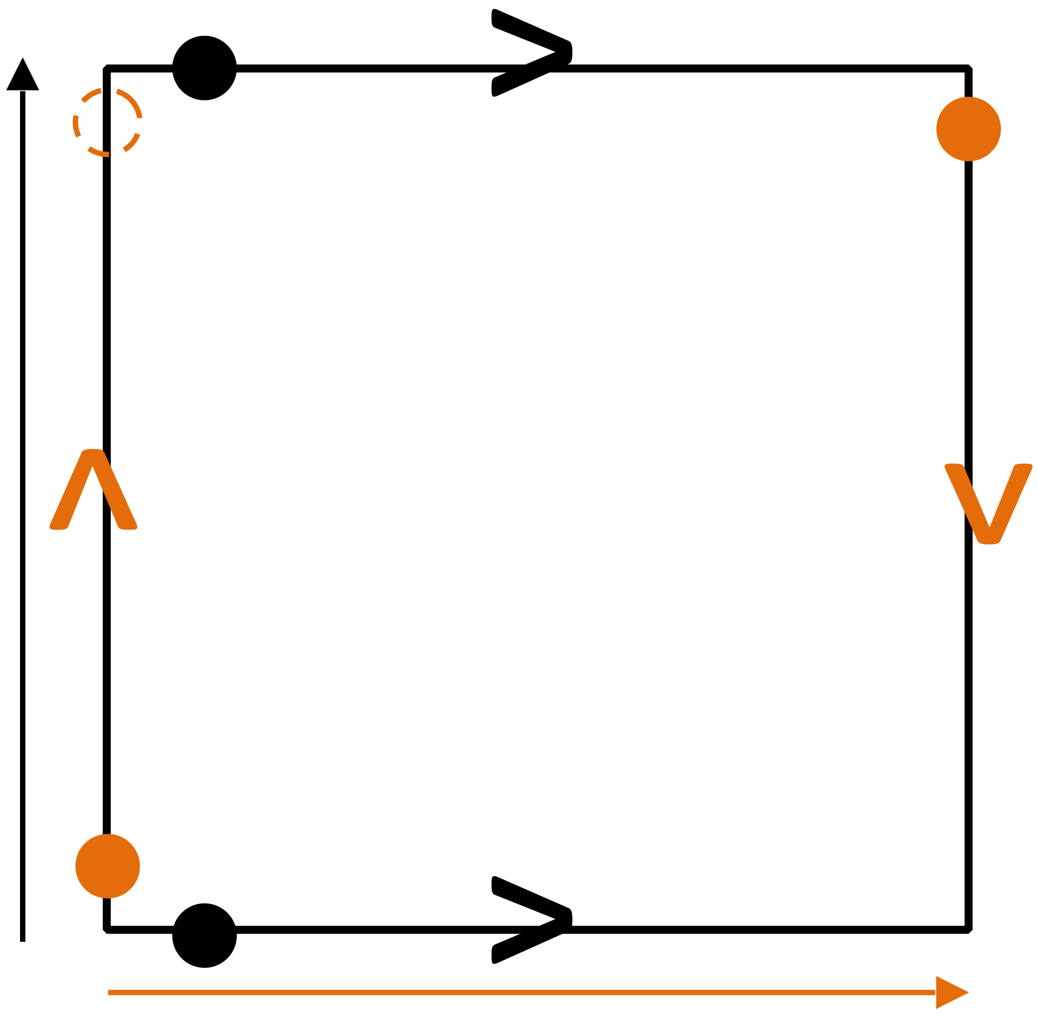

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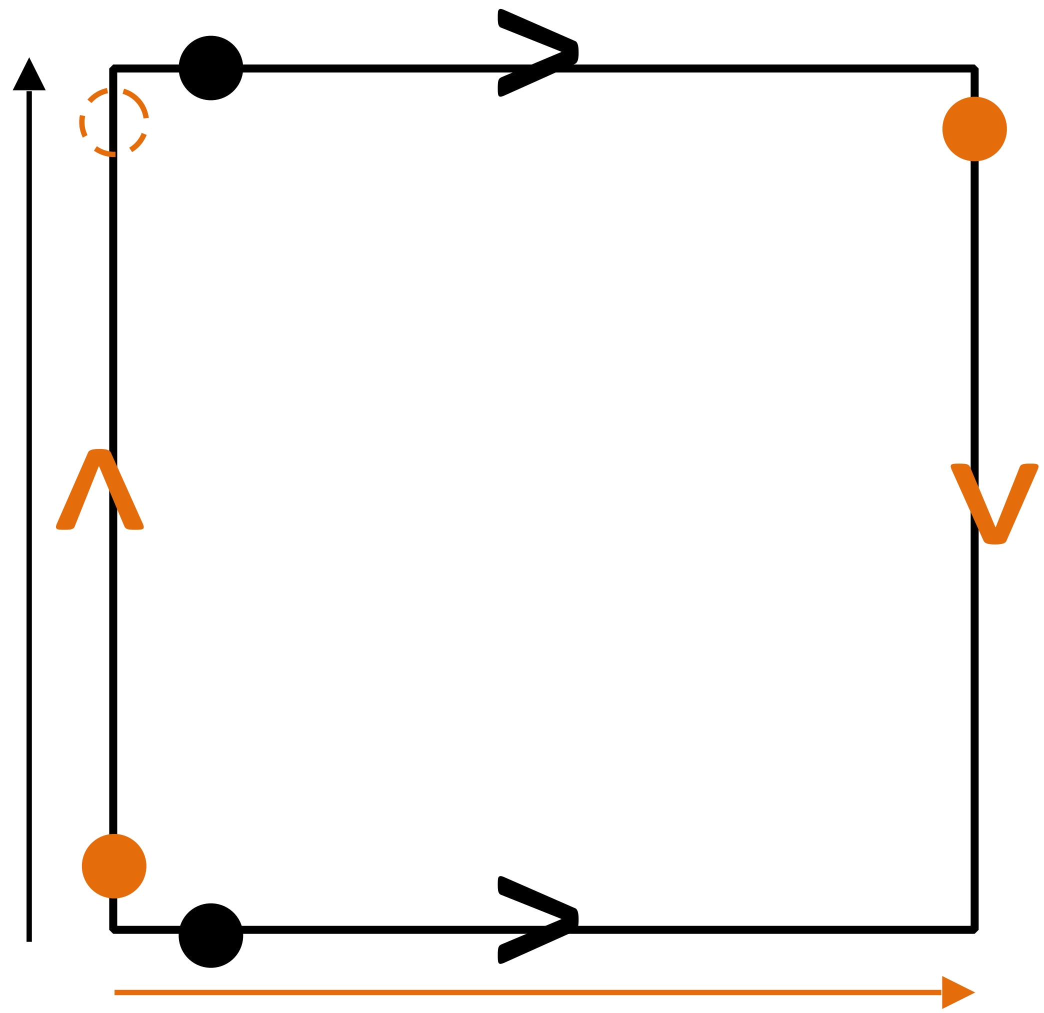

Klein bottle

Space group specific BC;
*half-integer #* of unit cells

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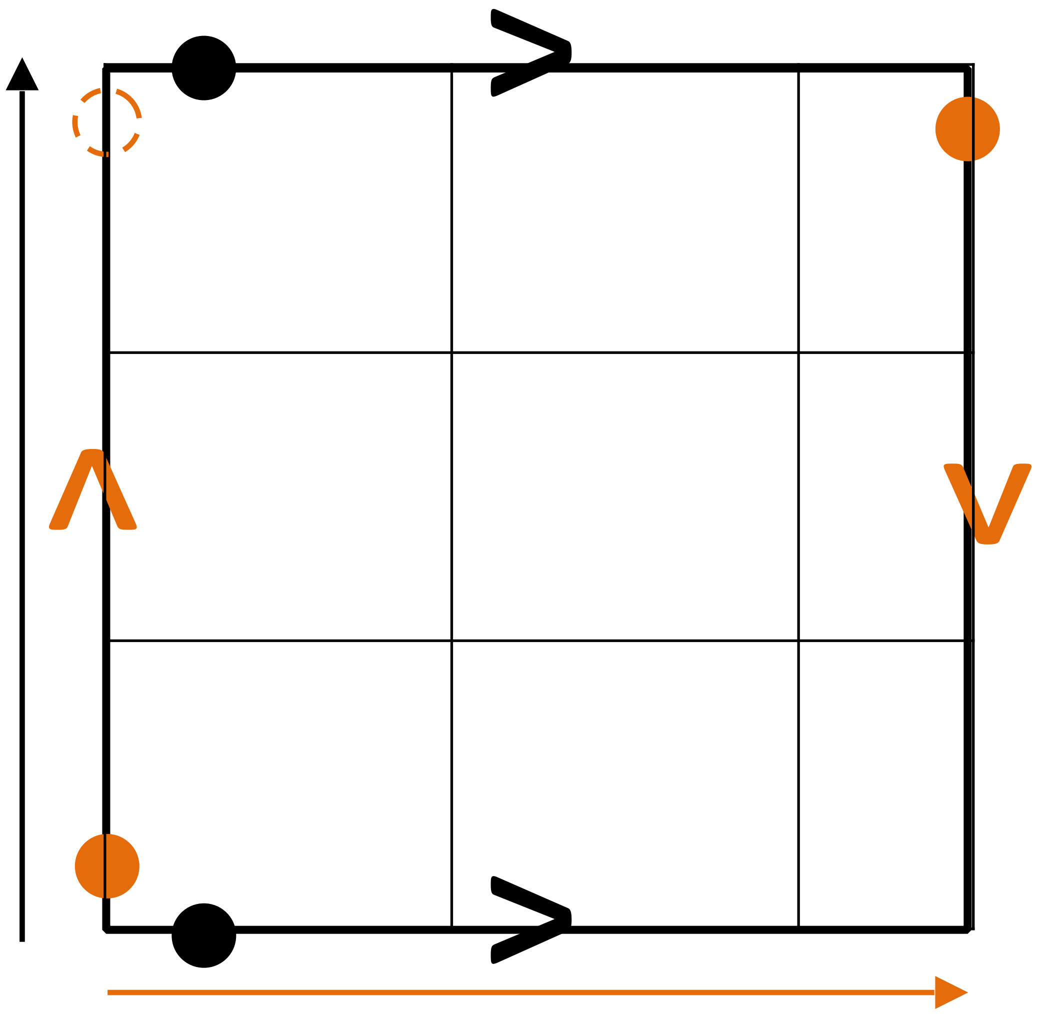

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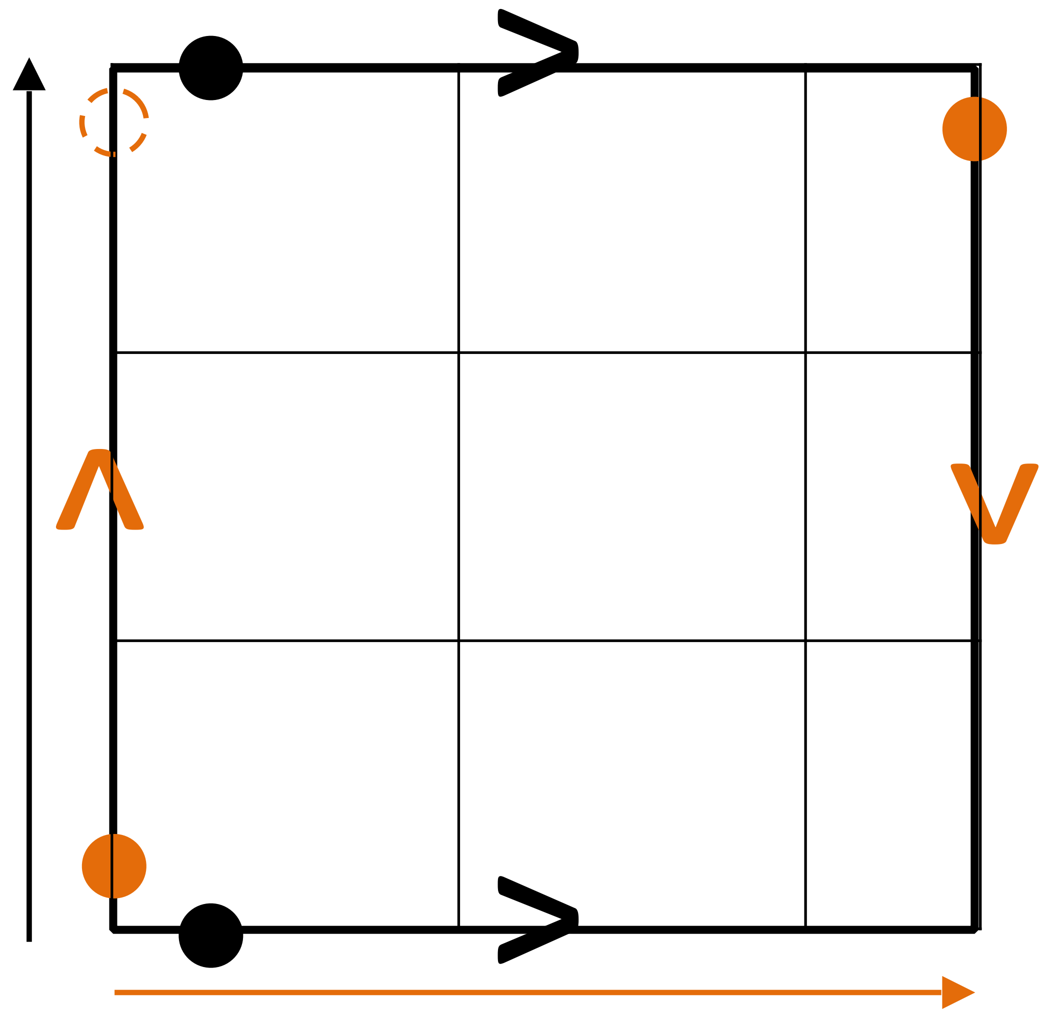

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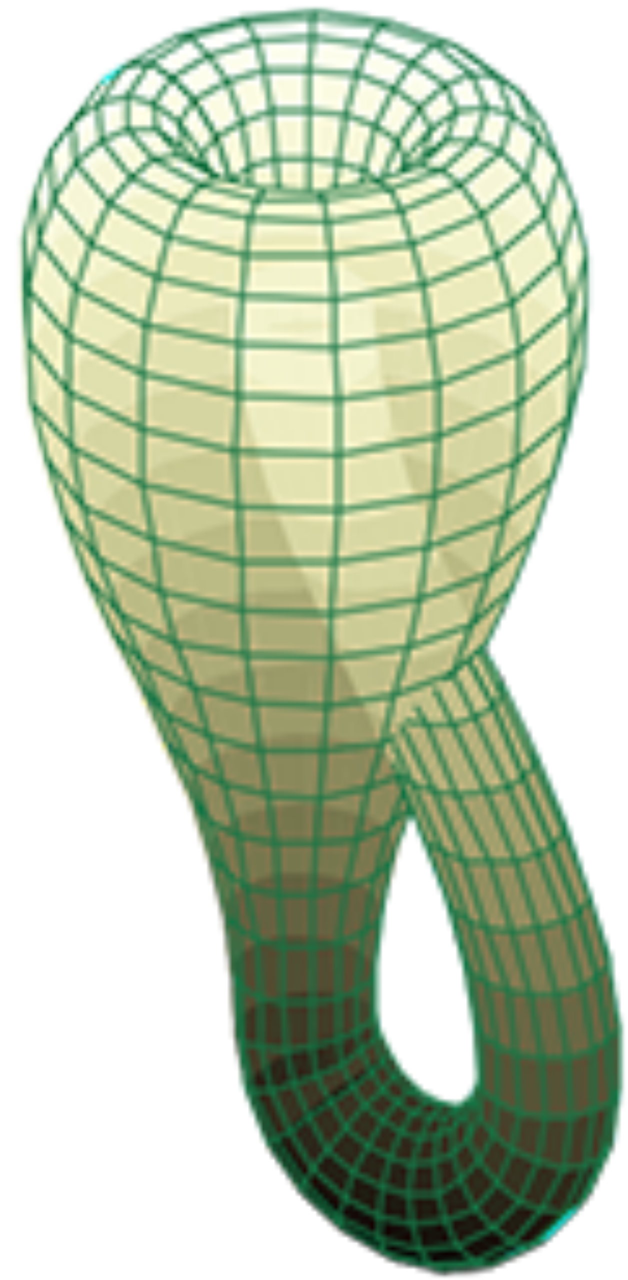

# Extension to non-Symmorphic space groups

- Compact space must be locally flat (like the torus).
- Only 10 such spaces in 3D - Biberbach spaces
- Can define spin on all these spaces (either Spin structure or Pin- structure permitted).
- Used to derive non-symmorphic bounds.

# Conclusion

- Introduced `filling enforced' quantum band insulator - filling forbids `atomic insulator'
- Established minimum filling for featureless insulators (`band insulators') with spin orbit coupling & interactions:
    - Symmorphic & non-Symmorphic lattices .
- Techniques can be used in new situations:

Symmorphic lattice with two S=1/2 per unit cell.
No trivial paramagnet due to reflection!
Can be trivial with charge fluctuations