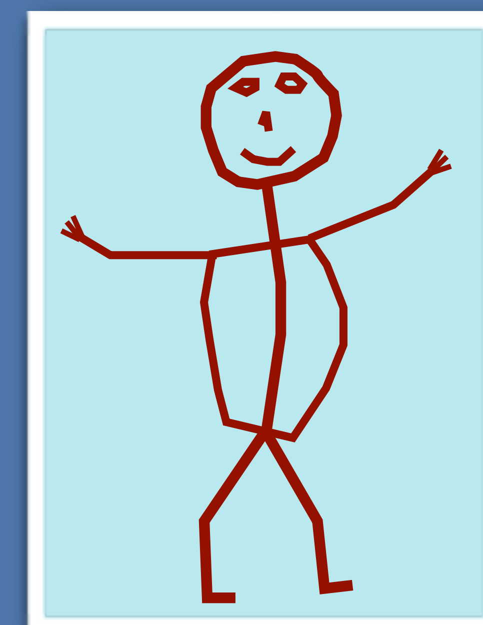
E	1	20/200
F P	2	20/100
T O Z	3	20/70
L P E D	4	20/50
P E C F D	5	20/40
E D F C Z P	6	20/30
F E L O P Z D	7	20/25
D E F P O T E C	8	20/20
L E F O D P C T	9	
F D P L T C E O	10	
P E Z O L C F T D	11	

Topological Obstructions to Band Insulator Behavior in Non-symmorphic Crystals

D. P. Arovas, UCSD



Siddharth Parameswaran
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Univ. Amsterdam → JHU

Ashvin Vishwanath
UC Berkeley

this is how I draw myself

Article : *Nature Physics* 9, 299 (2013)

Support : NSF , Simons Foundation , KITP , Aspen Center for Physics

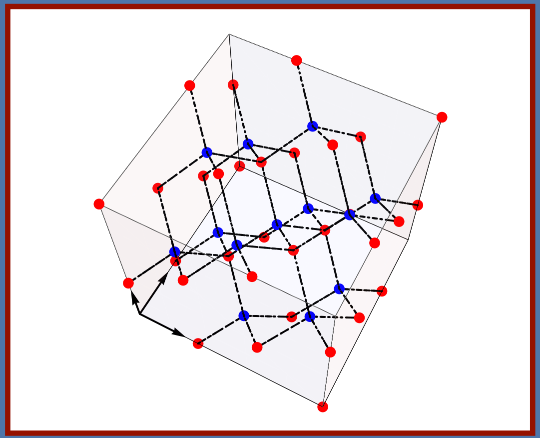
Phases of Matter

1. Classification by response functions:

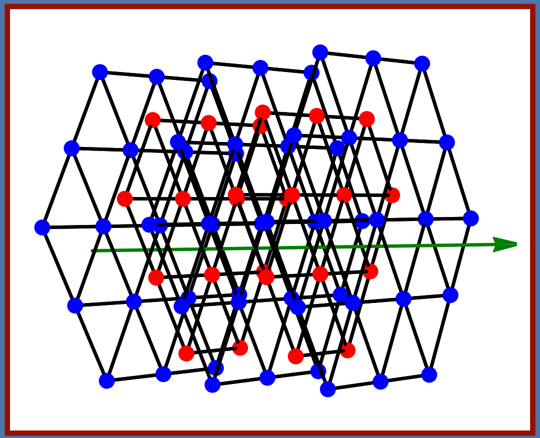
METAL

INSULATOR

2. Classification by crystalline symmetries:



DIAMOND

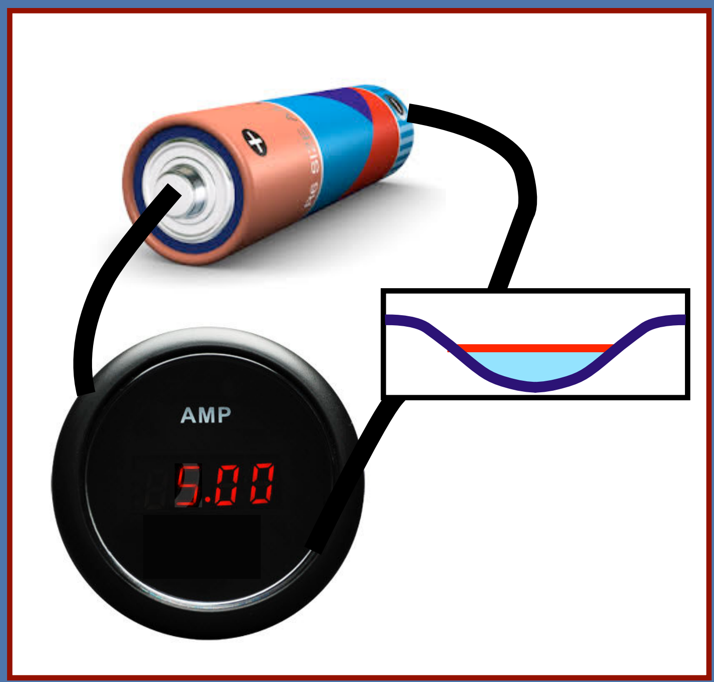


HCP

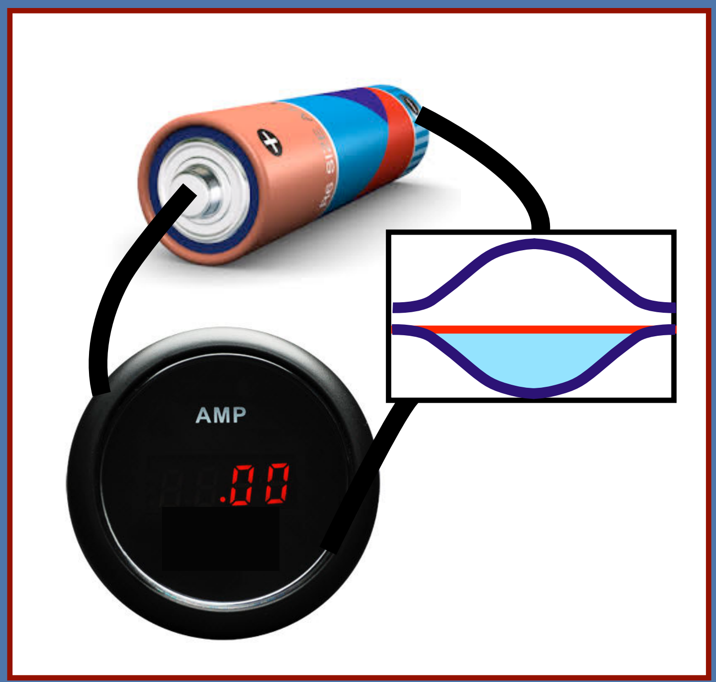
Band theory establishes a connection:

Bloch states: $\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r})\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$

Energy bands: $\varepsilon_n(\boldsymbol{k}) = \varepsilon_n(\boldsymbol{k}+\boldsymbol{K}) = \varepsilon_n(g\boldsymbol{k})$



METAL
some bands partially filled



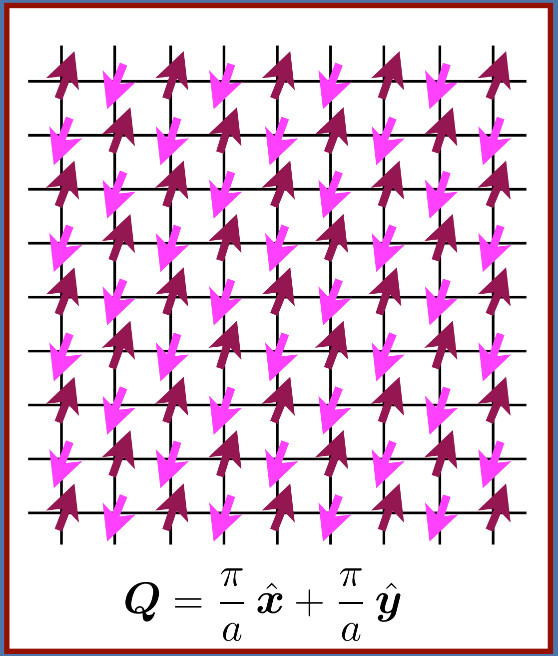
INSULATOR
all bands either filled or empty

noninteracting systems only!

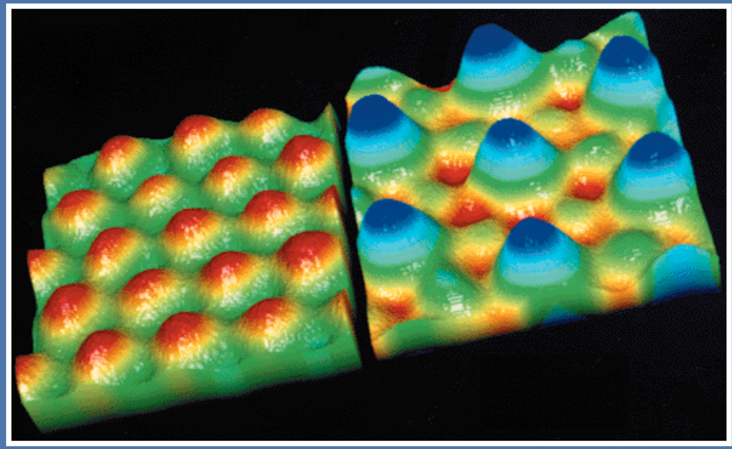
Effects of interactions

1) Benign : interacting ground state is adiabatically connected to noninteracting ground state from band theory.

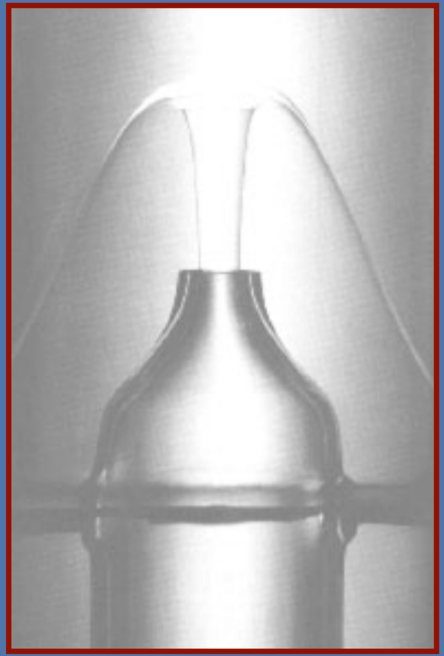
2) Essential : interacting ground state exhibits phenomenon of spontaneous symmetry breaking :



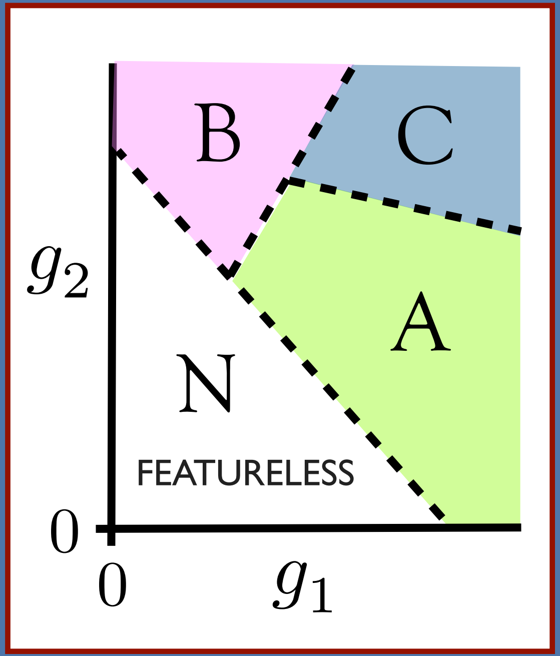
MAGNETS



DENSITY WAVES



SUPERFLUIDS

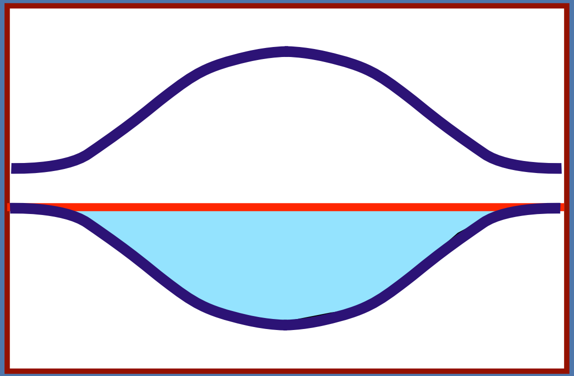


PHASE DIAGRAM

3) Any other possibilities?

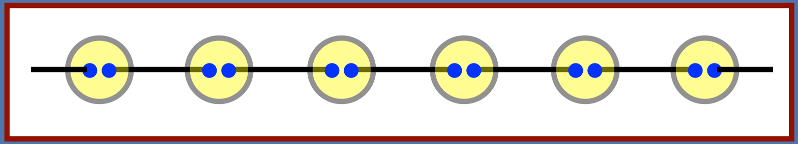
Can interactions produce a distinct symmetric phase not adiabatically connected to the noninteracting ground state?

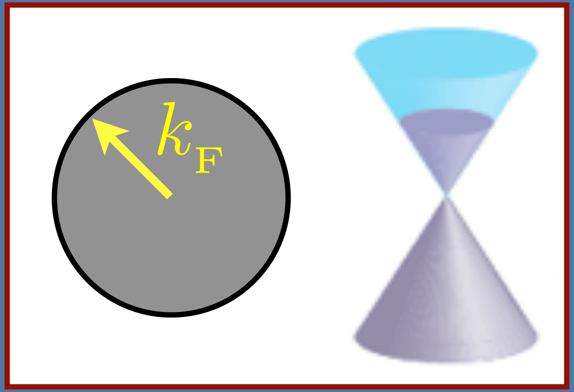
Examples of trivial phases without SSB:



band insulators
both topological and nontopological

quantum paramagnets
e.g. AKLT states

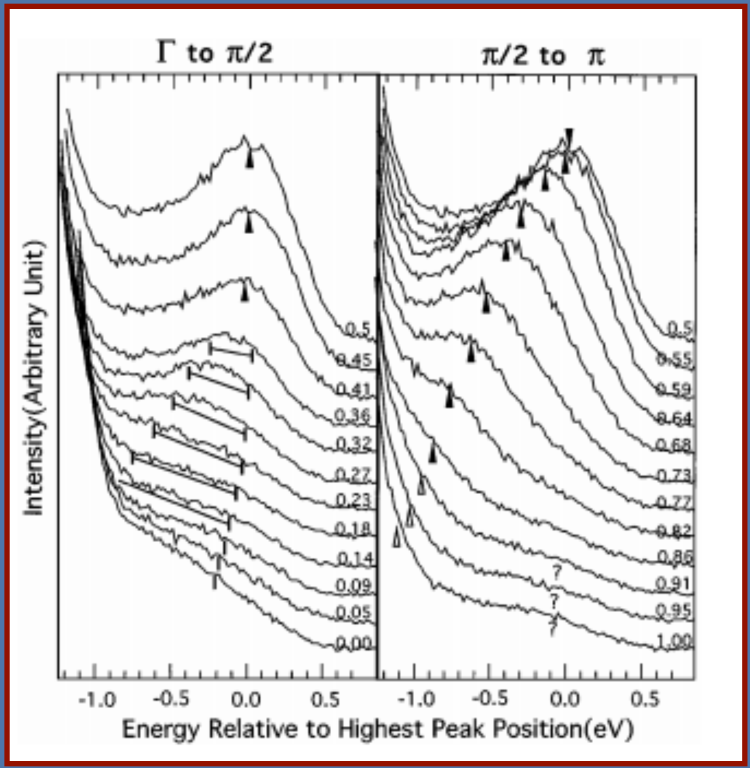




Fermi liquids
metals, semimetals

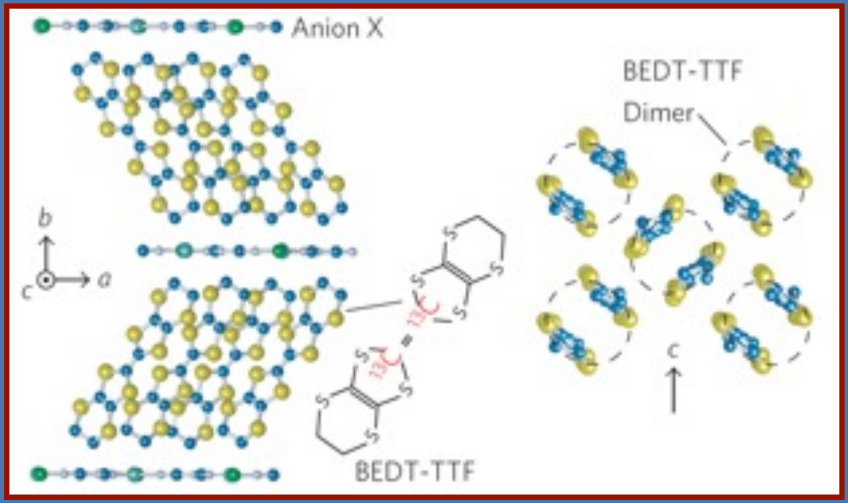
if gapped : unique ground state
if gapless : no fractionalization

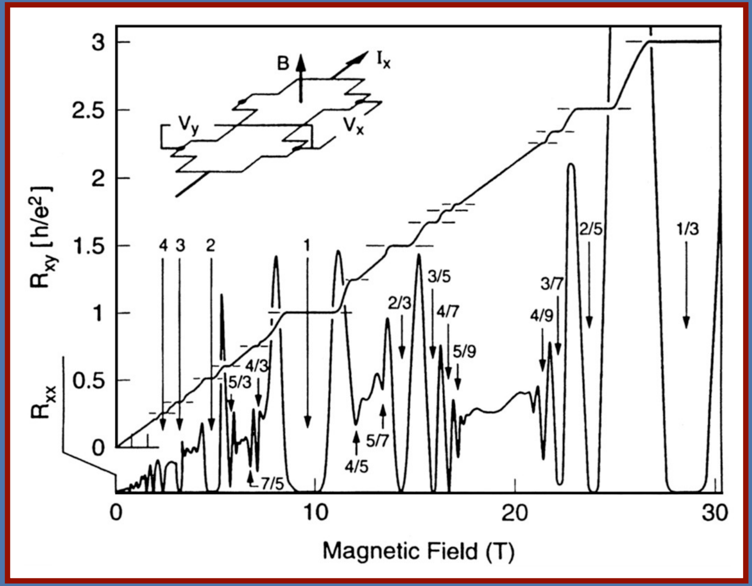
Examples of nontrivial phases without SSB:



Luttinger liquids
separation of spin and charge DOF

spin liquids
emergent gauge fields
fractionalization





FQHE
fractional charge and statistics

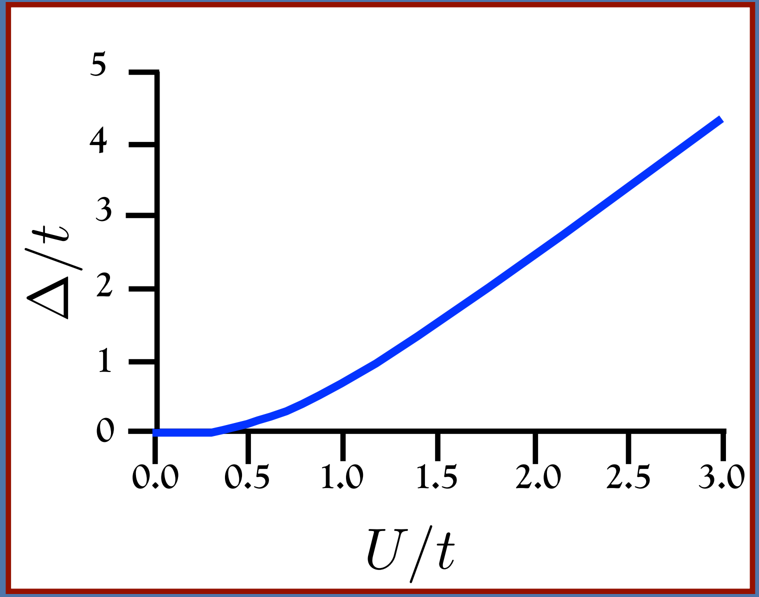
if gapped : degenerate vacua
all cases : fractionalization

Half-filled Hubbard model in d=1 dimension

$U \ll t$: *Umklapp* scattering relevant (g-ology)

$U \gg t$: strong coupling, $\Delta \propto U$

With $t = 1$: $\Delta = -4 + U + 8 \int_0^\infty \frac{d\omega}{\omega} \frac{J_1(\omega)}{1 + \exp(U\omega/2)}$



Spin-charge separation : spin metal + charge insulator

This state is **adiabatically disconnected** from the band insulator.

Filling factor : $\nu \equiv$ # electrons per cell per spin polarization

$\nu \in \mathbb{Z}$: adiabatic connection to band insulator

$\nu \in \mathbb{Z} + \frac{1}{2}$: Mott phase preserves all symmetries, but with no adiabatic connection to band insulator

At fractional filling, not even interactions can induce a unique symmetry-unbroken ground state.

This prompts the following question:

Q: If $\nu \in \mathbb{Z}$ is there always a band insulator?

A: No! For *nonsymmorphic* crystals, there is a topological obstruction to band insulator behavior unless the filling is ν is an integer multiple of the *non-symmorphic rank*, $\mathcal{S} \in \mathbb{Z}$

For $\nu \neq k \cdot \mathcal{S}$, the ground state must either be either

(i) gapless or (ii) topologically degenerate

Non-symmorphic crystallographic space groups

Basically, a space group S is nonsymmorphic if it includes *screw axes* or *glide planes*. Both of these operations involve *fractional translations* that are not within the Bravais lattice.

Formally, a crystallographic space group element $\{R\,,\boldsymbol{\tau}\}$ acts as

$$\{R\,,\boldsymbol{\tau}\}\boldsymbol{r} = R\boldsymbol{r} + \boldsymbol{\tau}$$

translation vector

point group matrix operation

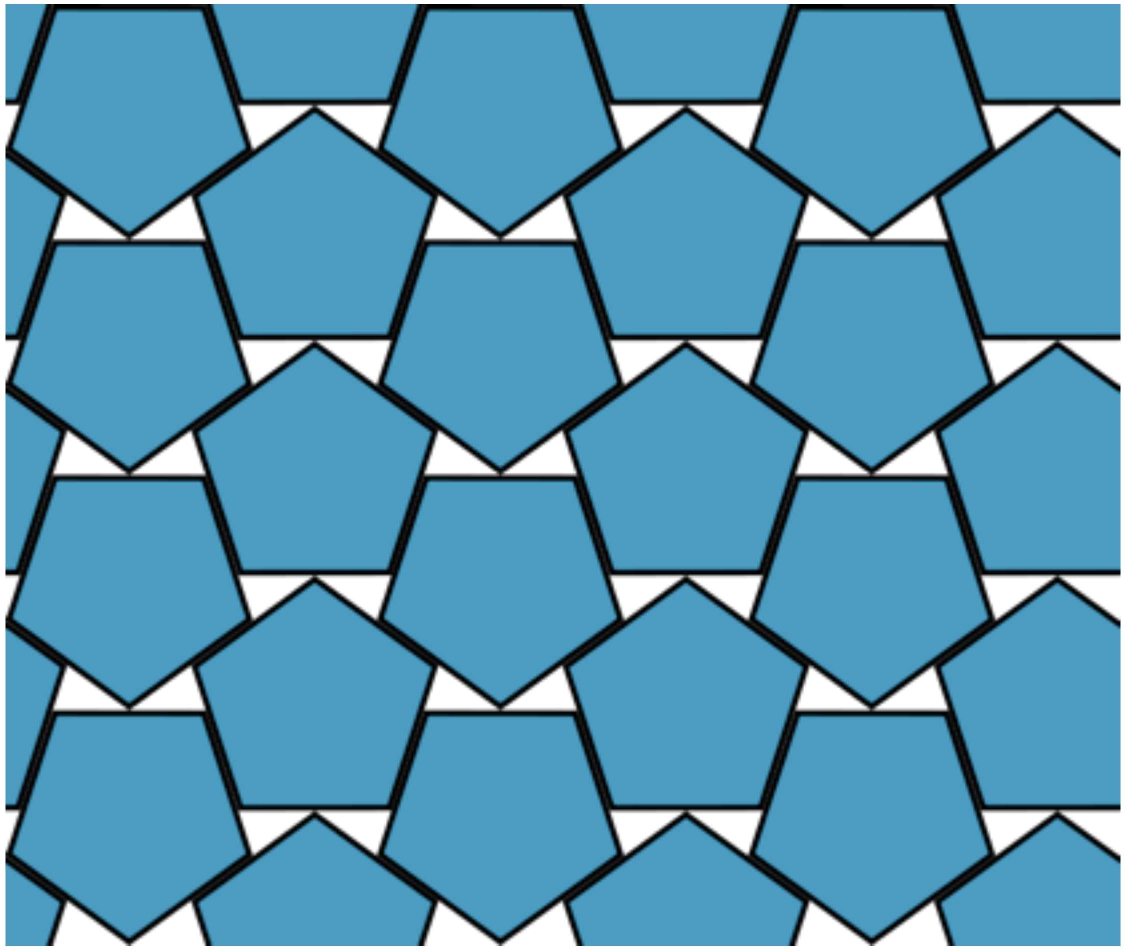
This forms a group under multiplication: $\{R,\boldsymbol{\tau}\}\{R',\boldsymbol{\tau}'\} = \{RR',R\boldsymbol{\tau}'+\boldsymbol{\tau}\}$

A space group is symmorphic when it is a semidirect product of the point group P and Bravais lattice translations T: $S = P \rtimes T$

A space group is nonsymmorphic when there is no possible choice of origin about which all its elements can be decomposed into a product of a lattice translation and a point group element.

Example : a lattice with a 2D glide line

space group $p4g$ (S. Parameswaran)



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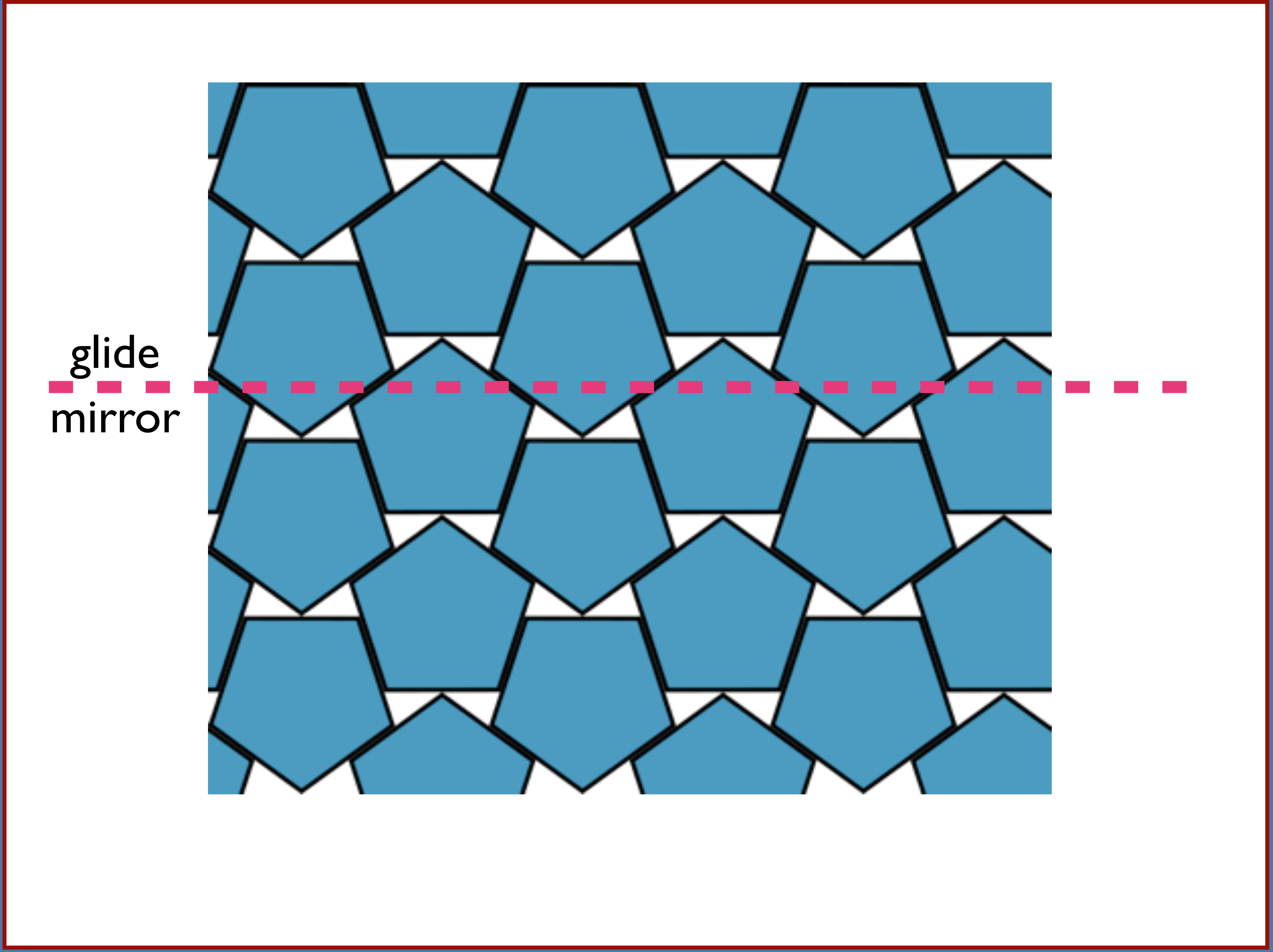

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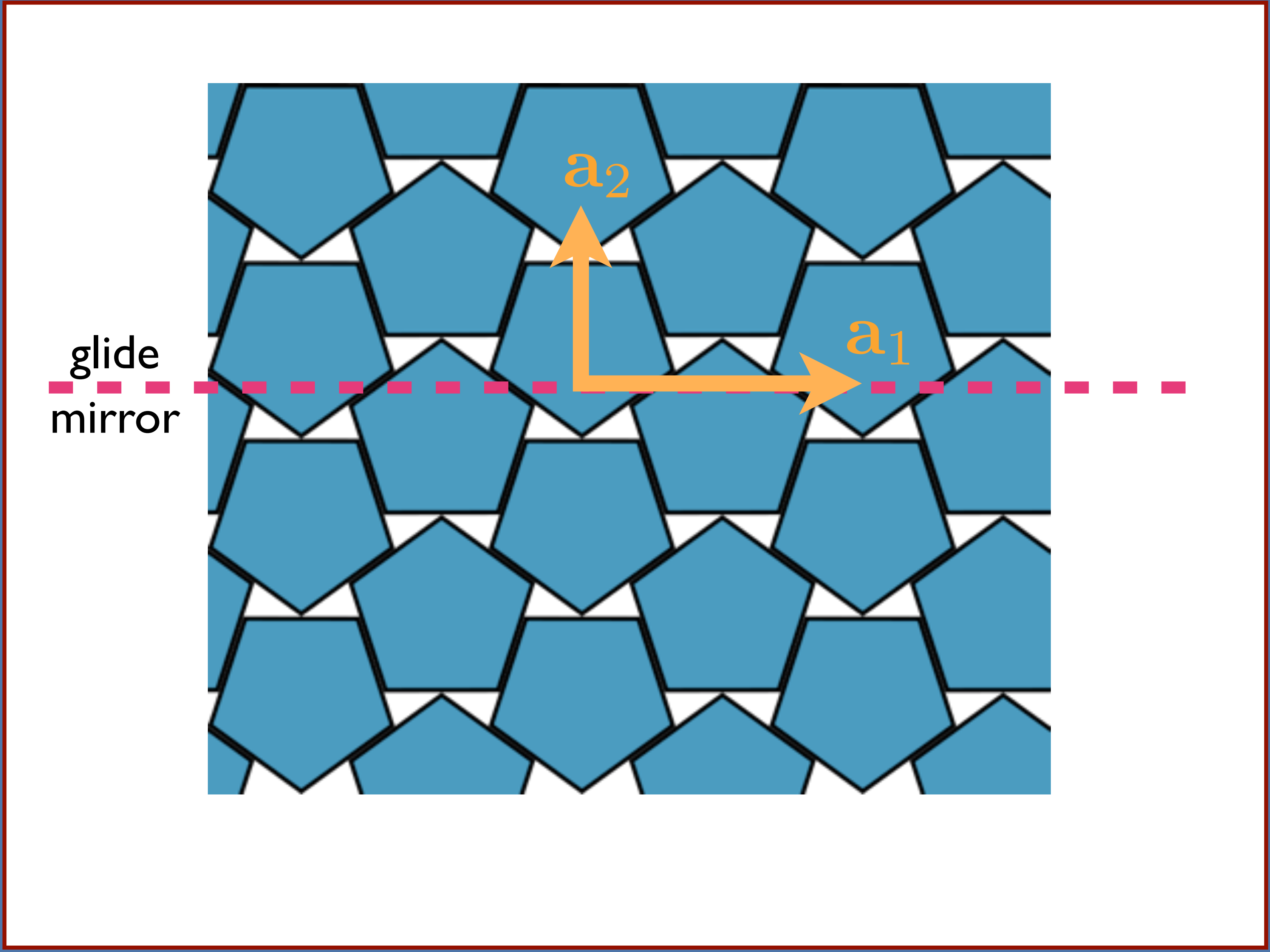

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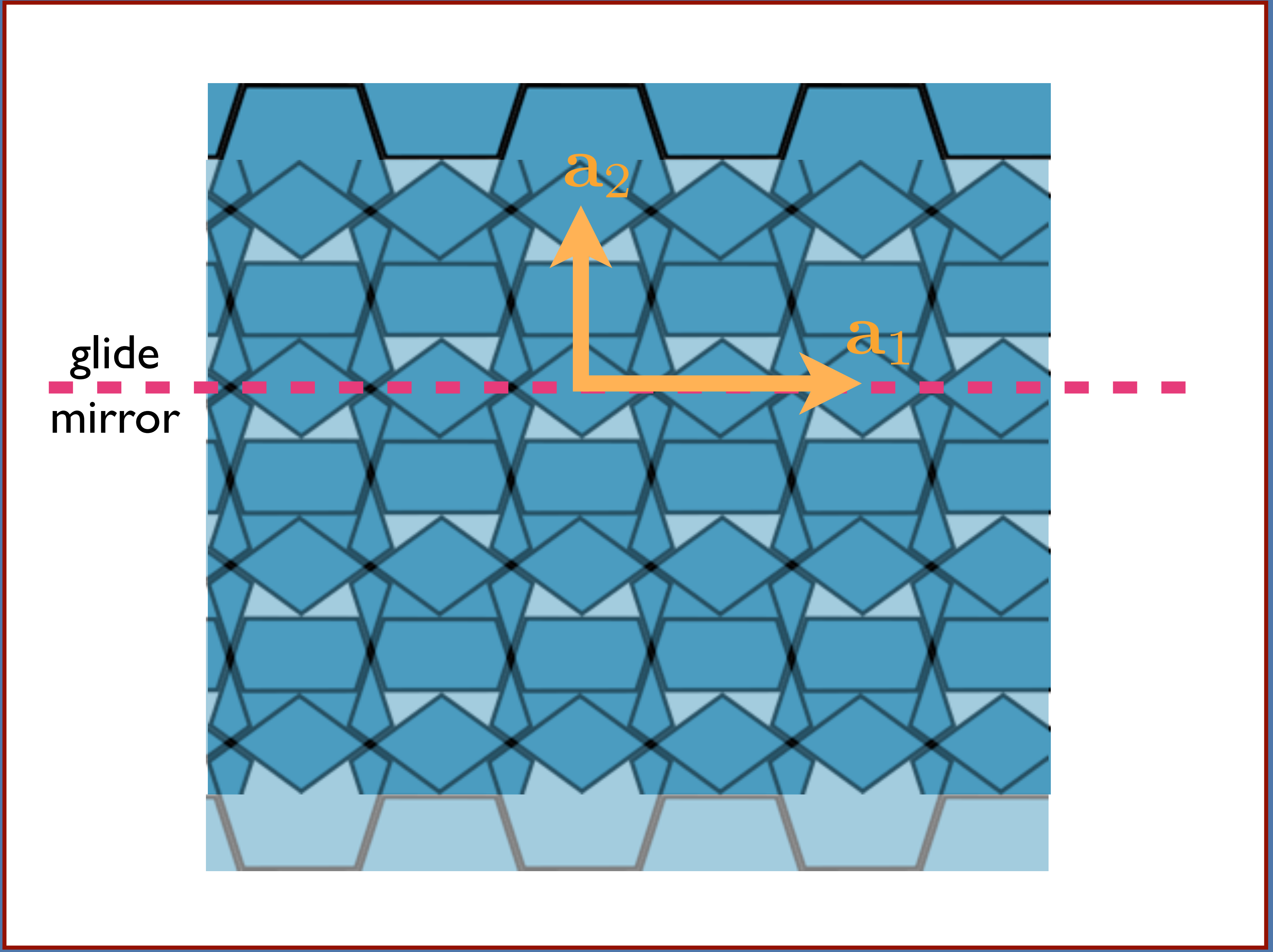

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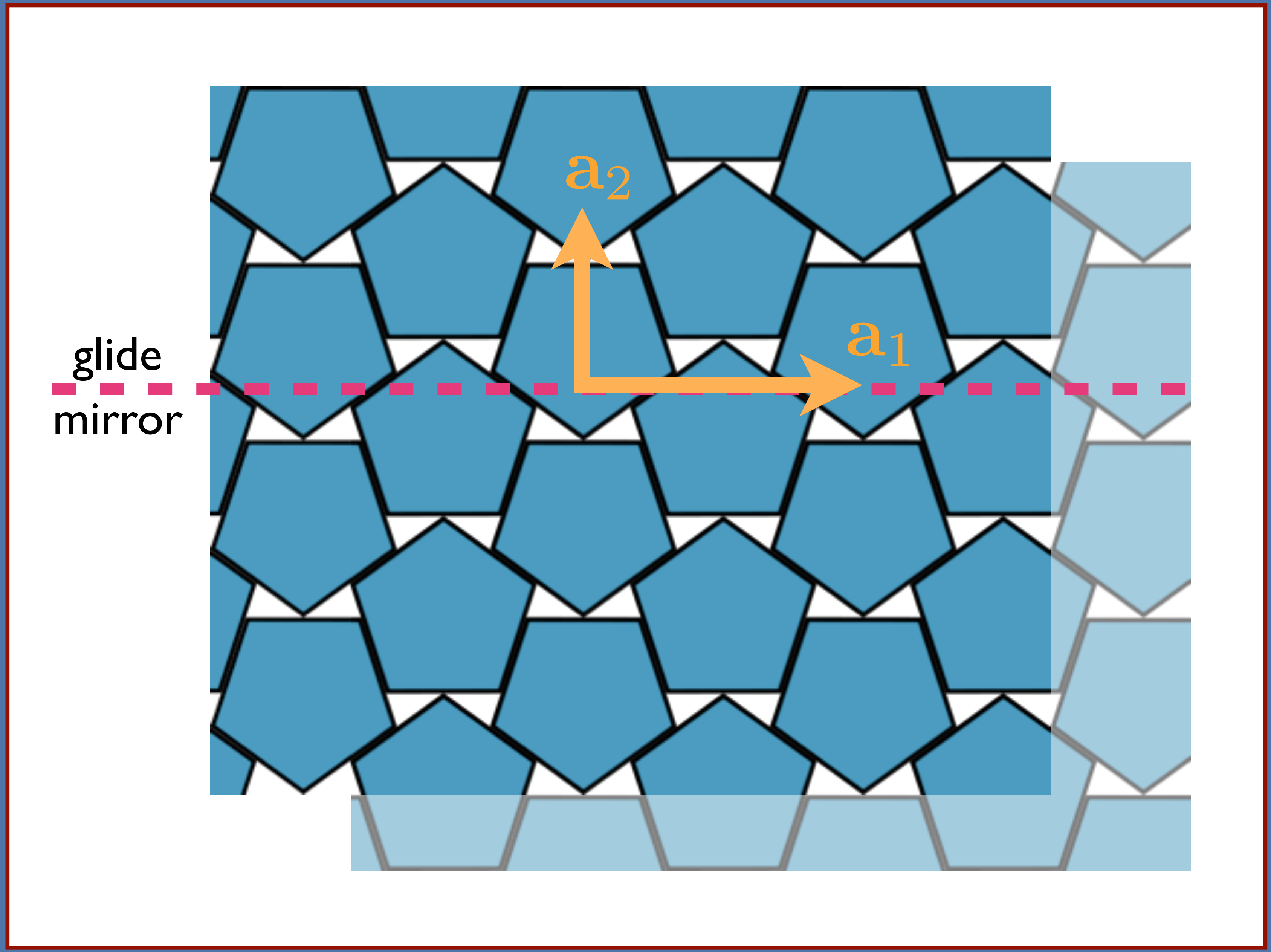
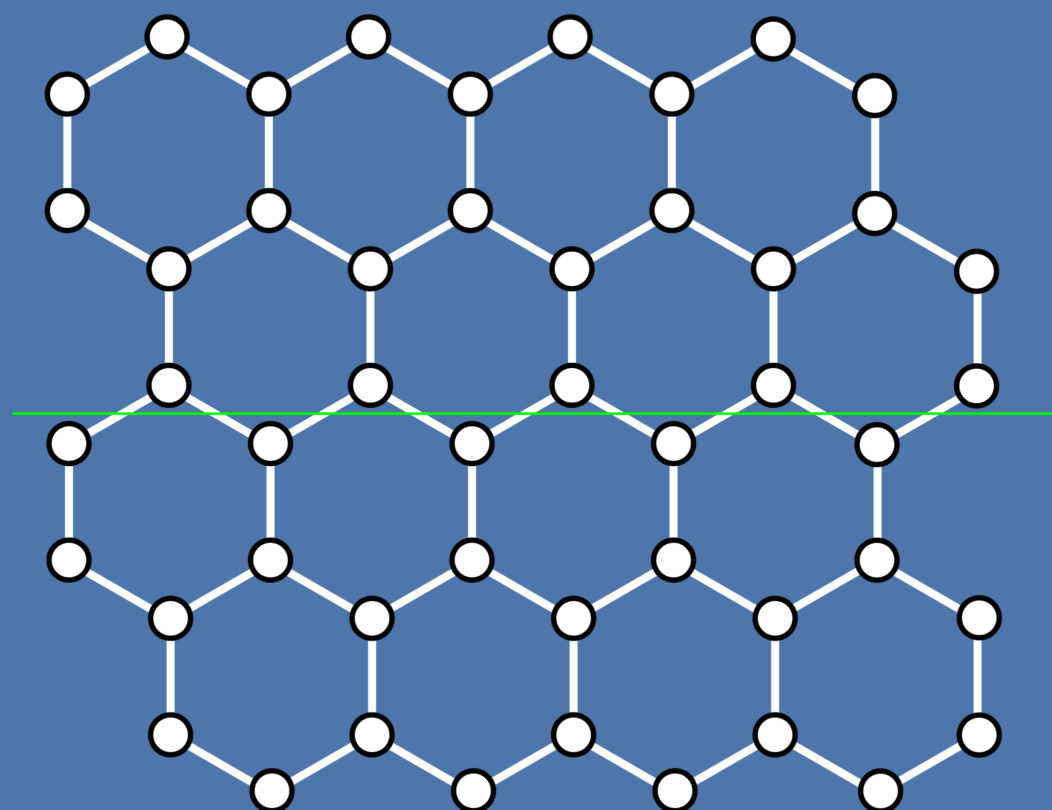


Glide operation : reflection in *x*-axis followed by translation by $\frac{1}{2}\boldsymbol{a}_1$

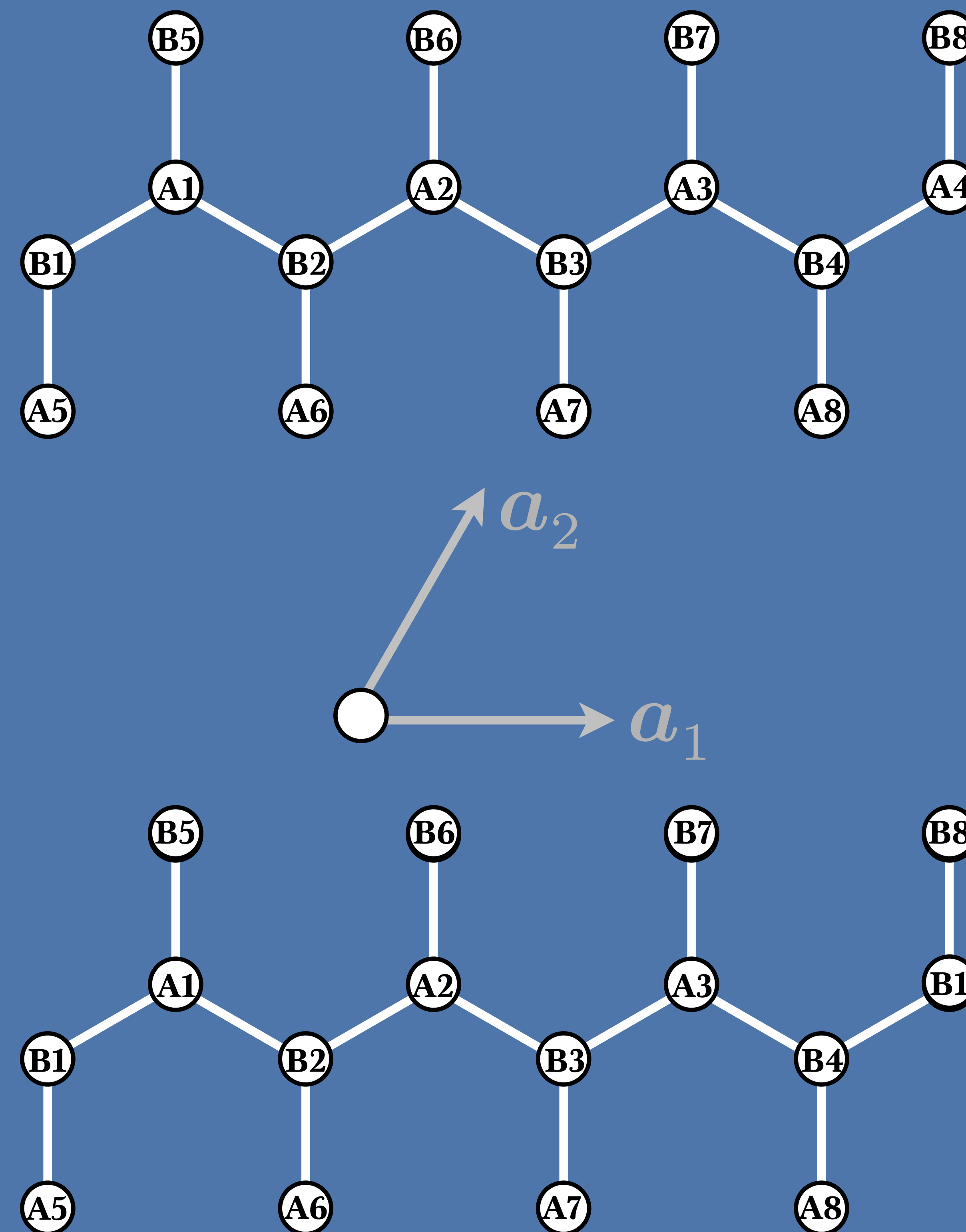
$$g = \left\{ I_x,\, \tfrac{1}{2}\boldsymbol{a}_1 \right\}$$

Essential vs. inessential <u>nonsymmorphic operations</u>

Graphene has a glide plane, yet its space group *p6m* is symmorphic!



The honeycomb glide is *inessential*, and may be written as an ordinary point group operation followed by a direct lattice vector translation.



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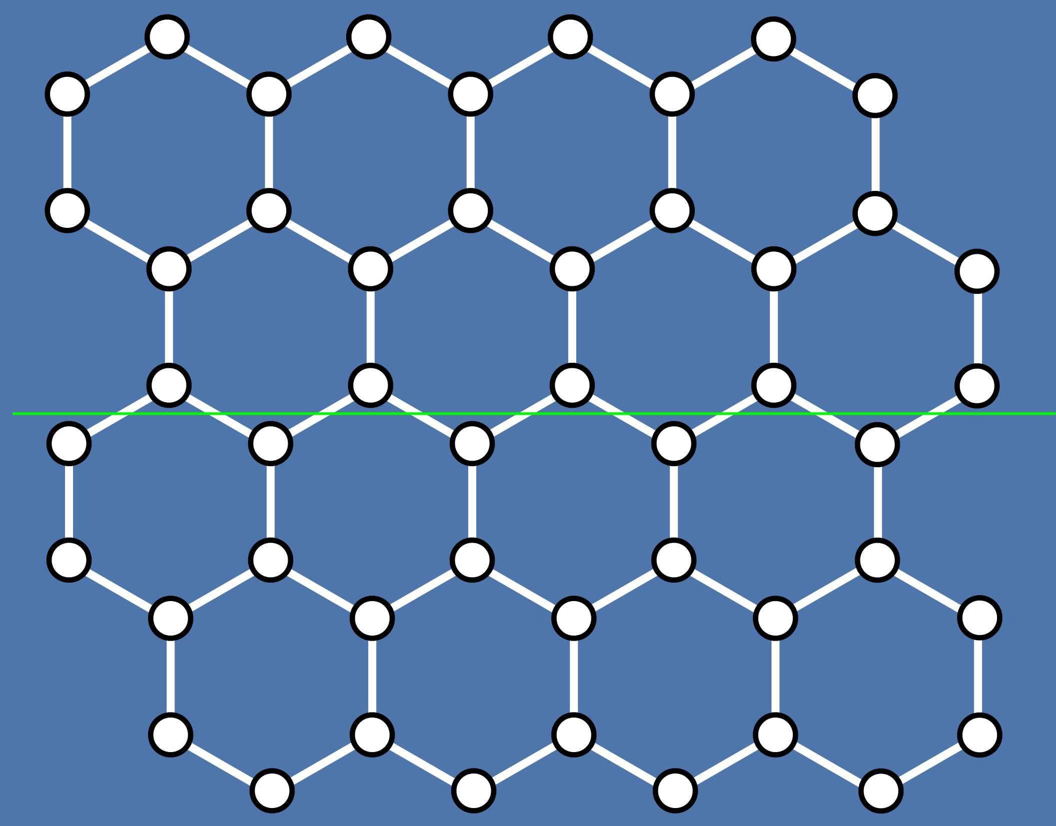

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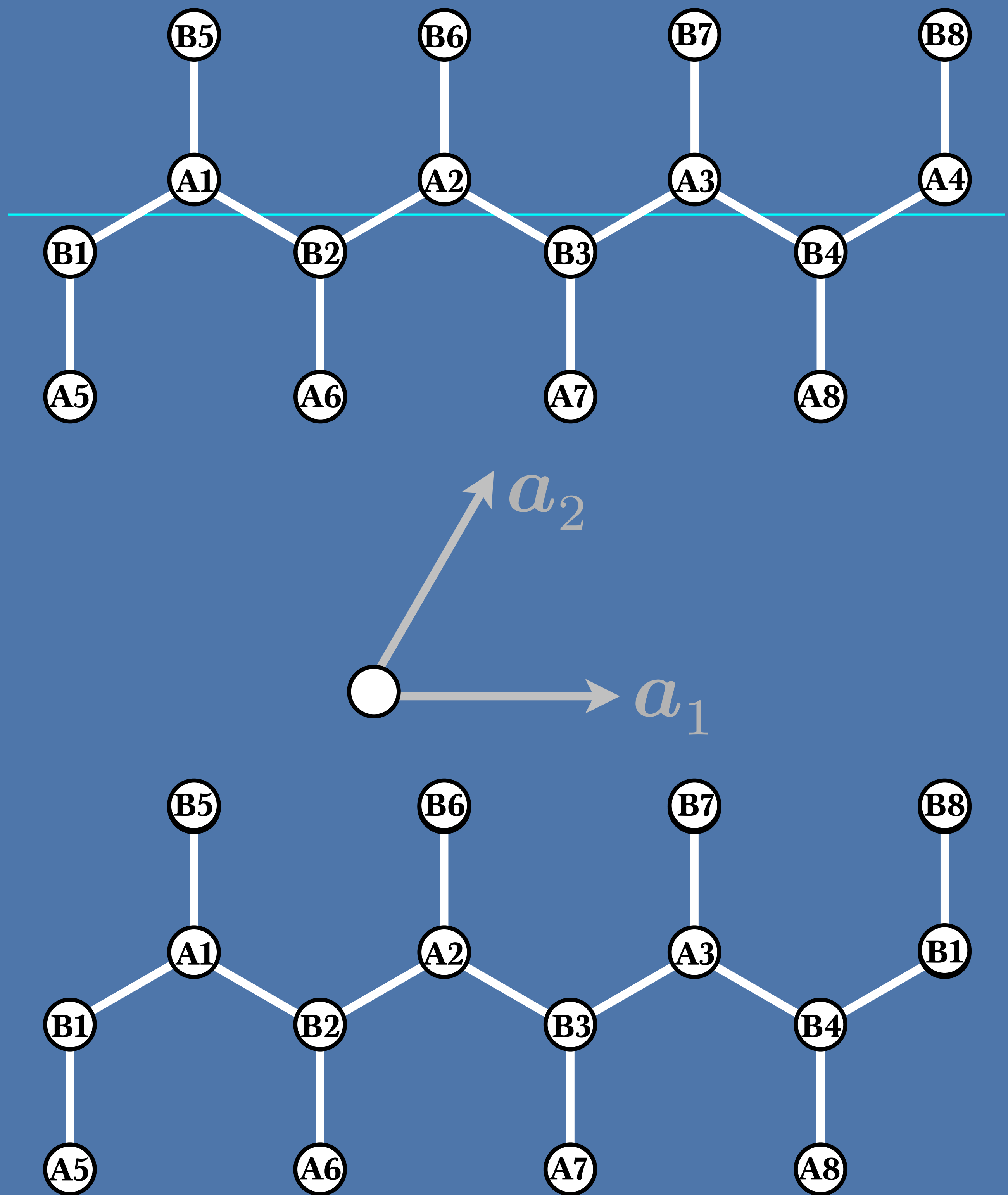

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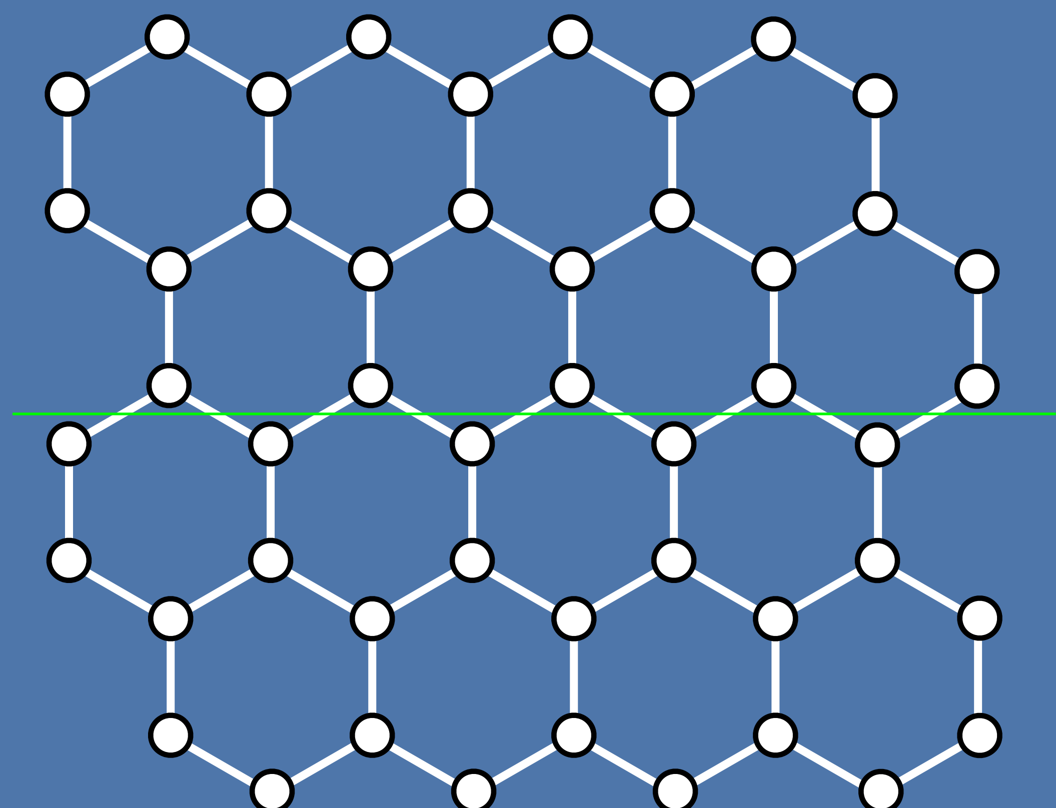

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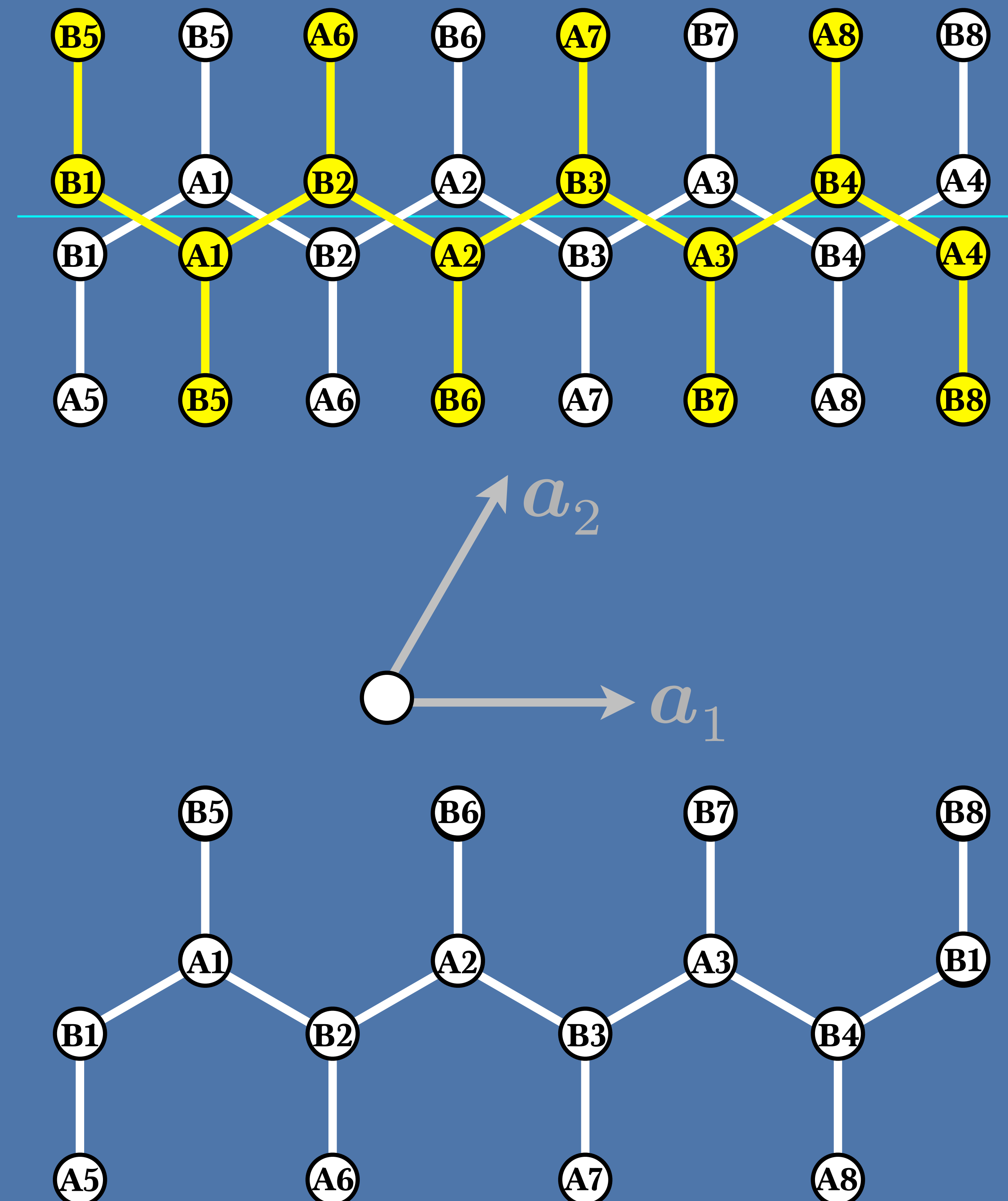

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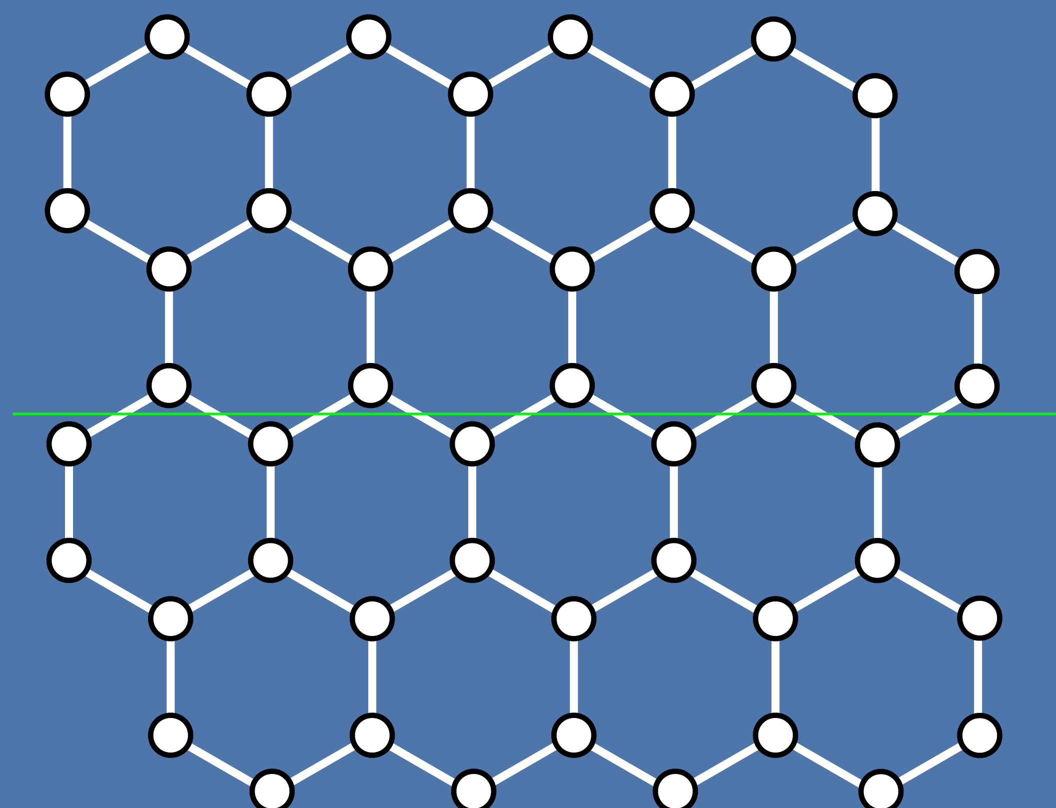

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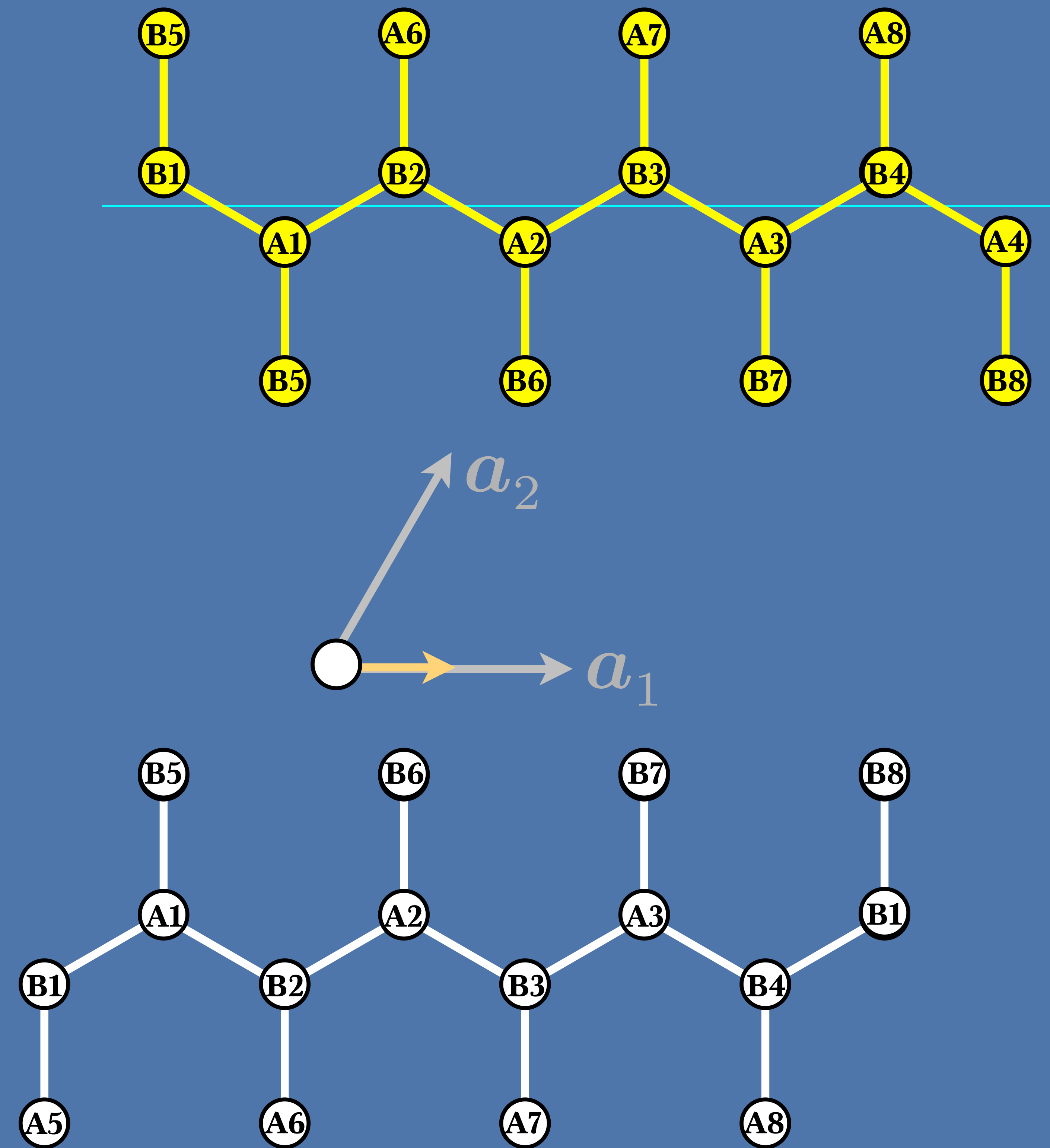
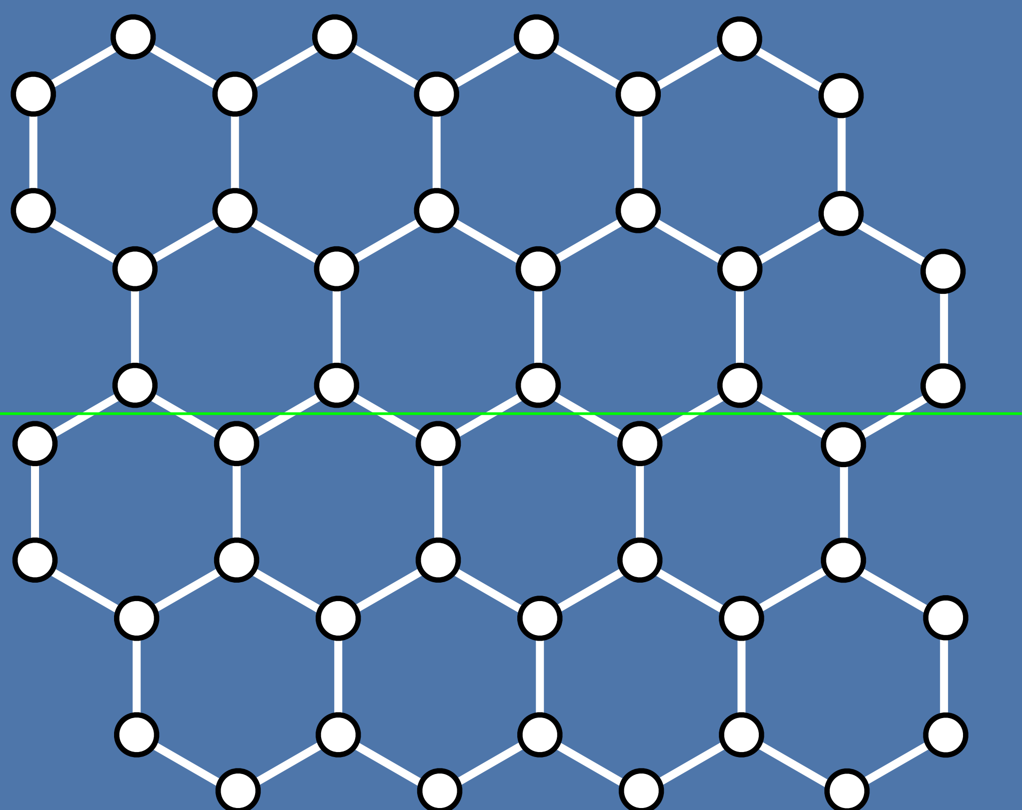


Essential vs. inessential nonsymmorphic operations

Graphene has a glide plane, yet its space group *p6m* is symmorphic!



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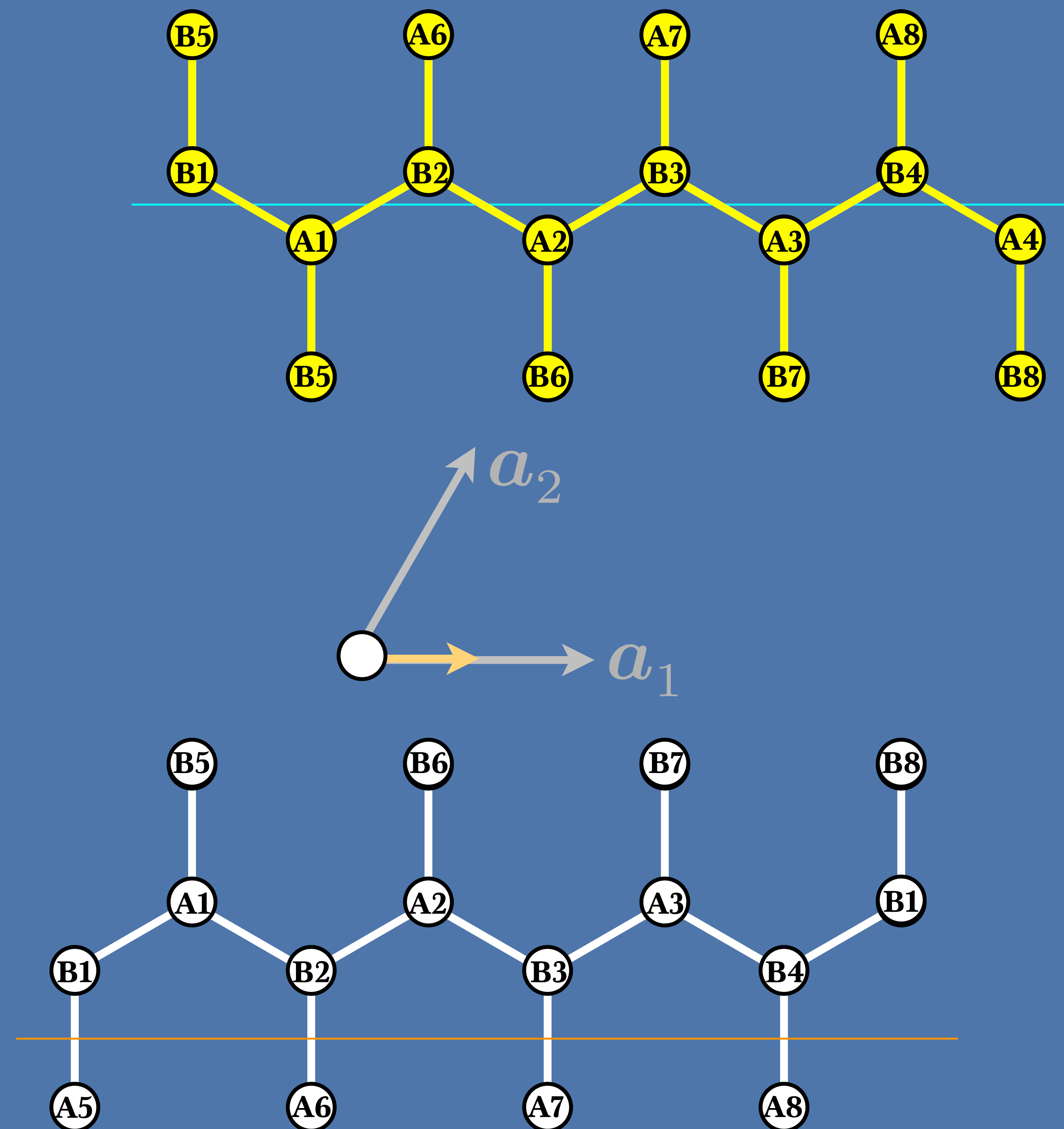

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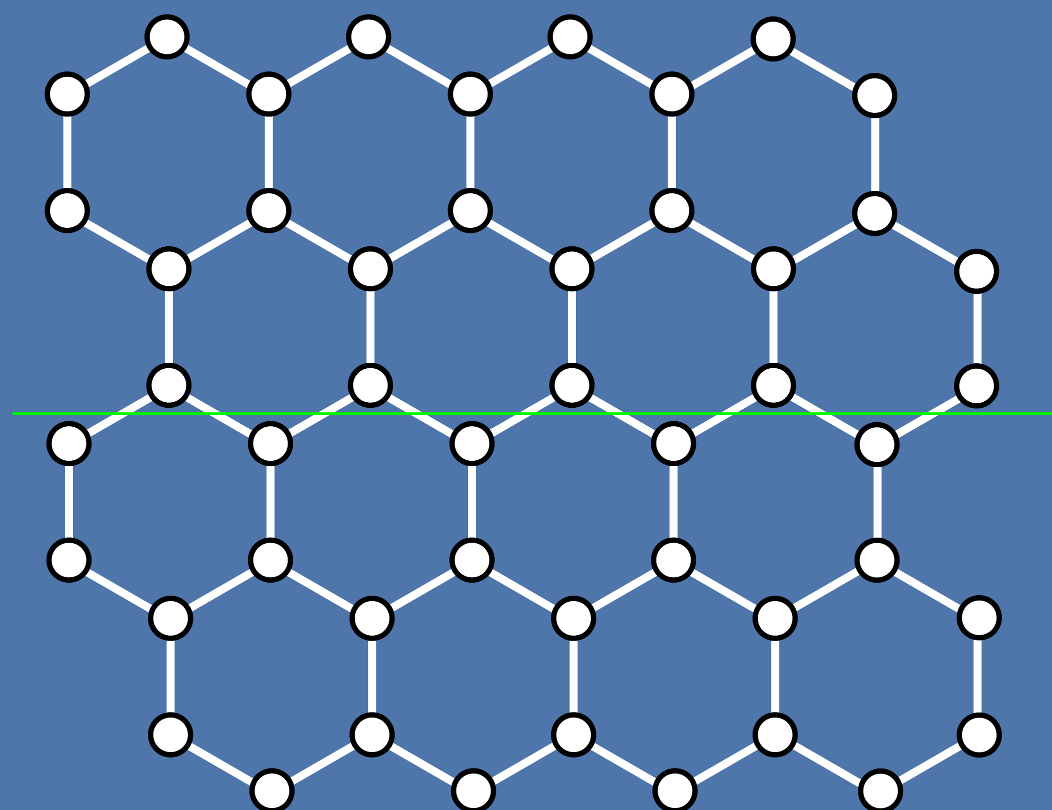

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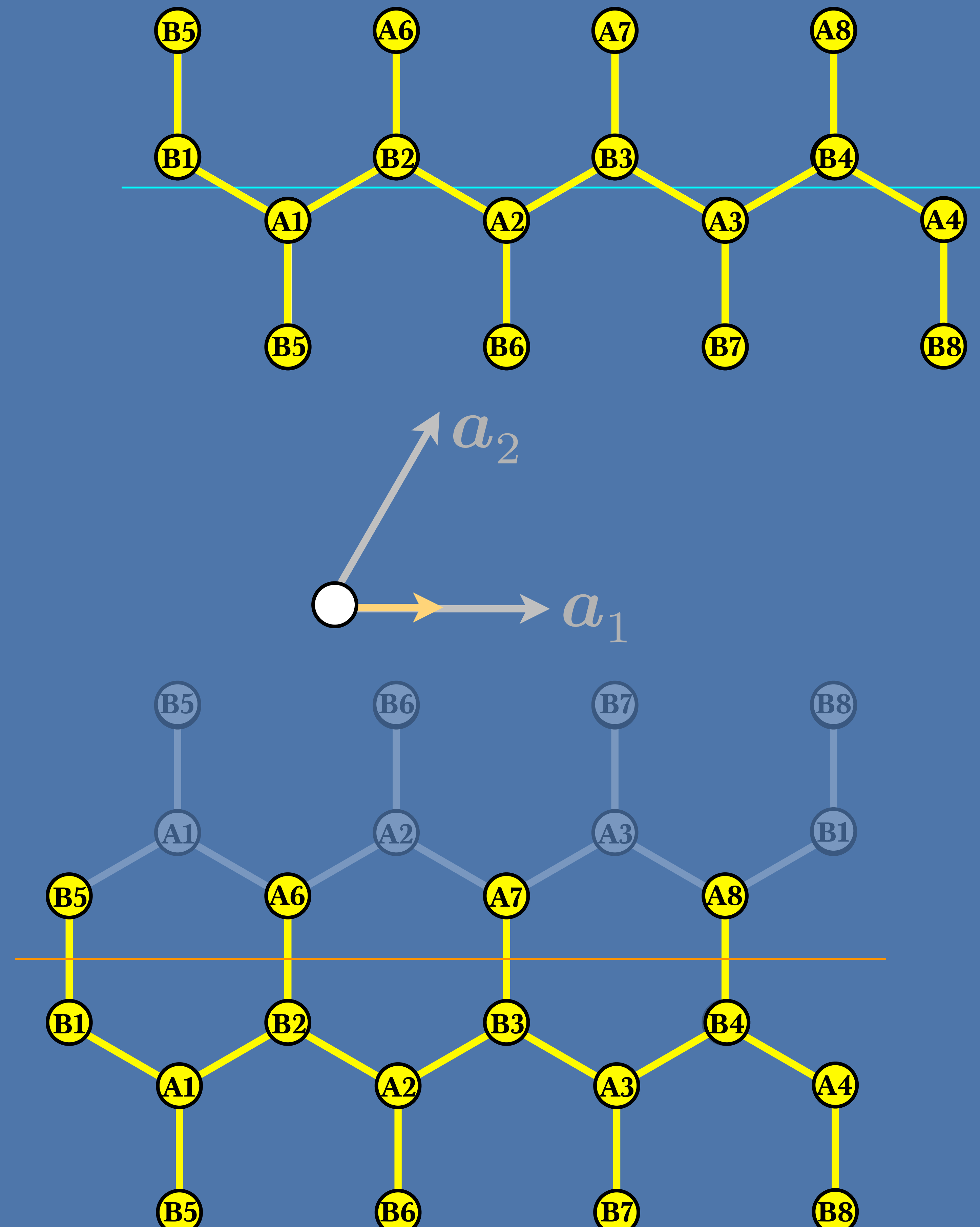

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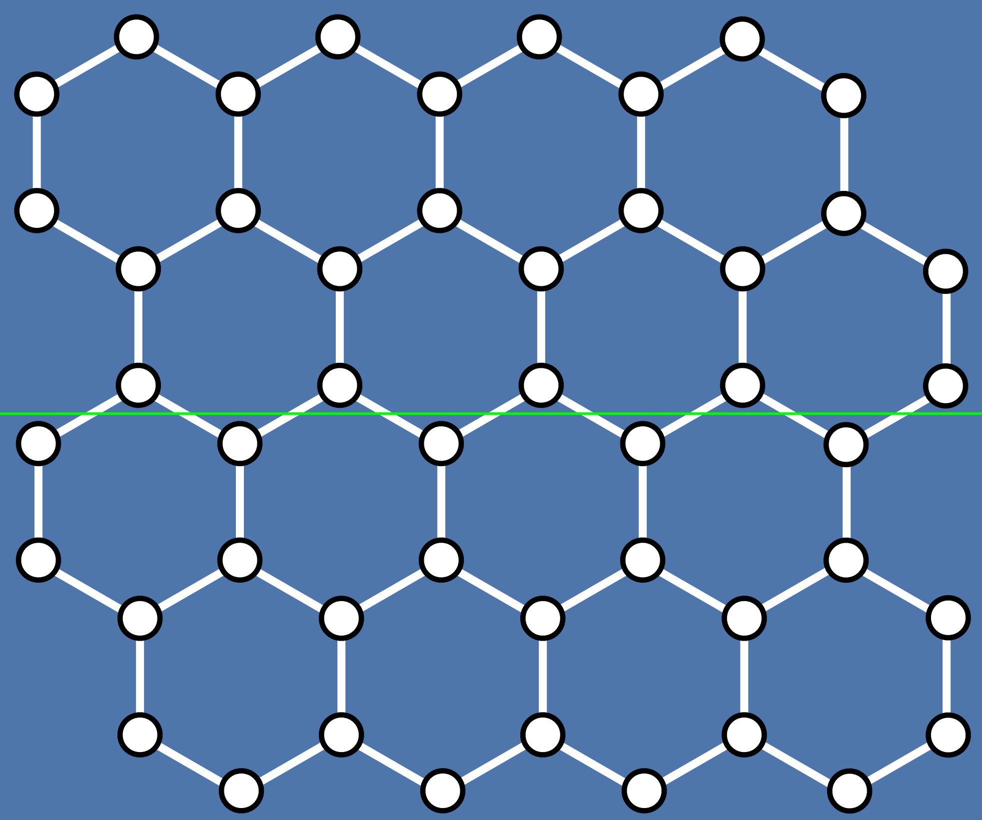

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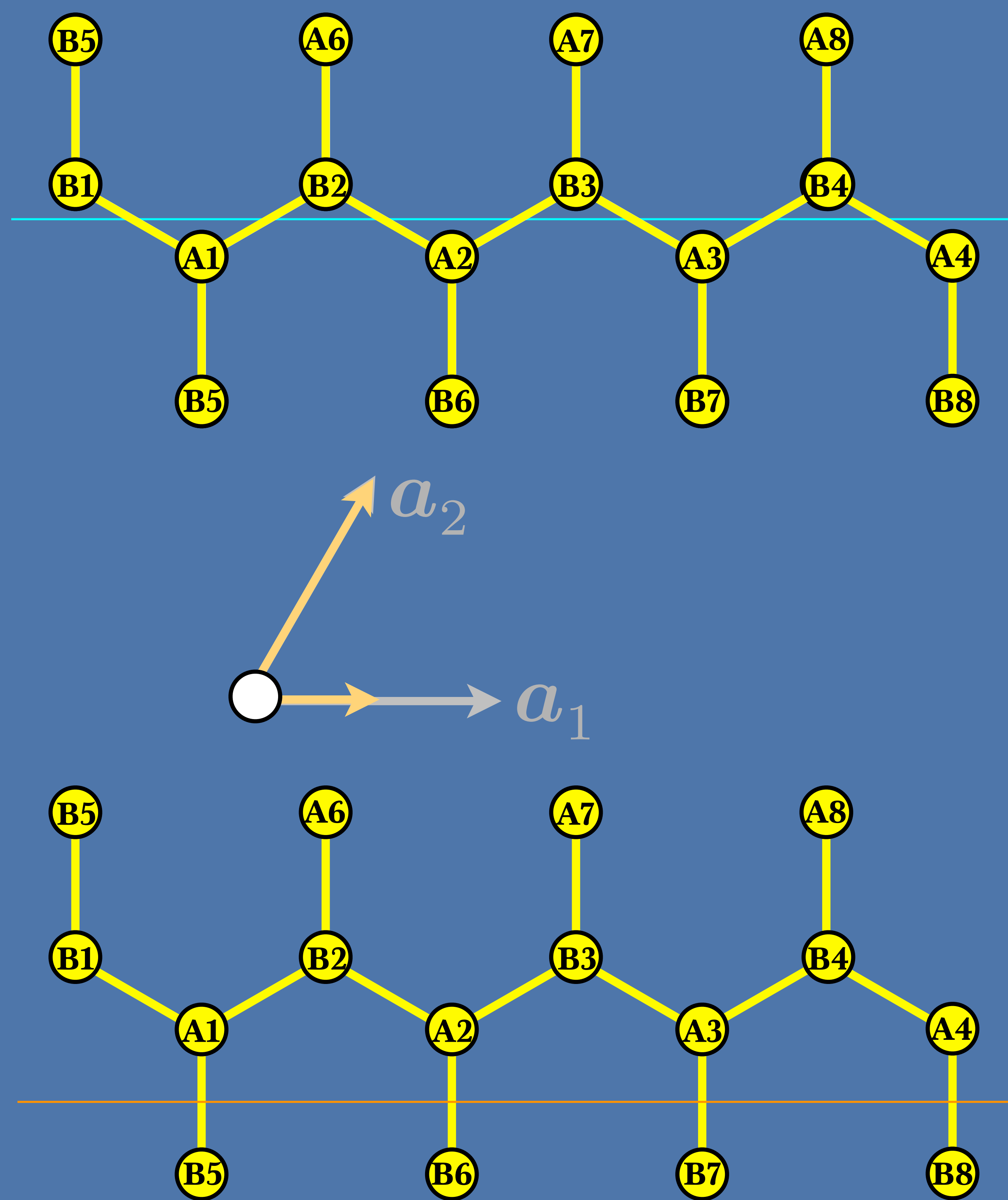
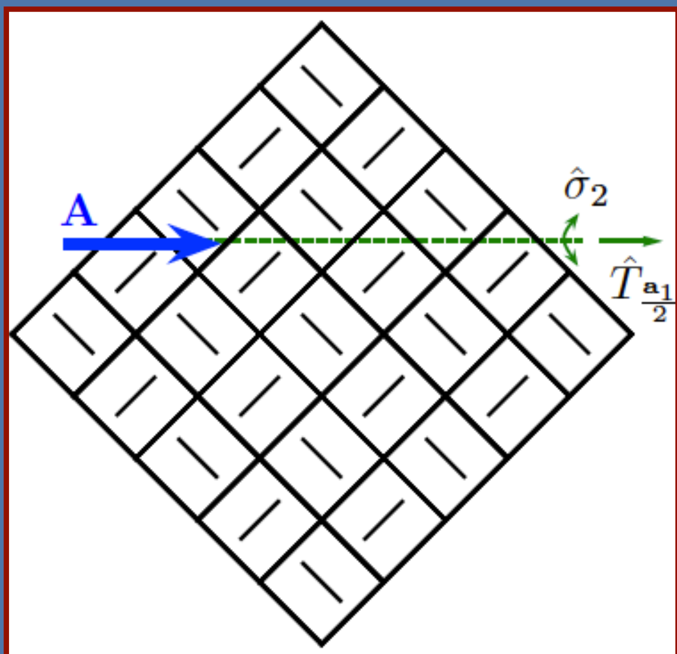
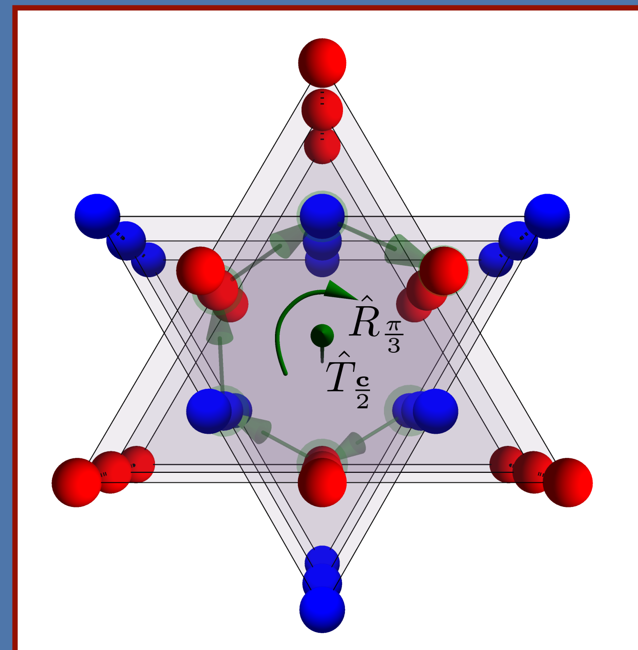


Ubiquity of nonsymmorphicity



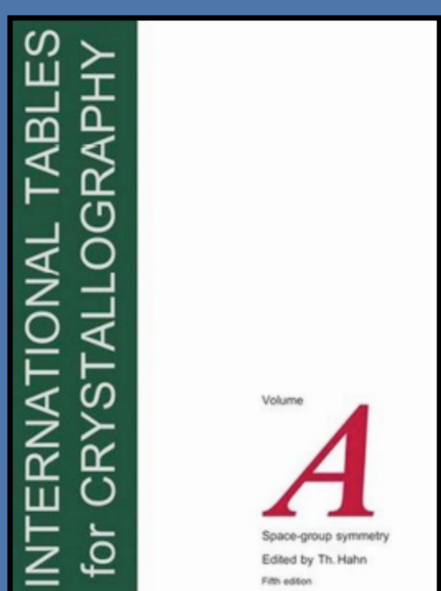
2D Shastry-Sutherland glide plane ; S=2



3D hexagonal close packed screw axis ; S=2

Table 1 | Some non-symmorphic groups and their ranks, colloquial structure names and representative materials.

d	Name	Examples	Space group	$\mathcal{S}$
2	Shastry–Sutherland	$SrCu_2(BO_3)_2$	*p4g*	2
3	hcp	Be, Mg, Zn	$P6_3/mmc$	2
3	Diamond	C, Si	$Fd\bar{3}m$	2
3	Pyrochlore	$Dy_2Ti_2O_7$ (spin ice)	$Fd\bar{3}m$	2
3	-	α-SiO_2, GeO_2	$P3_121$	3
3	-	$CrSi_2$	$P6_222$	3
3	-	$Pr_2Si_2O_7$, $La_2Si_2O_7$	$P4_1$	4
3	Hex. perovskite	$CsCuCl_3$	$P6_1$	6



CRYSTALLOGRAPHY	d=2	d=3
LATTICES	5	14
POINT GROUPS	10	32
SPACE GROUPS	17	230
SYMMORPHIC	13	73
NON-SYMMORPHIC	4	157

†Of the 157 nonsymmorphic three-dimensional space groups, 155 involve glide planes or screw axes, and two are exceptional cases.

Stickiness of nonsymmorphic energy bands

Results known from band theory. Bloch bands stick together in groups of S. Impossible to detach without breaking the symmetry.

PHYSICAL REVIEW B VOLUME 59, NUMBER 9 1 MARCH 1999-I

Connectivity of energy bands in crystals

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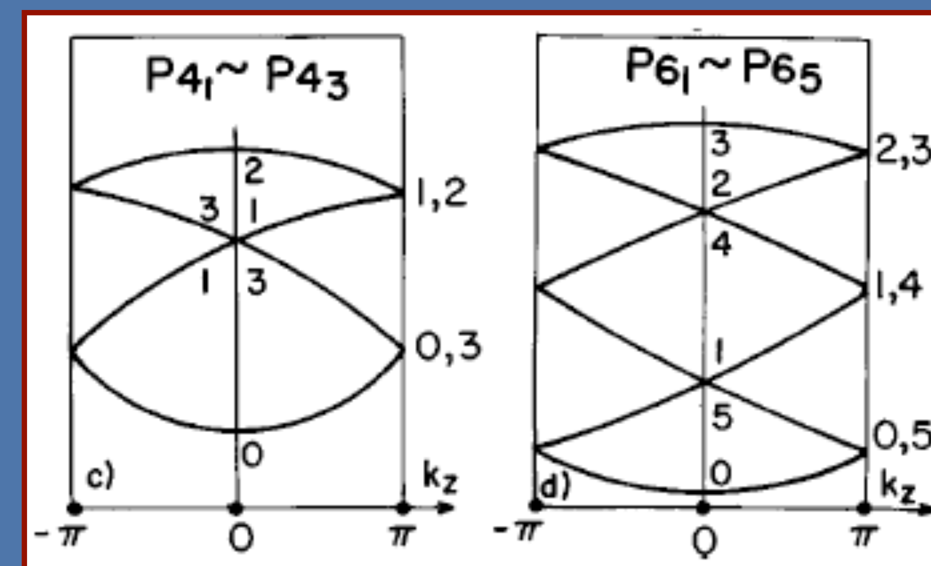
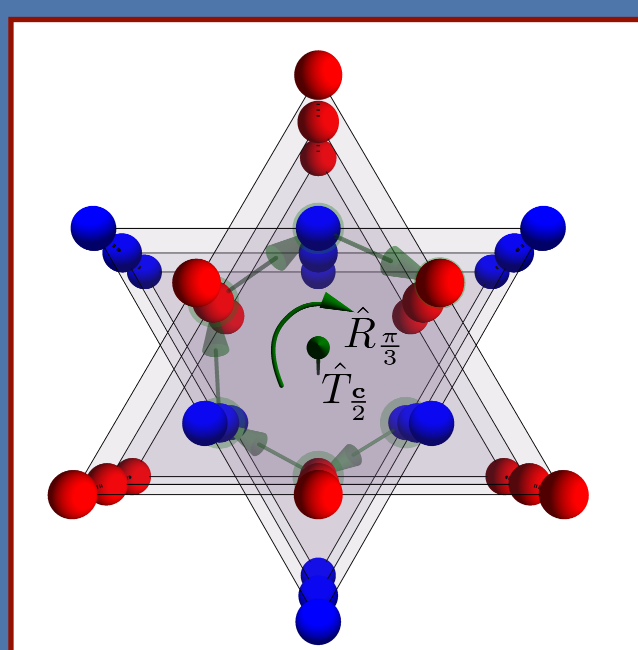
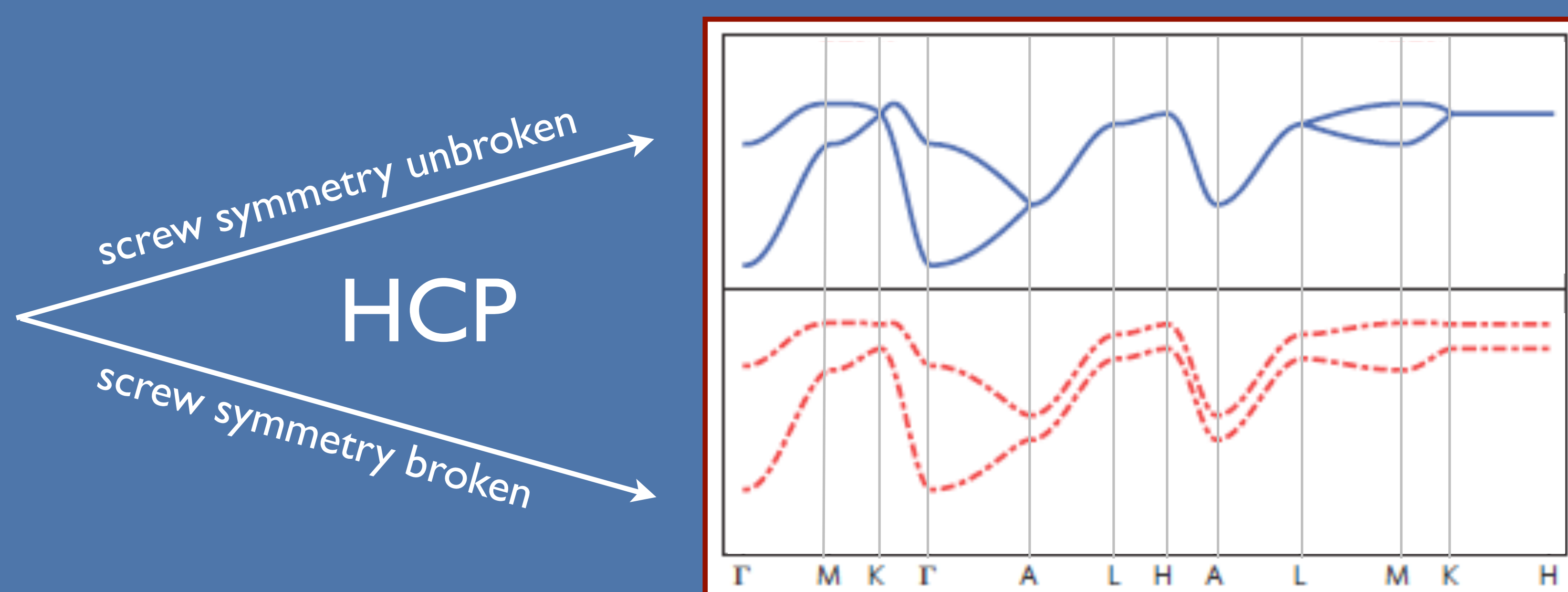
Department of Physics, Technion, Israel Institute of Technology, 32000 Haifa, Israel
(Received 30 September 1998)







Lieb-Schultz-Mattis-Oshikawa-Hastings theorem

Lieb, Schultz, Mattis (1961) / Altman and Auerbach (1998) / Oshikawa (2000) / Hastings (2004,2005)

"At fractional filling ν, a unique, gapped, featureless, insulating ground state is impossible."

$\nu \notin \mathbb{Z}$	unique	gapped	featureless	insulator	EXAMPLE
✓	✓	✓	✓	✓	NOT POSSIBLE
✓	✓	✗	✓	✗	METALLIC
✓	✓	✓	✗	✓	DENSITY WAVE
✓	✓	✗	✓	✓	SPIN-CHARGE SEPARATION
✓	✗	✓	✓	✓	TOPOLOGICAL ORDER
✗	✓	✓	✓	✓	BAND INSULATOR

Lieb-Schultz-Mattis argument

Consider an XXZ chain with periodic boundary conditions,

$$\hat{H} = \tfrac{1}{2} J_\perp \sum_{n=1}^{N} \left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+ \right) + J_z \sum_{n=1}^{N} S_n^z S_{n+1}^z$$

Suppose $|\Psi_0\rangle$ is the ground state, with $t\,|\Psi_0\rangle = e^{iK_0}|\Psi_0\rangle$.

Now apply the spin twist operator $U = \exp\left(\frac{2\pi i}{N} \sum_{j=1}^{N} j S_j^z \right)$ to $|\Psi_0\rangle$.

Find $t\,U\,t^\dagger = U\,e^{-2\pi i S_{\text{tot}}^z/N}\,e^{2\pi i S_1^z}$, so if $|\Psi_0\rangle$ is a spin singlet, then

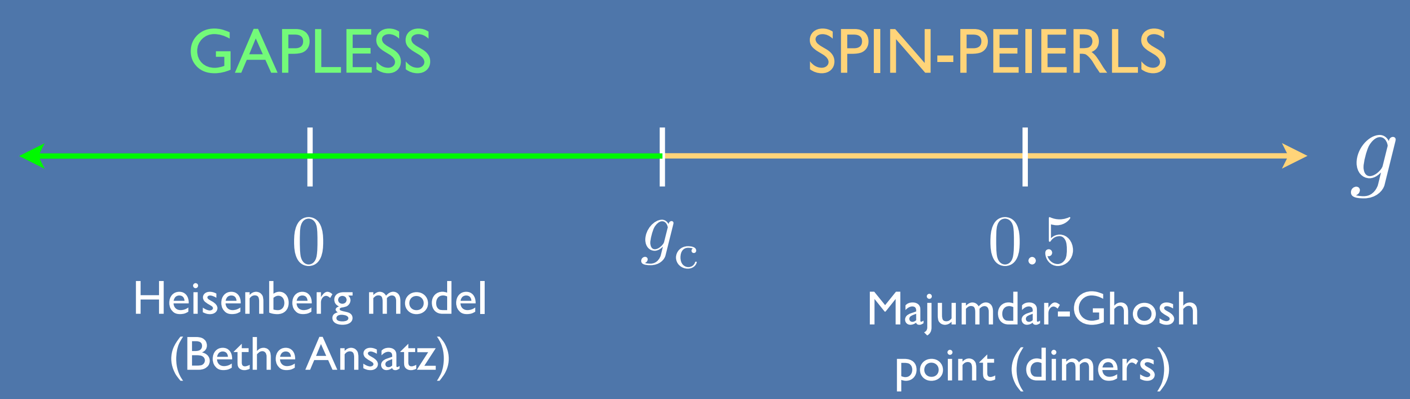
$$t\,|\Psi_1\rangle = e^{iK_1}|\Psi_1\rangle \quad \text{with} \quad |\Psi_1\rangle = U|\Psi_0\rangle \quad \text{and} \quad K_1 = K_0 + 2\pi S$$

$$U^\dagger S_n^+ S_{n+1}^- U = e^{2\pi i/N} S_n^+ S_{n+1}^- \quad ☞ \quad \langle \Psi_1 | \hat{H} | \Psi_1 \rangle = E_0 + \mathcal{O}(1/N)$$

Thus, we have found an orthogonal state $|\Psi_1\rangle$ which is degenerate with $|\Psi_0\rangle$ in the thermodynamic limit.

Example: next-nearest neighbor Heisenberg chain

$$\hat{H} = \sum_n \left[\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1} + g\, \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+2} \right]$$



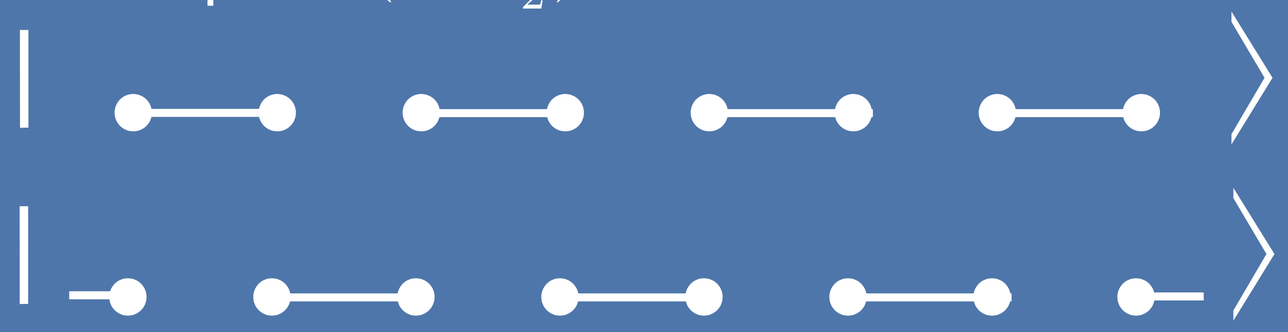
For $g < g_c \simeq 0.2411$, the spectrum is gapless.

For $g > g_c$, the system is in a spin-Peierls phase (doubly degenerate ground state with excitation gap)

Majumdar-Ghosh point $(g = \frac{1}{2})$:

$|A\rangle =$ | … $\rangle$

$|B\rangle =$ | … $\rangle$



$|A\rangle \pm |B\rangle$ has crystal momentum $0, \pi$

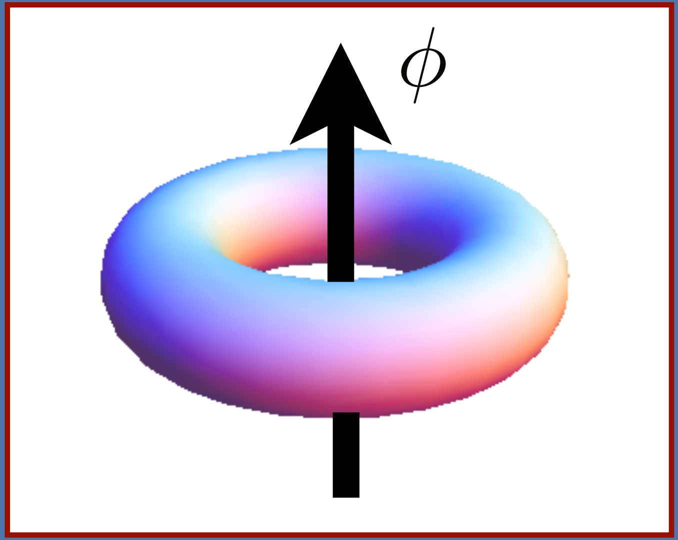
Oshikawa-Hastings extension of LSM theorem

The LSM argument works only in d=1 because

$$\langle\Psi_0|U^\dagger \hat{H} U|\Psi_0\rangle = E_0 - \tfrac{2\pi^2}{N^2}\langle\Psi_0|\hat{H}_\perp|\Psi_0\rangle = E_0 + \mathcal{O}(N^{d-2})$$

Oshikawa (2000) extended this argument to higher dimensions by examining the consequences of *adiabatic flux threading*. Place the system on a d-dimensional torus, and thread a flux ϕ through one of its cycles, resulting in a translationally-invariant $\hat{H}(\phi)$. Since $\big[\hat{H}(\phi), t\big] = 0$, the crystal momentum of the adiabatic ground state $|\Psi_0(\phi)\rangle$ is constant (0). Now define $|\Psi_1\rangle = U^\dagger|\Psi_0(2\pi)\rangle$, which must be a ground state of $\hat{H}(\phi=0)$, but with momentum

$$\Delta\boldsymbol{K} = 2\pi N_\perp \nu\, \hat{\boldsymbol{e}}$$



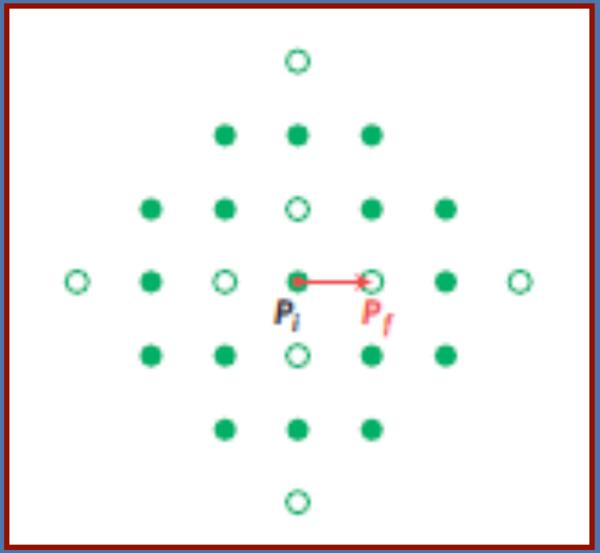
Here $\nu = \frac{p}{q}$ is the filling, and $N_\perp$ the number of sites in the transverse direction. If $\Delta\boldsymbol{K}$ not an RLV, then $\langle\Psi_0|\Psi_1\rangle = 0$.

The condition $\Delta \boldsymbol{K} \cdot \hat{\boldsymbol{e}} = 2\pi N_{\perp} \nu \neq 2\pi n$ requires $N_{\perp}$ and q to be relatively prime, and does not require *d=1*. In this case, the ground state *cannot be unique* at fractional filling.

At integer filling, $\Delta \boldsymbol{K}$ is a reciprocal lattice vector, hence the states $|\Psi_0\rangle$ and $|\Psi_1\rangle$ cannot be distinguished - or so it would seem!

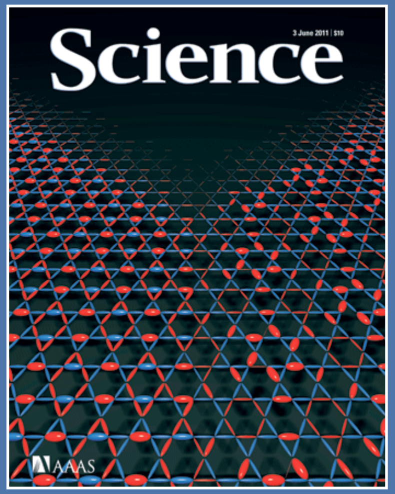
Some crystalline structures, however, exhibit *systematic extinctions* in their Bragg patterns. Such is the case with nonsymmorphic lattices. In such cases, $|\Psi_0\rangle$ and $|\Psi_1\rangle$ *can* be distinguished. This is the essential content of our observation.

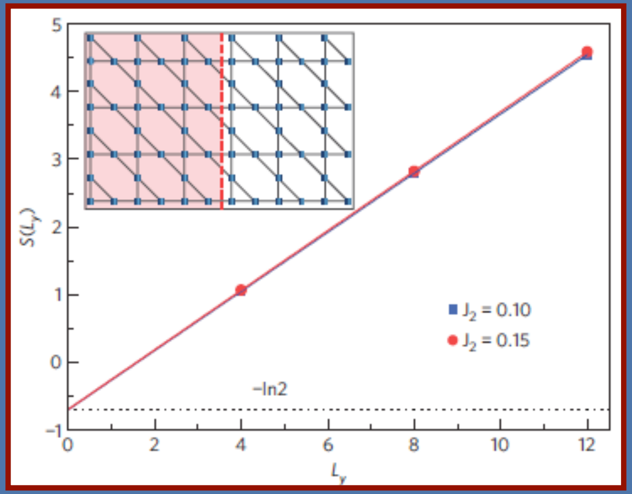
Fourier space crystallography and extinctions: Under a space group operation $\{R, \boldsymbol{\tau}\}$, the Fourier components of the density $n_{\boldsymbol{k}}$ transform as $n_{\boldsymbol{k}} \rightarrow n_{R\boldsymbol{k}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{\tau}}$. If $\boldsymbol{k}\cdot\boldsymbol{\tau} \neq 2\pi n$, then $n_{\boldsymbol{k}} = 0$.



Examples:

- For a $S = \frac{1}{2}$ Kagome lattice model with one electron per site, there are three sites per cell, hence $\nu = \frac{3}{2}$. With a featureless, gapped, insulating ground state, the system must exhibit topological degeneracy and fractionalization.





Yan, Huse, White (2011)
Jiang, Wang, Balents (2012)
chiral order? Capponi *et al.* (2013)

- For a $S = \frac{1}{2}$ honeycomb lattice model with one electron per site, there are two sites per cell, and the filling is $\nu = 1$. Is a featureless, gapped, insulating ground state necessarily a spin liquid? No. It could be a Mott insulator. Kimchi et al. (2013)

Gist of our argument (details in paper)

- First, we require a conserved U(1) charge, which could arise from spinless or spinful fermions, bosons, or magnets where S^z is a good quantum number. We then define

$$\nu \equiv \frac{\text{total U(1) charge}}{\text{number of unit cells}}$$

- Next, consider a nonsymmorphic SG operation $\hat{G} = \{R, \boldsymbol{\tau}\}$, where $\boldsymbol{\tau}$ is not in the direct lattice, and $R\boldsymbol{\tau} = \boldsymbol{\tau}$ (such as in a screw or glide). Now let $\boldsymbol{b}$ be the smallest reciprocal lattice vector for which $R\boldsymbol{b} = \boldsymbol{b}$. Now adiabatically thread a flux with vector potential $\boldsymbol{A} = \boldsymbol{b}/N$, which corresponds to a pure gauge.

- Starting with a ground state which is presumed to be an eigenstate of all symmetry operations, we must have $\hat{G}|\Psi_0\rangle = e^{i\Theta}|\Psi_0\rangle$. Let $|\tilde{\Psi}_0\rangle$ be the adiabatic image of $|\Psi_0\rangle$ after flux insertion. Flux threading commutes with $\hat{G}$.

- We 'pull back' to the original flux-less Hamiltonian via

$$\hat{U}_{\boldsymbol{b}} = \exp\left\{ \frac{i}{N} \int d^d r \, \boldsymbol{b} \cdot \boldsymbol{r} \, \hat{\rho}(\boldsymbol{r}) \right\}$$

where $\hat{\rho}(\boldsymbol{r})$ is the density operator for the U(1) charge. This removes the flux.

- Following Oshikawa (2000), define $|\Psi_1\rangle = \hat{U}_{\boldsymbol{b}}|\tilde{\Psi}_0\rangle$. Now $\hat{G}^{-1}\hat{U}_{\boldsymbol{b}}\hat{G} = \hat{U}_{\boldsymbol{b}}\, e^{i\boldsymbol{b}\cdot\boldsymbol{\tau}\, Q/N}$, where $Q = \nu N N_\perp$ is the total U(1) charge. Furthermore, $\boldsymbol{\tau}$ is fractional, hence

$$\boldsymbol{b}\cdot\boldsymbol{\tau} = 2\pi t/\mathcal{S}_G$$

where t and $\mathcal{S}_G$ are relatively prime. We therefore conclude that $\langle\Psi_0|\Psi_1\rangle = 0$ whenever $t\nu N_\perp/\mathcal{S}_G$ is fractional. We can always choose $N_\perp$ so that it is relatively prime to $\mathcal{S}_G$. We conclude that adiabatic flux insertion and removal generates a distinct ground state whenever the filling ν is not an integer multiple of $\mathcal{S}_G$.

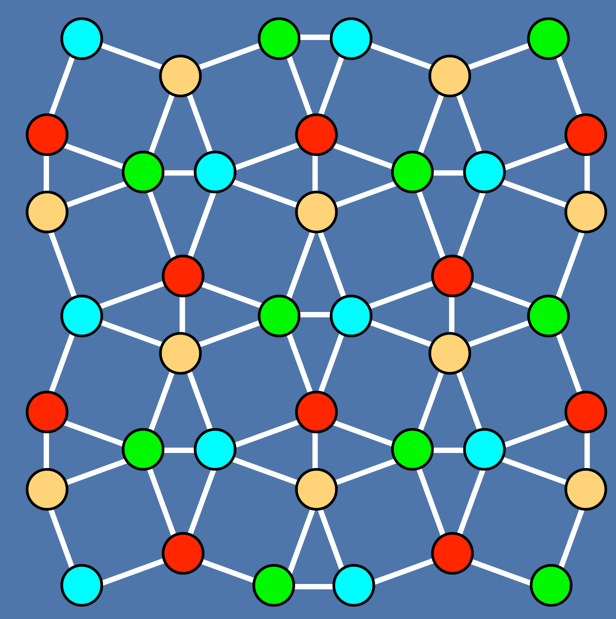
- The least common multiple of the $\{\mathcal{S}_G\}$ must divide the nonsymmorphic rank $\mathcal{S}$.

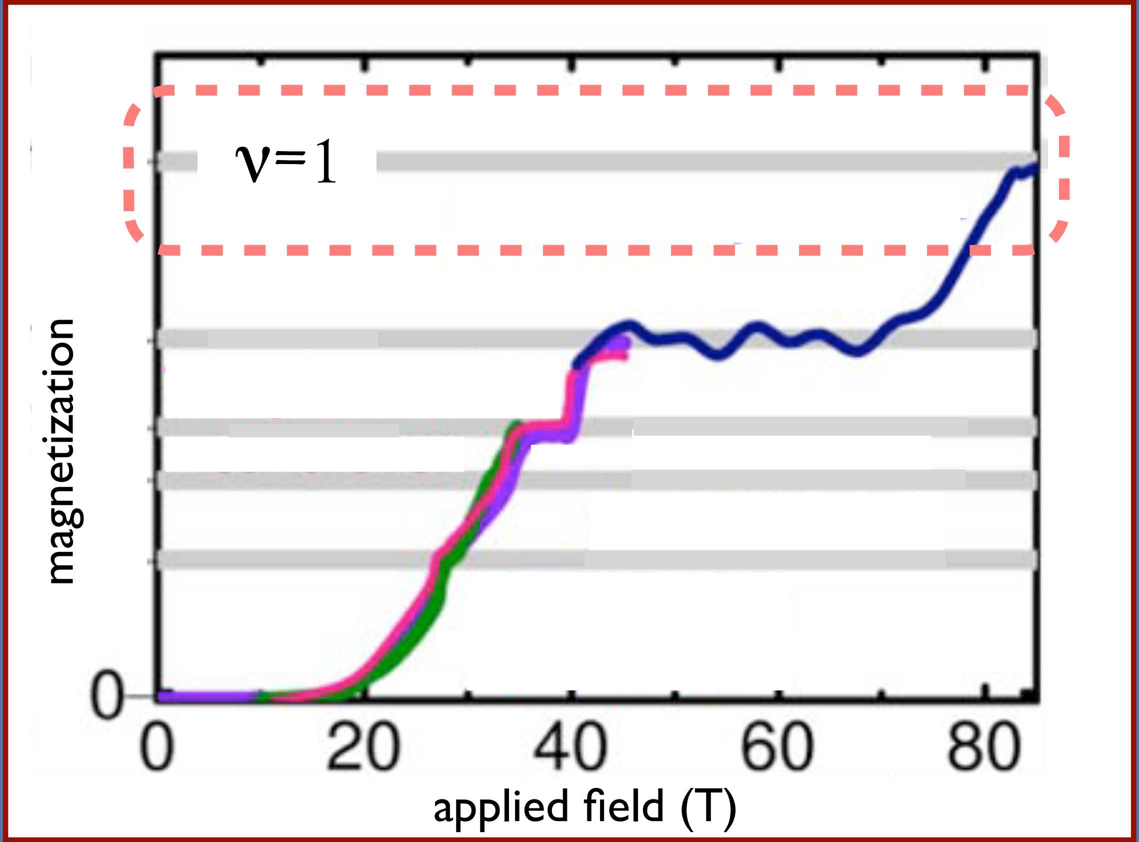
- A necessary consequence:

  Both diamond and pyrochlore lattices have space group $Fd\bar{3}m$, for which $\mathcal{S} = 2$. For interacting electrons with one e^- per site, one has $\nu = 1$ for diamond, and $\nu = 2$ for pyrochlore. Thus, a trivial insulator at this filling is impossible on the diamond lattice, but possible on the pyrochlore lattice.

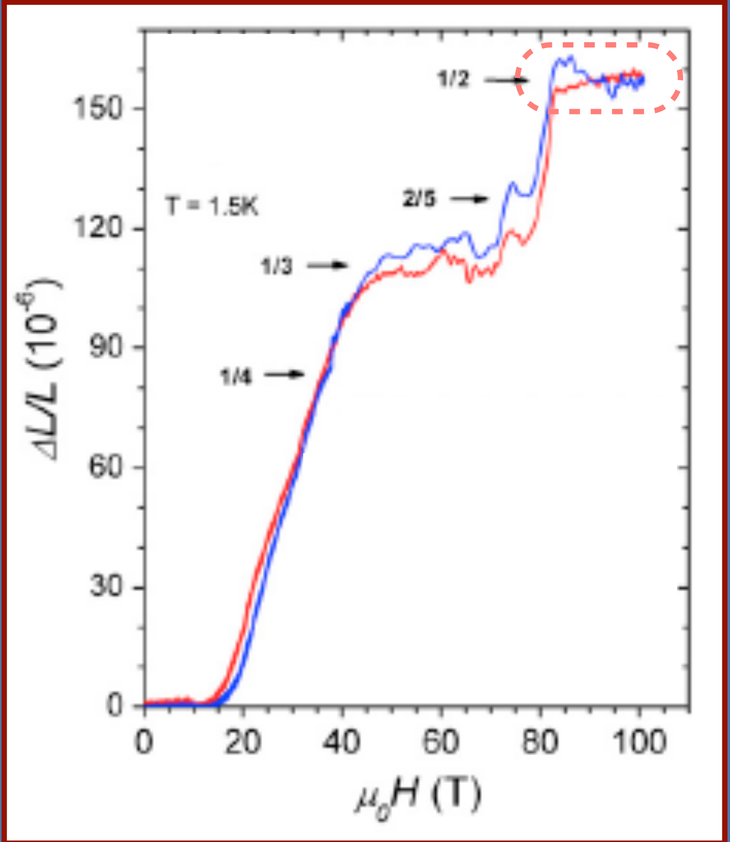
Magnetization plateaux in $SrCu_2(BO_3)_2$

- $CuBO_3$ layers form Shastry-Sutherland lattice
- In a field, SCBO exhibits a magnetization plateau at half the saturation value $\rightarrow \nu = 1$
- Accordingly, since S_{SSL}=2, the plateau state must be topologically ordered, or else break a symmetry. [See Momoi and Totsuka (2000)]





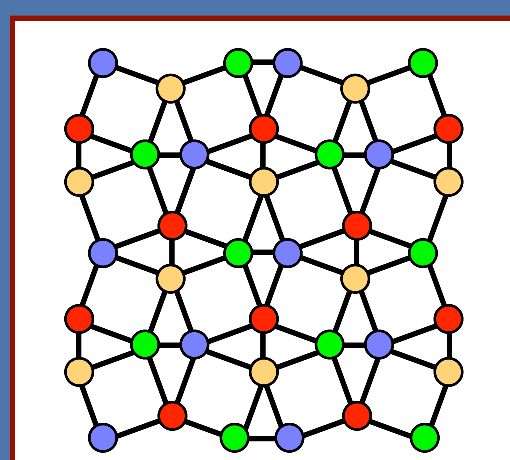
Jaime *et al.* (PNAS, 2012)



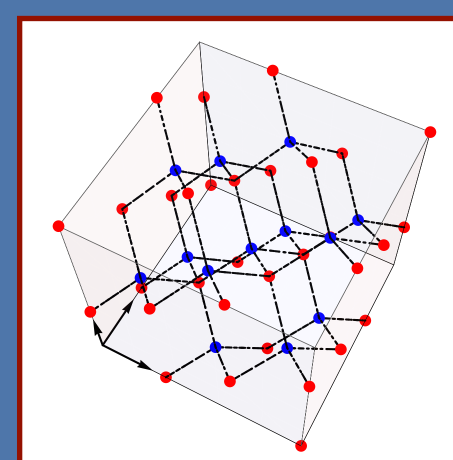
Sebastian *et al.* (PNAS, 2008)

Summary

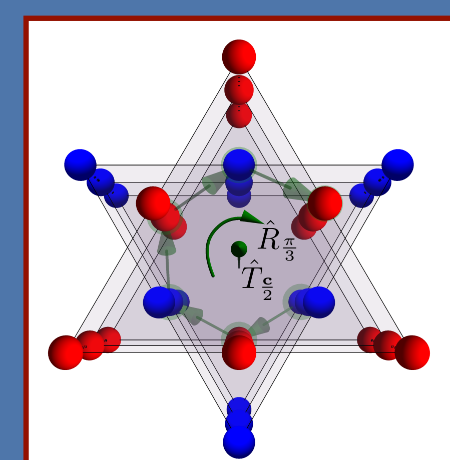
- Basic question: is there always a band insulator for $\nu \in \mathbb{Z}$? NO!
- Discrete invariant of space group: nonsymmorphic rank $\mathcal{S}$
  - quantum of filling for featureless insulators
  - Bloch bands stick in groups of $\mathcal{S}$ and can't be unstuck without breaking symmetry
  - implications for band theory, interacting Bose and Fermi systems, topological degeneracy, fractionalization
  - 157 of 230 three-dimensional space groups are nonsymmorphic $(\mathcal{S} > 1)$



$p4g$



$Fd\bar{3}m$



$P6_3/mmc$

- Questions: time-reversal? spin-orbit? quasicrystals? defects?