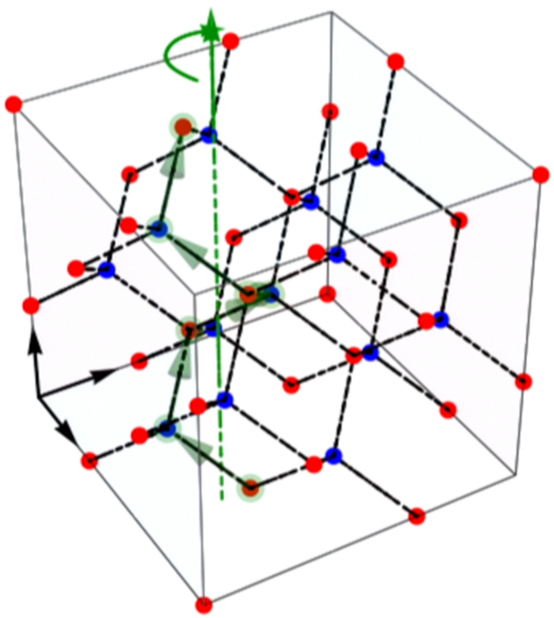
Title: Fractionalization from Crystallography

Date: Nov 18, 2014 03:30 PM

URL: http://pirsa.org/14110132

Abstract: A featureless insulator is a gapped phase of matter that does not exhibit fractionalization or other exotic physics, and thus has a unique ground state. The classic albeit non-interacting example is an electronic band insulator. A standard textbook argument tells us that band insulators require an even number of electrons -- an integer number for each spin -- per unit cell. I will explore the converse question: given such an 'integer filling', is a featureless insulating state possible? I will demonstrate that in most three-dimensional crystals, an insulating ground state cannot be unique -- and hence cannot be featureless -- except at certain special fillings fixed by the crystalline space group. This result, which remains valid more generally for interacting systems of fermions, bosons, or spins (as long as they have a conserved U(1) charge), relies on a combination of topological 'flux insertion' arguments and elementary crystallographic ideas. I will explore its implications through examples ranging from band theory, where it leads to the identification of protected semimetals, to frustrated magnetism, where it suggests new venues for spin liquid physics.

Fractionalization from Crystallography



Siddharth Parameswaran
University of California, Irvine

Condensed Matter Seminar, Perimeter Institute, November 18, 2014

SIMONS FOUNDATION

Collaborators

Ashvin Vishwanath

UC Berkeley

Ari Turner

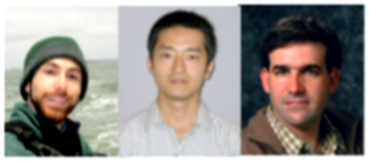
UvA (Amsterdam) → JHU

Dan Arovas

UC San Diego

S.P., Turner, Arovas & Vishwanath, *Nature Physics* **9**, 299 (2013)

+ related work w/ Itamar Kimchi, Fa Wang, Dan Stamper-Kurn



S.P., Kimchi, Turner, Stamper-Kurn & Vishwanath, *Phys. Rev. Lett.* **110**, 125301 (2013)

Kimchi, S.P., Turner, Wang & Vishwanath, *PNAS* **110**, 16378 (2013)

Overview

Introduction: Classifying phases

metals vs. insulators, symmetry and fractionalization

Why are Mott insulators 'special'?

topological order and spin-charge separation

Hastings-Oshikawa-Lieb-Schultz-Mattis theorem

Mott Physics and Crystal Symmetry

constraints from crystallography

'non-symmorphic rank' of a space group

Implications and Applications

identifying new Mott insulators

'required' band touchings

Classifying Phases

One simple way

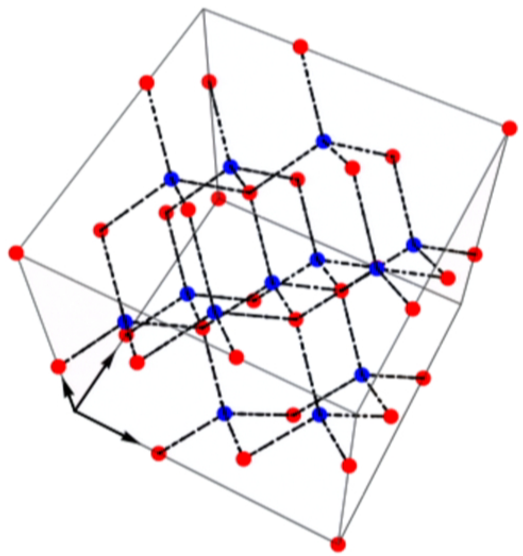
Metals

Insulators

Images: http://wikipedia.com, http://www.androidspin.com, http://www.nauticexpo.com

Classifying Phases

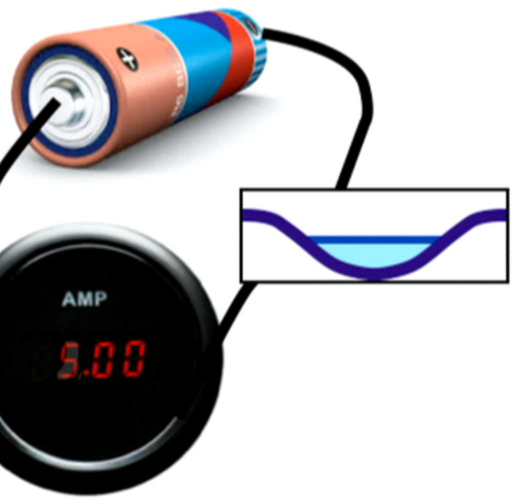
Another way: symmetries



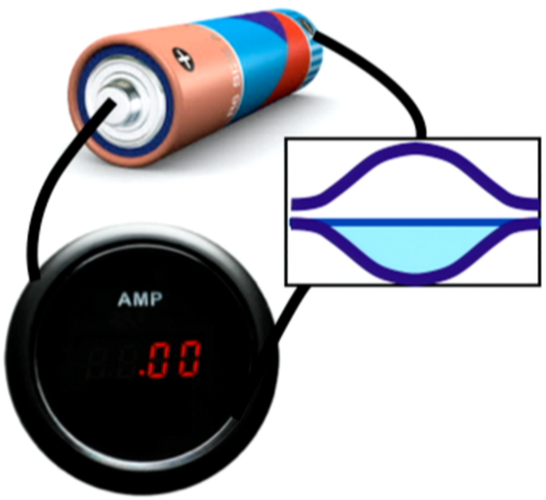
e.g. all crystals in one of 230 space groups

Band theory involves both

Bloch's theorem + Schrödinger equation ⇒ energy bands



Metals: partially filled bands



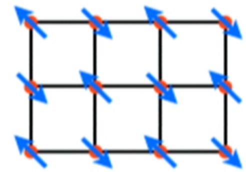
Insulators: filled bands

(without interactions)

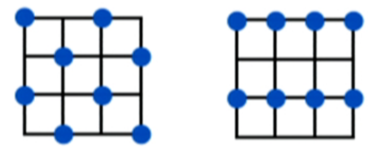
Add Interactions: Symmetry Breaking

magnets
- ferro-

- antiferro-



charge density waves

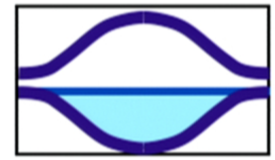


superfluids

Can there be distinct phases, even w/o symmetry breaking?

Featureless Phases with No Symmetry Breaking

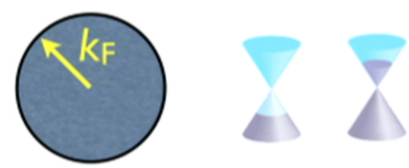
band insulators (incl. topological)



'quantum paramagnets'

e.g. spin-1 'AKLT' chain

metals, semimetals

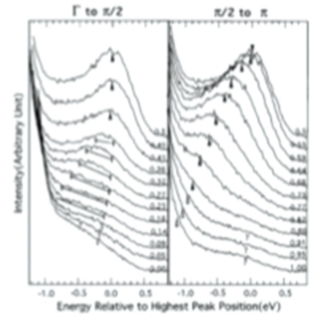


if gapped, unique g.s.; if gapless, no fractionalization

Fractionalized Phases with No Symmetry Breaking

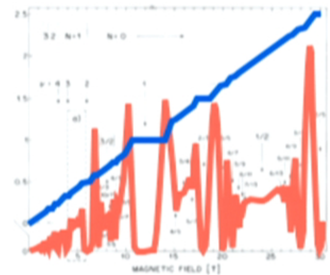
Spin-charge separation in 1D

'Luttinger liquid': $v_{\rm spin} \neq v_{\rm charge}$



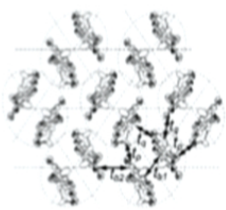
Fractional quantum Hall effect

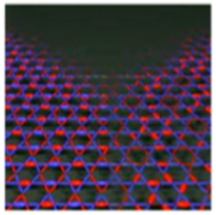
fractionalized charge and statistics



Gapped/gapless Quantum Spin Liquids

gapped spinons/thermal metal, charge insulator





if gapped, degenerate g.s.; all cases, fractional quantum numbers

Detecting Fractionalization

Fractionalized phases encode physics in entanglement

[Gapped case: Kitaev & Preskill '06; Levin & Wen '06]

Hard to measure!

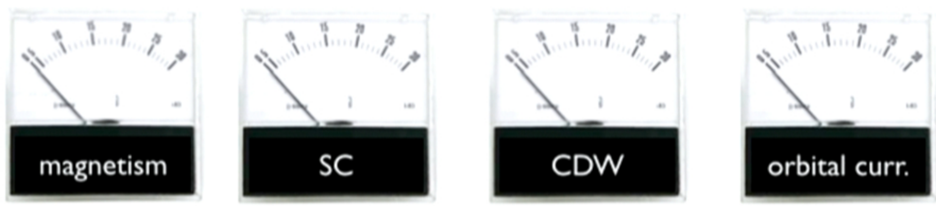
Detecting Fractionalization

Fractionalized phases encode physics in entanglement

[Gapped case: Kitaev & Preskill '06; Levin & Wen '06]

Hard to measure!

Suppose we check all symmetries, and they're unbroken.

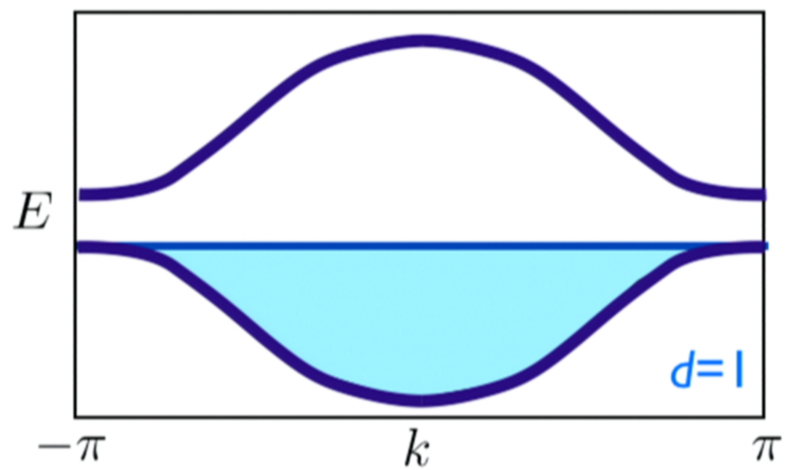


• • •

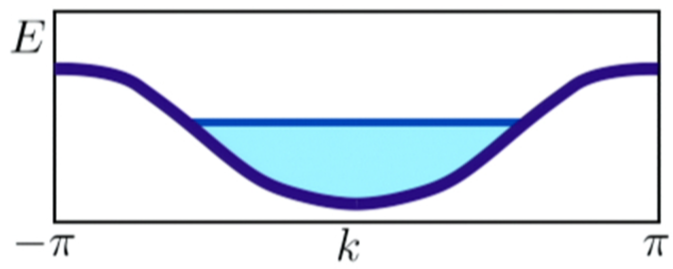
When is the system in an interesting phase?

Example #1: Band Insulators

- Gapped
- Breaks no symmetries
- Unique ground state (periodic system)



Example #2: half-filling + Hubbard U



$d=1$

$U \gg t$: Heisenberg AF

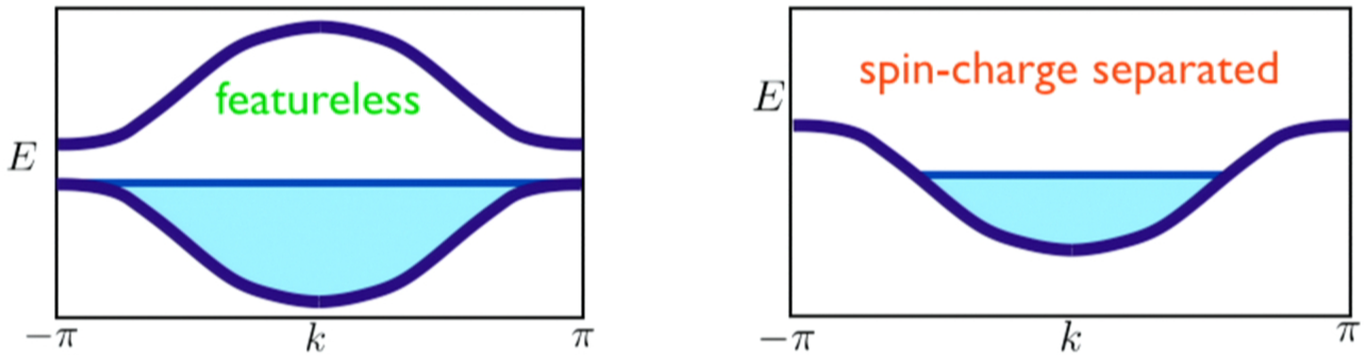
$$H \approx \frac{t^2}{U} \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

Spin-1/2 Heisenberg chain is gapless [Lieb, Schulz, Mattis '61]

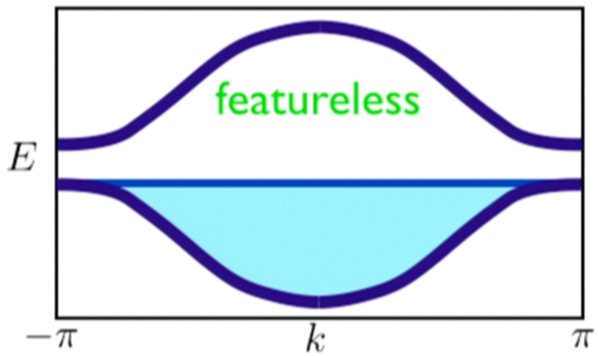
Charge insulator, spin metal: spin-charge separation!

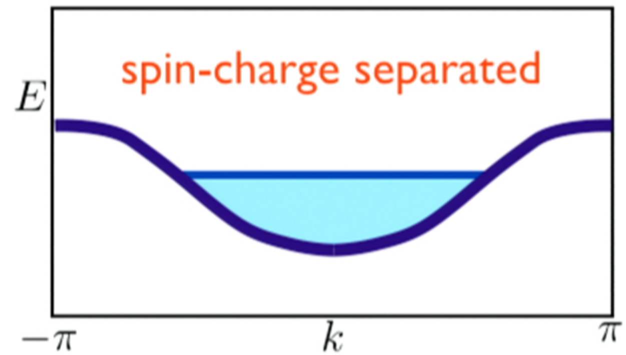
(actually, charge gap for all $U \neq 0$) [Lieb & Wu '68]

Why are they different?



Why are they different?





different <u>filling</u>

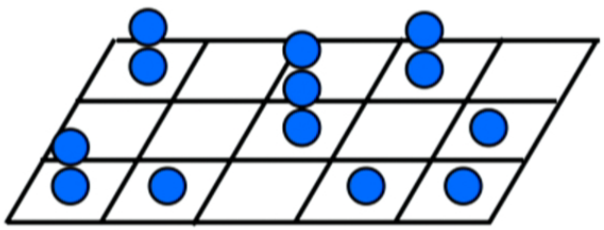
Integer filling: adiabatic connection to band insulator
(even if particular case needs interactions)

Fractional filling: no adiabatic continuity to band insulator
(unless a symmetry is broken and redefines unit cell)

Can 'no adiabatic continuity to band insulator' be made precise?

Minimal requirements:

crystal structure



conserved global U(1) charge

$$\sum \#(\bullet) = N$$

Need both to define *filling*:

$$\nu = \frac{\text{total charge}}{\text{number of unit cells}}$$

Hastings-Oshikawa-Lieb-Schultz-Mattis 'Theorem'

At fractional filling,
unique, gapped, translationally invariant* insulating ground state
is impossible

*shorthand: 'featureless'

Hastings-Oshikawa-Lieb-Schultz-Mattis 'Theorem'

At fractional filling,
unique, ~~gapped,~~ translationally invariant* ~~insulating~~ ground state
is ~~im~~possible

What are alternatives?

remain metallic (charge travels freely)

*shorthand: 'featureless'

Hastings-Oshikawa-Lieb-Schultz-Mattis 'Theorem'

At fractional filling,
unique, ~~gapped,~~ translationally invariant* ~~insulating~~ ground state
is ~~im~~possible

What are alternatives?

remain metallic (charge travels freely)

*shorthand: 'featureless'

Hastings-Oshikawa-Lieb-Schultz-Mattis ‘Theorem’

At fractional filling,
unique, gapped, ~~translationally invariant~~* insulating ground state
is ~~im~~possible

What are alternatives?

remain metallic (charge travels freely)

break symmetry (redefine ‘filling’)

*shorthand: ‘featureless’

Hastings-Oshikawa-Lieb-Schultz-Mattis 'Theorem'

At fractional filling,
unique, ~~gapped~~ translationally invariant* insulating ground state
is ~~im~~possible

What are alternatives?

remain metallic (charge travels freely)

break symmetry (redefine 'filling')

insulate, remain gapless (e.g. spin-charge separation)

*shorthand: 'featureless'

Hastings-Oshikawa-Lieb-Schultz-Mattis 'Theorem'

At fractional filling,
~~unique~~, gapped, translationally invariant* insulating ground state
is ~~im~~possible

What are alternatives?

remain metallic (charge travels freely)

break symmetry (redefine 'filling')

insulate, remain gapless (e.g. spin-charge separation)

ground state degeneracy = 'topological order'

*shorthand: 'featureless'

Hastings-Oshikawa-Lieb-Schultz-Mattis 'Theorem'

At fractional filling,
~~unique~~, gapped, translationally invariant* insulating ground state
is ~~im~~possible

What are alternatives?

remain metallic (charge travels freely)

break symmetry (redefine 'filling')

insulate, remain gapless (e.g. spin-charge separation)

ground state degeneracy = 'topological order'

Strict definition of 'no adiabatic continuity'; involves fractionalization.

*shorthand: 'featureless'

At fractional unit cell filling:

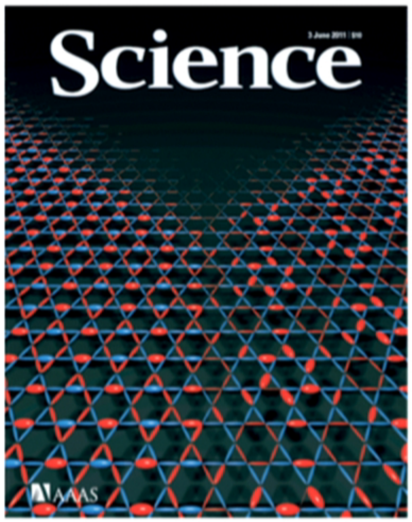
Gap + No Symmetry Breaking $\Rightarrow$ fractionalization

Strongly constrains possible phases

At fractional unit cell filling:

Gap + No Symmetry Breaking ⇒ fractionalization

Strongly constrains possible phases



e.g. Kagome Lattice Heisenberg Model

DMRG: gap + no symmetry breaking

half-integer filling ⇒ not featureless

g.s. = Z_2 quantum spin liquid

[Yan, Huse, White, *Science* '11]

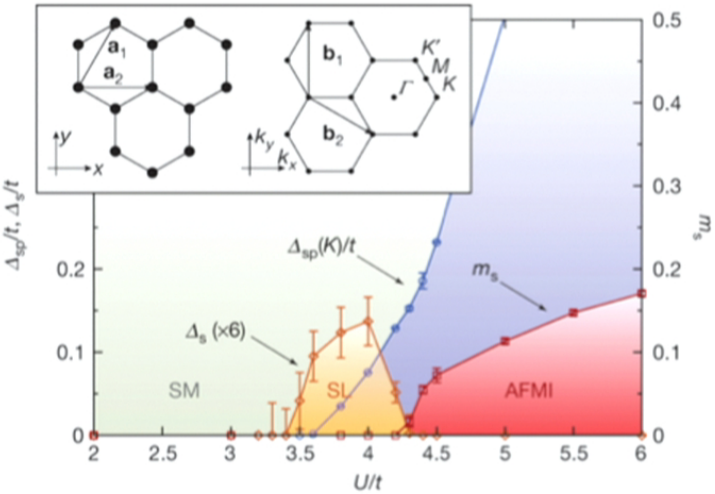
[smoking gun: entanglement entropy: Jiang, Wang, Balents, *Nat. Phys.* '12]

At integer unit cell filling:

Gap + No Symmetry Breaking ⇒ ???

At integer unit cell filling:

Gap + No Symmetry Breaking ⇒ ???



e.g. Honeycomb Hubbard Model

[Meng, et al., *Nature* '10]

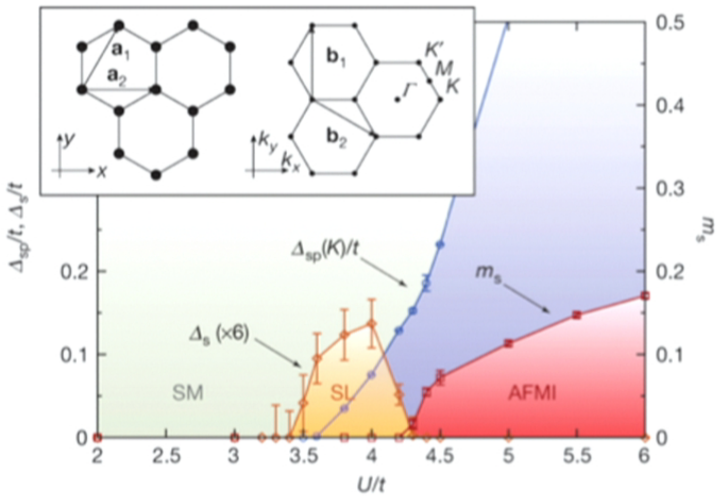
QMC: gap + no symmetry breaking

integer unit cell filling

fractionalized spin liquid?

At integer unit cell filling:

Gap + No Symmetry Breaking ⇒ ???



e.g. Honeycomb Hubbard Model

[Meng, et al., *Nature* '10]

QMC: gap + no symmetry breaking

integer unit cell filling

fractionalized spin liquid?

Not necessarily!

e.g. can construct 'featureless' SU(2) -symmetric fermion insulator with no fractionalization

[I. Kimchi, S.P., *et al. PNAS* **110**, 16378 (2013)]

Fractional filling: no ‘featureless’ phase allowed

This Talk

When is a featureless phase forbidden at integer filling?

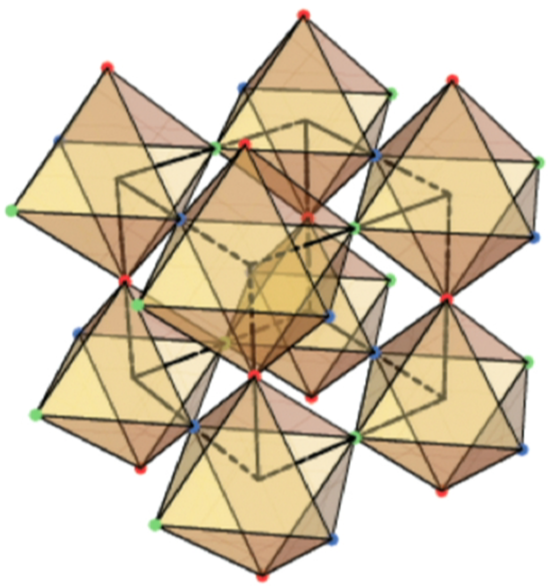
Related band theory problem

Related band theory problem

<u>given</u> exactly <u>one</u> spinless fermion per unit cell

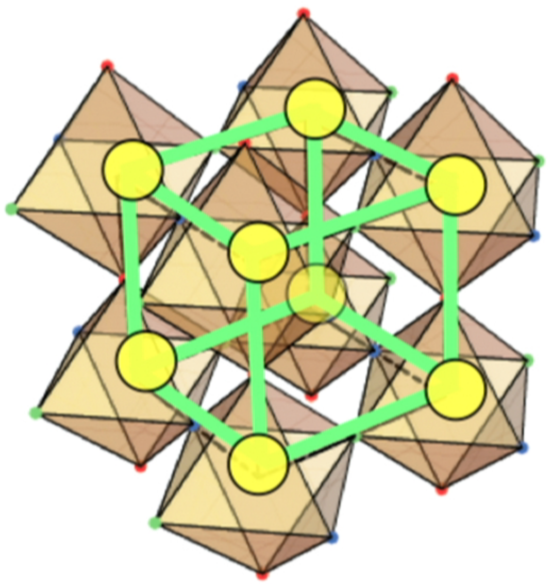
+ a <u>specified</u> crystal

+ freedom to



Related band theory problem

given exactly one spinless fermion per unit cell



+ a specified crystal

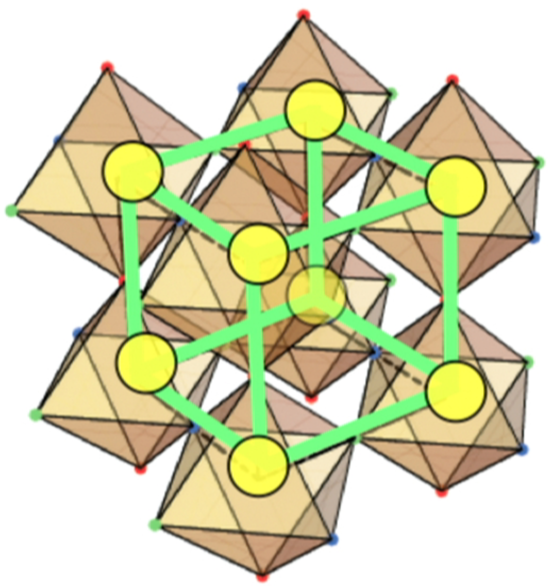
+ freedom to

- add sites*
- change hopping

*Freedom to add sites removes 'tight binding' constraints

Related band theory problem

given exactly one spinless fermion per unit cell



+ a specified crystal

+ freedom to

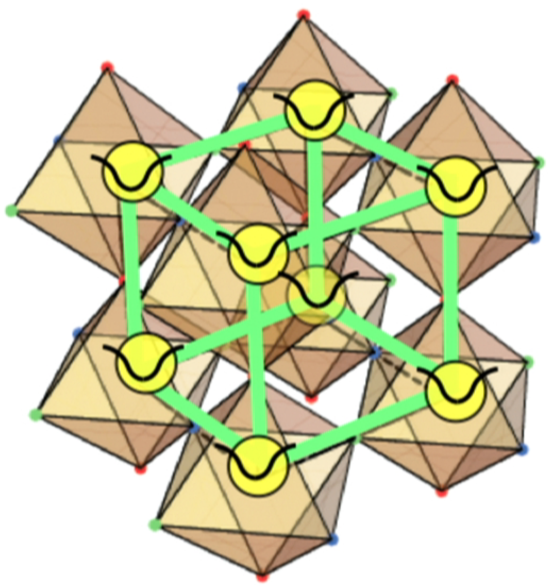
- add sites*

- change hopping

*Freedom to add sites removes 'tight binding' constraints

Related band theory problem

given exactly one spinless fermion per unit cell



+ a specified crystal

+ freedom to

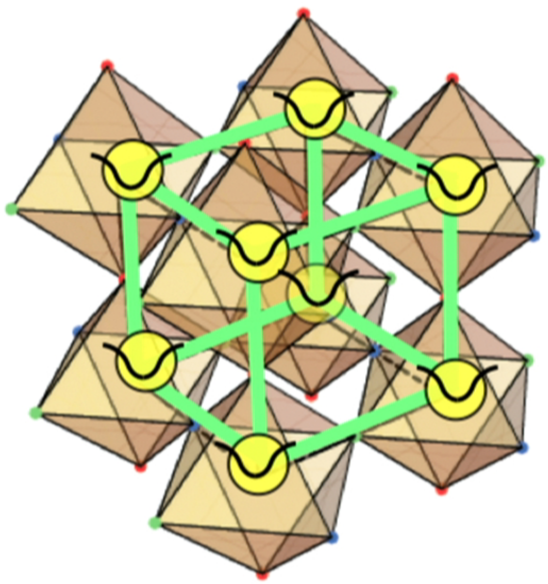
- add sites*
- change hopping
- tune onsite terms

*Freedom to add sites removes 'tight binding' constraints

Related band theory problem

given exactly one spinless fermion per unit cell

+ a specified crystal



+ freedom to

- add sites*
- change hopping
- tune onsite terms

Can we always find a band insulator?

*Freedom to add sites removes 'tight binding' constraints

Flux Insertion

Flux Insertion: 'Laughlin' Arguments

Idea: prove non-uniqueness of g.s. by constructing degenerate state

Flux Insertion: 'Laughlin' Arguments

Idea: prove non-uniqueness of g.s. by constructing degenerate state

How to get another state?

Conserved charge ⇒ 'magnetic' flux

Thread 2π flux (=1 'flux quantum')

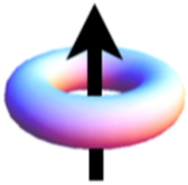
Usually: $\Delta E = E(2\pi) - E(0) \neq 0$; insulator: $\Delta E \rightarrow 0$ as $L \rightarrow \infty$

Flux Insertion: 'Laughlin' Arguments

Idea: prove non-uniqueness of g.s. by constructing degenerate state

How to get another state?

Conserved charge ⇒ 'magnetic' flux

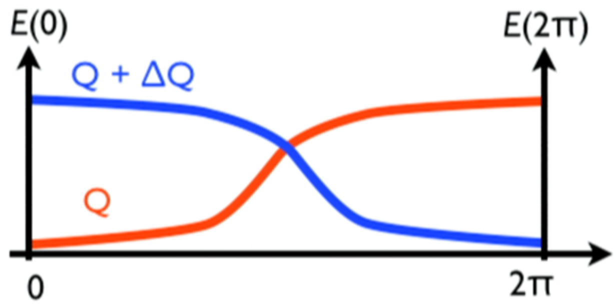


Thread 2π flux (=1 'flux quantum')

Usually: $\Delta E = E(2\pi) - E(0) \neq 0$; insulator: $\Delta E \to 0$ as $L \to \infty$

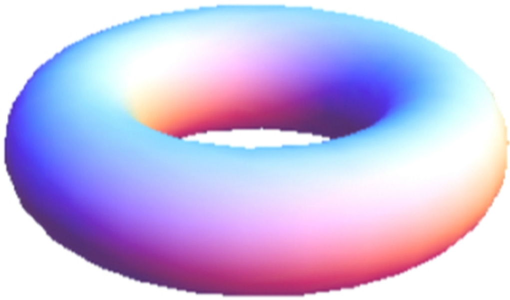
Obtain degenerate state; is it really distinct?

Look for a quantum number 'Q' that changed in the cycle



Poor man's 'Proof' of LSMHO

System on torus, in ground state



[Oshikawa, PRL '04]

['Rigorized' by Hastings, PRB '05, Europhys B '07]

Poor man's 'Proof' of LSMHO

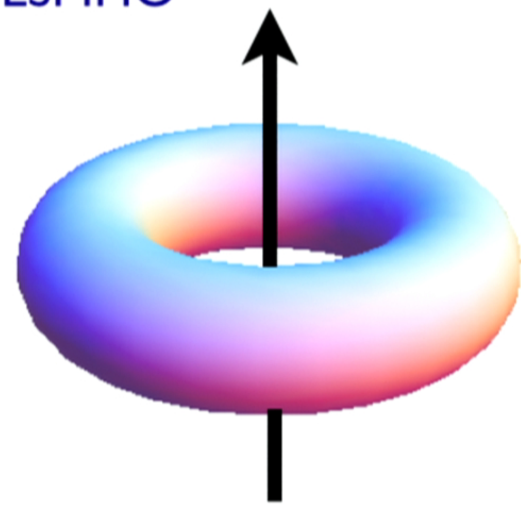
System on torus, in ground state

Thread quantum of flux, follow g.s.

(insulator: energy unchanged)

$$|\Psi_0\rangle \rightarrow |\tilde{\Psi}_0\rangle$$

degenerate;
is it different?



[Oshikawa, PRL '04]

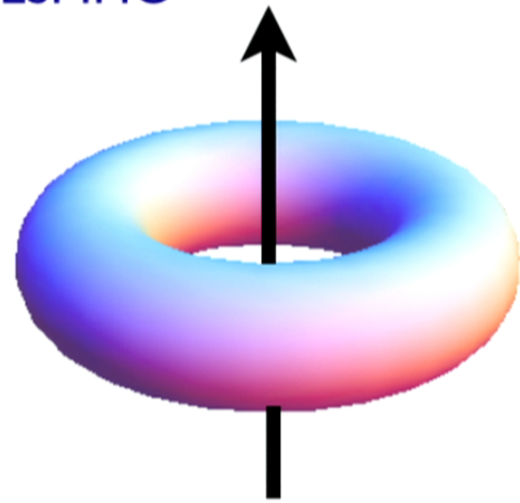
['Rigorized' by Hastings, PRB '05, Europhys B '07]

Poor man's 'Proof' of LSMHO

System on torus, in ground state

Thread quantum of flux, follow g.s.
(insulator: energy unchanged)

$$|\Psi_0\rangle \rightarrow |\tilde{\Psi}_0\rangle$$ degenerate; is it different?



Faraday's law ⇒ $\Phi(t)$ induces E-field
⇒ force on charges

[Oshikawa, PRL '04]

['Rigorized' by Hastings, PRB '05, Europhys B '07]

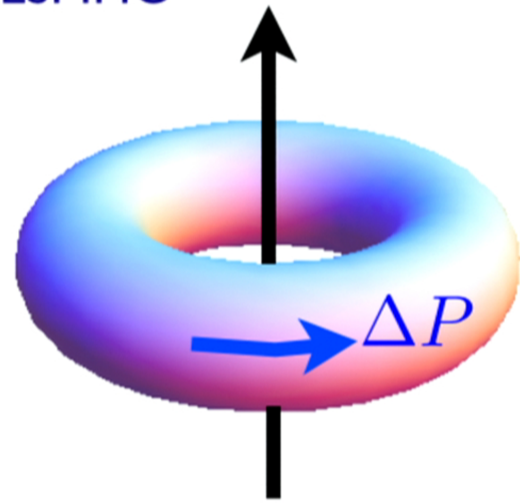
Poor man's 'Proof' of LSMHO

System on torus, in ground state

Thread quantum of flux, follow g.s.

(insulator: energy unchanged)

$$|\Psi_0\rangle \rightarrow |\tilde{\Psi}_0\rangle$$ degenerate; is it different?



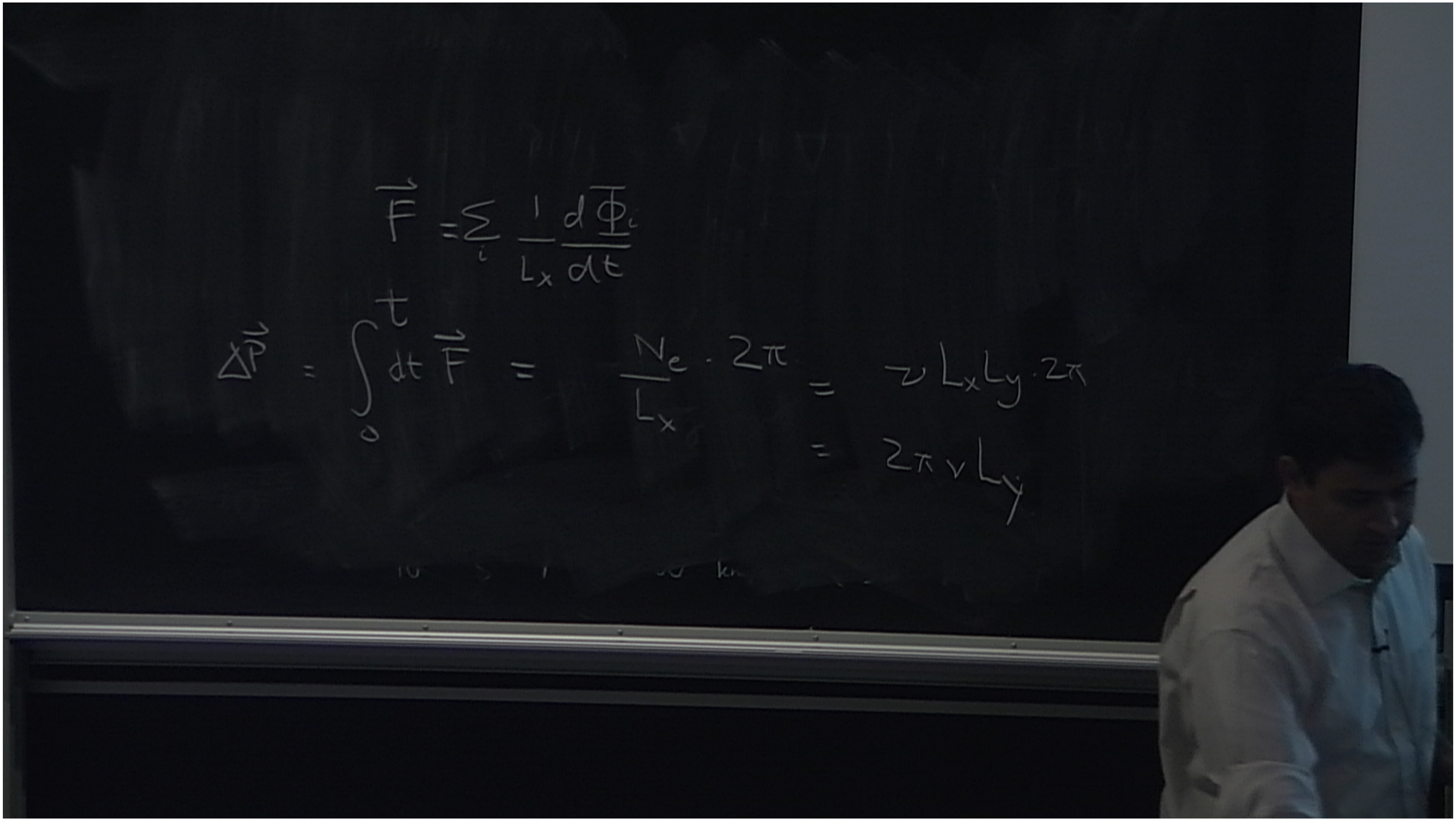
Faraday's law ⇒ $\Phi(t)$ induces E-field

⇒ force on charges

⇒ $\Delta P = 2\pi N_y \nu$

[Oshikawa, PRL '04]

['Rigorized' by Hastings, PRB '05, Europhys B '07]


$\vec{F} = \sum_i \frac{1}{L_x} \frac{d\Phi_i}{dt}$
$\Delta \vec{P} = \int_0^t dt\, \vec{F} = \frac{N_e}{L_x} \cdot 2\pi = \nu L_x L_y \cdot 2\pi$
$= 2\pi \nu L_y$

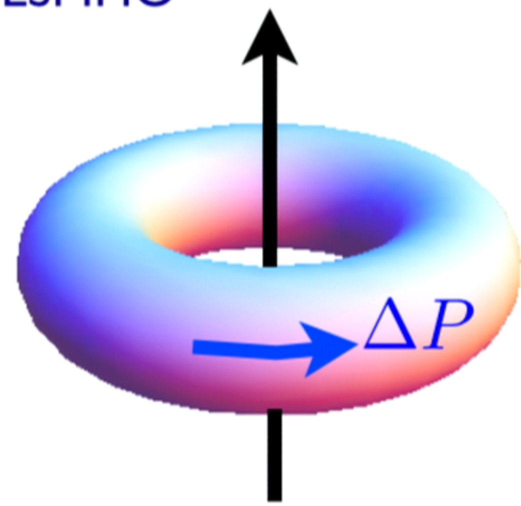
Poor man's 'Proof' of LSMHO

System on torus, in ground state

Thread quantum of flux, follow g.s.

(insulator: energy unchanged)

$|\Psi_0\rangle \to |\tilde{\Psi}_0\rangle$ degenerate; is it different?



[Oshikawa, PRL '04]

['Rigorized' by Hastings, PRB '05, Europhys B '07]

Faraday's law ⇒ Φ(*t*) induces *E*-field

⇒ force on charges

⇒ $\Delta P = 2\pi N_y \nu$

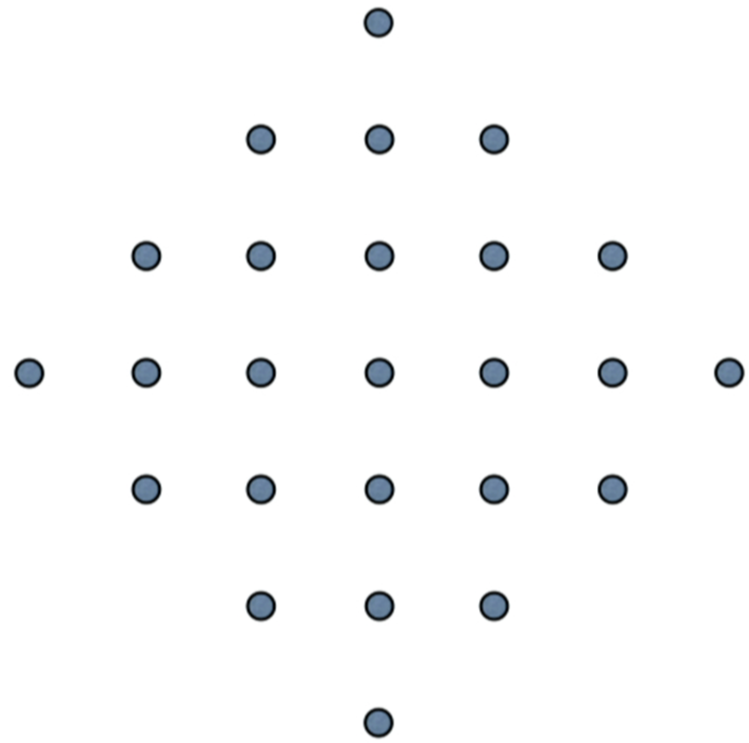
$\Delta P \neq 2\pi n \Rightarrow$ crystal momentum changed, $\langle \Psi_0 | \tilde{\Psi}_0 \rangle = 0$

g.s. can't be unique at fractional ν!

Flux threading: reciprocal lattice picture

$$|\Psi_0\rangle \longrightarrow |\tilde{\Psi}_0\rangle$$

$$\Delta P = 2\pi N_y \nu$$



[Paramekanti, Vishwanath, PRB '05]

N_y odd

Flux threading: reciprocal lattice picture

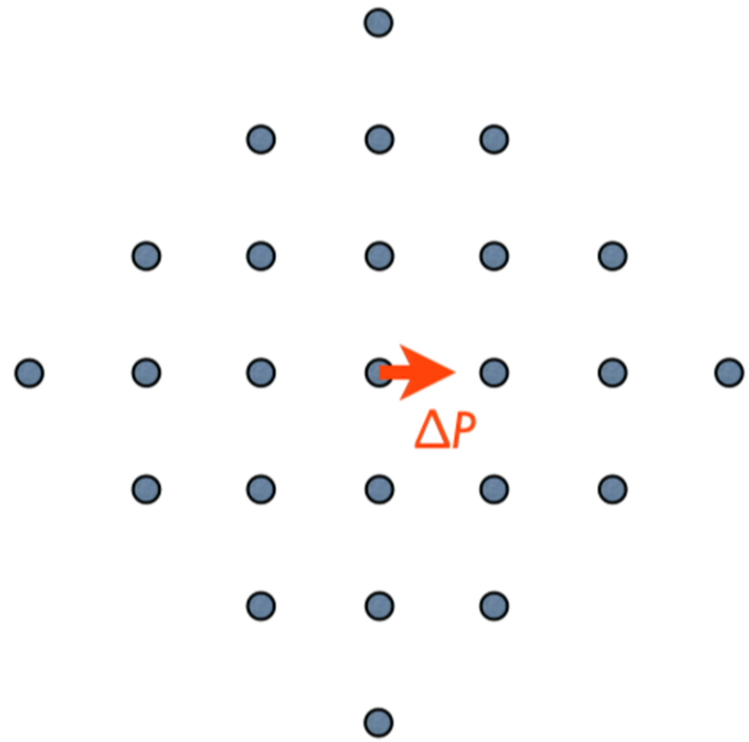
$|\Psi_0\rangle \longrightarrow |\tilde{\Psi}_0\rangle$

$\Delta P = 2\pi N_y \nu$

ν=1/2

$|\Psi_0\rangle, |\tilde{\Psi}_0\rangle$

distinguishable

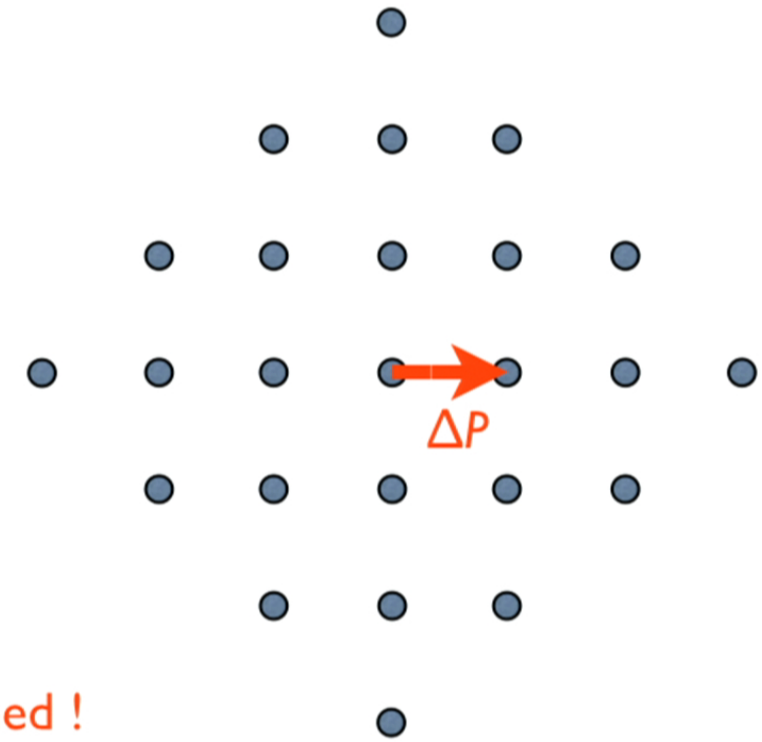


[Paramekanti, Vishwanath, PRB '05]

N_y odd

Flux threading: reciprocal lattice picture

$|\Psi_0\rangle \longrightarrow |\tilde{\Psi}_0\rangle$



$\Delta P = 2\pi N_y \nu$

ν=1

Δ*P* at Bragg peak

$|\Psi_0\rangle, |\tilde{\Psi}_0\rangle$ can't be distinguished !

[Paramekanti, Vishwanath, PRB '05]

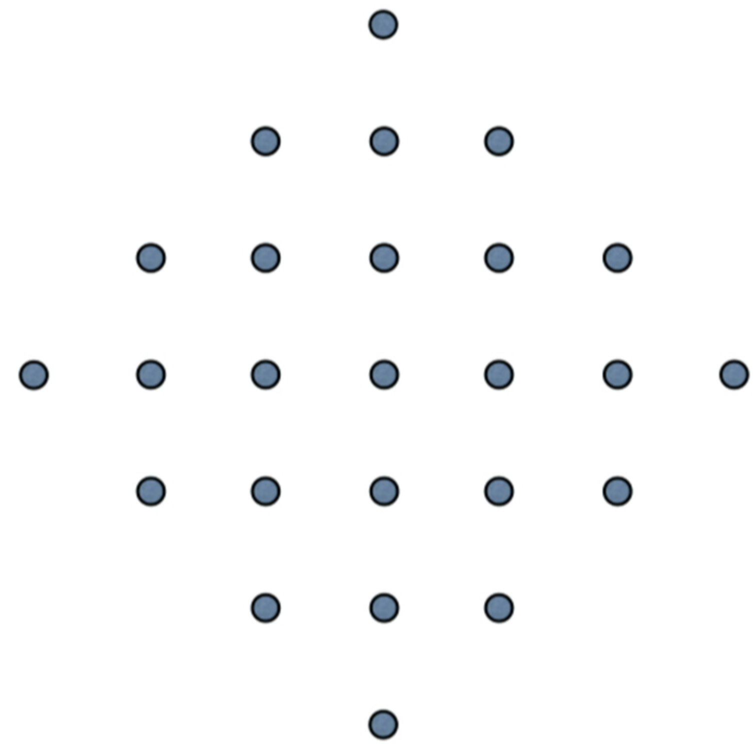
N_y odd

Flux threading: reciprocal lattice picture

$|\Psi_0\rangle \longrightarrow |\tilde{\Psi}_0\rangle$

$e^{iP} \longrightarrow e^{i(P+\Delta P)}$

$$\Delta P = 2\pi N_y \nu$$



[Paramekanti, Vishwanath, PRB '05]

N_y odd

Flux threading: reciprocal lattice picture

Clue: Bragg extinctions

$$|\Psi_0\rangle \longrightarrow |\tilde{\Psi}_0\rangle$$

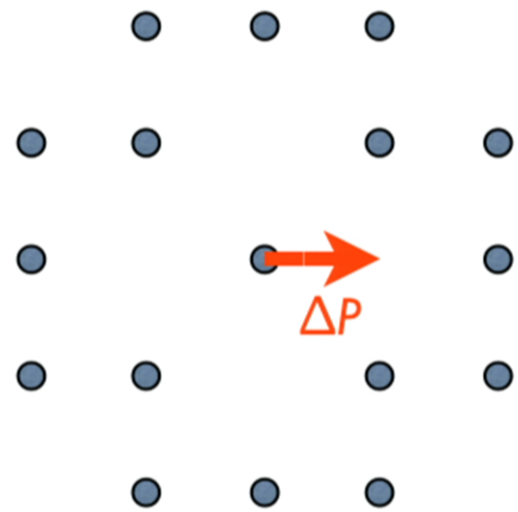
$$e^{iP} \longrightarrow e^{i(P+\Delta P)}$$

$$\Delta P = 2\pi N_y \nu$$

$\nu = 1$

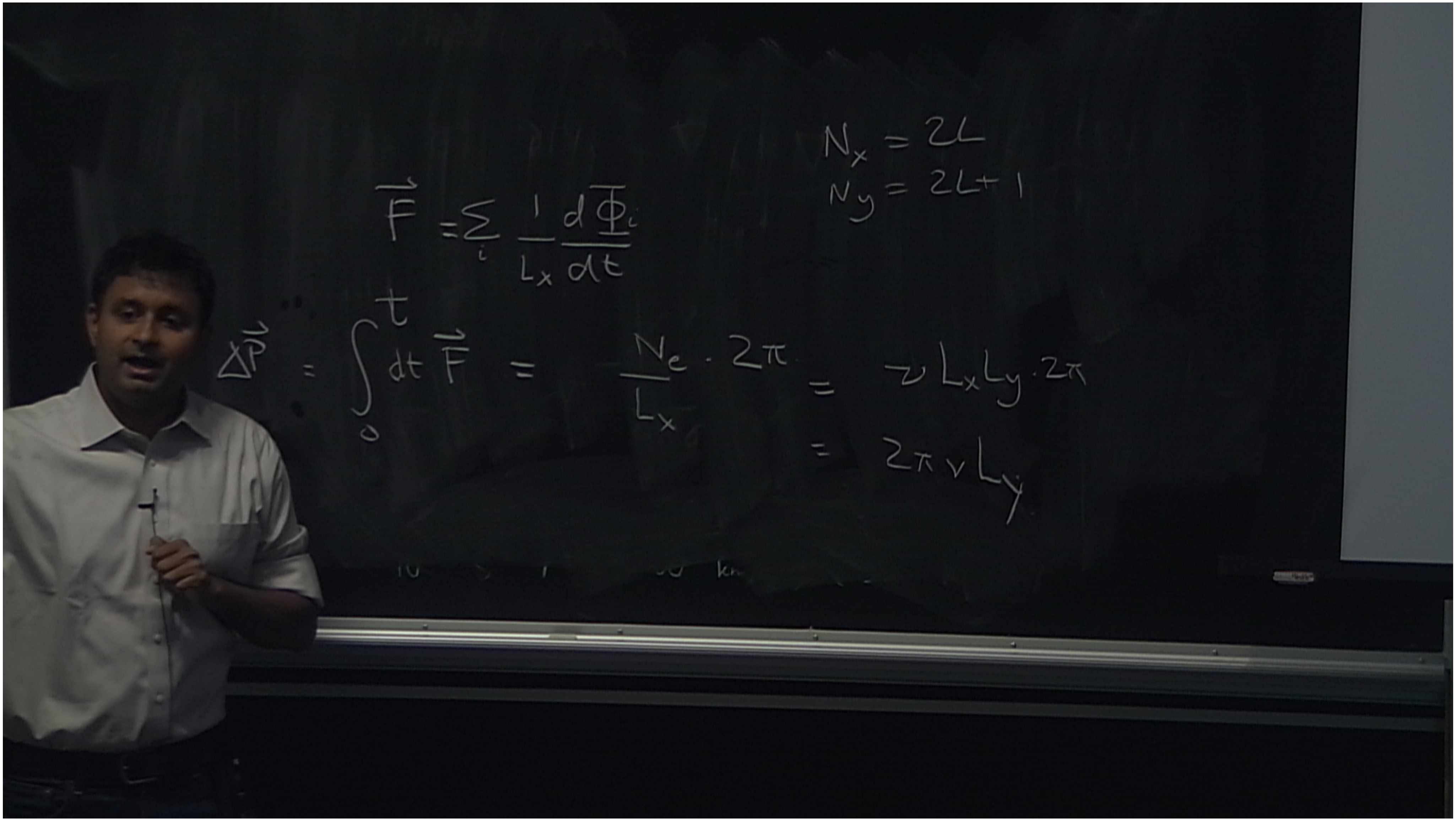
ΔP at [redacted]

$|\Psi_0\rangle, |\tilde{\Psi}_0\rangle$ distinguishable



[S.P., et. al., Nat. Phys. **9**, 299]

N_y odd


$N_x = 2L$
$N_y = 2L+1$
$\vec{F} = \sum_i \frac{1}{L_x} \frac{d\Phi_i}{dt}$
$\Delta\vec{P} = \int_0^t dt\, \vec{F} = \frac{N_e}{L_x} \cdot 2\pi = \nu L_x L_y \cdot 2\pi$
$= 2\pi \nu L_y$

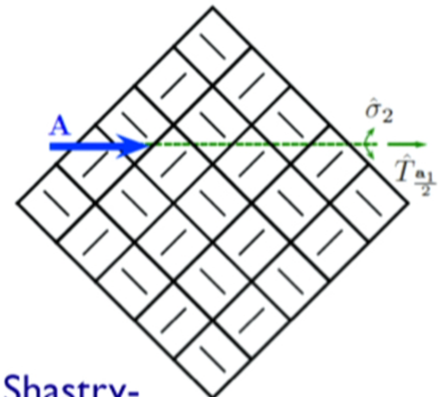
From Extinctions to Crystallography

Crystals with missing peaks: non-symmorphic

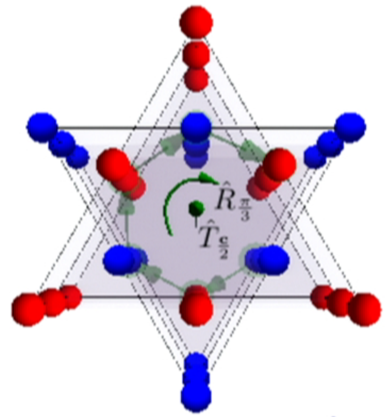
loosely: 'glide mirrors' and/or 'screw rotations'

(reflection/rotation × transl. by fraction of lattice vector)

special symmetry produces
destructive interference,
'kills' Bragg peaks



Shastry-
Sutherland



hcp

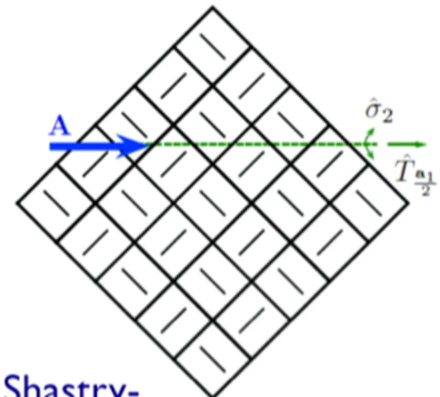
From Extinctions to Crystallography

Crystals with missing peaks: non-symmorphic

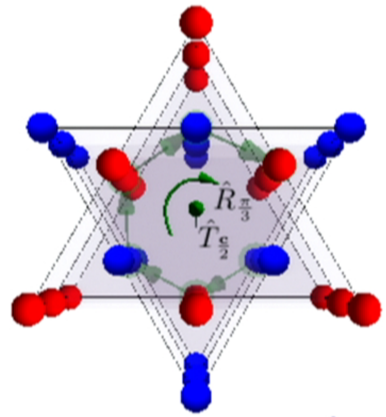
loosely: 'glide mirrors' and/or 'screw rotations'

(reflection/rotation × transl. by fraction of lattice vector)

special symmetry produces destructive interference, 'kills' Bragg peaks



Shastry-Sutherland



hcp

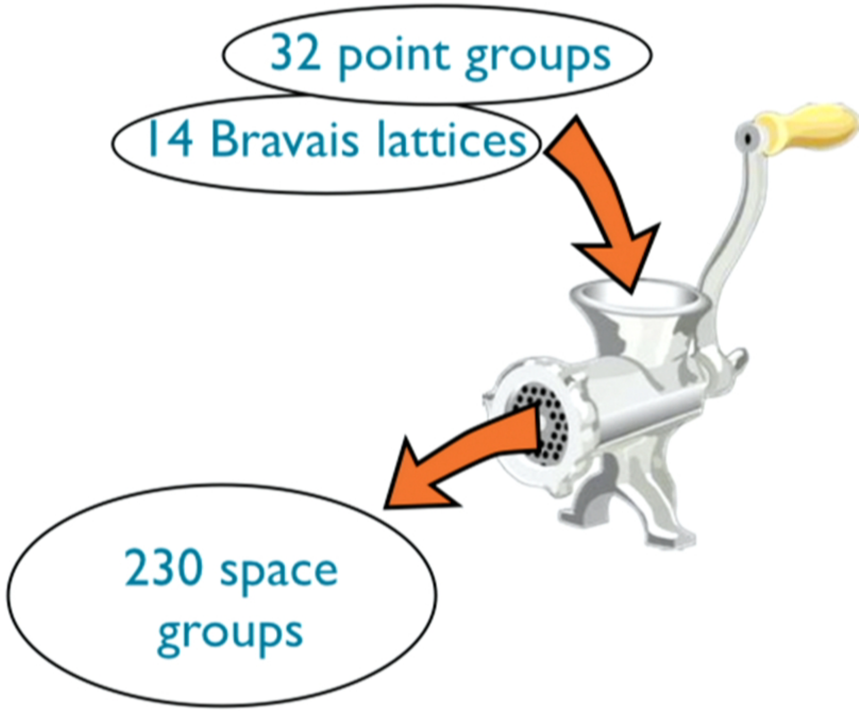
Crystallography in 60 seconds

Fyodorov, Schönflies, Barlow

Crystallography in 60 seconds

Fyodorov, Schönflies, Barlow

Crystallography in 60 seconds

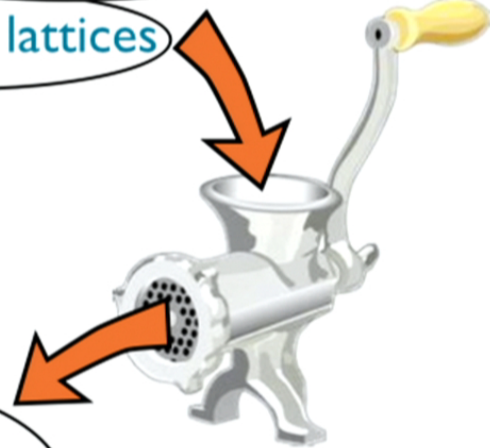


Fyodorov, Schönflies, Barlow

Crystallography in 60 seconds

32 point groups

14 Bravais lattices

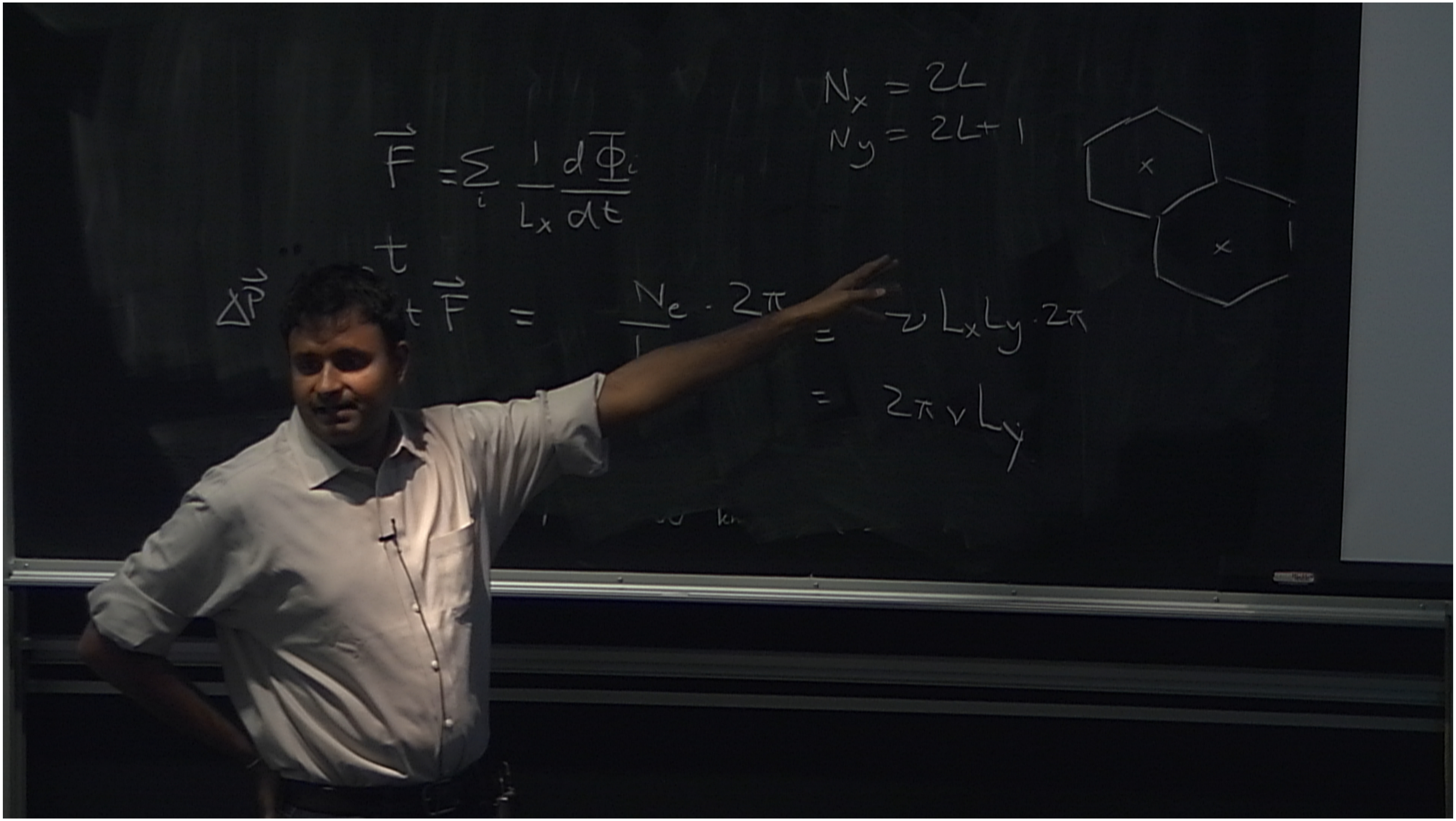


230 space groups

Fyodorov, Schönflies, Barlow

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

if not: non-symmorphic 157

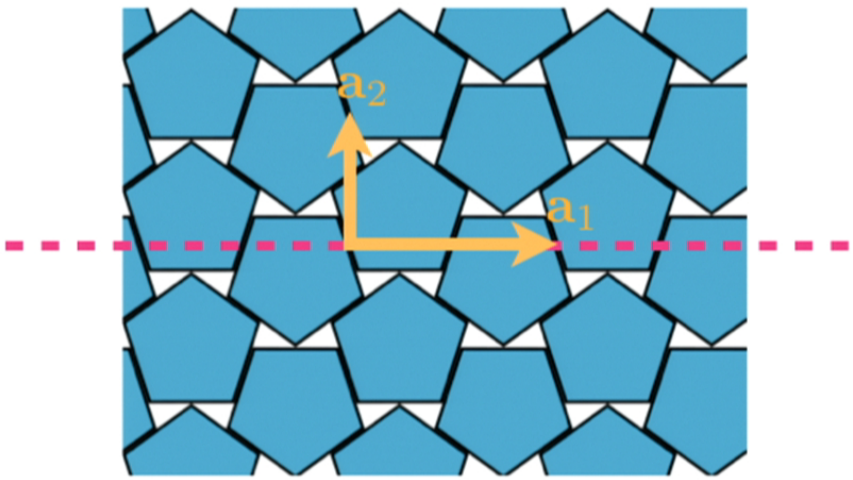


$\vec{F} = \sum_i \frac{1}{L_x} \frac{d\Phi_i}{dt}$
$N_x = 2L$
$N_y = 2L+1$
$\Delta\vec{P}$
$t\,\vec{F}$
$= \frac{N_e \cdot 2\pi}{L}$
$= \nu L_x L_y \cdot 2\pi$
$= 2\pi \nu L_y$

Nonsymmorphic Symmetries

Point-group operations accompanied by non-lattice translations

2D: glide mirrors

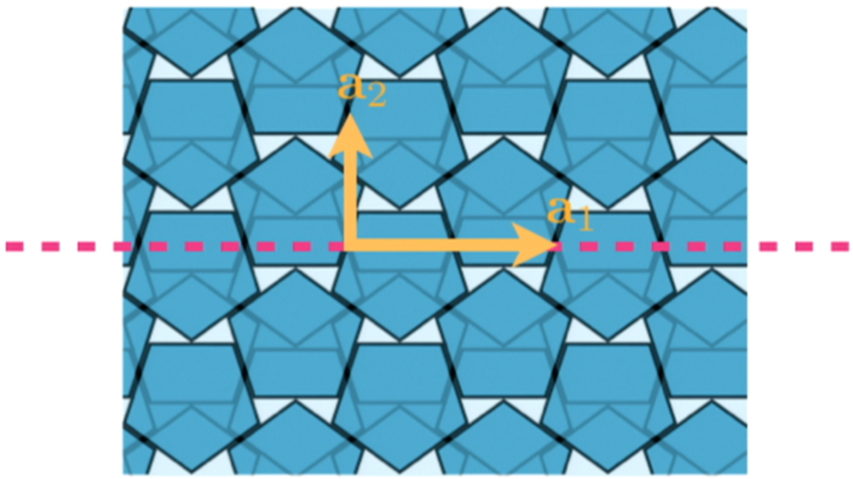


same space group ‘p4g’ as Shastry-Sutherland

Nonsymmorphic Symmetries

Point-group operations accompanied by non-lattice translations

2D: glide mirrors

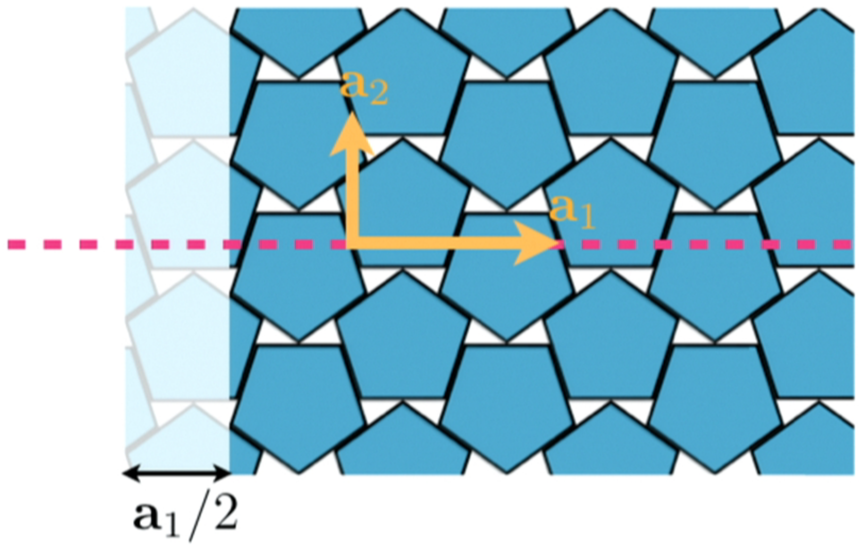


same space group 'p4g' as
Shastry-Sutherland

Nonsymmorphic Symmetries

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

2D: glide mirrors

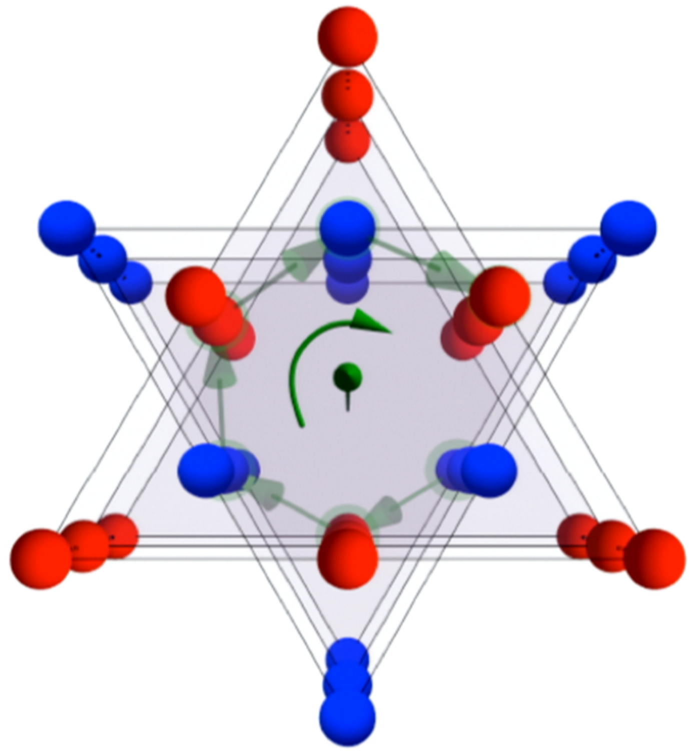


same space group 'p4g' as
Shastry-Sutherland

Nonsymmorphic Symmetries

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

3D: also screw rotations



hcp or 'p6/mmc'

'Nonsymmorphic Rank'

Run argument for various flux insertions/symmetries

Find smallest S so that if ν multiple of S, unique g.s. allowed

‘Nonsymmorphic Rank’

Run argument for various flux insertions/symmetries

Find smallest S so that if ν multiple of S, unique g.s. allowed

S is a property of space group: ‘nonsymmorphic rank’

'Nonsymmorphic Rank'

Run argument for various flux insertions/symmetries

Find smallest S so that if ν multiple of S, unique g.s. allowed

S is a property of space group: 'nonsymmorphic rank'

Crystallography $\Rightarrow S = 1,2,3,4$ or 6.

‘Nonsymmorphic Rank’

Run argument for various flux insertions/symmetries

Find smallest S so that if ν multiple of S, unique g.s. allowed

S is a property of space group: ‘nonsymmorphic rank’

Crystallography $\Rightarrow S = 1,2,3,4$ or 6.

73 symmorphic space groups: $S=1$

157 non-symmorphic space groups: $S>1$

'Nonsymmorphic Rank'

Run argument for various flux insertions/symmetries

Find smallest S so that if ν multiple of S, unique g.s. allowed

S is a property of space group: 'nonsymmorphic rank'

Crystallography $\Rightarrow S = 1,2,3,4$ or 6.

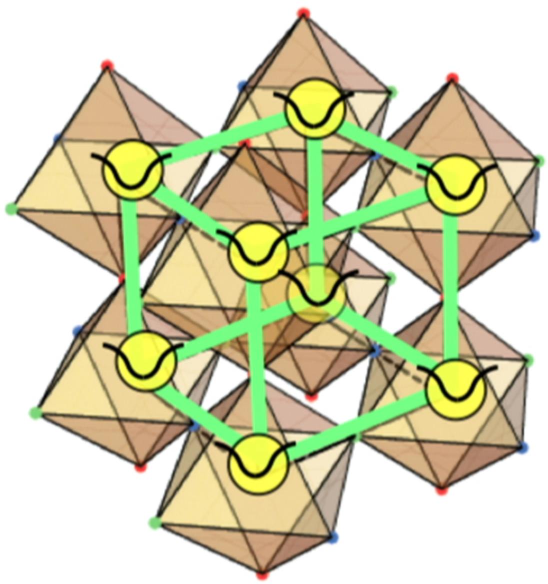
73 symmorphic space groups: $S=1$

157 non-symmorphic space groups: $S>1$

S = minimum filling where featureless insulator is allowed!

Related band theory problem

given exactly one spinless fermion per unit cell



+ a specified crystal

+ freedom to

- add sites*
- change hopping
- tune onsite terms

Can we always find a band insulator?

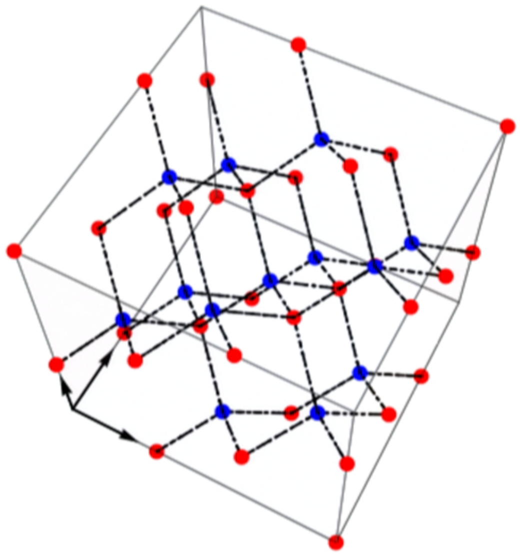
*Freedom to add sites removes 'tight binding' constraints

No!

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

No!

one (spinless) fermion per unit cell
not always sufficient

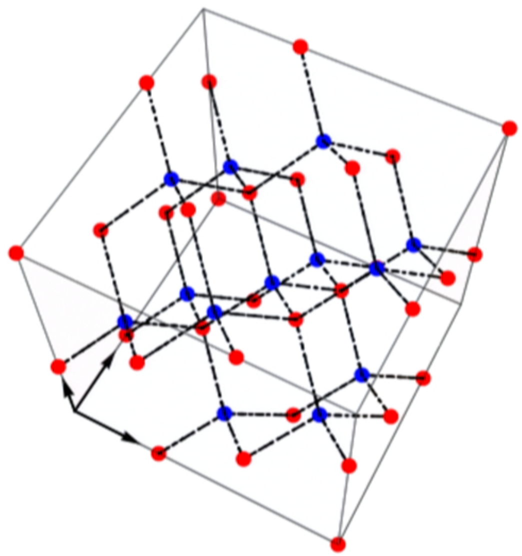


e.g. diamond lattice

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

No!

one (spinless) fermion per unit cell
not always sufficient



e.g. diamond lattice

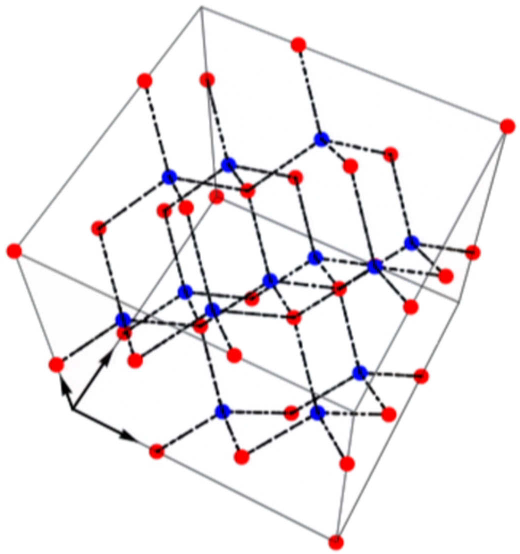
band insulators <u>only</u>
when filling is a multiple of 2

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

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

No!

one (spinless) fermion per unit cell
not always sufficient



e.g. diamond lattice

band insulators only
when filling is a multiple of 2

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

Band insulator only if filling = multiple of *S*

[S.P., *et. al., Nat. Phys.* **9**, 299]

#1: Band-Sticking Constraints

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

#1: Band-Sticking Constraints

Band insulators are featureless: no symmetry breaking, unique g.s.

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

#1: Band-Sticking Constraints

Band insulators are featureless: no symmetry breaking, unique g.s.

In nonsymmorphic crystals: <u>forbidden</u> except at special fillings

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

#1: Band-Sticking Constraints

Band insulators are featureless: no symmetry breaking, unique g.s.

In nonsymmorphic crystals: forbidden except at special fillings

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

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

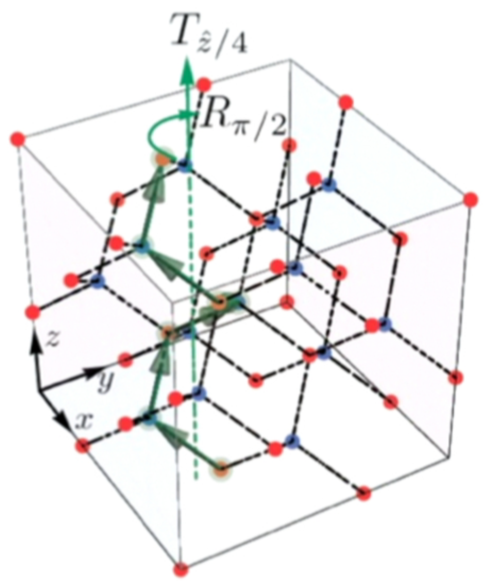
#1: Band-Sticking Constraints

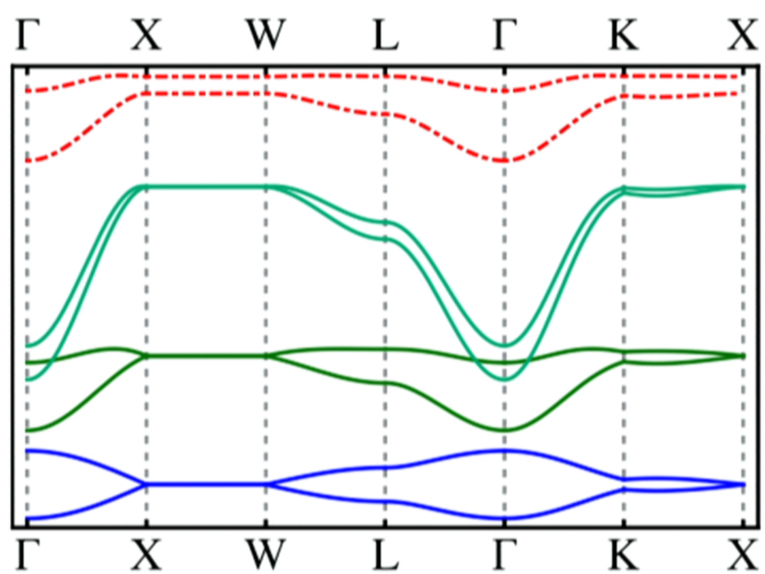
Band insulators are featureless: no symmetry breaking, unique g.s.

In nonsymmorphic crystals: forbidden except at special fillings

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

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





[S.P., *et. al.*, *Nat. Phys.* **9**, 299] [Hints in band theory literature: Herring; König & Mermin; Michel & Zak...]

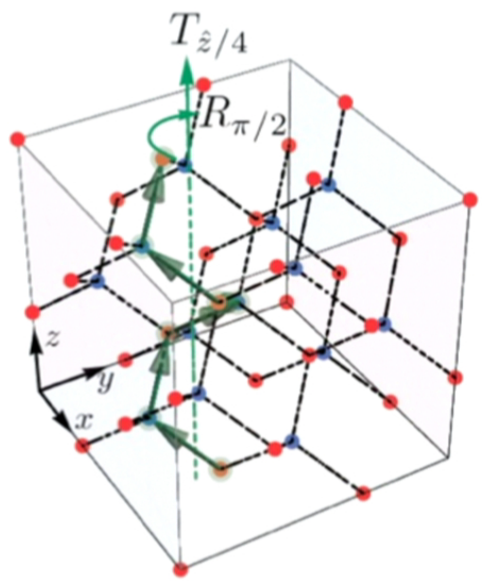
#1: Band-Sticking Constraints

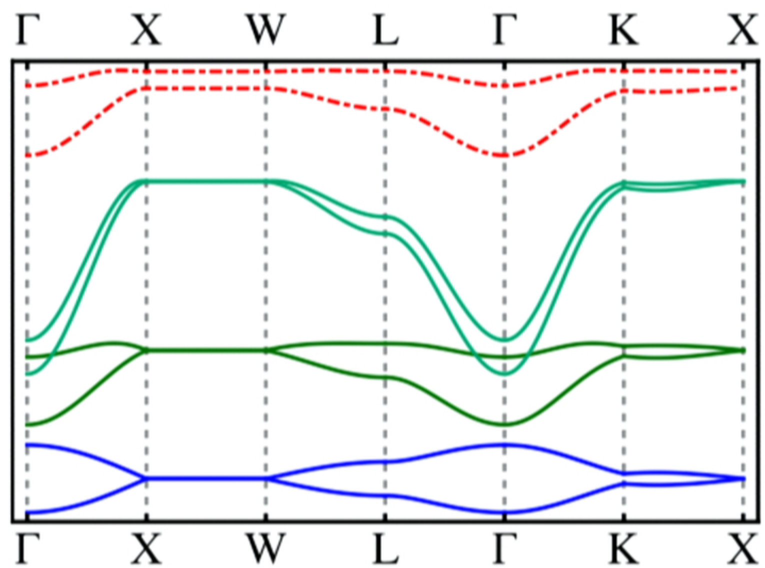
Band insulators are featureless: no symmetry breaking, unique g.s.

In nonsymmorphic crystals: <u>forbidden</u> except at special fillings

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

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





[S.P., *et. al.*, *Nat. Phys.* **9**, 299] [Hints in band theory literature: Herring; König & Mermin; Michel & Zak...]

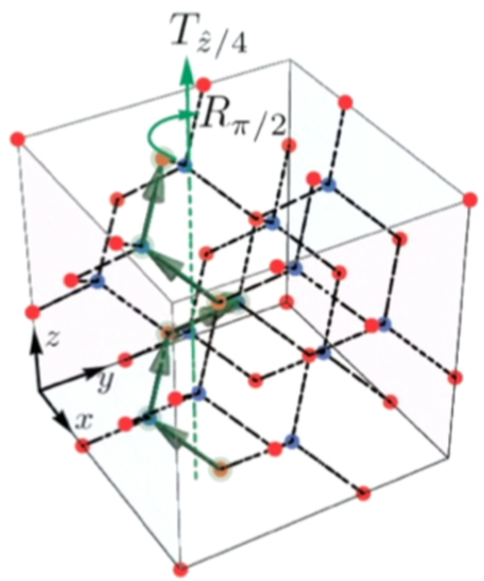
#1: Band-Sticking Constraints

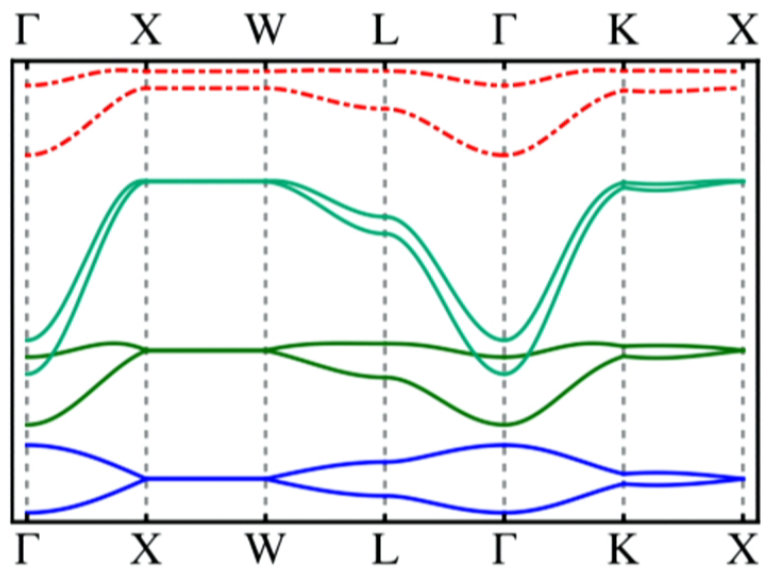
Band insulators are featureless: no symmetry breaking, unique g.s.

In nonsymmorphic crystals: <u>forbidden</u> except at special fillings

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

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





[S.P., *et. al.*, *Nat. Phys.* **9**, 299] [Hints in band theory literature: Herring; König & Mermin; Michel & Zak...]

#2: Searching for Spin Liquids

All our argument required was a conserved U(1) charge

99]

#2: Searching for Spin Liquids

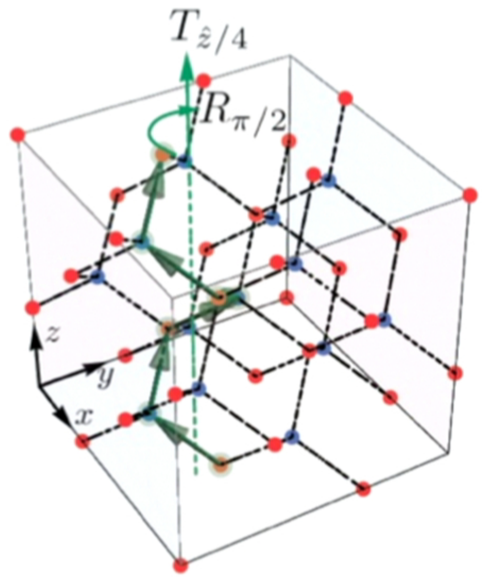
All our argument required was a conserved U(1) charge

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

#2: Searching for Spin Liquids

All our argument required was a conserved U(1) charge

For spin systems: conserved S_z

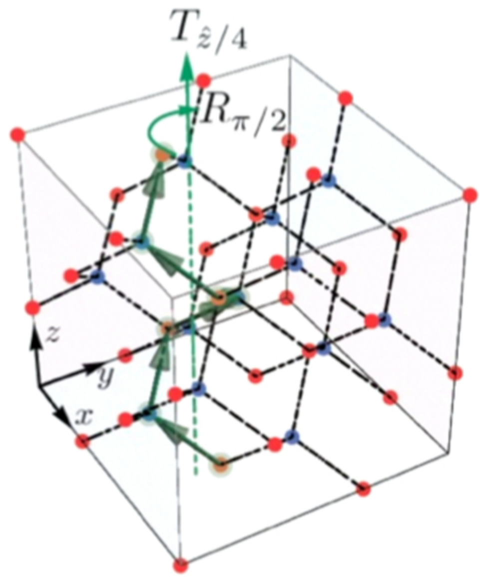


[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

#2: Searching for Spin Liquids

All our argument required was a conserved U(1) charge

For spin systems: conserved S_z



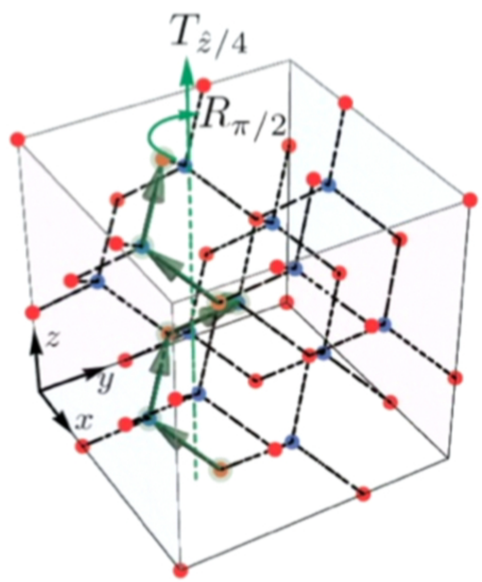
e.g. spin-1/2 moments, diamond lattice

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

#2: Searching for Spin Liquids

All our argument required was a conserved U(1) charge

For spin systems: conserved S_z



e.g. spin-1/2 moments, diamond lattice

(occurs in materials: A-site spinels)

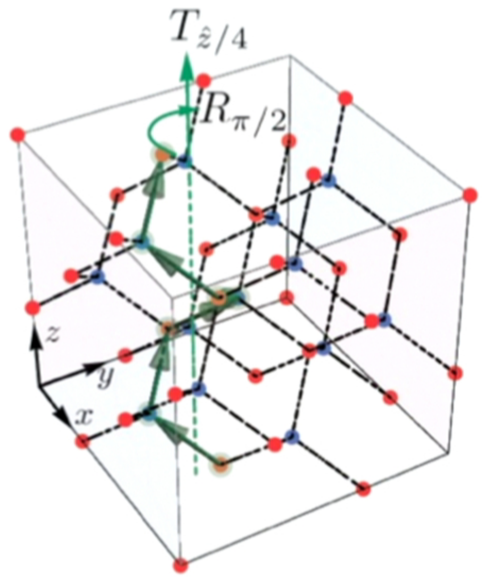
Spin-gapped gs must break symmetry, or be a spin liquid

[S.P., et. al., *Nat. Phys.* **9**, 299]

#2: Searching for Spin Liquids

All our argument required was a conserved U(1) charge

For spin systems: conserved S_z



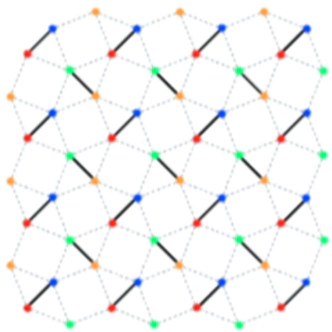
e.g. spin-1/2 moments, diamond lattice

(occurs in materials: A-site spinels)

Spin-gapped gs must break symmetry,
or be a spin liquid

[S.P., et. al., *Nat. Phys.* **9**, 299]

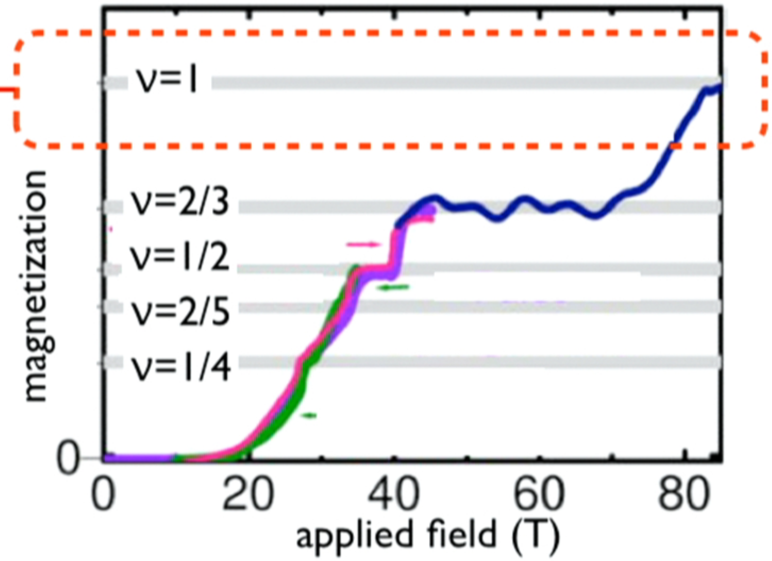
#3: Magnetization Plateaus



$SrCu(BO_3)_2$
(Shastry-Sutherland)

'filling' $\nu = 2 \times \frac{\text{Magnetization}}{\text{Sat. Magnetization}}$

<u>ν=1</u>
broken symmetry
<u>or</u> spin liquid!



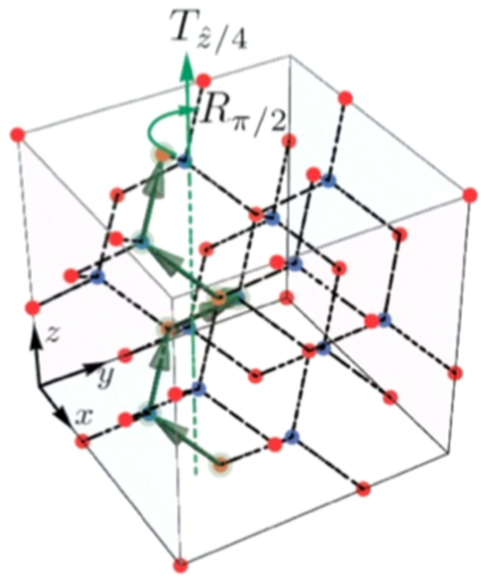
[<u>S.P.</u>, *et. al.*, *Nat. Phys.* **9**, 299]

[S.E. Sebastian *et. al.*, *PNAS* '08]

#2: Searching for Spin Liquids

All our argument required was a conserved U(1) charge

For spin systems: conserved S_z



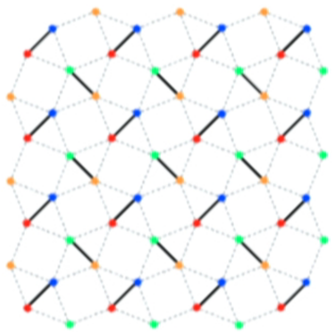
e.g. spin-1/2 moments, diamond lattice

(occurs in materials: A-site spinels)

Spin-gapped gs must break symmetry, or be a spin liquid

[S.P., et. al., Nat. Phys. 9, 299]

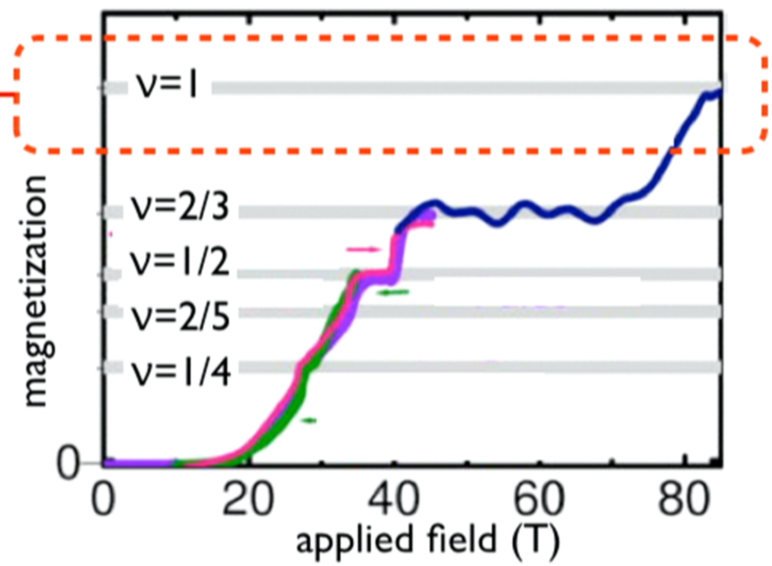
#3: Magnetization Plateaus



$SrCu(BO_3)_2$
(Shastry-Sutherland)

'filling' $\nu = 2\times \frac{\text{Magnetization}}{\text{Sat. Magnetization}}$

ν=1
broken symmetry
or spin liquid!



[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

[S.E. Sebastian *et. al.*, *PNAS* '08]

Viewed from perspective of real space, preserving symmetry rests on where to place 'center of charge'

(work with bosons for simplicity)

On non-symmorphic lattice, such choice always breaks symmetry

On symmorphic lattice, such a choice is always possible

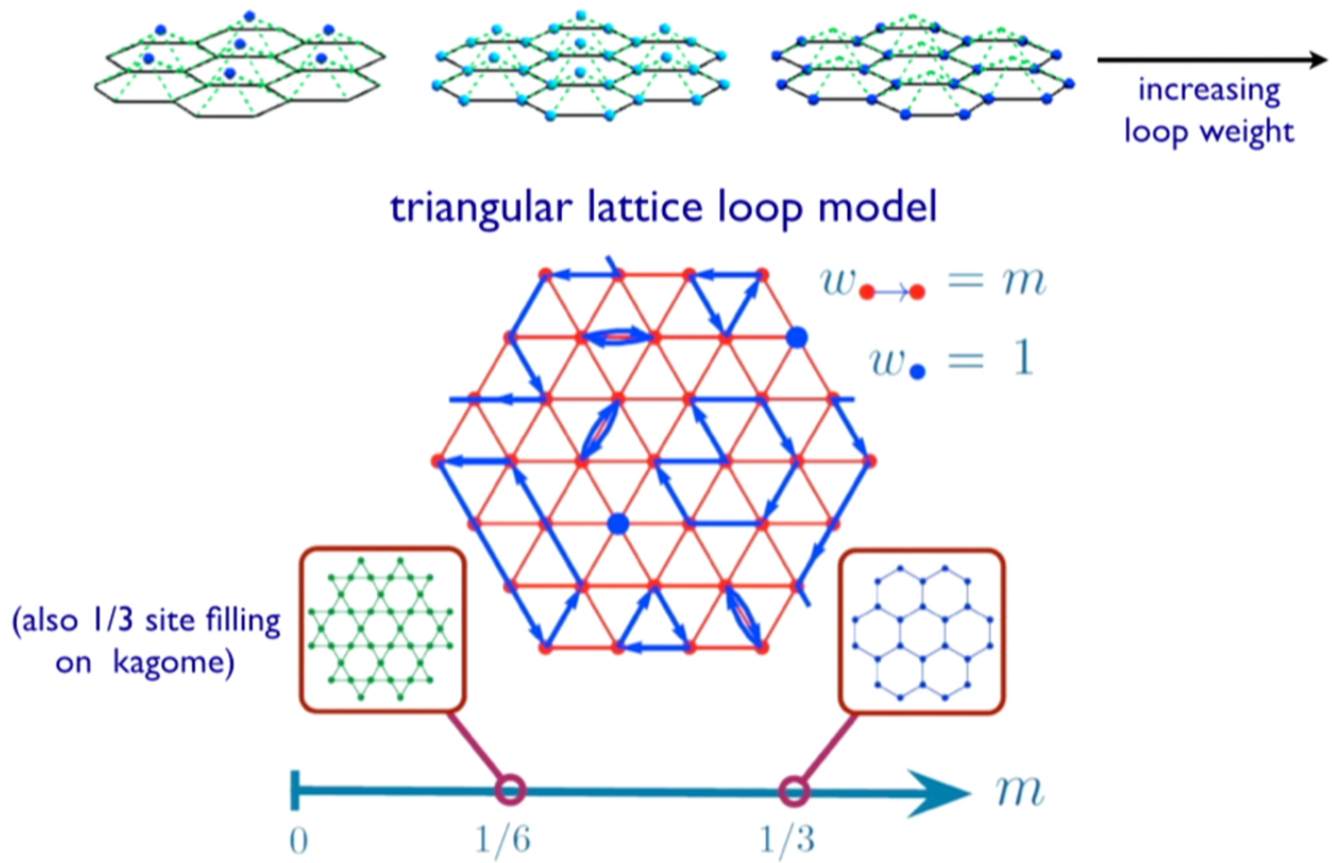
but

particular tight-binding lattice may not have 'site' at symmetry center

On such lattices, we can construct 'quantum' Bose insulators

Honeycomb Lattice Example

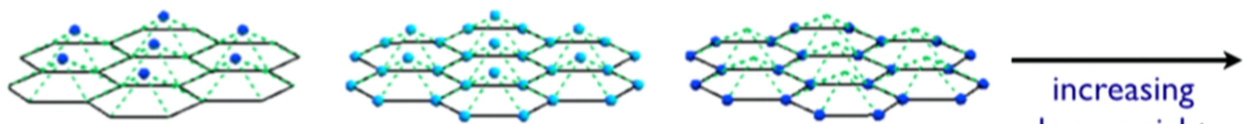
Symmorphic: 1 boson per unit cell (half-site-filling)



[S.P., et. al., *PRL* **110**, 125301(2013); I. Kimchi, S.P., et. al., *PNAS* **110** 16378 (2013)]

Honeycomb Lattice Example

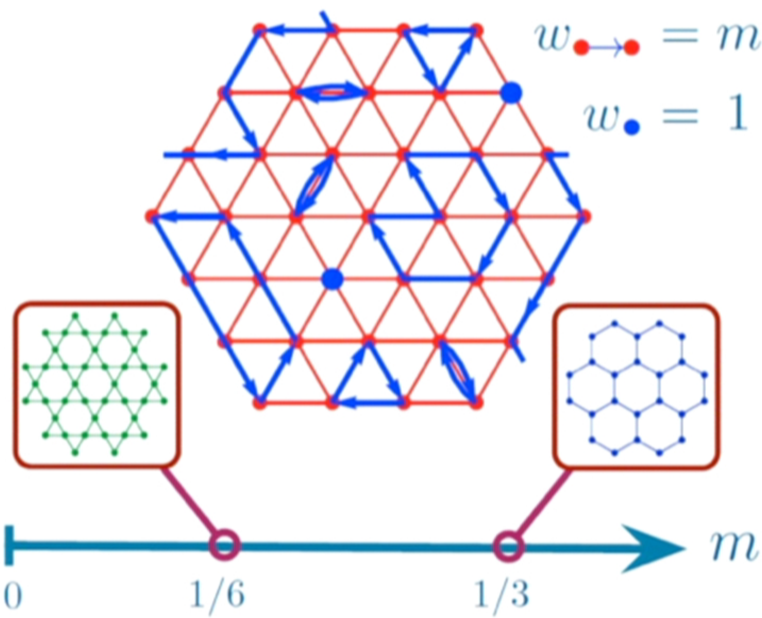
Symmorphic: 1 boson per unit cell (half-site-filling)



increasing
loop weight

triangular lattice loop model

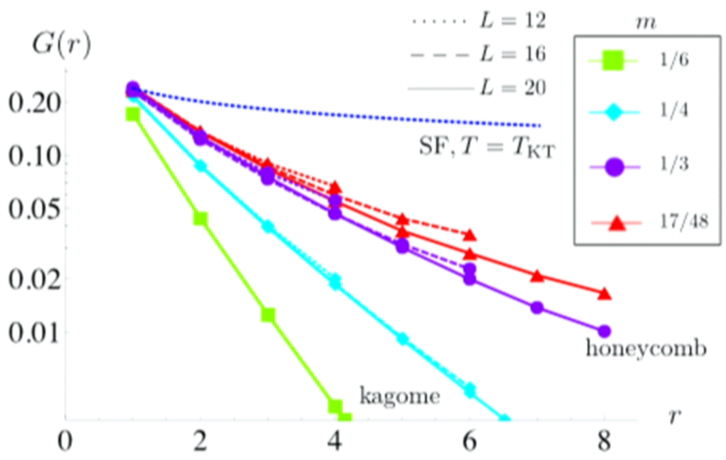
(also 1/3 site filling
on kagome)



[S.P., *et. al.*, *PRL* **110**, 125301(2013); I. Kimchi, S.P., *et. al.*, *PNAS* **110** 16378 (2013)]

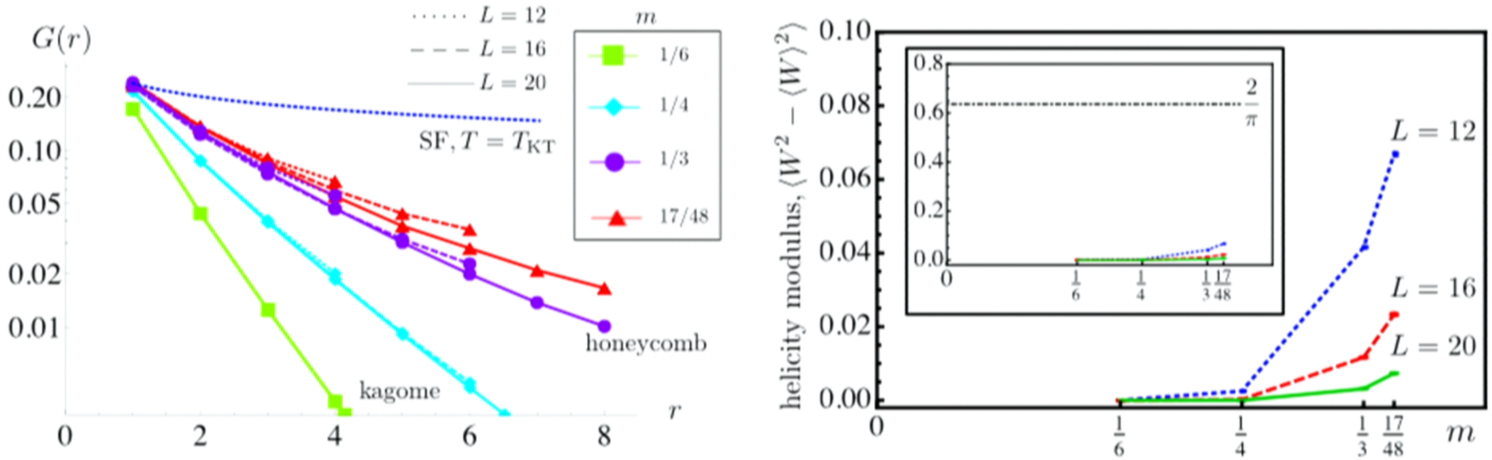
Honeycomb Lattice Example

Monte Carlo Results from Loop model



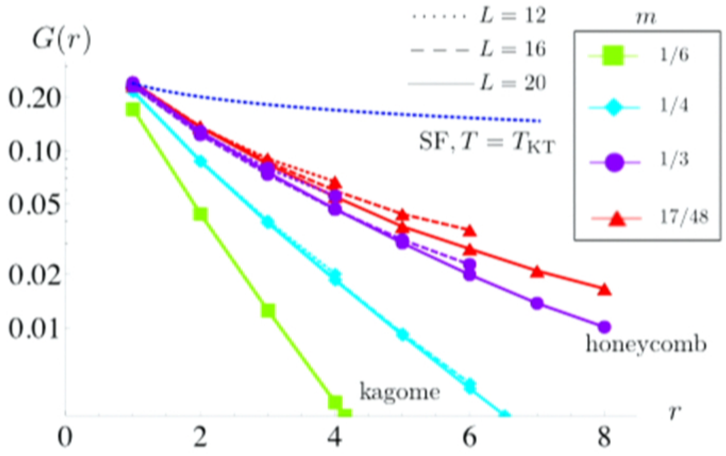
Honeycomb Lattice Example

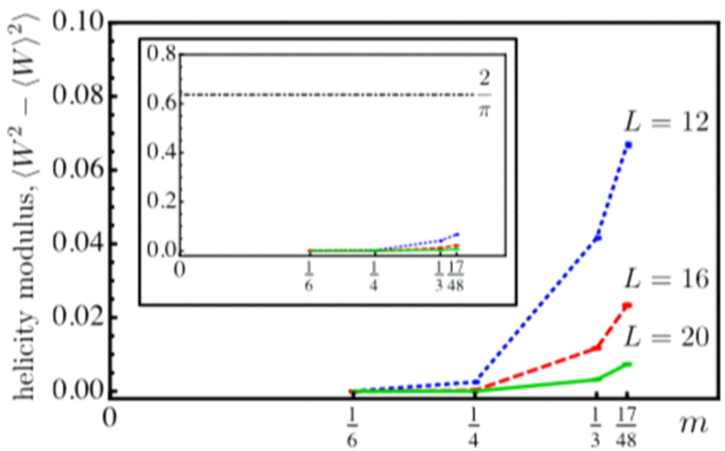
Monte Carlo Results from Loop model

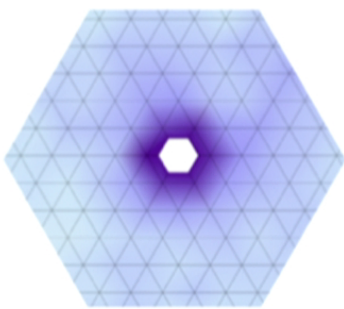


Honeycomb Lattice Example

Monte Carlo Results from Loop model







Exponential decaying boson correlations (no SF)

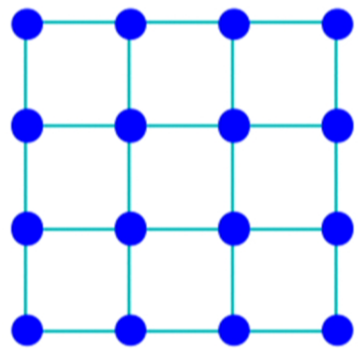
No discrete symmetry breaking

‘Many-Body Polarization’ Arguments (Briefly)

‘Many-Body Polarization’ Arguments (Briefly)

How do we build an insulator?

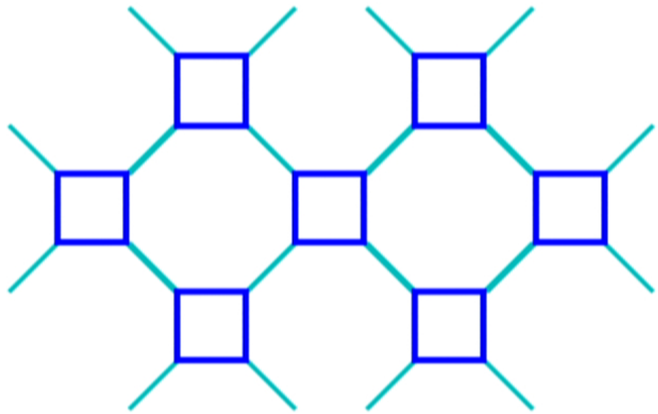
I particle per unit cell



classical particles,
fixed number/site

How do we build an insulator?

1 particle per unit cell

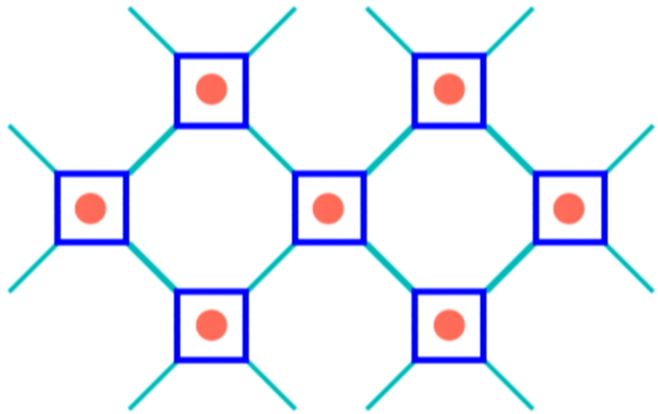


'molecular orbitals'

Can be formalized in terms of polarization

How do we build an insulator?

1 particle per unit cell



'molecular orbitals'

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

Can be formalized in terms of polarization

Polarization Approach

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, which are localized in disconnected regions of the many-particle configuration space and have essentially vanishing overlap. This property is the analog of localization for a single particle and leads directly to the electrical properties characteristic of insulators. An Appendix deals with a soluble model exhibiting a transition between an insulating and a conducting state.

Polarization Approach

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, which are localized in disconnected regions of the many-particle configuration space and have essentially vanishing overlap. This property is the analog of localization for a single particle and leads directly to the electrical properties characteristic of insulators. An Appendix deals with a soluble model exhibiting a transition between an insulating and a conducting state.

Flux threading, sensitivity to b.c.s, and polarization: all related

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

Polarization Approach

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, which are localized in disconnected regions of the many-particle configuration space and have essentially vanishing overlap. This property is the analog of localization for a single particle and leads directly to the electrical properties characteristic of insulators. An Appendix deals with a soluble model exhibiting a transition between an insulating and a conducting state.

Flux threading, sensitivity to b.c.s, and polarization: all related

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

Can interpret LSMHO in terms of polarization

Nakamura & Voit; Ortiz, Martin

Polarization Approach

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, which are localized in disconnected regions of the many-particle configuration space and have essentially vanishing overlap. This property is the analog of localization for a single particle and leads directly to the electrical properties characteristic of insulators. An Appendix deals with a soluble model exhibiting a transition between an insulating and a conducting state.

Flux threading, sensitivity to b.c.s, and polarization: all related

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

Can interpret LSMHO in terms of polarization

Nakamura & Voit; Ortiz, Martin

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

Combining Polarization and Fourier Crystallography

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

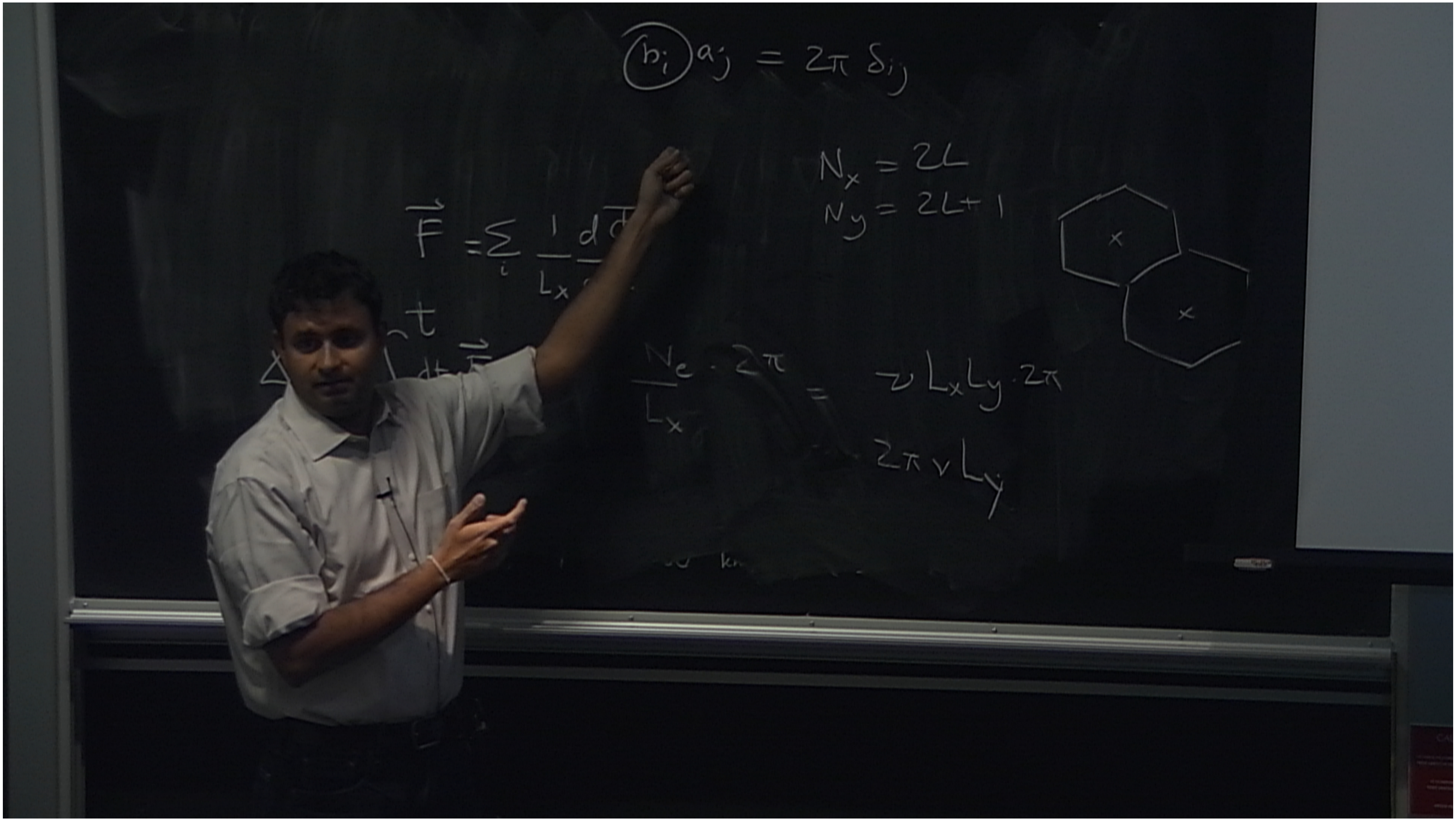
'twist operator': $\hat{U}_{\mathbf{k}} = e^{i\int d^3r(\mathbf{k}\cdot\mathbf{r})\hat{\rho}(\mathbf{r})}$

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

$$\mathbb{P}_{\mathbf{k}} \propto \arg\langle\Psi_0|\hat{U}_{\mathbf{k}}|\Psi_0\rangle$$

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

[S.P., *et. al.*, *Nat. Phys.* **9**, 299]

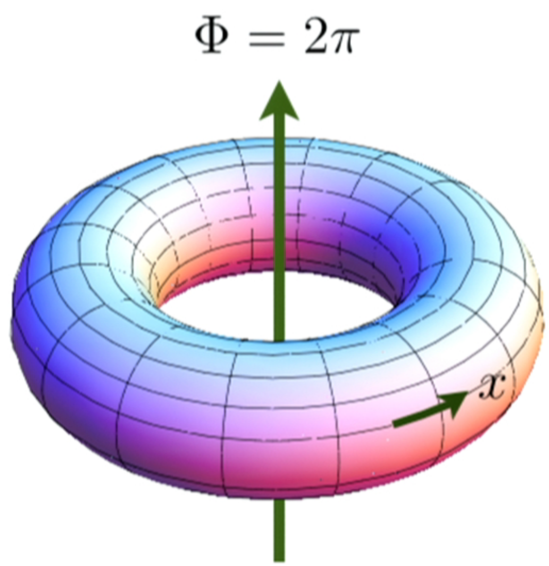


$b_i a_j = 2\pi \delta_{ij}$
$N_x = 2L$
$N_y = 2L+1$
$\vec{F} = \sum_i \frac{1}{L_x} \frac{d}{}$
$\frac{N_e \cdot 2\pi}{L_x} =$
$\nu L_x L_y \cdot 2\pi$
$2\pi \nu L_y$

Flux threading (Fractional Filling)

1. Thread 2π flux through 'handle'

$|\Psi_0\rangle \longrightarrow |\Psi$



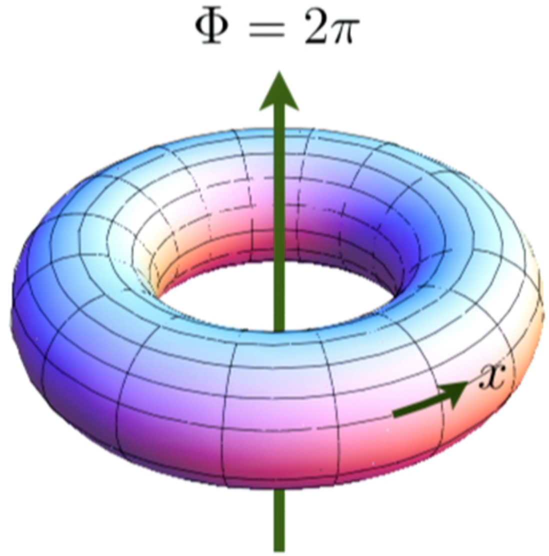
[Oshikawa, PRL **84**, 1535 (2000)]

Flux threading (Fractional Filling)

1. Thread 2π flux through 'handle'

$$|\Psi_0\rangle \longrightarrow |\Psi'_0\rangle$$

spectrum returns to itself



2. Gauge away inserted flux

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

$$|\Psi'_0\rangle$$

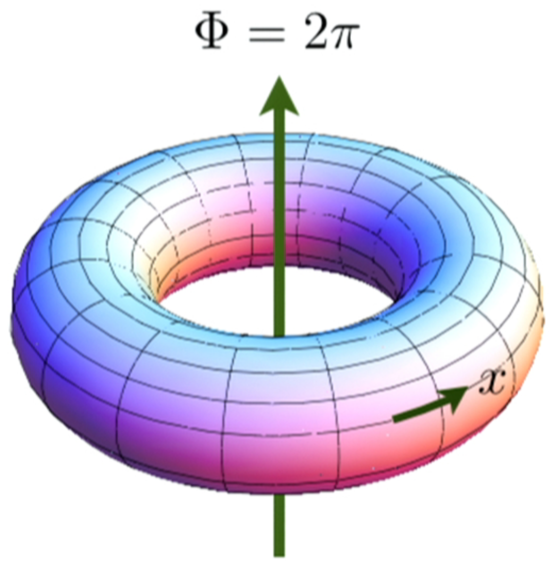
[Oshikawa, PRL **84**, 1535 (2000)]

Flux threading (Fractional Filling)

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 $|\Psi_0\rangle$

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

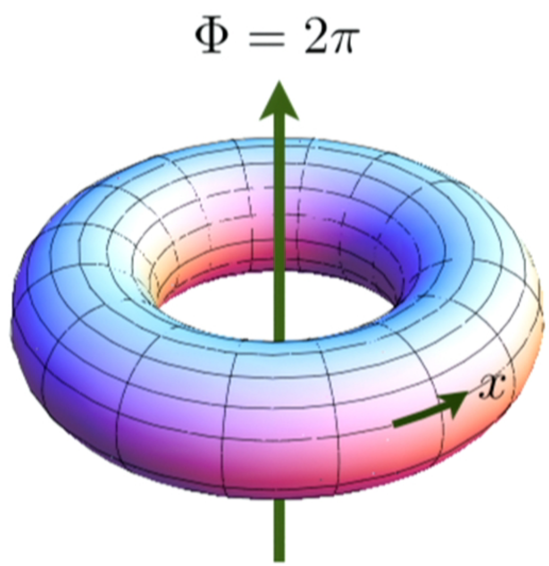
[Oshikawa, PRL **84**, 1535 (2000)]

Flux threading (Fractional Filling)

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')

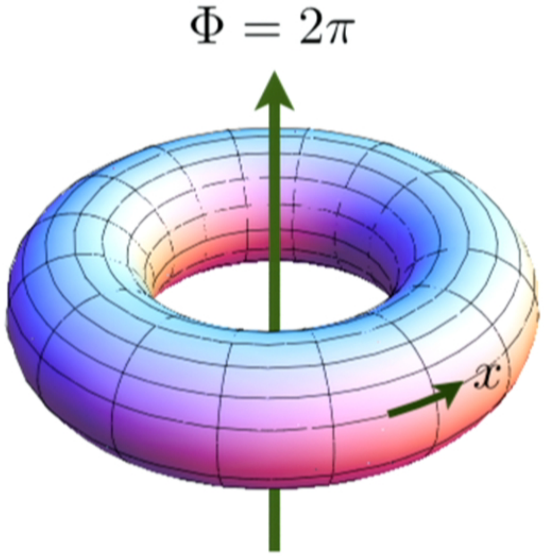
[Oshikawa, PRL **84**, 1535 (2000)]

Flux threading (Unit Filling)

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 $|\Psi_0\rangle$

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

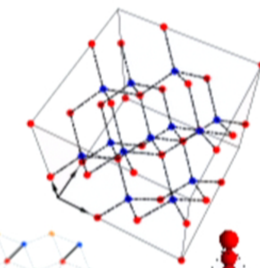
[SP, Turner, Arovas, Vishwanath, in progress]

Summary

<u>Basic Question</u>: can we constrain g.s. at <u>integer</u> filling?

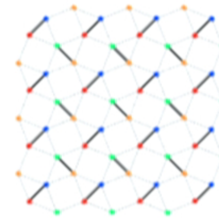
Symmetry invariant of space group: Nonsymmorphic Rank *S*

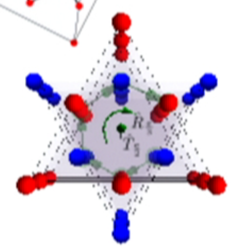
- minimum filling for featureless insulator
- Bloch bands 'stick' in groups of (at least) *S*
- implications: band theory, spin systems, fractionalization...



157/230 3D space groups have *S*>1

- hexagonal close packing (P6/mmc, *S*=2)
- diamond, pyrochlore (Fd3m, *S*=2)





Alternative Route: Polarization + Fourier-Space crystallography

time reversal? spin-orbit? quasicrystals?

Also: non-symmorphicity crucial for 'true' Crystalline TIs

[C-X Liu & R-X Zhang, arXiv:1308.4717]

<u>S.P.</u>, Turner, Arovas & Vishwanath, *Nature Physics* **9**, 299

[cf. also R.Roy, arXiv:1212.2944]