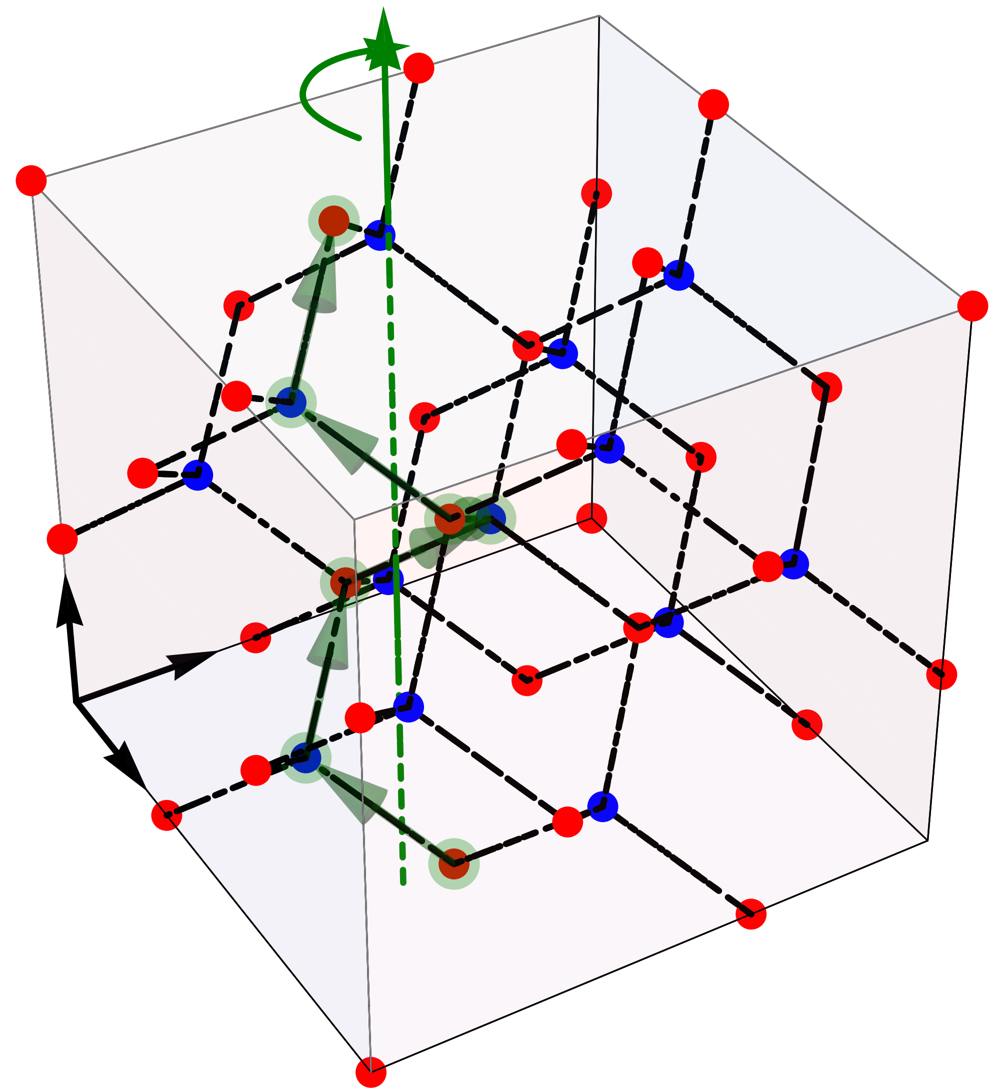
When can insulators be 'featureless'?



Sid Parameswaran
University of California, Berkeley

Frustrated Magnetism and Quantum Spin Liquids, KITP, September 20, 2012

SIMONS FOUNDATION

Collaborators

Ashvin Vishwanath

UC Berkeley

Ari Turner

UC Berkeley→Amsterdam

Dan Arovas

UC San Diego

Itamar Kimchi

UC Berkeley → KITP Grad Fellow
→ UC Berkeley (we hope!)

Dan Stamper-Kurn

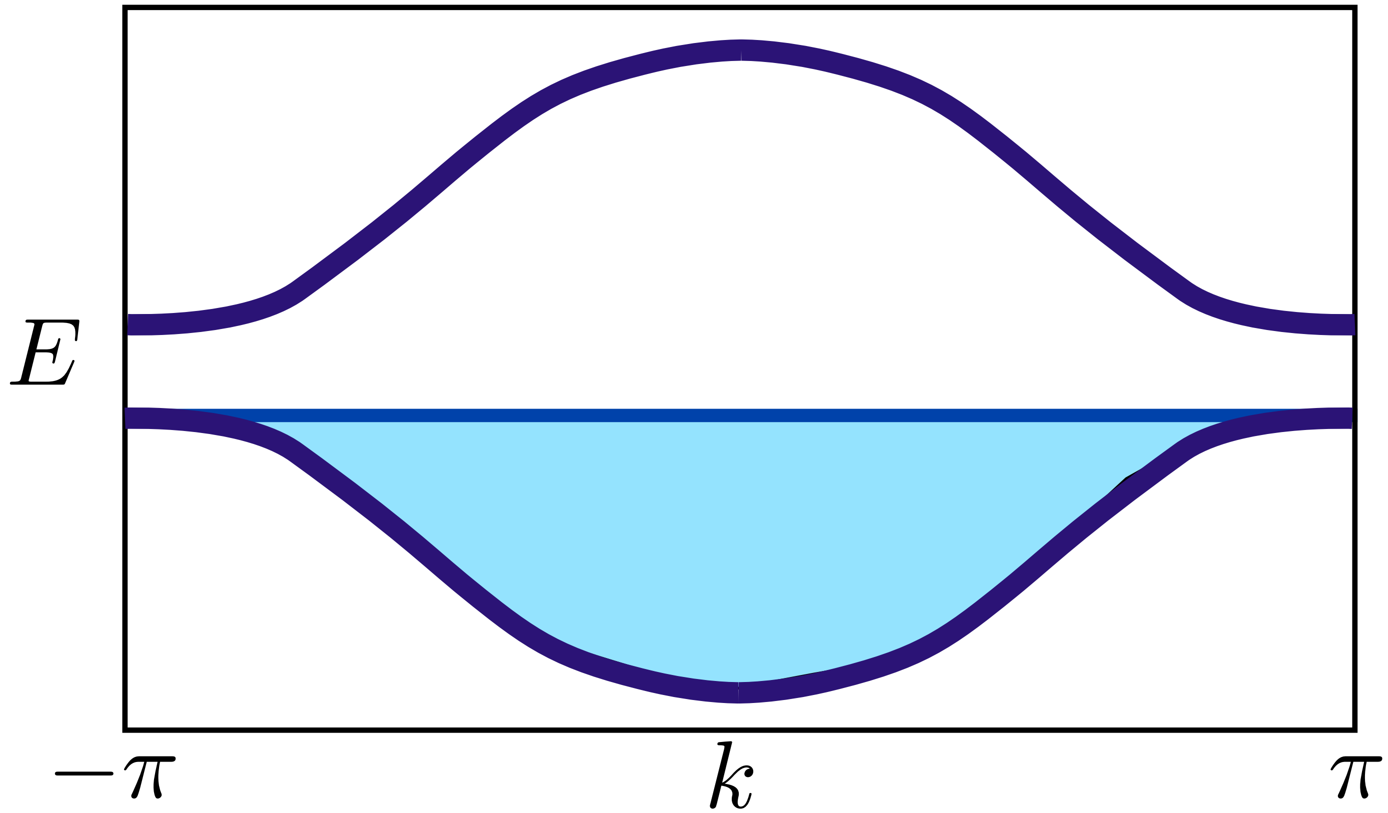
UC Berkeley

Featureless Insulators

The Invisible Man, HG Wells, Signet Ed.

- Gapped
- Break no symmetries
- Unique gs on torus
- No fractionalization

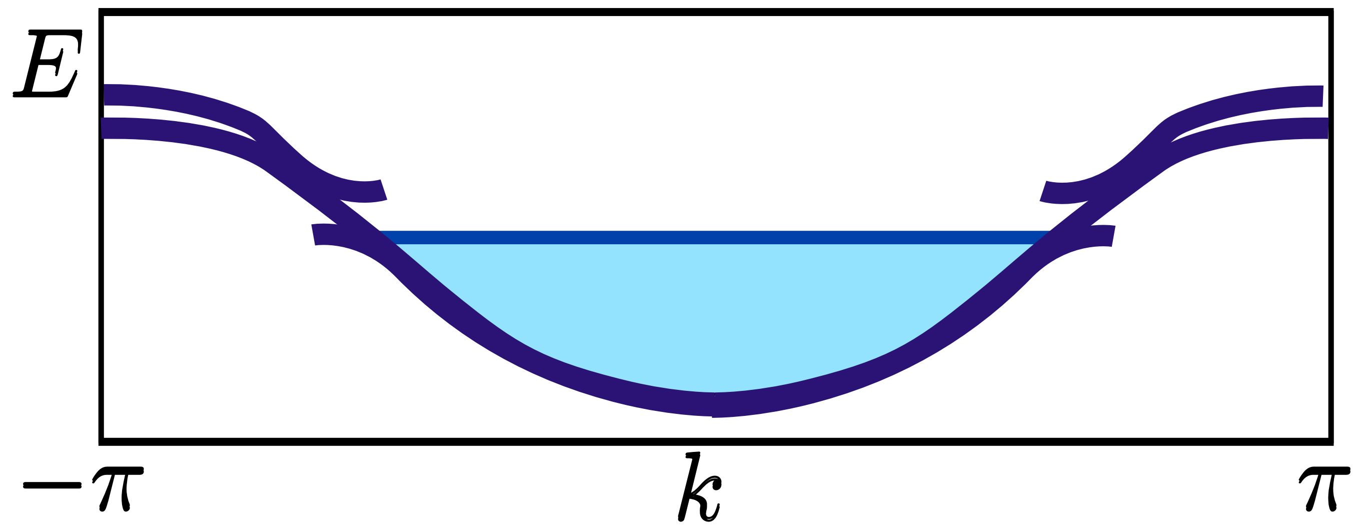
Classic example: band insulator

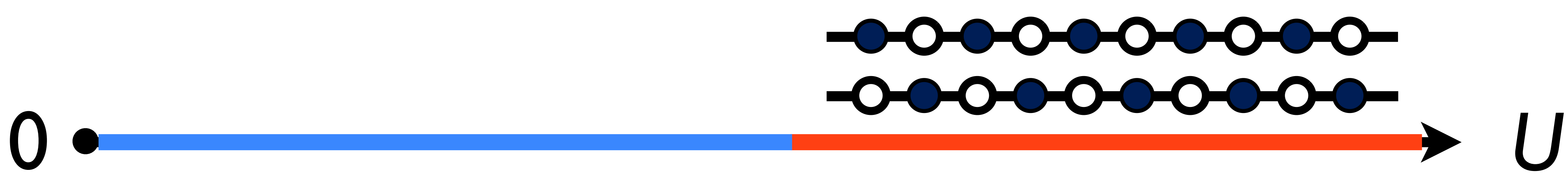


Classic counter-example: half-filled 1D spinless Hubbard model

For small U, metal is stable
To open a gap: dimerize

Luttinger liquid
+ umklapp





Featureless state is ruled out

d=1: Lieb-Schultz-Mattis Theorem

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.

Generalization: models with conserved U(1)
(e.g. particle number, S_z)

At fractional charge per unit cell, ground state is either gapless or breaks symmetry

(Featureless state is ruled out)

d>1: Hastings' Theorem

d=1, fractional filling: gaplessness vs. symmetry breaking

d>1, fractional filling: can also have 'exotic' insulator
preserves symmetry, but has GS degeneracy

Topologically ordered state

In d>1, at fractional filling of a unit cell,
insulating GS cannot be featureless

Gap + no S.B. ⇒ Topological order

[Hastings, PRB **69**, 104431 (2004); EPL **70,** 824 (2005)]

Son of Man, Rene Magritte

What is it good for?

At fractional unit cell filling:

Gap + No Symmetry Breaking ⇒ Topological Order!

absence of symmetry breaking is *sufficient* condition

SCIENCE VOL 332 3 JUNE 2011 1173

Spin-Liquid Ground State of the $S = 1/2$ Kagome Heisenberg Antiferromagnet

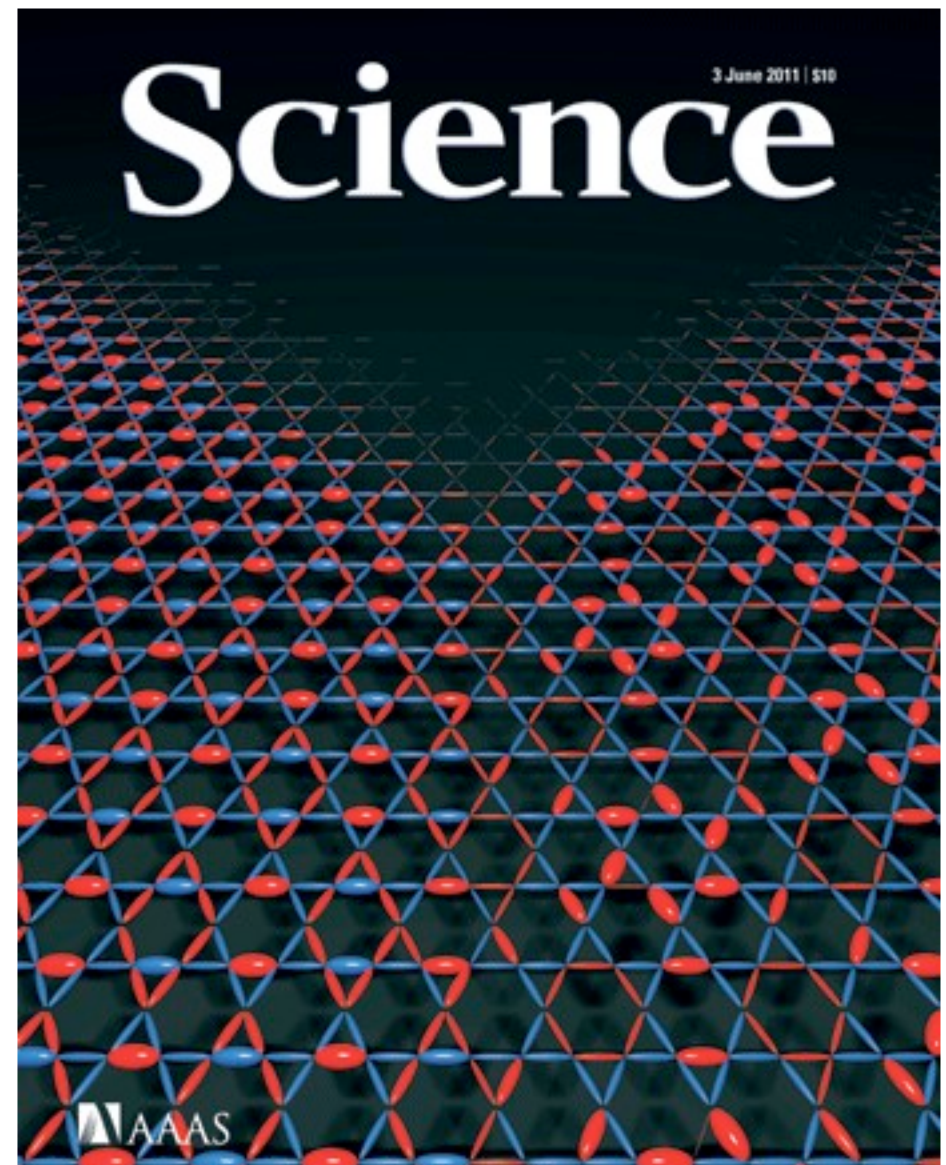
Simeng Yan,[1] David A. Huse,[2,3] Steven R. White[1]*

half-integer unit cell filling

no symmetry breaking

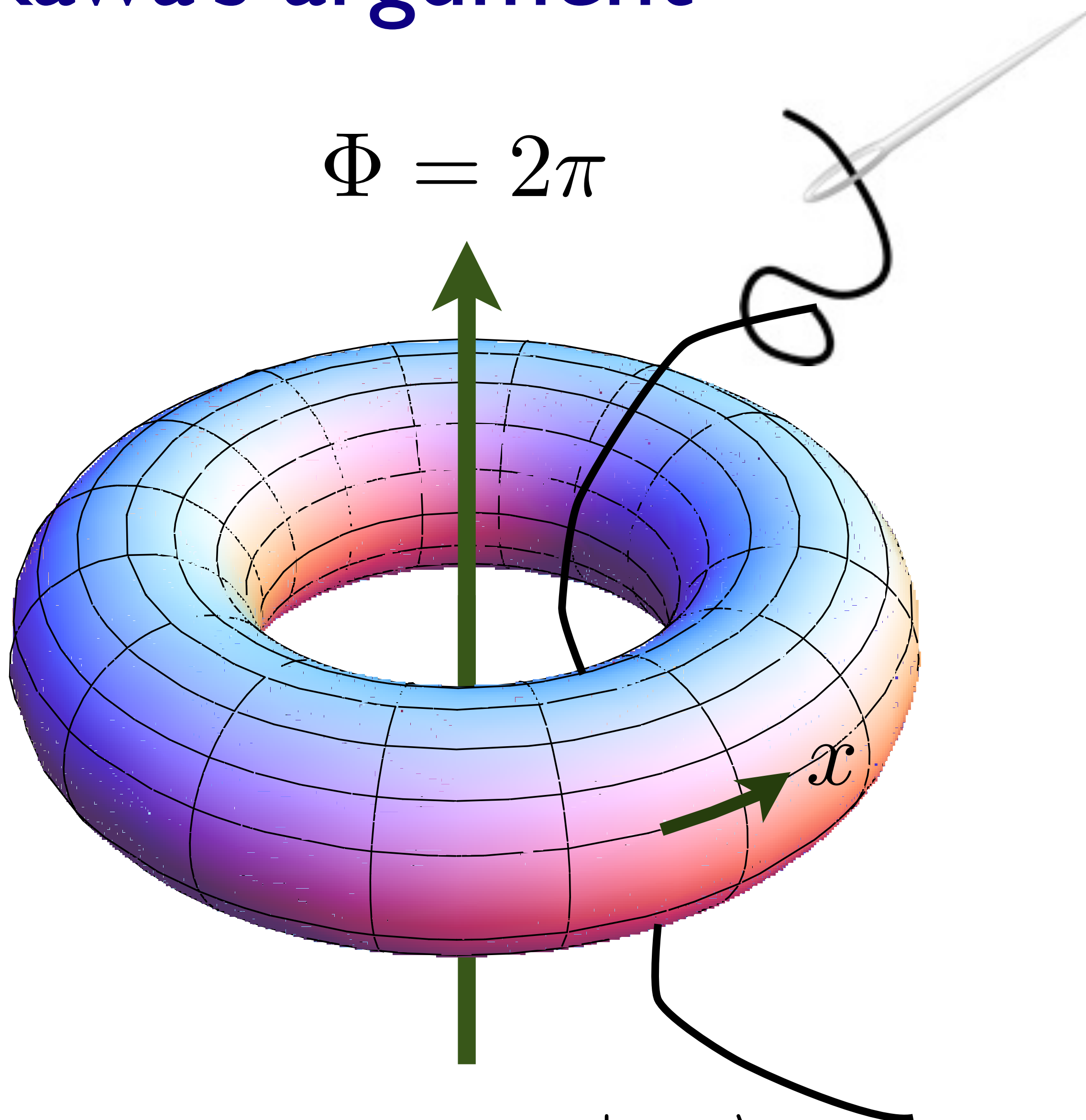
spin liquid

[smoking gun: entanglement entropy
Jiang, Wang, Balents, arXiv 1205.4289]



Flux threading & Oshikawa's argument

1. Thread 2π flux through 'handle'



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

spectrum returns to itself

2. Gauge away inserted flux

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

$|\Psi_0'\rangle \longrightarrow \hat{U}|\Psi_0'\rangle$ Energy very close* to $|\Psi_0\rangle$

At filling p/q : flux removal doesn't commute with translation

$$\hat{U}^{-1}\hat{T}_x\hat{U} = \hat{T}_x e^{i2\pi\frac{V}{L}\frac{p}{q}}$$

Insulating ground state always degenerate.

(*not quite rigorous, but intuition similar to Hastings')

[Oshikawa, PRL **84**, 1535 (2000)]

Translations constrain possibilities at fractional unit cell filling.

What (if anything) constrains possibilities at <u>integer</u> unit cell filling?

An example:

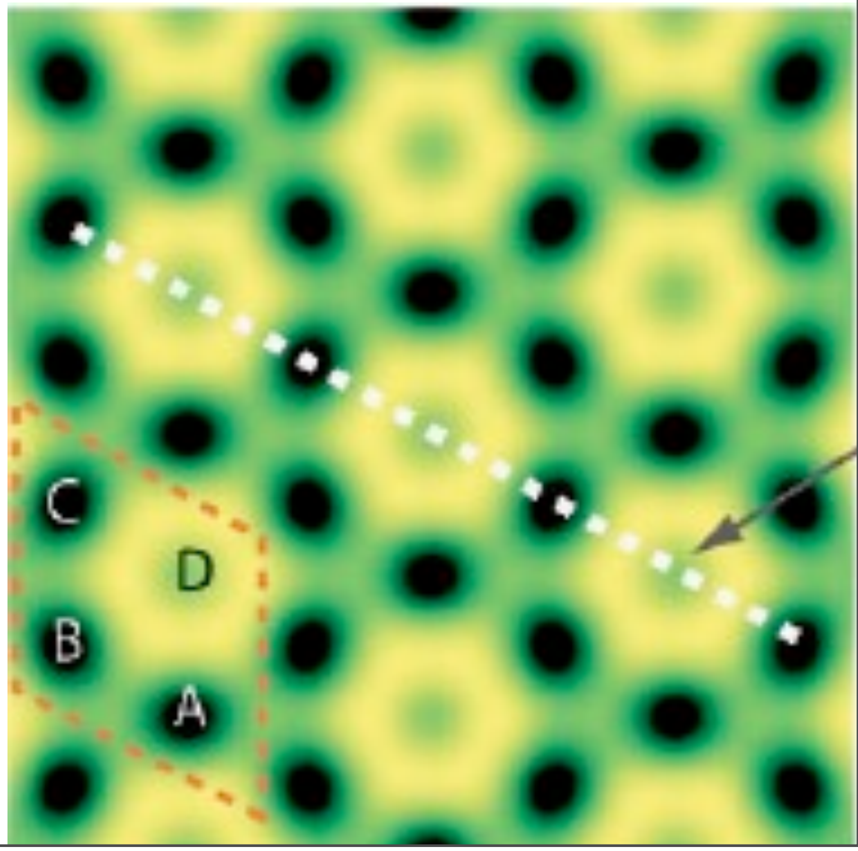
Bosonic Mott insulators on non-Bravais lattices,
integer unit cell filling but fractional site filling;

(also related magnetization plateaus for XXZ models)

PRL 108, 045305 (2012) PHYSICAL REVIEW LETTERS week ending 27 JANUARY 2012

Ultracold Atoms in a Tunable Optical Kagome Lattice

Gyu-Boong Jo,[1] Jennie Guzman,[1] Claire K. Thomas,[1] Pavan Hosur,[1] Ashvin Vishwanath,[1,2] and Dan M. Stamper-Kurn[1,2]
[1]*Department of Physics, University of California, Berkeley California 94720, USA*
[2]*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*



NATURE | Vol 464 | 8 April 2010

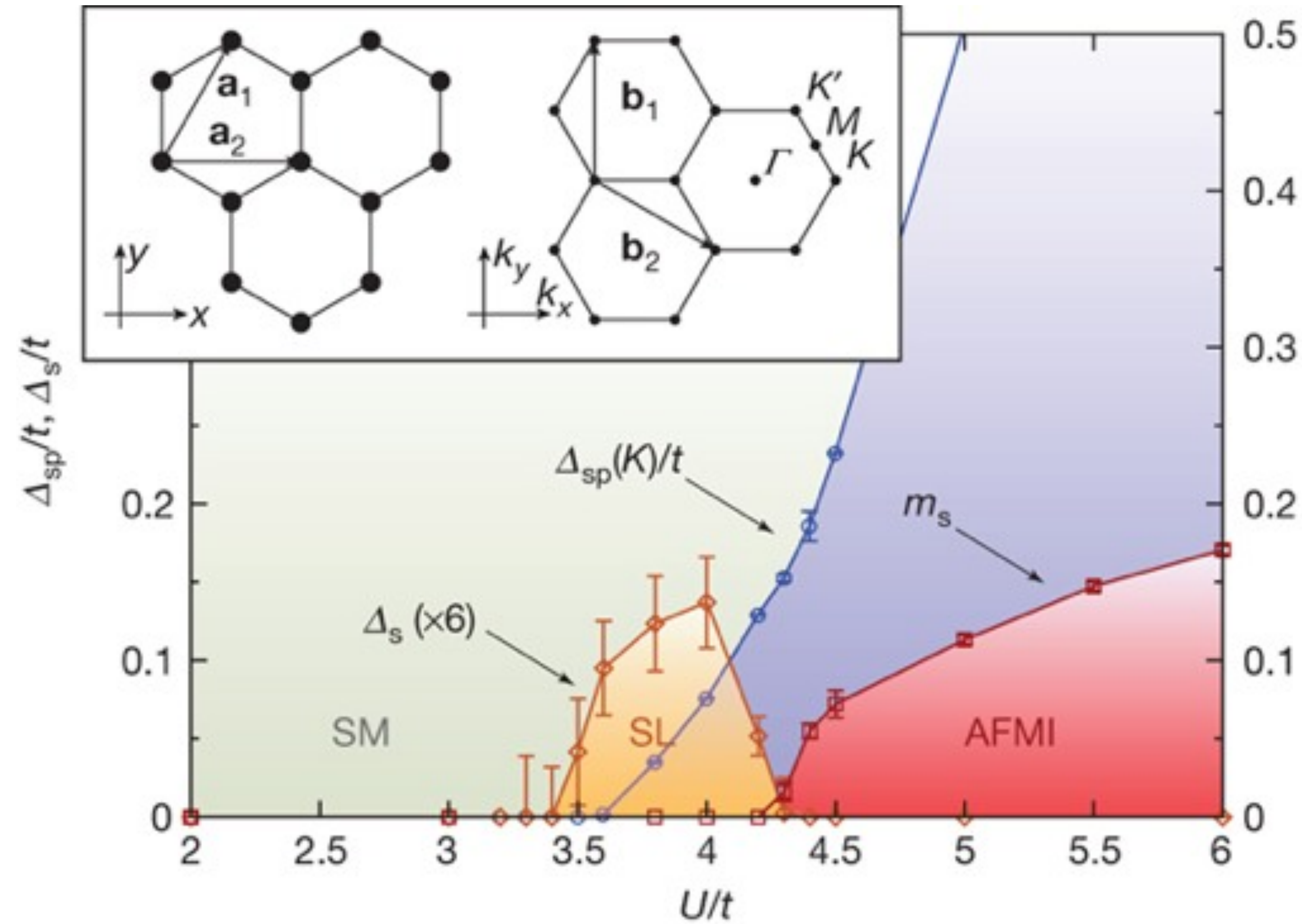
Quantum spin liquid emerging in two-dimensional correlated Dirac fermions

Z. Y. Meng[1], T. C. Lang[2], S. Wessel[1], F. F. Assaad[2] & A. Muramatsu[1]

integer unit cell filling

no symmetry breaking

is it a spin liquid?



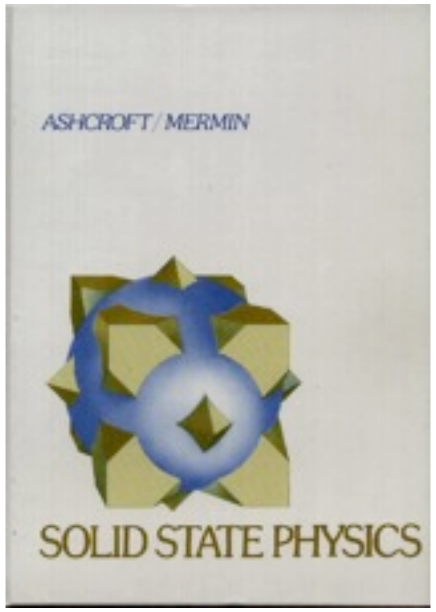
Often no obvious featureless wavefn. Is there a general principle?

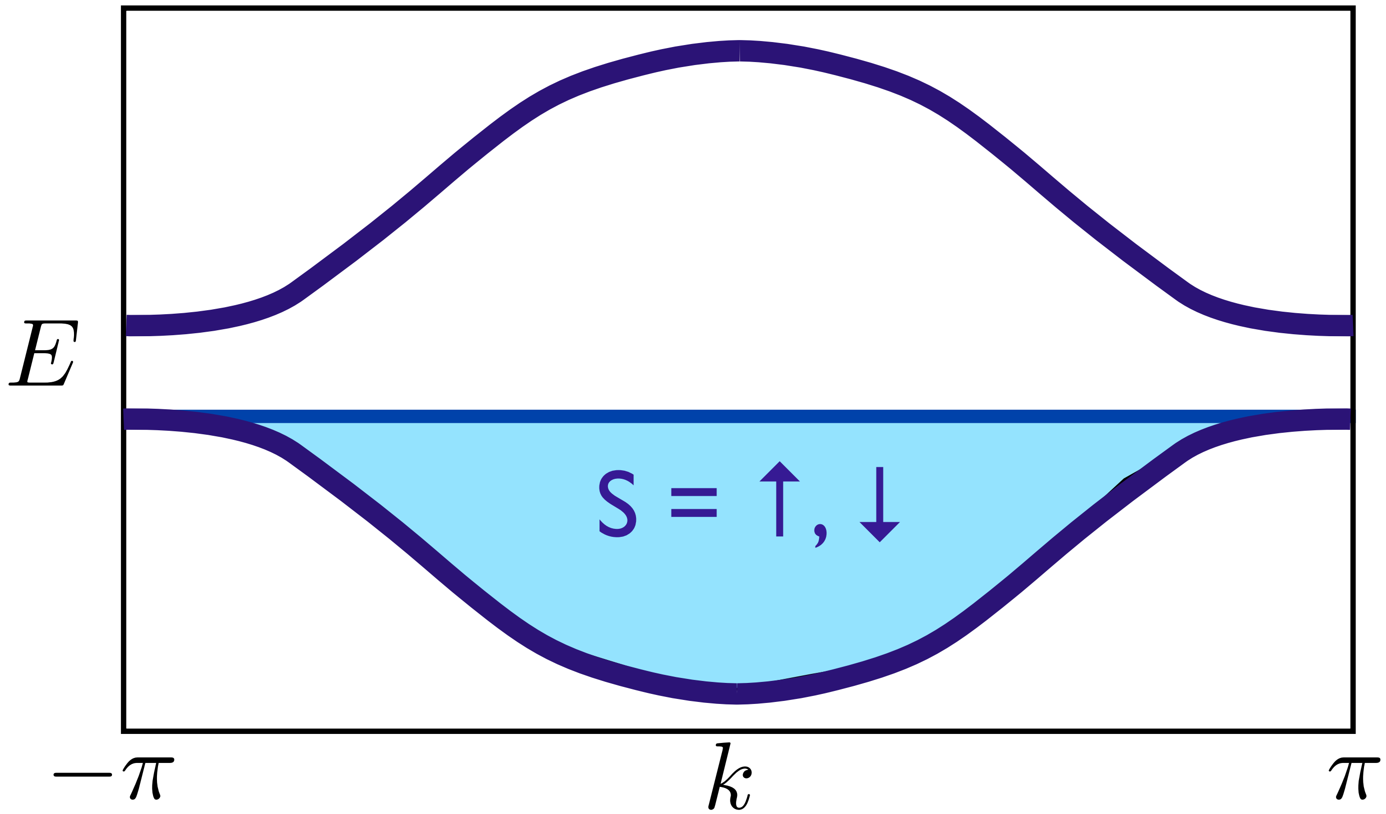
What is the non-interacting intuition?

for a moment: spinful electrons

Some textbook band theory

even # of electrons per unit cell
necessary condition for band insulator



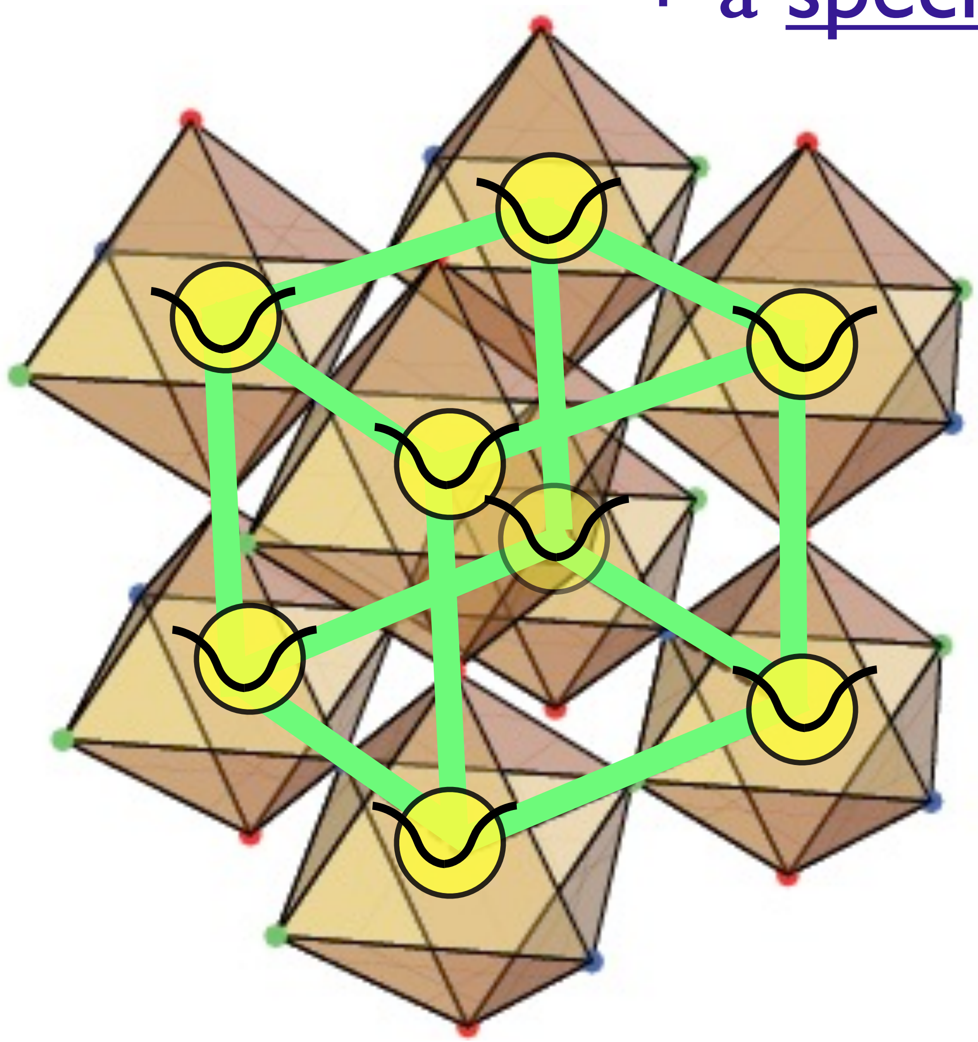


What is the non-interacting intuition?

Non-Textbook Challenge

given an even number of electrons per unit cell

+ a specified crystal (no spin-orbit)



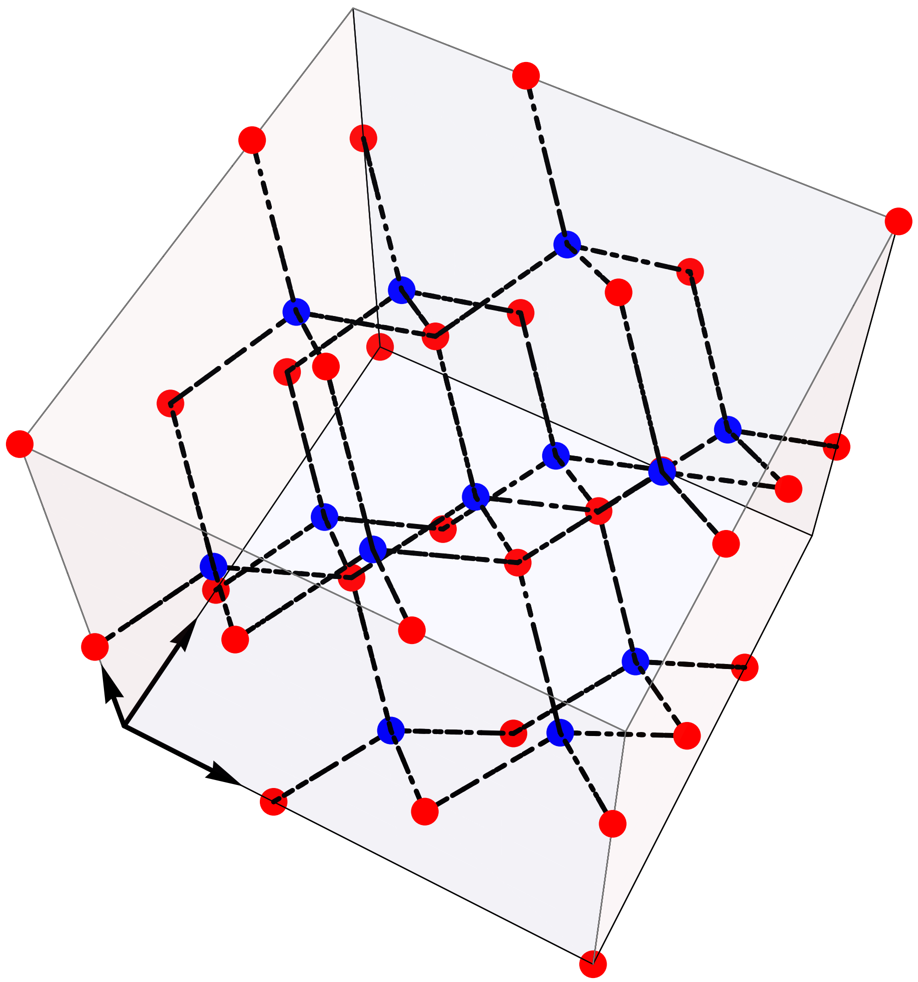
- add sites
- change hopping
- tune onsite terms

(preserve crystal symmetry
+ time reversal)

Can you always find a band insulator?

No!

even number of electrons per unit cell
not always sufficient



eg. diamond lattice

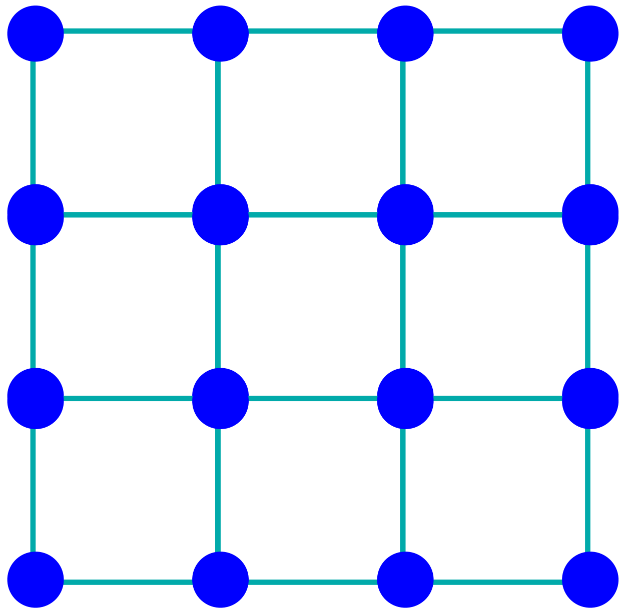
band insulators <u>only</u>
when filling is a multiple of 4

for each crystal, can associate integer S (often>1)

Band insulator only if filling = multiple of 2S

How do we build a Featureless Mott insulator?

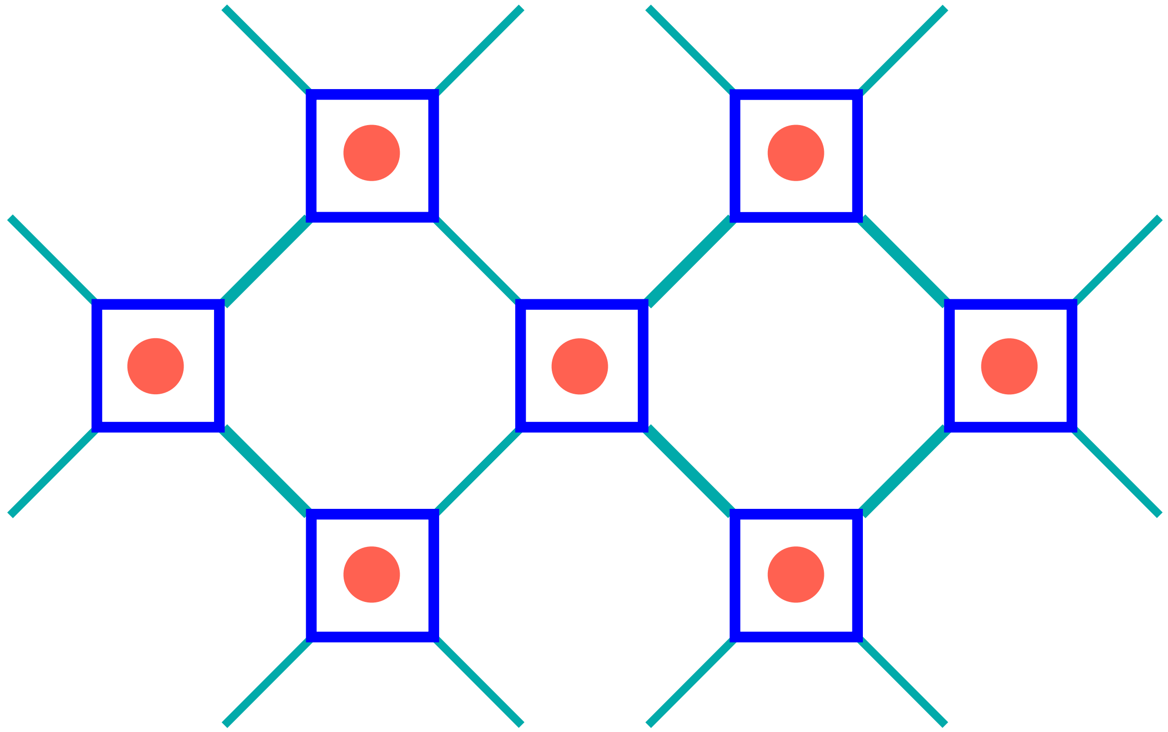
1 boson per unit cell



classical particles,
fixed number/site

How do we build a Featureless Mott insulator?

1 boson per unit cell



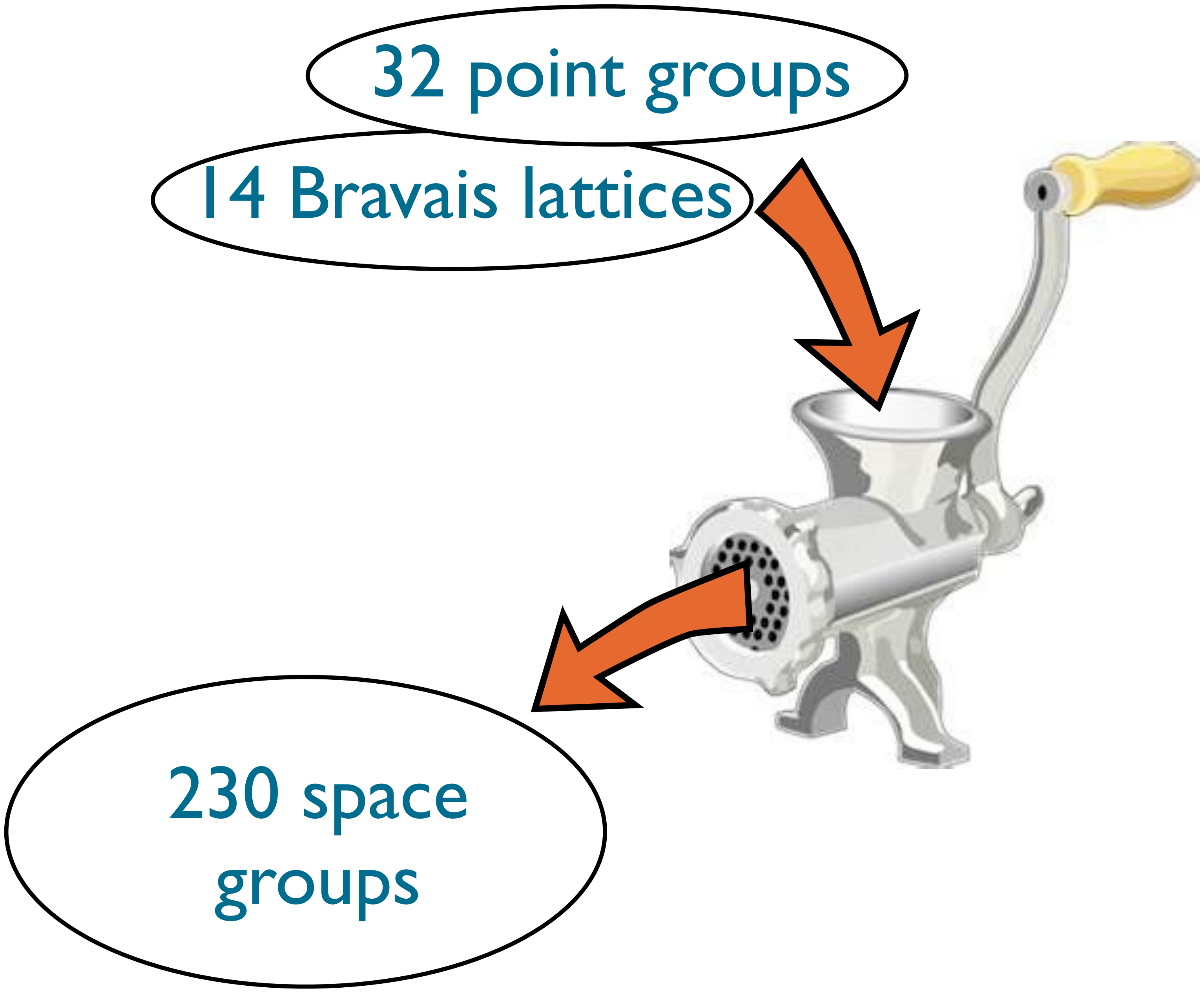
'molecular orbitals'

Intuition: 'center of charge' at high-symmetry point

Are there lattices where unit cell has no points with full symmetry?

We need some 19th century physics!

Crystallography in 60 seconds



Fyodorov, Schönflies, Barlow

if there is a point with full PG symmetry: symmorphic 73

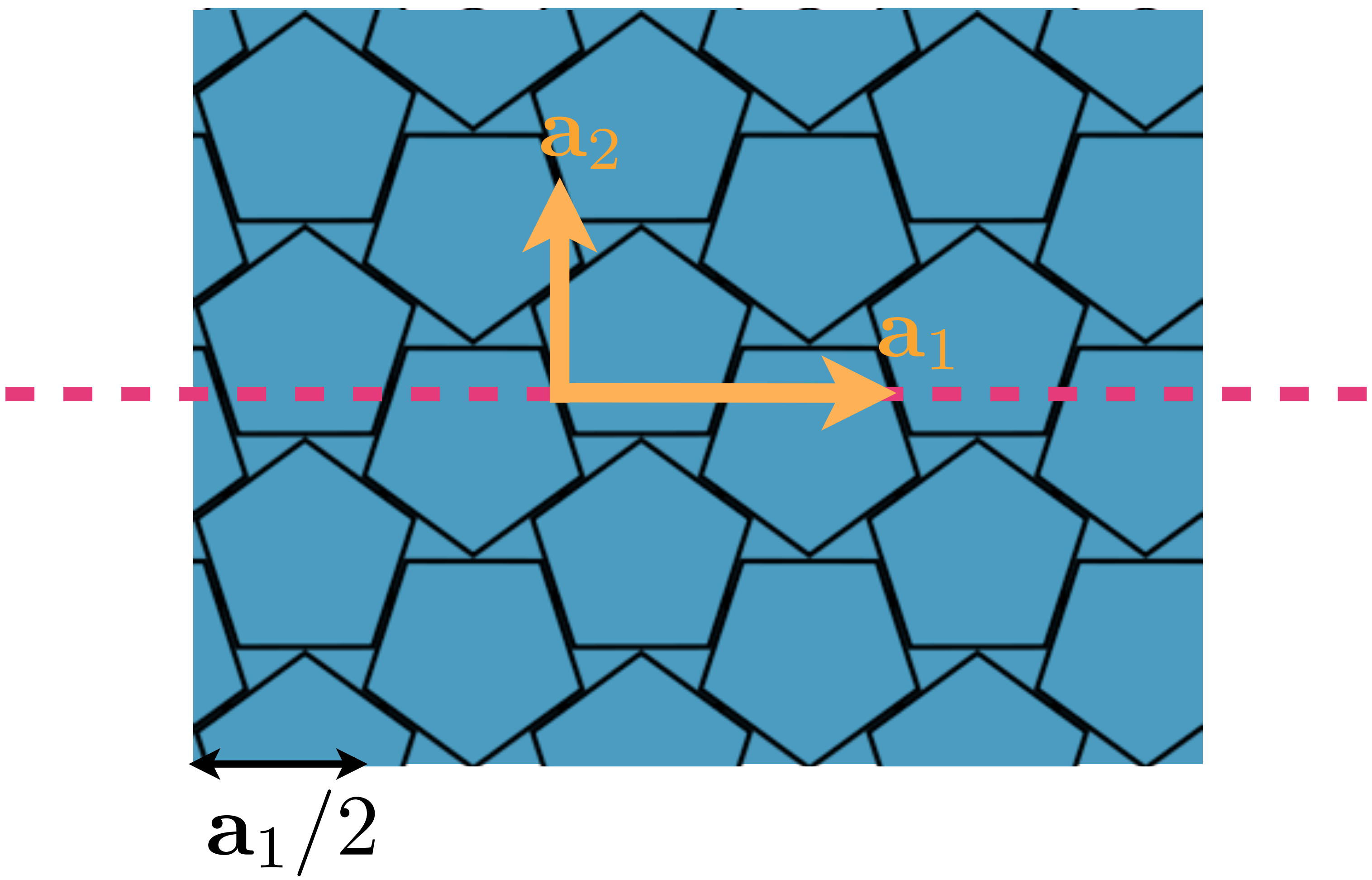
if not: non-symmorphic 157

Suggests we look at nonsymmorphic crystals more closely

Nonsymmorphic Symmetries

Point-group operations accompanied by non-lattice translations

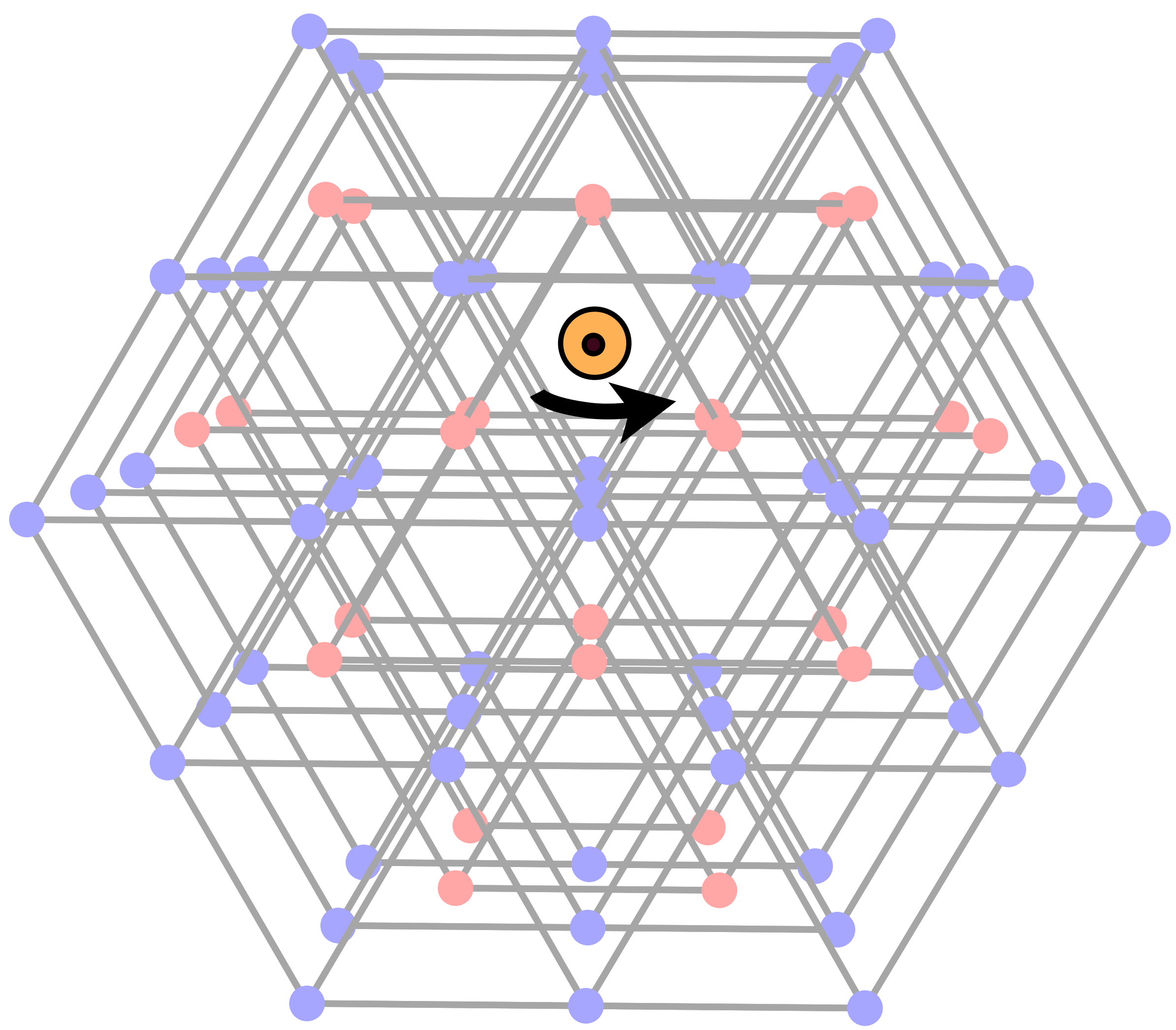
2D: glide mirrors

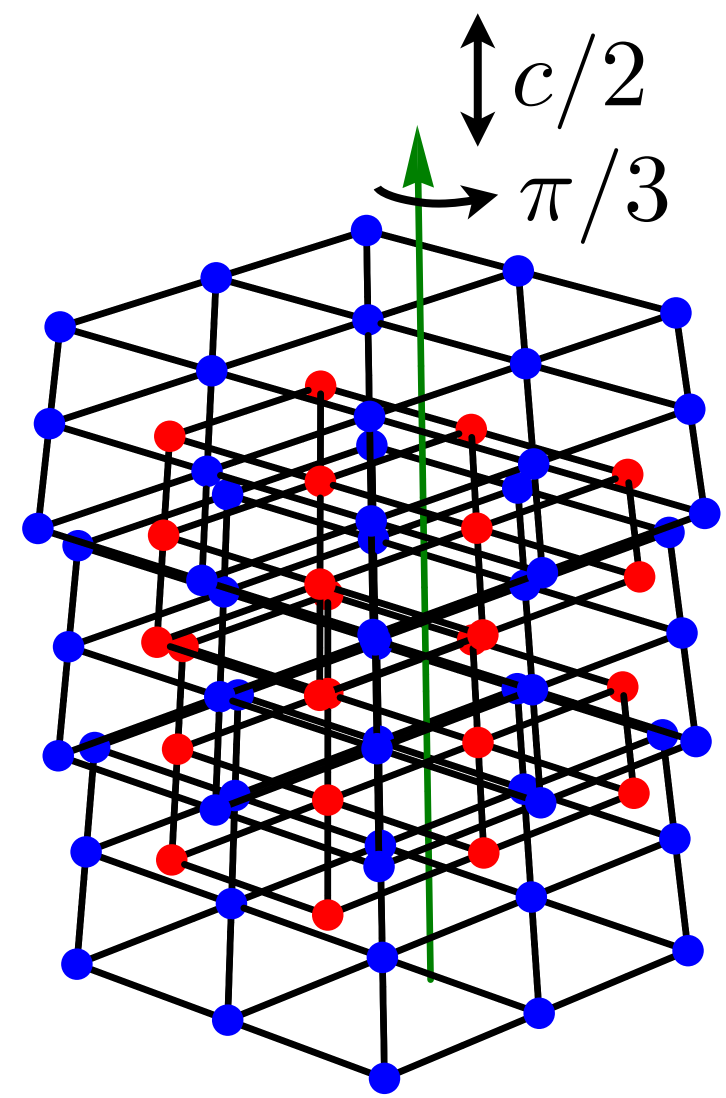


Nonsymmorphic Symmetries

Point-group operations accompanied by <u>non-lattice</u> translations

3D: screw rotations



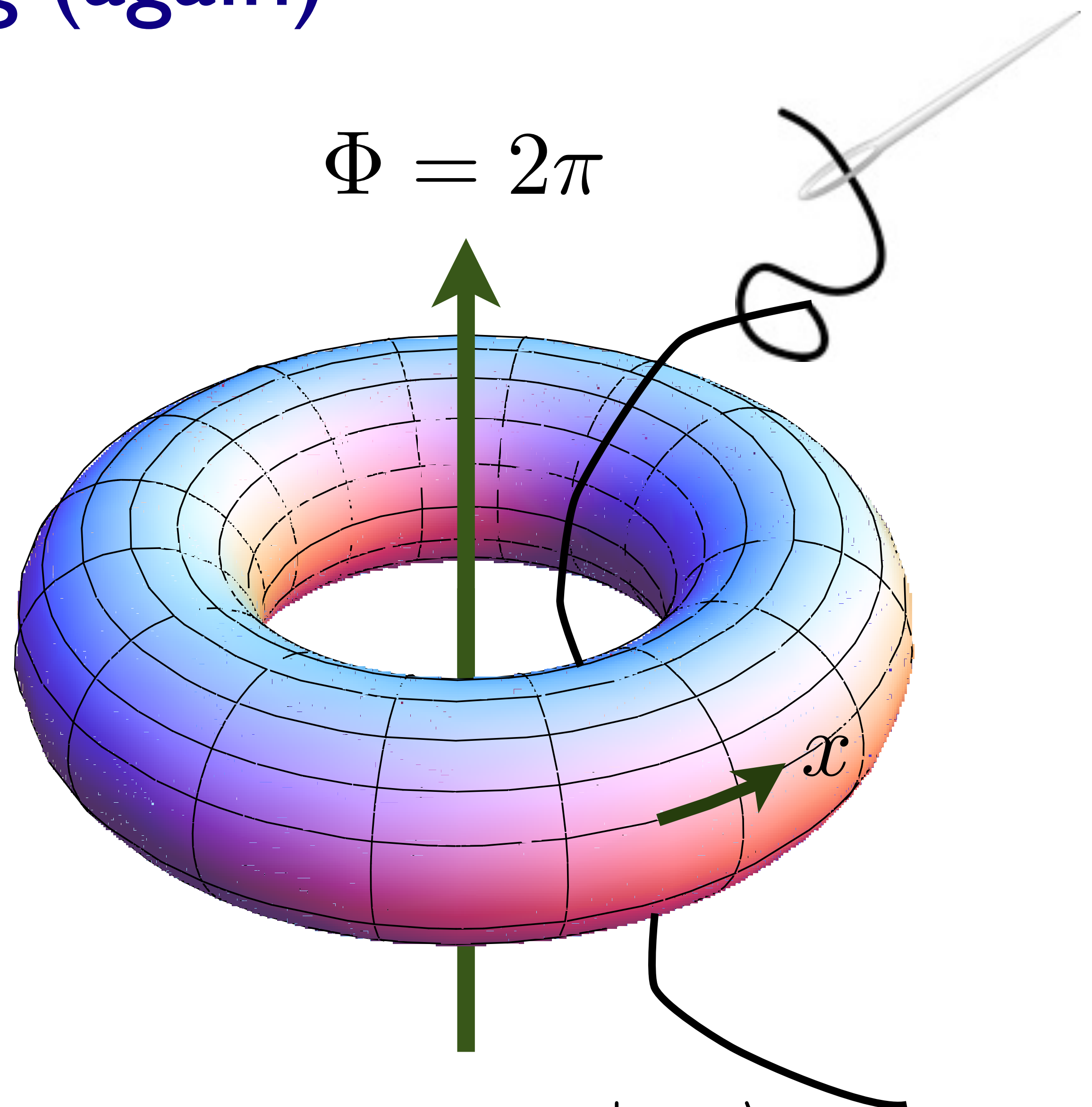


Flux threading (again)

1. Thread 2π flux through 'handle'

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

spectrum returns to itself



2. Gauge away inserted flux

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

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

Energy very close* to $|\Psi_0\rangle$

At filling 1: flux removal doesn't commute with nonsymm. op.

$$\hat{U}\hat{G}\hat{U}^{-1} = \hat{G}e^{2\pi i \frac{r}{s} L^2}$$

Insulating ground state always degenerate.

(*not quite rigorous, but intuition similar to Hastings') [SP, Turner, Arovas, Vishwanath, in progress]

Nonsymmorphic Rank

[SP, Turner, Arovas, Vishwanath, in progress]

Take a glide or screw, G

Keep acting with it until it becomes removable.

$$\hat{G}^{\mathcal{S}_G} = \{\text{lattice translation}\} \times \{\text{ PG operation}\}$$

$\mathcal{S}_G$ = nonsymmorphic rank of g

(can obtain using simple geometry)

Nonsymmorphic rank of space group, $\mathcal{S}$ = l.c.m.($\mathcal{S}_G$) for all G

What (if anything) constrains possibilities at <u>integer</u> unit cell filling?

A: Featureless insulators ruled out unless filling is multiple of $\mathcal{S}$

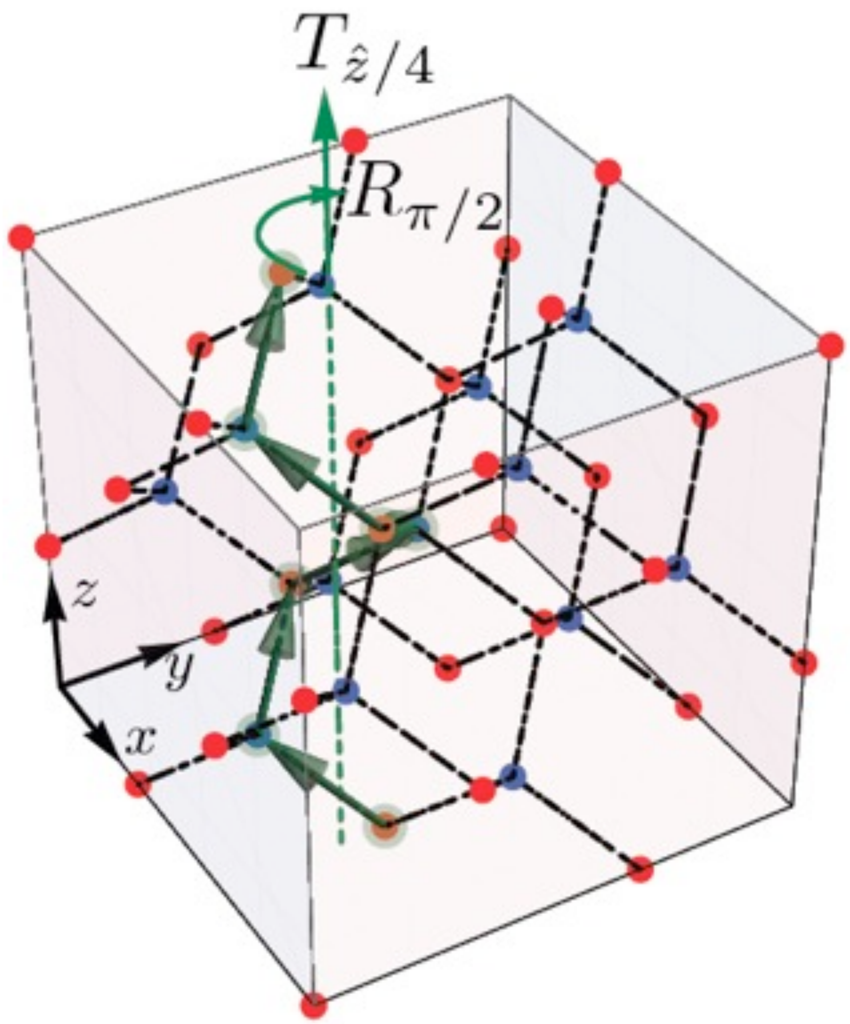
What is the non-interacting intuition?

Band insulators are featureless

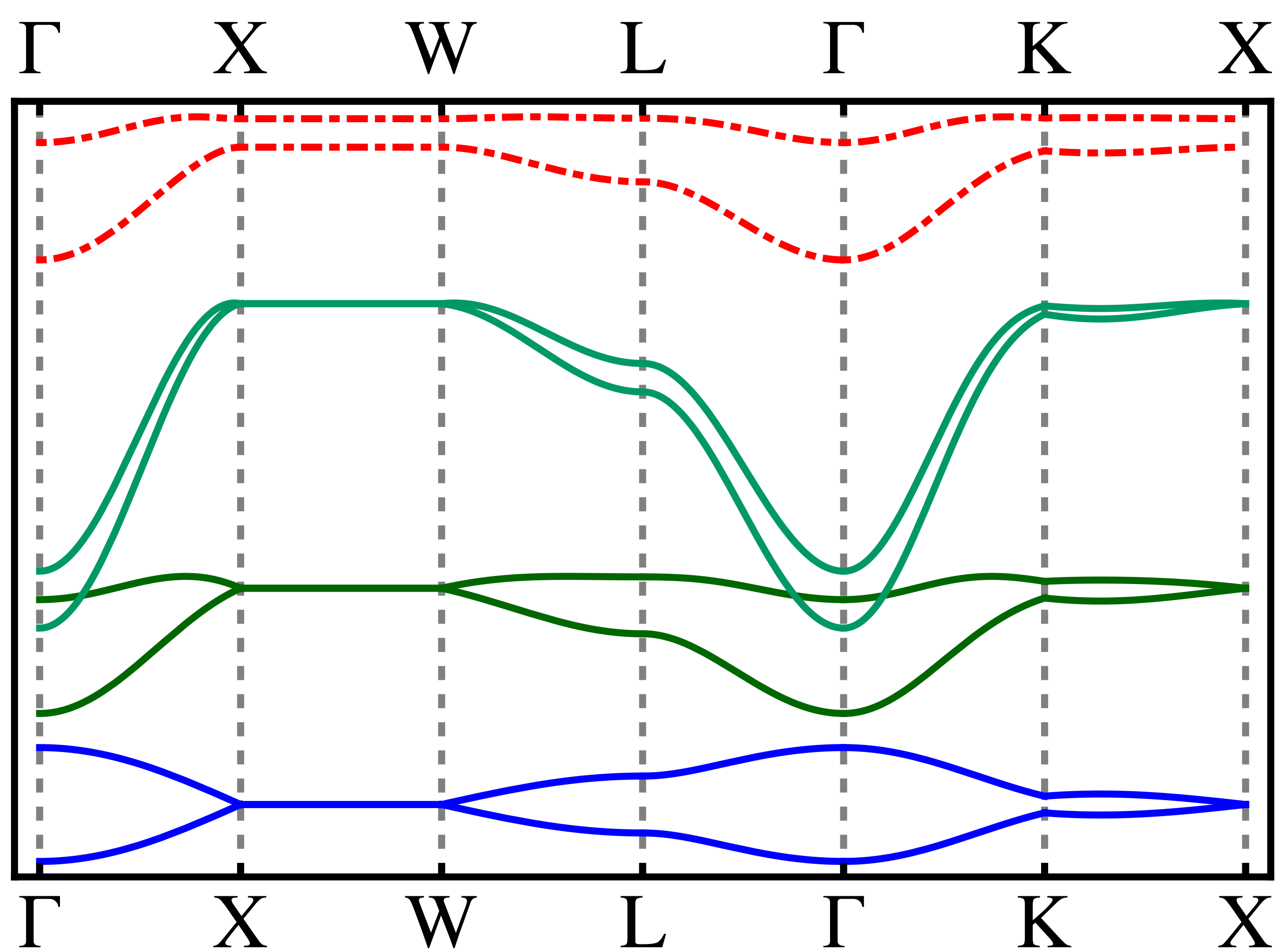
In nonsymmorphic crystals: forbidden except at special fillings

Bands 'stick together' in multiples of $\mathcal{S}$

e.g. diamond lattice $\mathcal{S} = 2$



[SP, Turner, Arovas, Vishwanath, in progress]



[Hints in band theory literature: Herring; König & Mermin; Michel & Zak...]

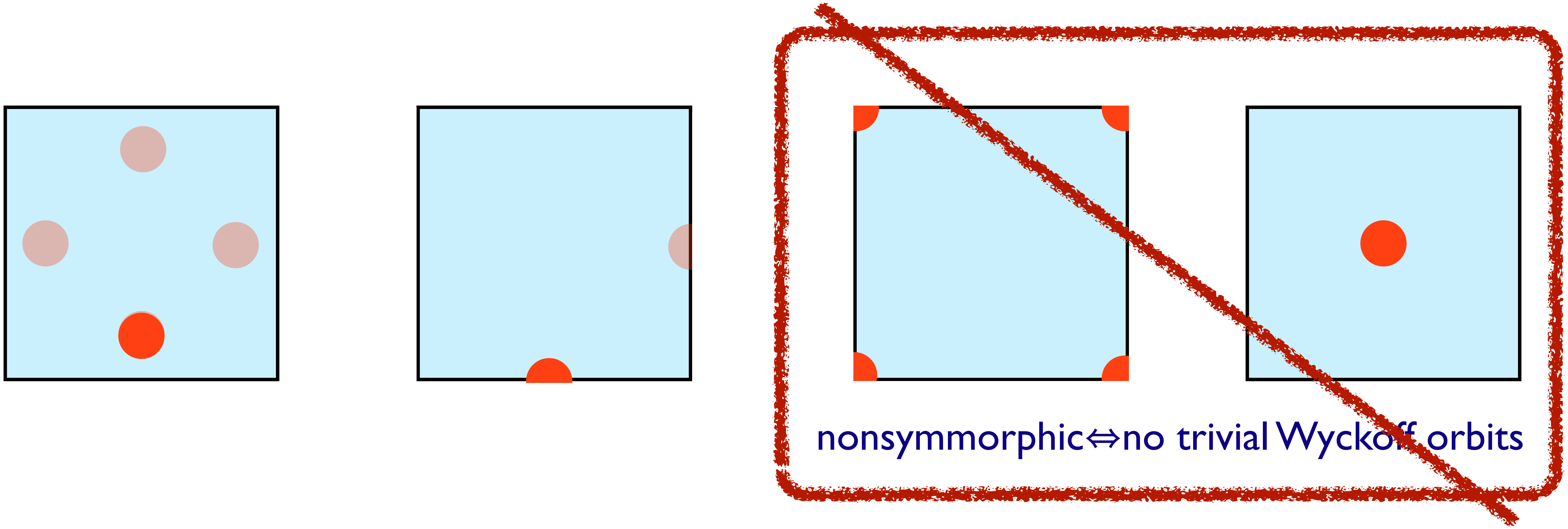
Crystallographic ('Wyckoff') Orbits

pick a point, act with PG (modulo lattice translations)

eventually 'orbit' will close

size of orbit can't be bigger than order of group

but can be smaller



$$\frac{\text{size of smallest orbit}}{\text{nonsymmorphic rank}} = \text{integer}$$ (1 in most cases)

Hard to construct featureless states. Is there a general principle?

(for simplicity: bosons + assume S = size of smallest orbit)

$\mathcal{S}$ bosons per unit cell

one boson on each position in the minimal Wyckoff orbit

What if tight-binding lattice does not have sites there?

symmetrically delocalize onto nearby sites

individual bosonic orbitals may now overlap

need to calculate correlations

overlap expansion of wavefunction

$\Rightarrow$ classical loop model on Bravais lattice

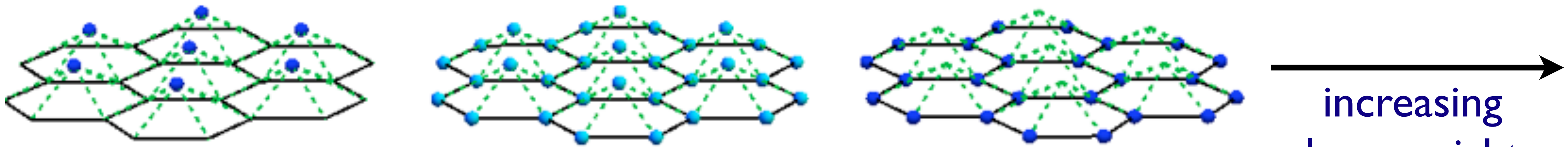
Can check the Wyckoff orbit size for all 230 space groups against the predicted nonsymmorphic rank (simple exercise)

SPACE GROUP NONSYMMORPHIC RANKS 9/19/12 1

ITC #	Hermann-Maguin Symbol	NS Rank	$\lvert W_c \rvert$ (size of orbit in cryst. cell)	Divisor (number of prim. cells/cryst. cell)	$\lvert W_p \rvert$ (orbit in prim. cell)
TRICLINIC					
1	P1	1	1	1	1
2	$P\bar{1}$	1	1	1	1
MONOCLINIC					
3	P2	1	1	1	1
NS 4	$P12_11$	2	2	1	2
5	C121	1	2	2	1
6	P1m1	1	1	1	1
NS 7	P1c1	2	2	1	2
8	C1m1	1	2	2	1
NS 9	C1c1	2	4	2	2
10	P12/m1	1	1	1	1
NS 11	$P12_1/m1$	2	2	1	2
12	C12/m1	1	2	2	1

Honeycomb Lattice Example

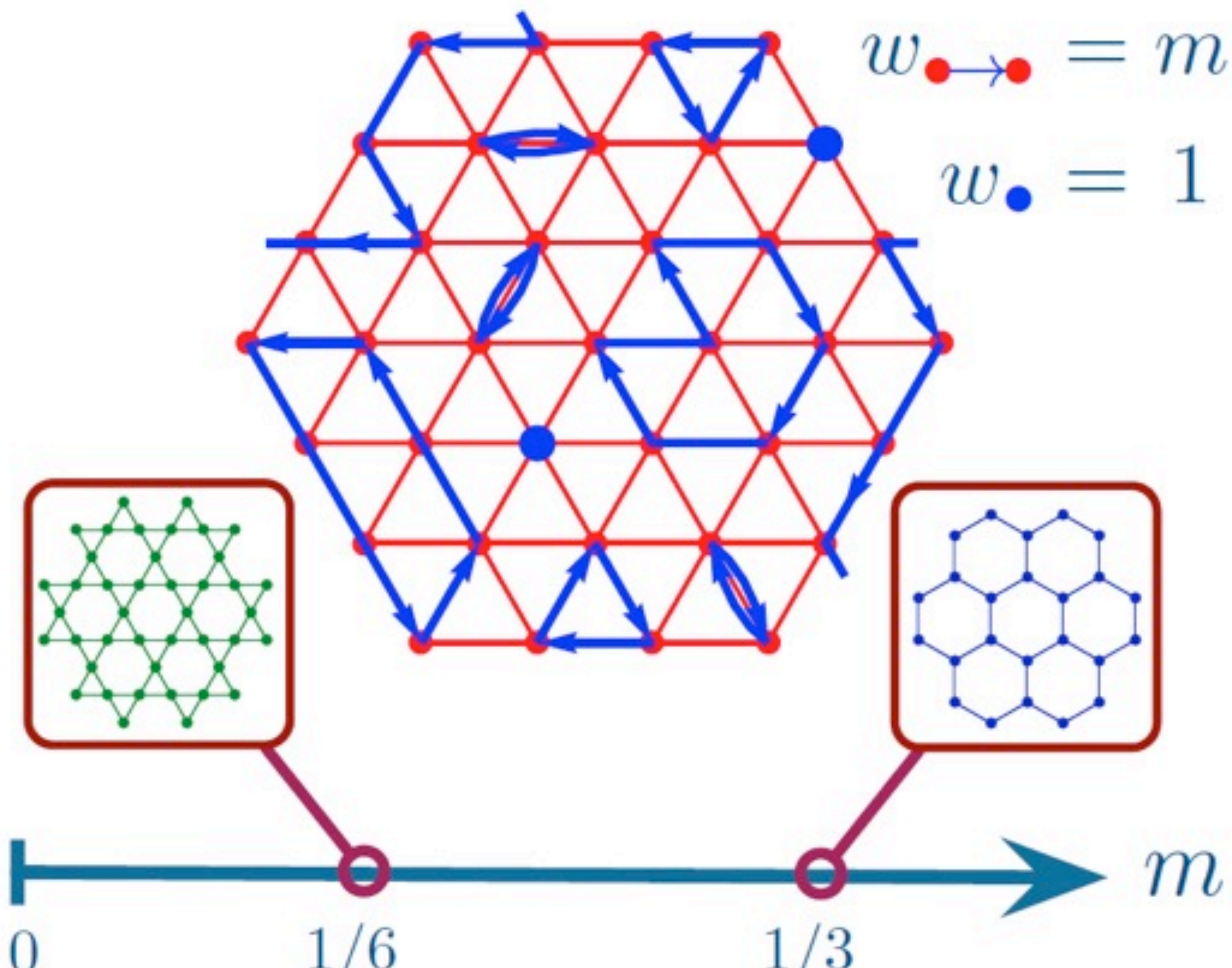
Symmorphic: 1 boson per unit cell (half-site-filling)



increasing loop weight

triangular lattice loop model

(also 1/3 site filling on kagome)

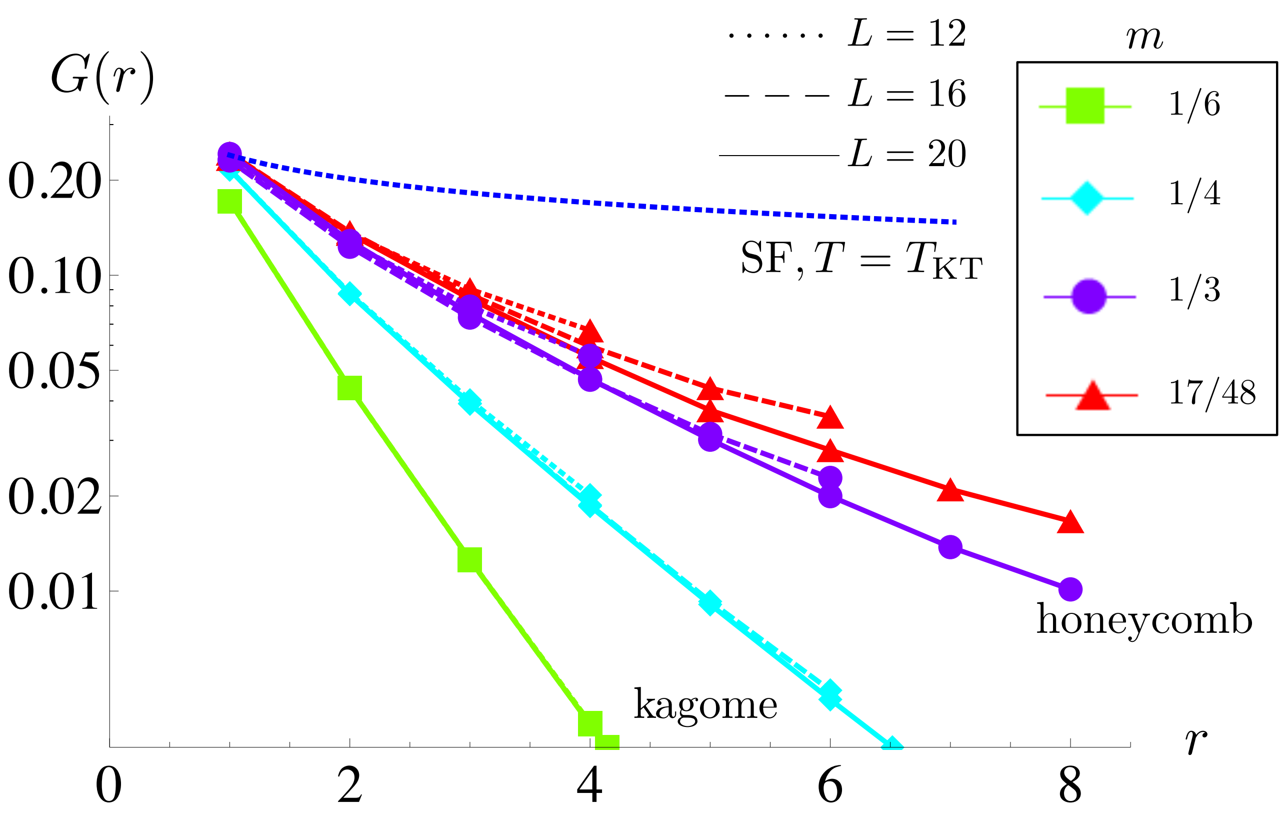


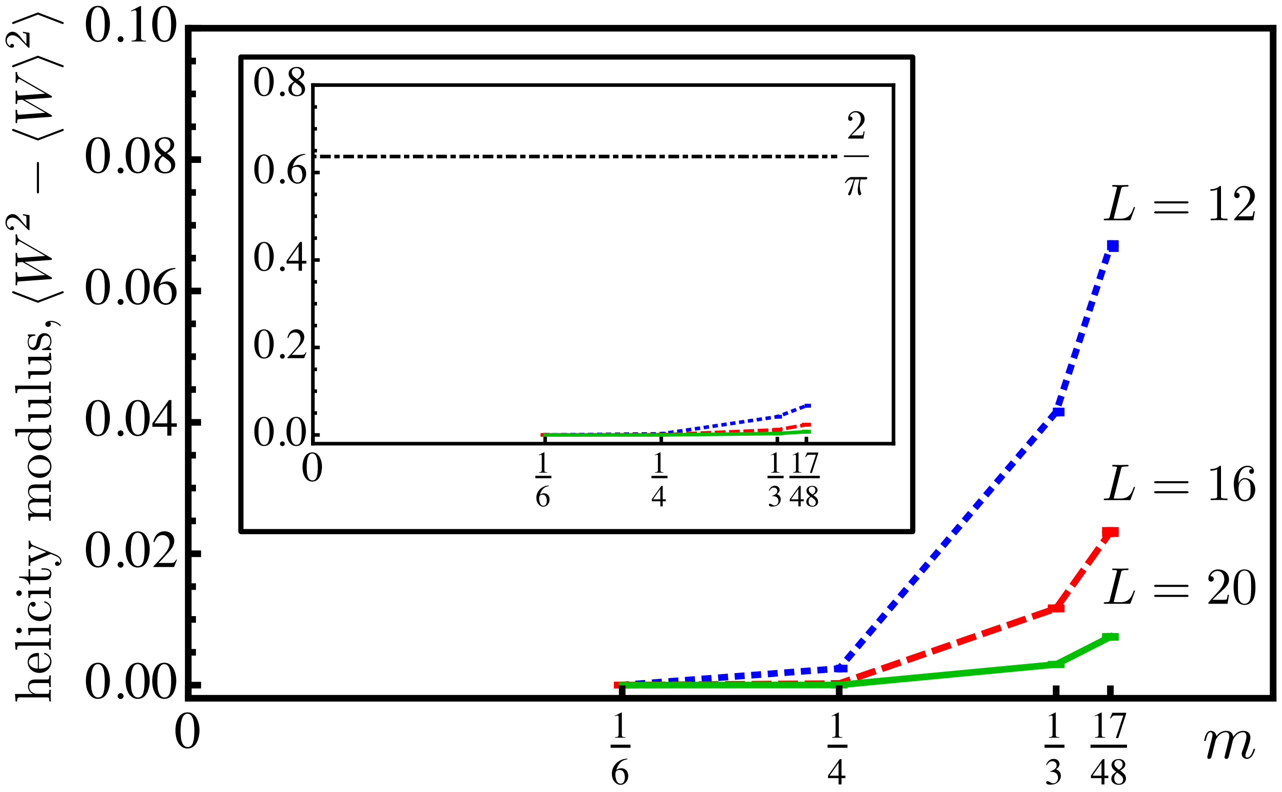
[Kimchi, SP, Turner, Vishwanath, arXiv: 1207.0498]

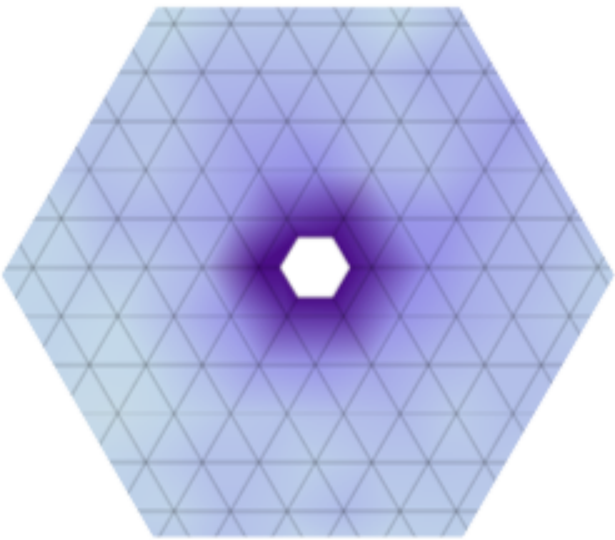
Honeycomb Lattice Example

[Kimchi, SP, Turner, Vishwanath, arXiv: 1207.0498]

Monte Carlo Results from Loop model







Exponential decaying boson correlations (no SF)

No discrete symmetry breaking

We don't (yet) have a parent Hamiltonian.

related Wannier approach: 1/3 kagome WF + parent Hamiltonian, fails for HC
[SP, Kimchi, Turner, Stamper-Kurn, Vishwanath, arXiv: 1206.1072]

Polarization Picture & Fourier Space Approach

[SP, Turner, Arovas, Vishwanath, in progress]

Can interpret LSM/Hastings/Oshikawa in terms of polarization

Nakamura & Voit; Ortiz, Martin

$$\mathbb{P}_i = \frac{e}{2\pi L^2} \lim_{L\to\infty} \arg \langle \Psi_0 | e^{i\int d^3r (\mathbf{b}_i \cdot \mathbf{r})\hat{\rho}(\mathbf{r})} | \Psi_0 \rangle$$

(sensitivity to BCs equivalent to flux threading)

Kohn; Resta & Sorella, Souza, Wilkens & Martin, Ortiz & Martin...

Generalize: allowed BCs (pure gauge) live on reciprocal lattice

'twist operator': $\hat{U}_{\mathbf{k}} = e^{i\int d^3r (\mathbf{k}\cdot\mathbf{r})\hat{\rho}(\mathbf{r})}$

$$\mathbf{k} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$$

Transformation of twist ops. under space group is equivalent to 'Fourier space crystallography'

- allows alt. derivation, also 'exceptional space groups'

[Fourier space crystallog. : Mermin, Rev. Mod. Phys. **64**, 3 (1992); König &Mermin, PRB **56**, 13607 (1997); PNAS **96**, 3502 (1999);]

Summary

Symmetry invariant of a space group: Nonsymmorphic Rank $\mathcal{S}$

minimum filling for featureless insulator

Bloch bands 'stick' in groups of (at least) $\mathcal{S}$

divisor of size of minimum Wyckoff orbit

[SP, Turner, Arovas, Vishwanath, in progress]

157/230 space groups have $\mathcal{S} > 1$

hexagonal close packing (P6/mmc, S=2)

diamond, pyrochlore (Fd3m, S=2)

Suggests algorithm for constructing featureless phases

[Kimchi, SP, Turner, Vishwanath, arXiv:1207.0498]

Alternative Route: Polarization + Fourier-Space crystallography

cf. also R.Roy, to appear

time reversal?

spin-orbit? quasicrystals?

Flux threading & Oshikawa's argument: Technical

Assume gs respects translations (along x)

$$\hat{T}_x|\Psi_0\rangle = e^{iP_x^0}|\Psi_0\rangle \qquad \hat{U} = e^{2\pi i \sum_{\mathbf{r}} \frac{x_{\mathbf{r}}}{L}\hat{\rho}_{\mathbf{r}}}$$

$$|\Psi_0\rangle \xrightarrow{\text{thread flux}} |\Psi_0'\rangle \xrightarrow{\text{gauge tr.}} \hat{U}|\Psi_0'\rangle$$

$$P_x^0 \qquad P_x^0 \qquad P_x^0 + ??2\pi\lfloor L_y L_z \frac{p}{q}\rfloor$$

At filling p/q : $\hat{U}^{-1}\hat{T}_x\hat{U} = \hat{T}_x e^{i2\pi\frac{V}{L}\frac{p}{q}}$

If $L_y L_z \frac{p}{q}$ is not an integer $|\Psi_0\rangle$, $\hat{U}|\Psi_0'\rangle$ are orthogonal.

Insulating ground state always degenerate.

[Oshikawa, PRL **84**, 1535 (2000)]