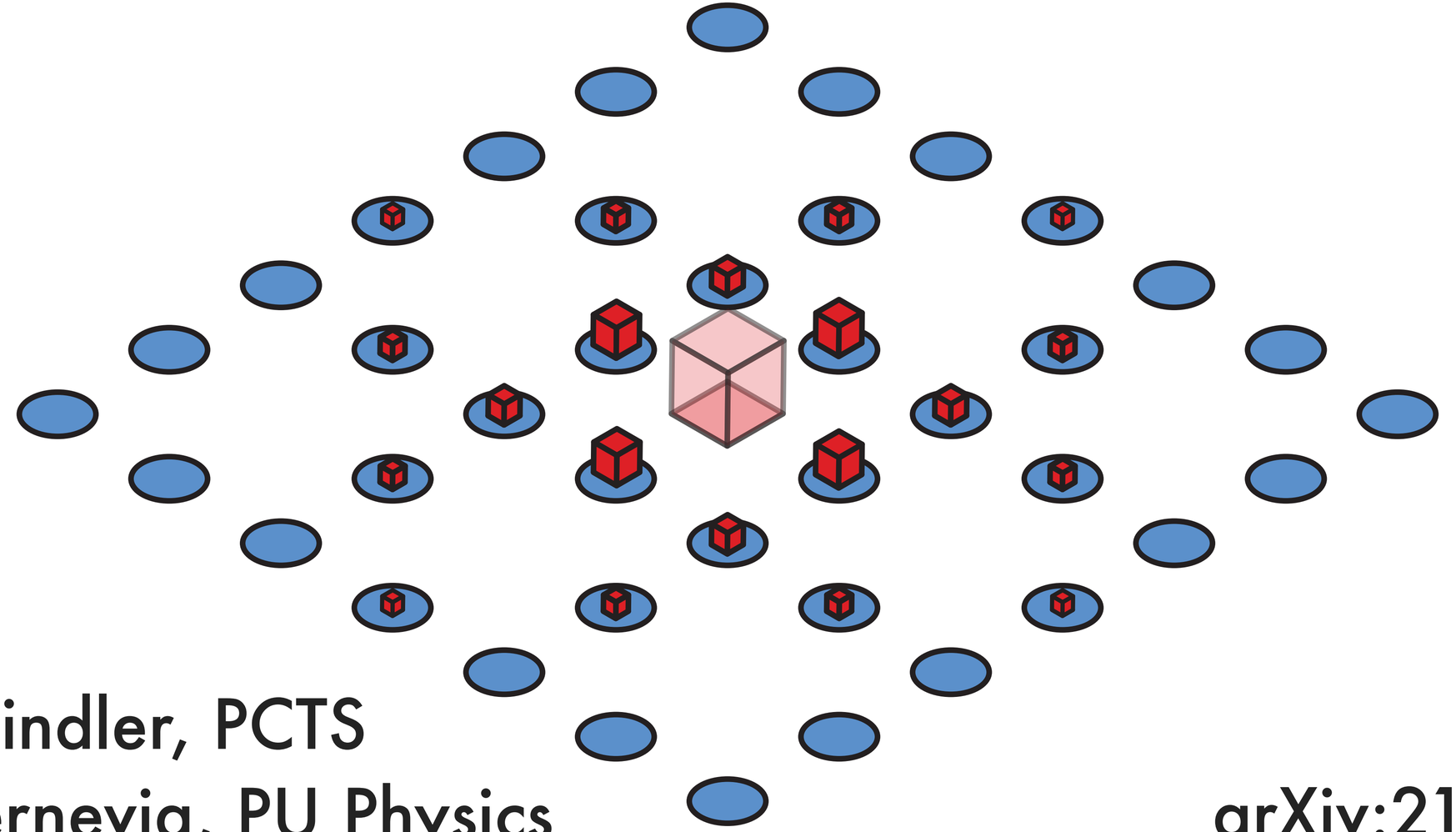
Non-Compact Atomic Insulators



Frank Schindler, PCTS
Andrei Bernevig, PU Physics

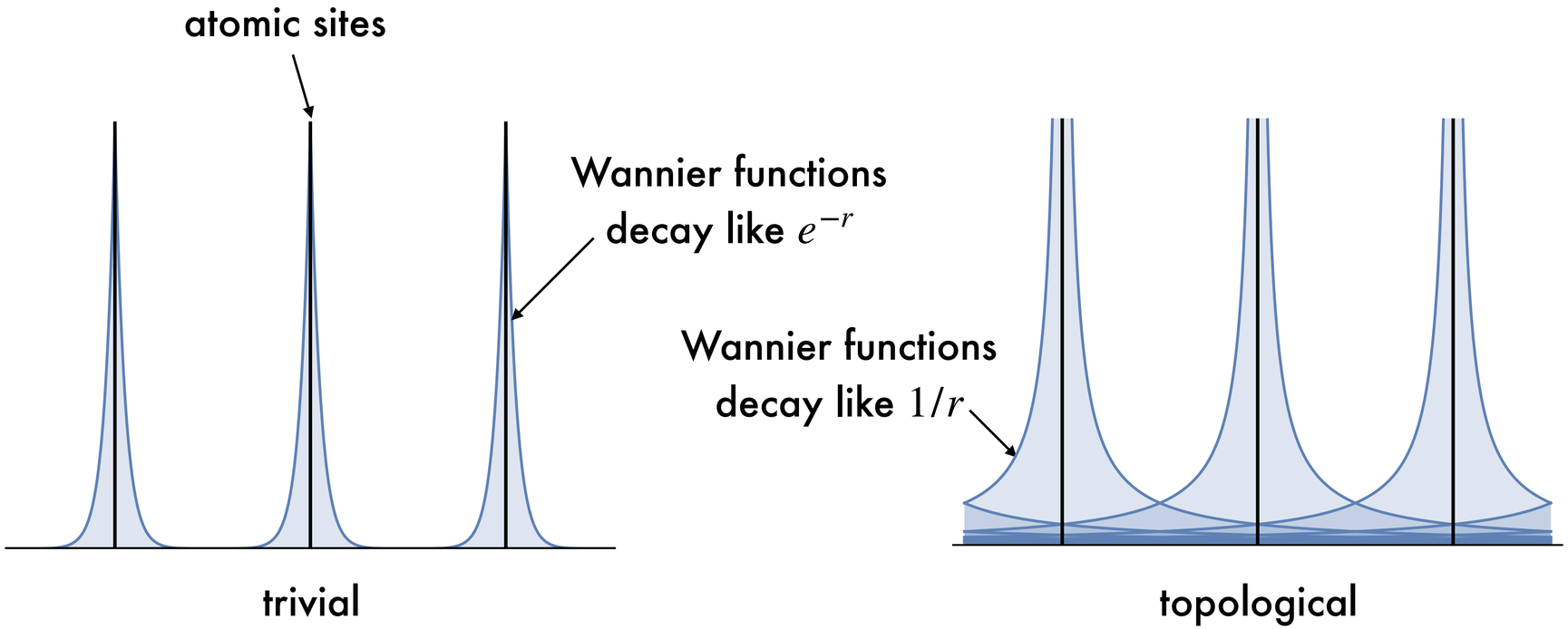
arXiv:2107.13556

Real-space picture of band topology

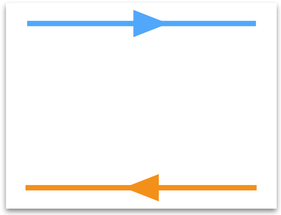
Insulators have **momentum** space topological invariants, e.g. the Chern number $C = \int \mathrm{d}^2k\, F$

Uncertainty principle: global properties in **momentum** space $\Longleftrightarrow$ local properties in **real** space

Wannier function $W_R = \int \mathrm{d}k\, e^{\mathrm{i}kR} \Psi_k$ ← Bloch function



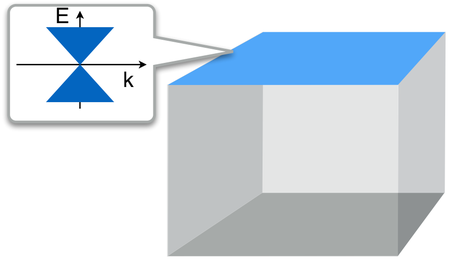
2D Chern Insulator



No exponentially localizable Wannier functions

Brouder, C., et al. (2007). Physical review letters, 98(4), 046402

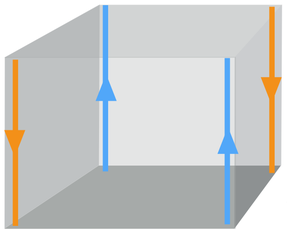
3D Topological Insulator



No exponentially localizable Wannier functions that satisfy time-reversal symmetry

Soluyanov, A. A., & Vanderbilt, D. (2011). Physical Review B, 83, 035108

3D Higher-Order TI



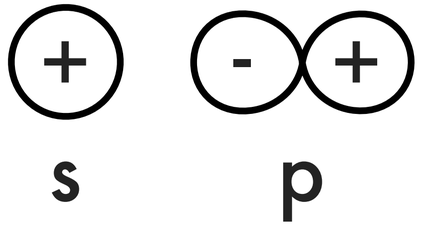
No exponentially localizable Wannier functions that satisfy crystalline symmetry

Topology as a Wannier Obstruction

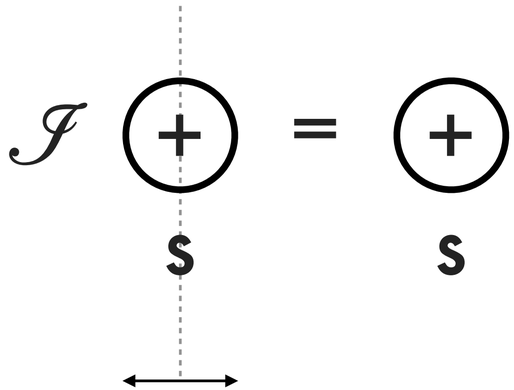
unified picture of topological insulators, obstructed atomic limits, fragile phases, …

Are there Wannier obstructions beyond exponential localization?

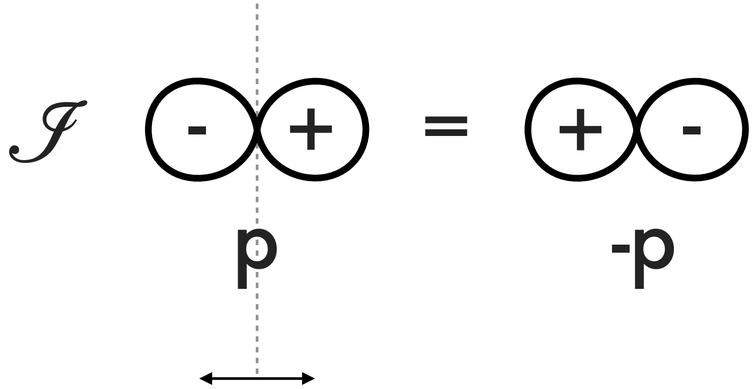
Orbital symmetry

s and p orbitals 

have opposite inversion eigenvalues



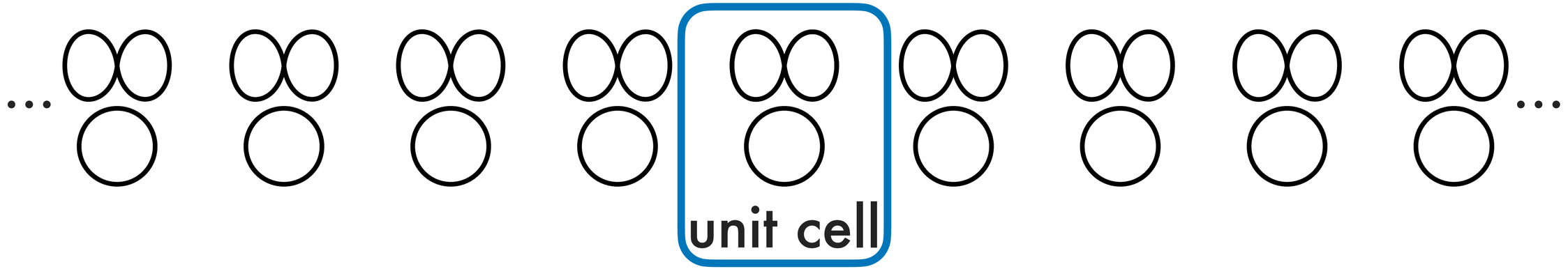
s has eigenvalue +1



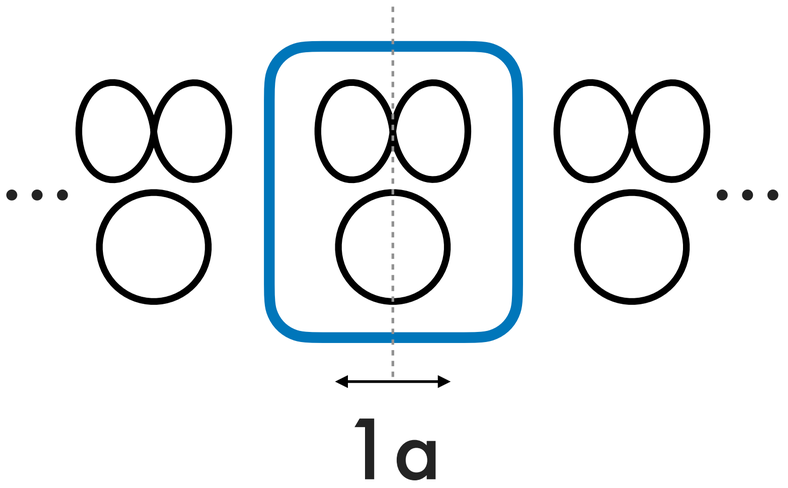
p has eigenvalue -1

Crystal symmetry

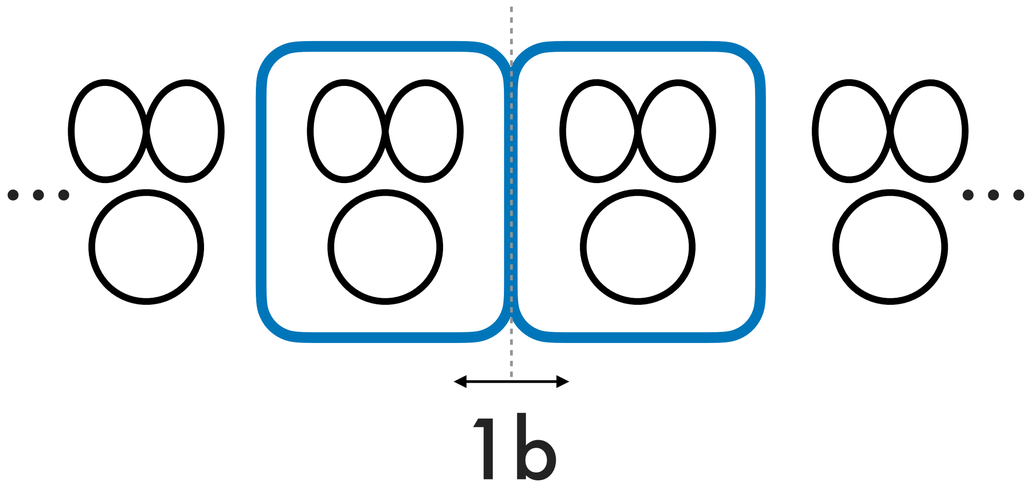
Let's build a 1D crystal out of s and p orbitals



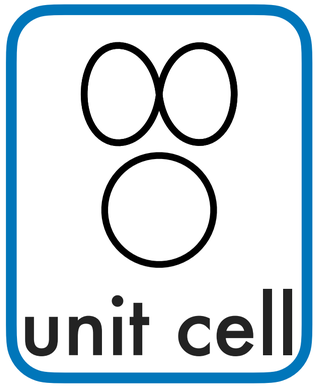
There are two inversion centers of the infinite lattice:



and

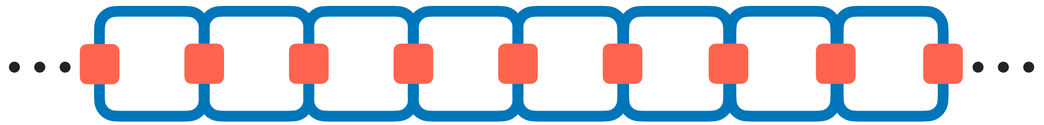


Constructing an insulator

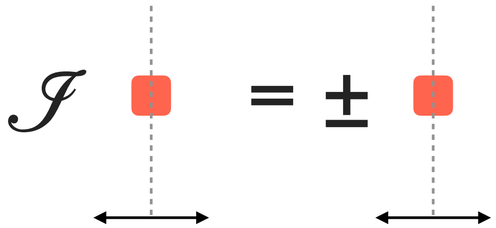
At half-filling, each 

provides a single electron

Two insulating limits where electrons are localized:

 and 

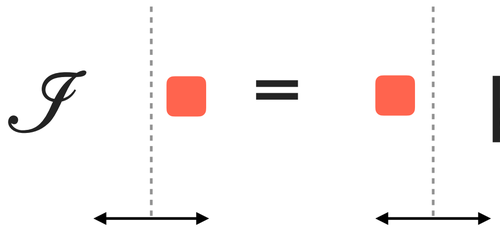
These are **topologically** distinct when enforcing inversion symmetry



+ for s

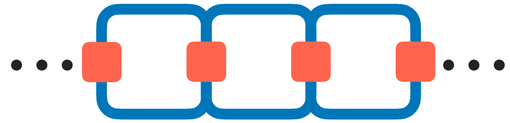
- for p

we cannot move 



breaks symmetry

(Obstructed) atomic insulators

We use the terminology  and 

unobstructed atomic insulator

obstructed atomic insulator

electrons localized **on** atoms

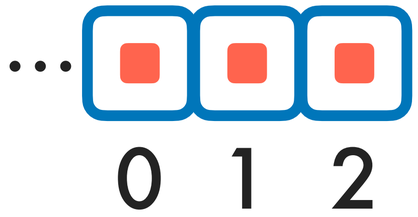
electrons localized **away** from atoms

previous terminology: ~~trivial~~ ~~topological~~

the term topological is now reserved for insulators without a localized electron picture – these exist in 2D or higher

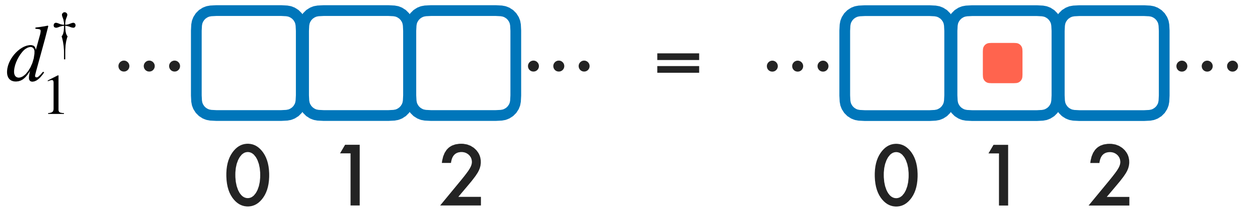
Unobstructed ground state

Given an atomic insulator, how do we construct its ground state?



$= \ldots d_0^\dagger d_1^\dagger d_2^\dagger \ldots |0\rangle$

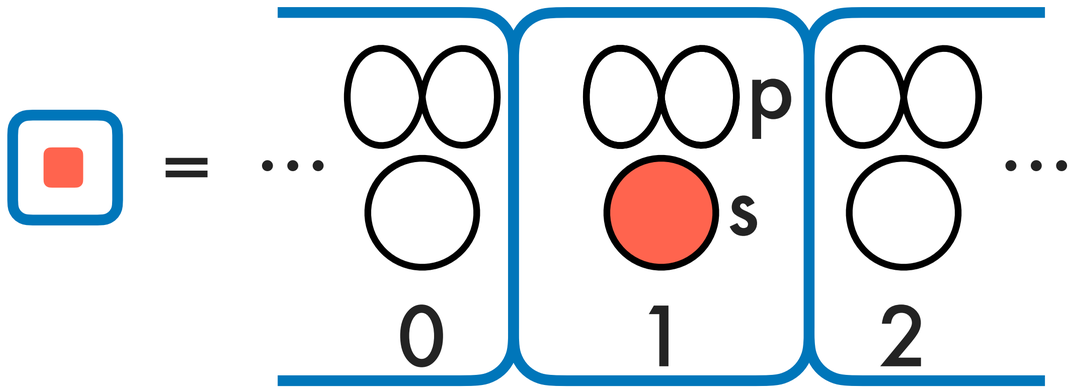
$d_1^\dagger$ creates an electron centered at unit cell 1



What does this really mean?

It means that

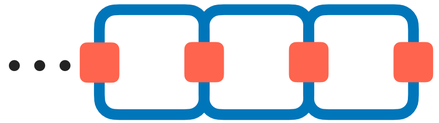
$d_1^\dagger = c_{1,s}^\dagger$



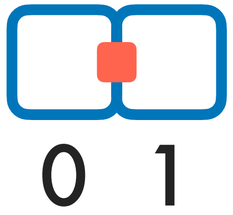
if ■ has s-character (inversion eigenvalue 1)

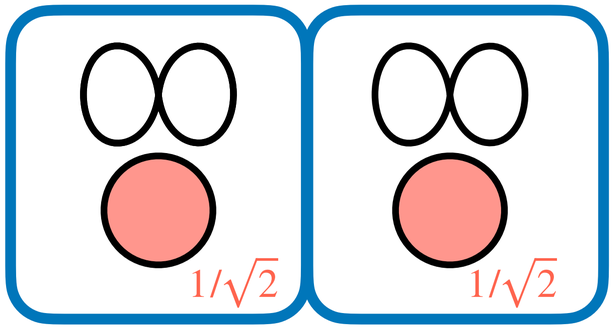
Obstructed ground state

We have seen that  can be obtained by occupying the s-orbital in every unit cell

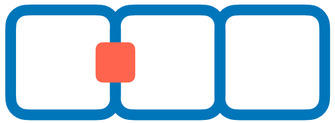
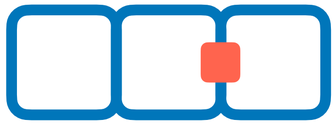
What about 

$= \ldots d^\dagger_{-1/2} d^\dagger_{1/2} d^\dagger_{3/2} d^\dagger_{5/2} \ldots |0\rangle$?

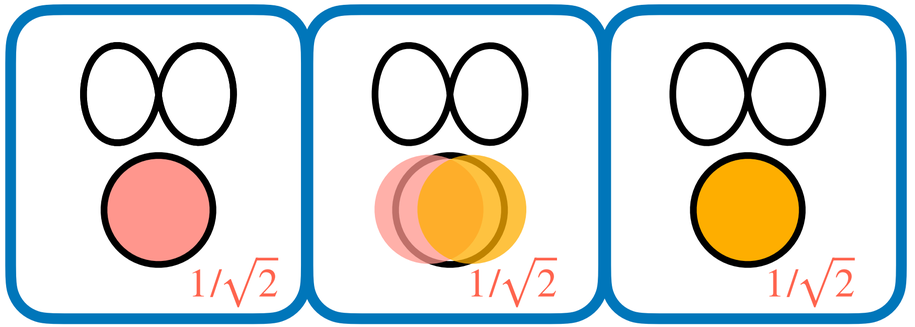
Naively, 

$=$ 

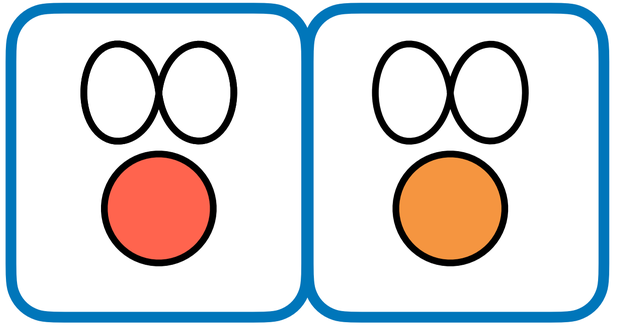
so that $d^\dagger_{1/2} = \dfrac{c^\dagger_{0,s} + c^\dagger_{1,s}}{\sqrt{2}}$

BUT: $\langle \ldots$  $\ldots | \ldots$  $\ldots \rangle \neq 0$

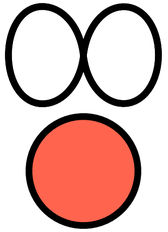
local electron states not orthogonal!

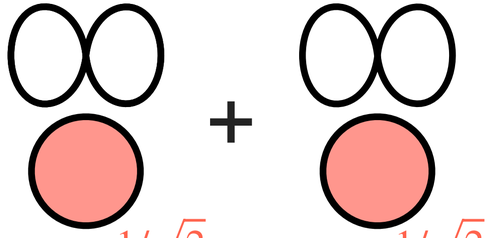


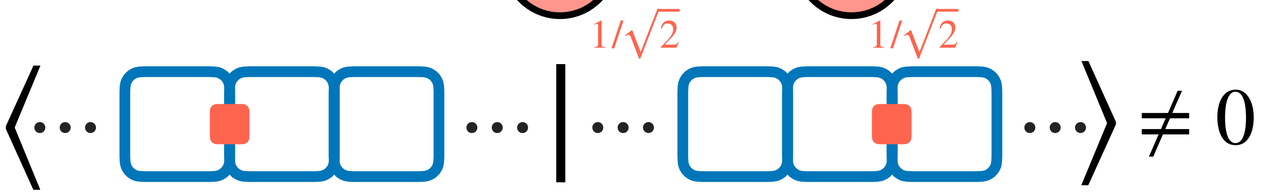
Wannier states are orthogonal

Recall: for the unobstructed case,  there is no overlap!

→ perfect orthogonality: 

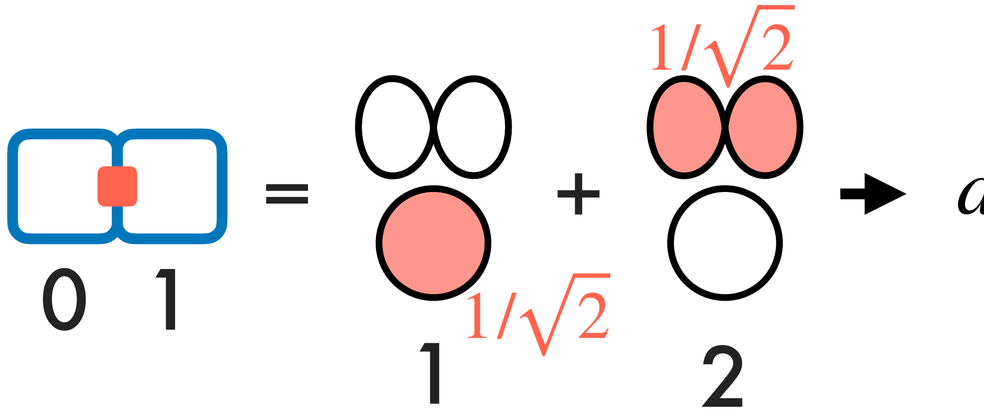
Technically, this means that the states  form a **Wannier basis**.

On the other hand, the states  do not.



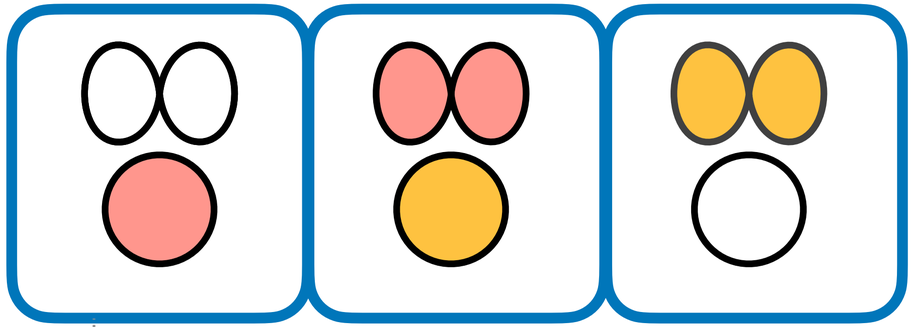
A naive orthogonal solution

What about this obstructed state:



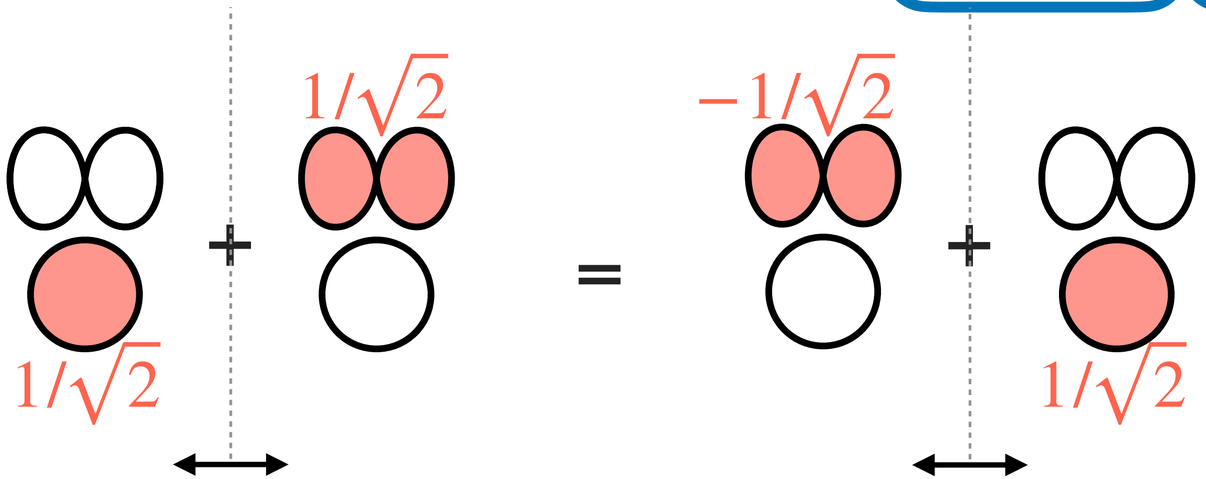
$$\rightarrow \quad d^{\dagger}_{1/2} = \frac{c^{\dagger}_{0,s} + c^{\dagger}_{1,p}}{\sqrt{2}} \quad ?$$

It is orthogonal to all translates:



✓

BUT: $\mathscr{I}$

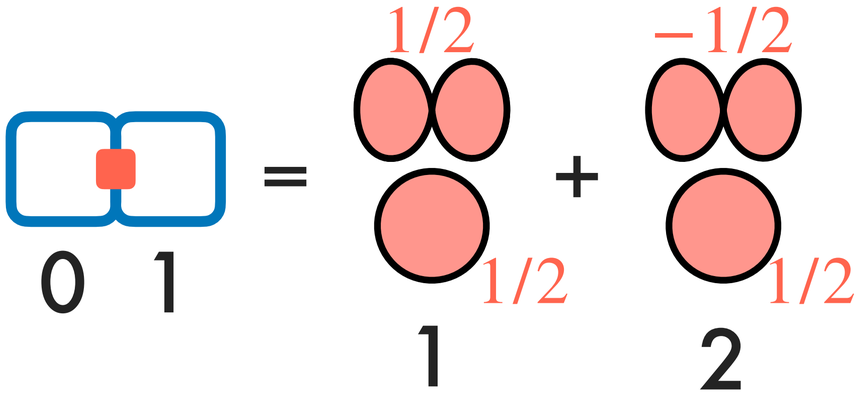


state breaks inversion

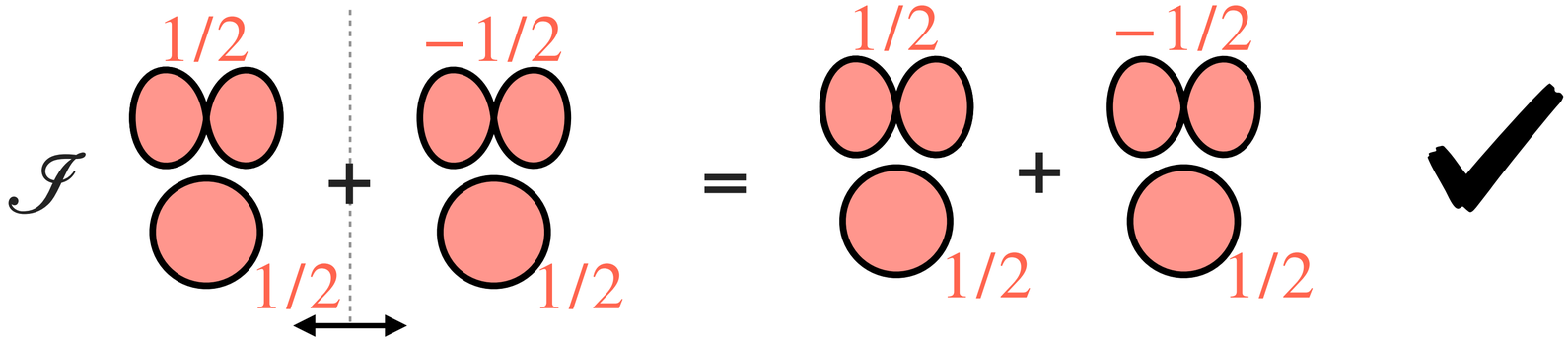
✗

A compact atomic insulator

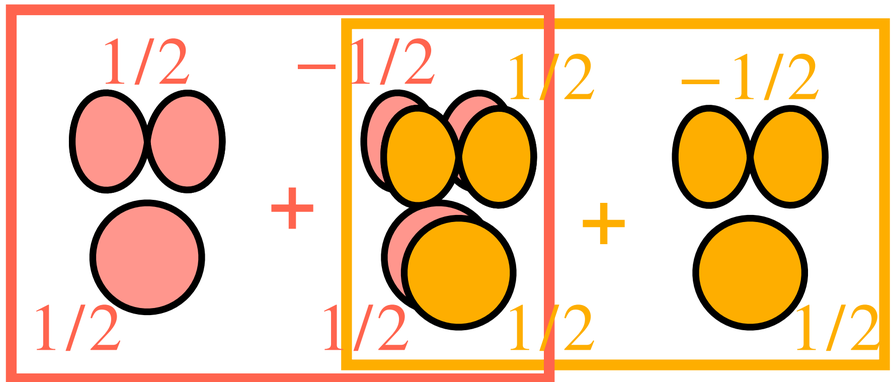
Here's a nontrivial solution:



Inversion:



Orthogonality:

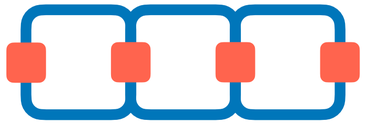


$= 1/4 - 1/4 = 0$

this is the **SSH** model

Compactness

We have seen that …  … admits a trivial **finite-range, symmetric and orthogonal = compact** set of Wannier states

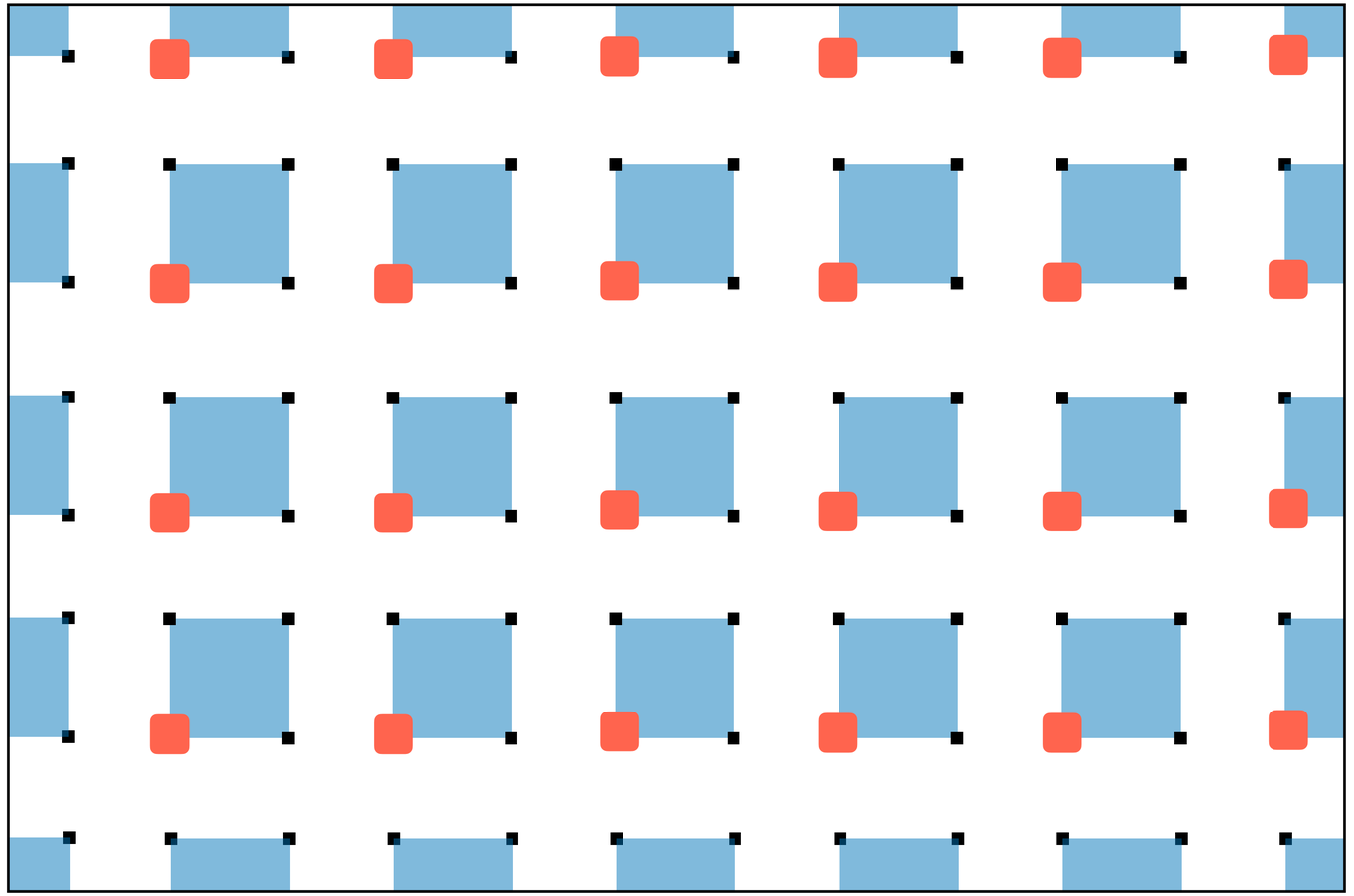
while …  … admits a nontrivial **compact** Wannier basis.

In fact, **every unobstructed** atomic insulator is **compact**.

So is every **obstructed** atomic insulator in **1D**. But not in **D≥2**!

A 2D obstructed atomic insulator

Consider the lattice



unit cell:

s orbital

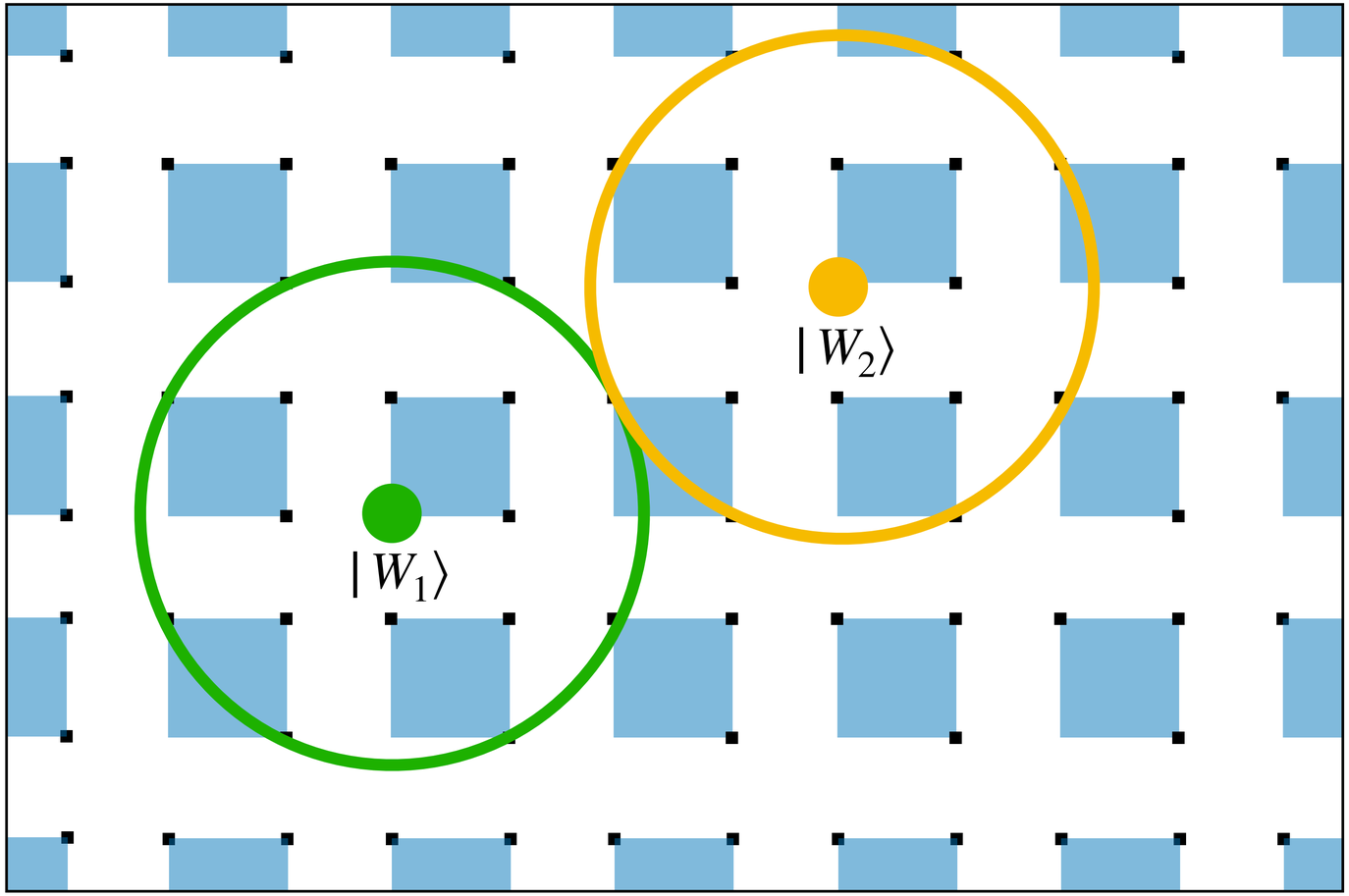
s orbital

s orbital

We want to build an insulator out of obstructed

s electrons.

Non-Compactness



finite-range assumption:

$$\langle W_1 | \blacksquare \rangle \neq 0$$

inversion symmetry:

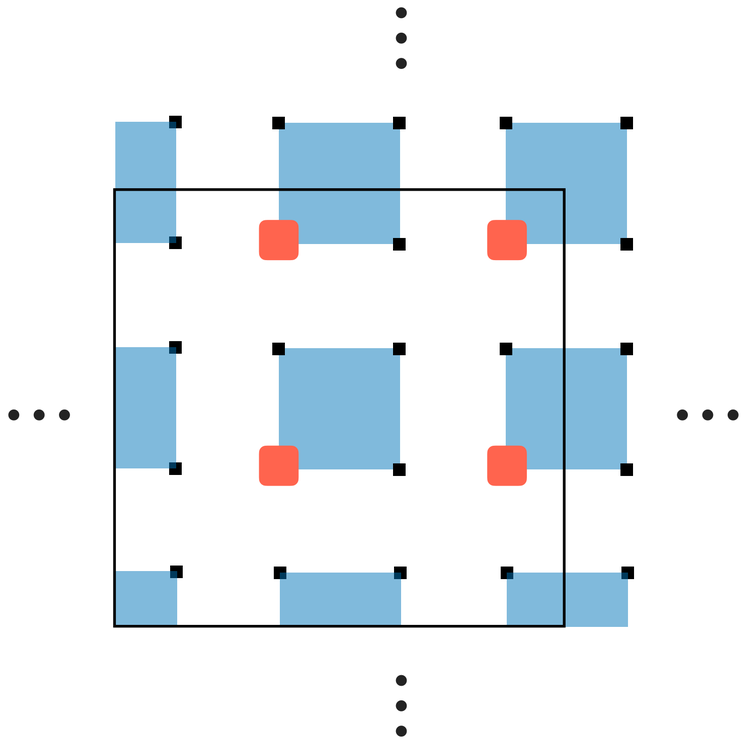
$$\langle W_2 | \blacksquare \rangle = \langle W_2 | \mathscr{I}^\dagger \mathscr{I} | \blacksquare \rangle = \langle W_1 | \blacksquare \rangle \neq 0$$

$$\langle W_1 | W_2 \rangle = \langle W_1 | \blacksquare \rangle \langle \blacksquare | W_2 \rangle \neq 0$$

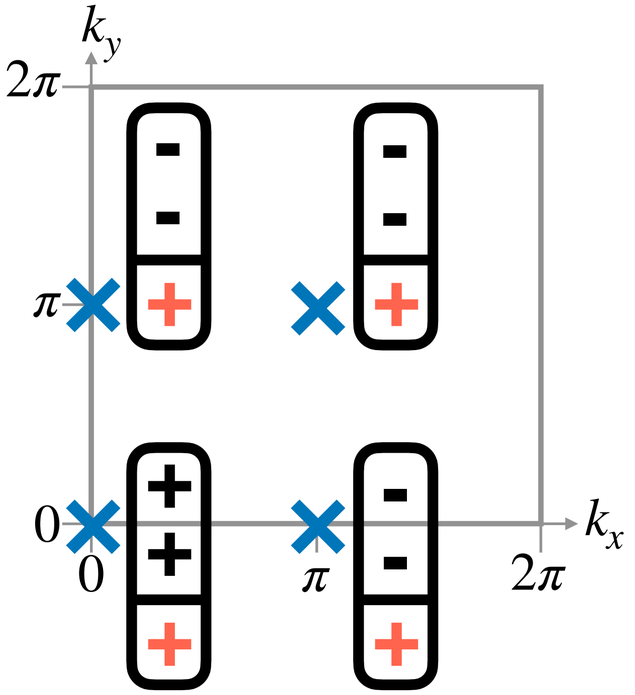
there is no finite-range, orthogonal, inversion-symmetric Wannier basis

Momentum-space picture

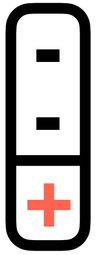
in momentum space,



turns into

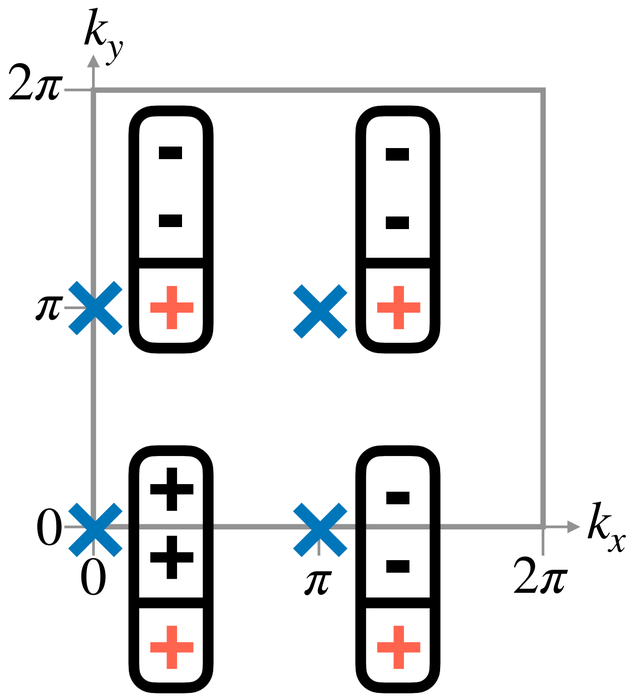


×: inversion-symmetric momenta

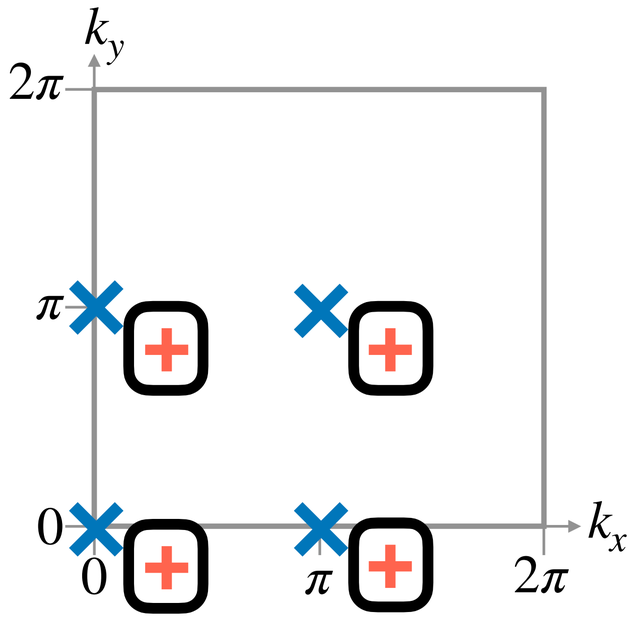
Here,  empty
occupied

are the **inversion eigenvalues** of the 3 bands.

What's universal here?

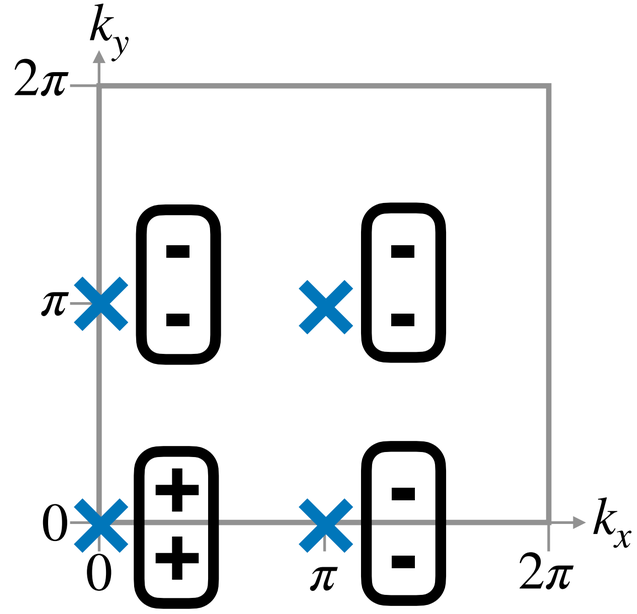


=



obstructed
atomic insulator

$\oplus$

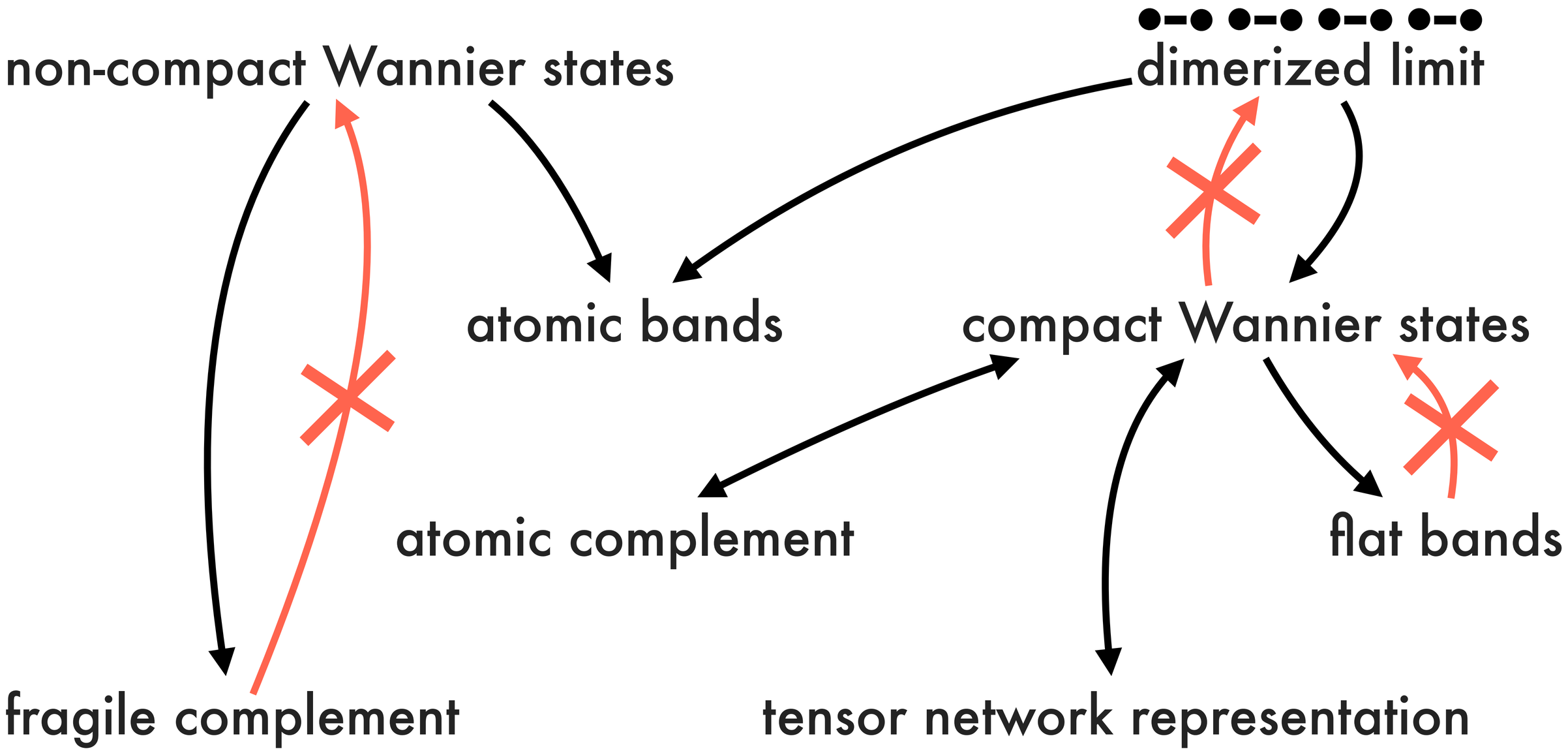


not any atomic insulator!
(fragile) topological

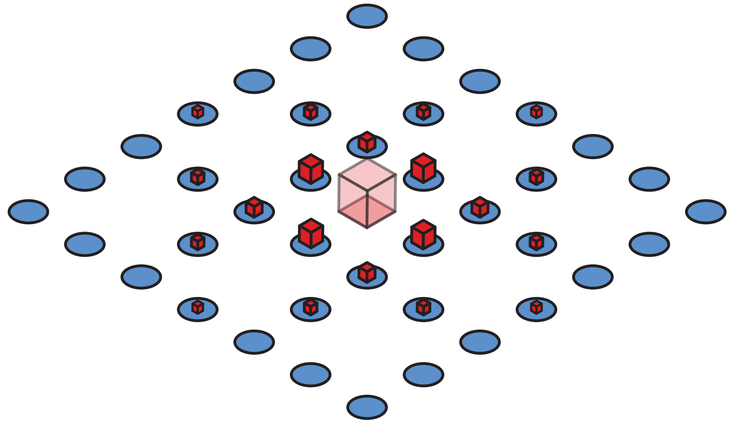
arXiv 2107.13556: general proof that the **complement** of inversion-symmetric **fragile bands** must be **non-compact**

and lots of other technical stuff…

Bird's-eye view of our paper



Why should we care about non-compactness?



1. **generalization** of the highly successful exponential/ algebraic Wannier localization dichotomy
2. guaranteed nontrivial **quantum geometry**, shows up in observables such as the superfluid weight
3. new no-go theorems about **tensor network** representability, beyond Chern #

Thank you for your attention!