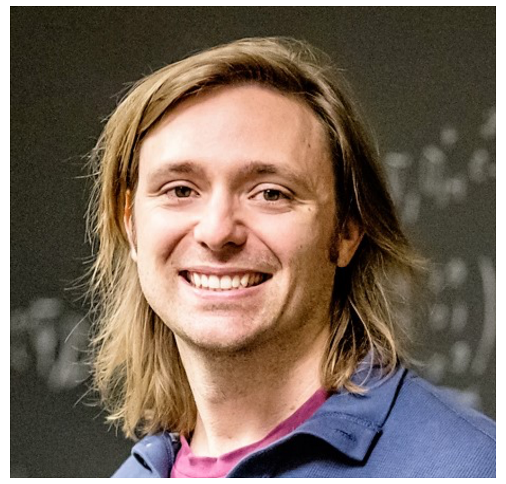
Boundary obstructed topological phases

Raquel Queiroz
Weizmann Institute of Science
July 27, 2020

Boundary obstructed topological phases

Eslam Khalaf, Wladimir Benalcazar, Taylor Hughes, RQ 1908.00011





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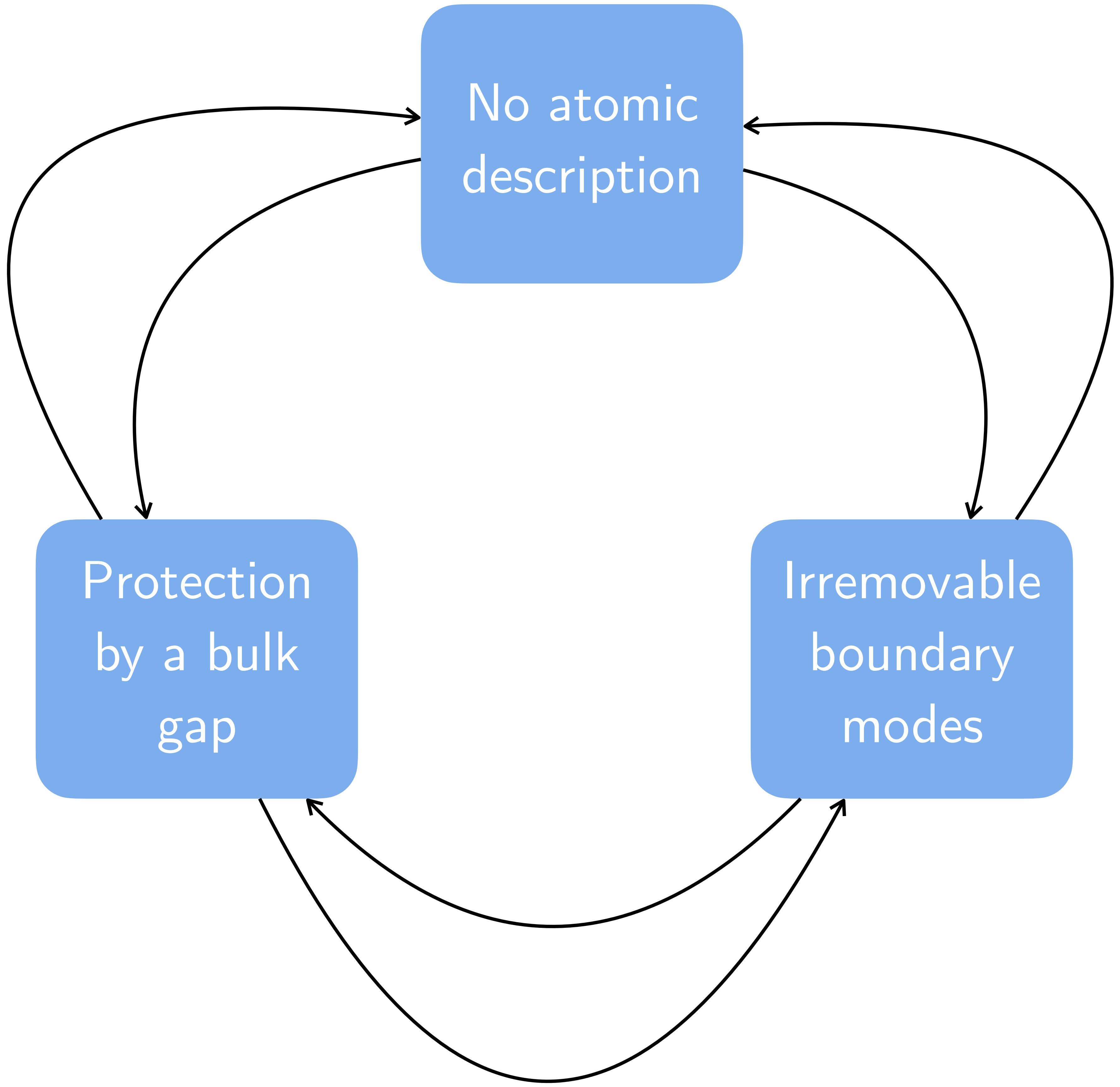
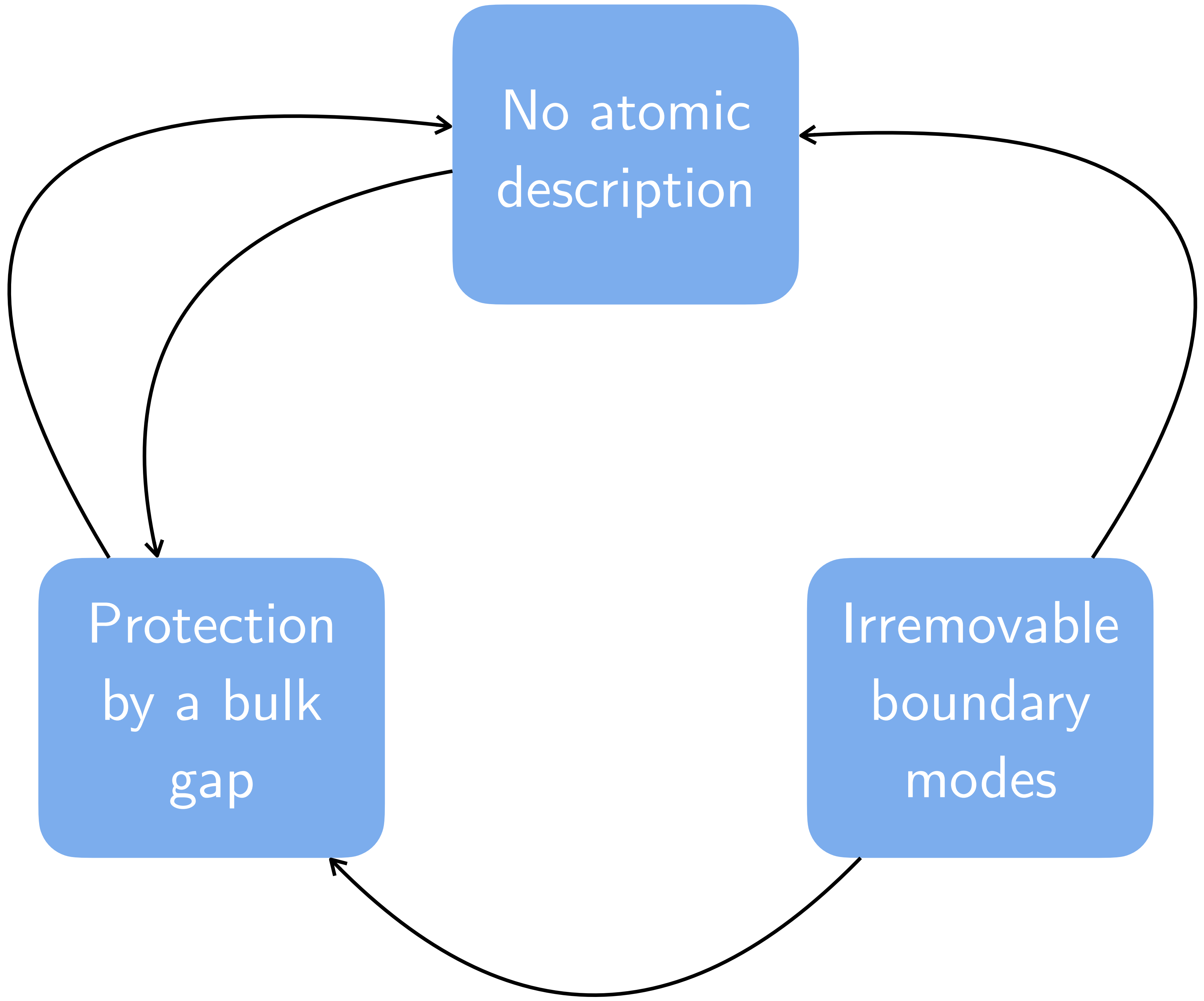
Topological obstructions in crystalline systems



→ Internal symmetry: all directions hold

Topological obstructions in crystalline systems



→ Internal symmetry: all directions hold

→ Crystalline symmetry: subtleties arise

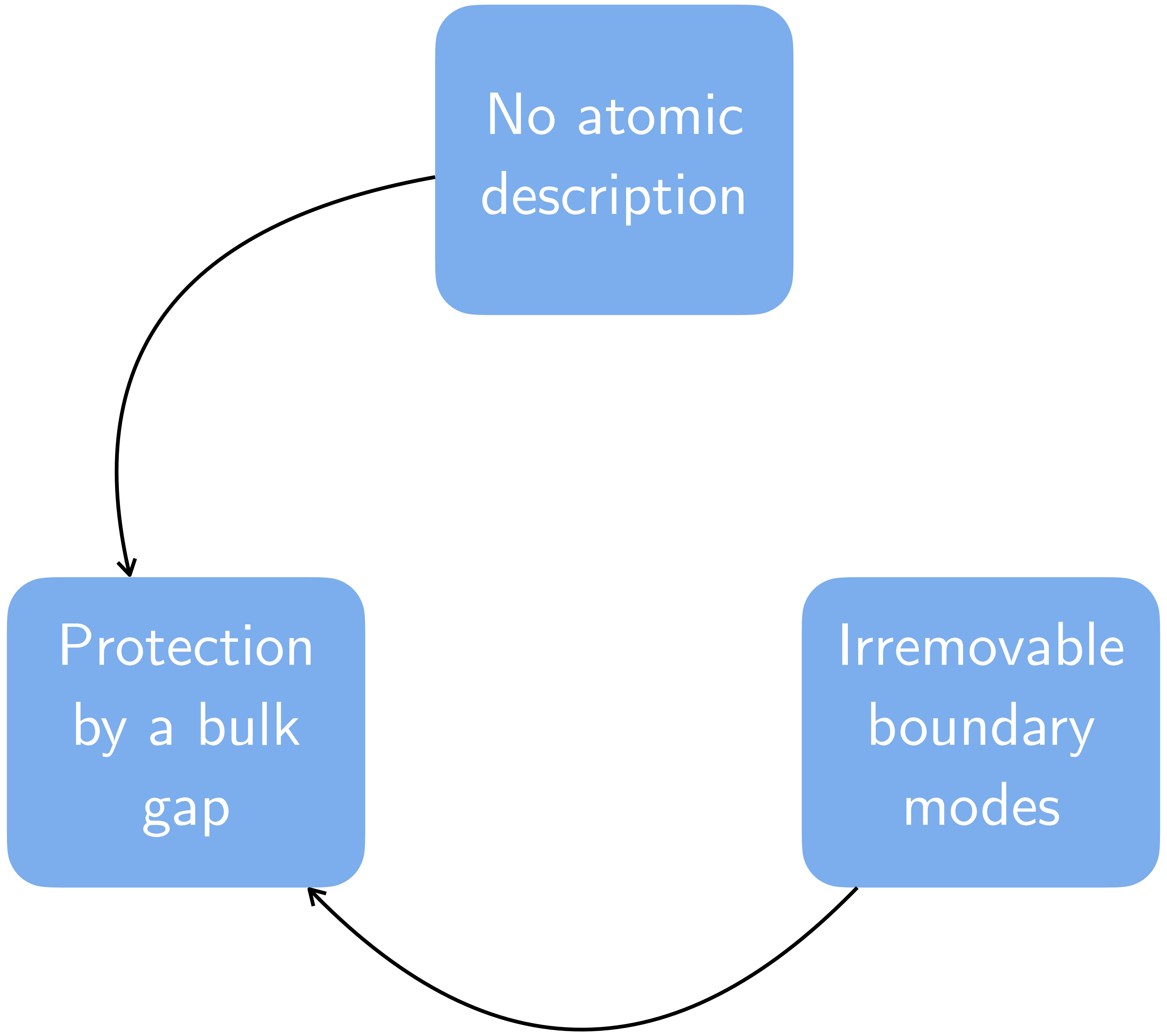
→ Fragile topological phases [Po et al 2017]:

→ No atomic description

→ Removable boundary charge

→ Protected by bulk gap closing

Topological obstructions in crystalline systems



- → Internal symmetry: all directions hold
- → Crystalline symmetry: subtleties arise
  - → Fragile topological phases [Po et al 2017]:
    - → No atomic description
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  - → Obstructed atomic phases [Bradlyn et al 2017]:
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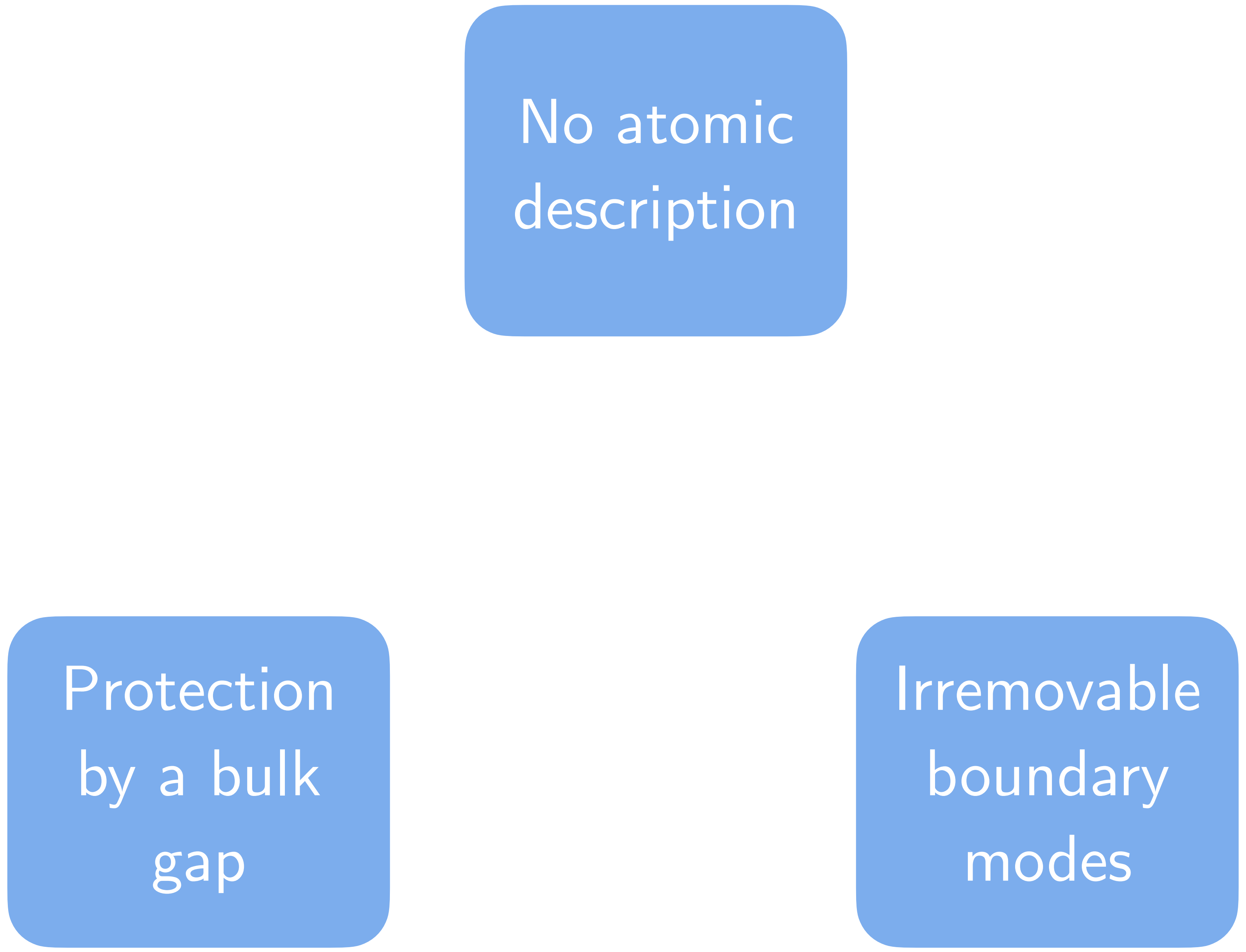
Topological obstructions in crystalline systems



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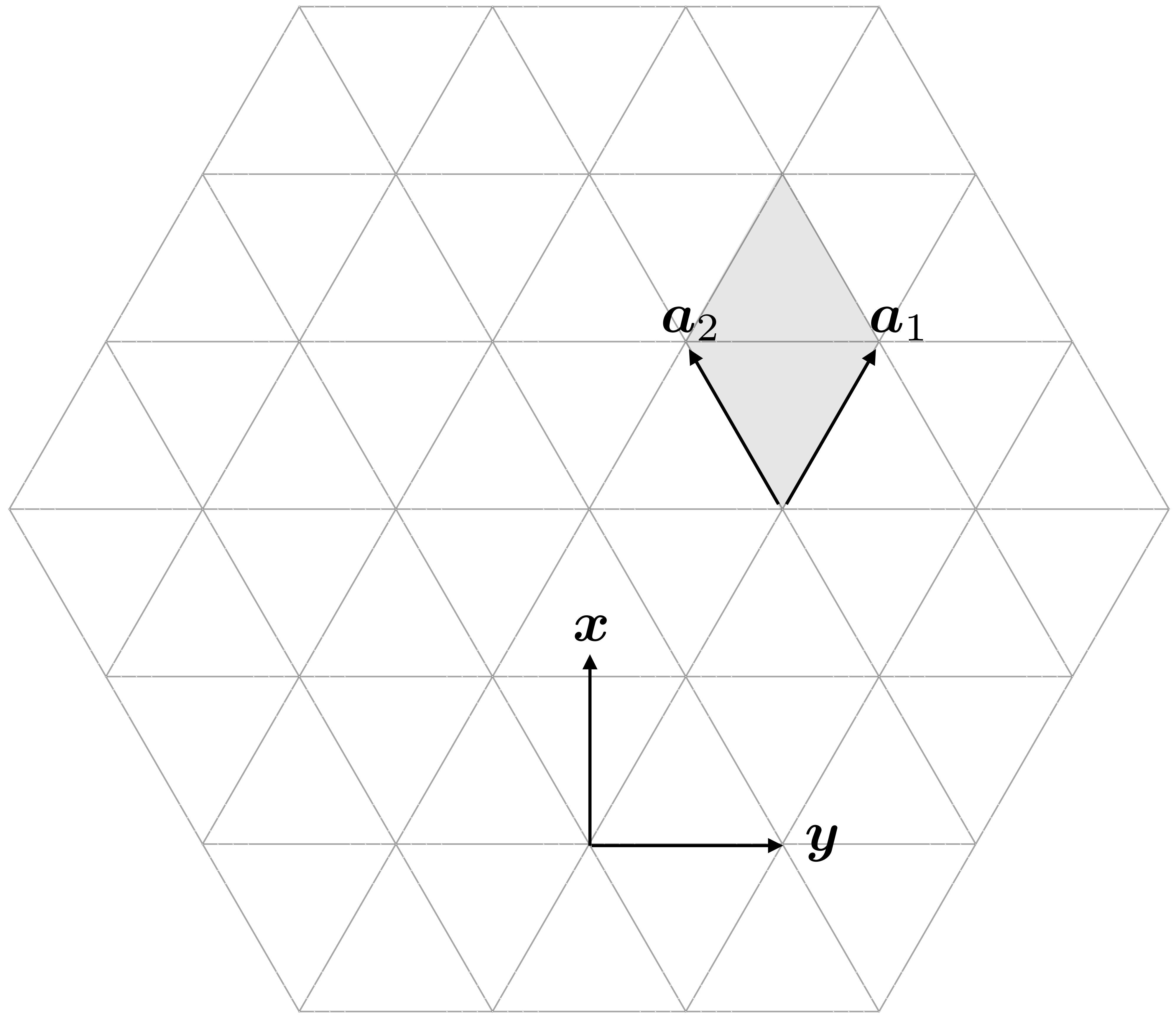
introduction

Basics of crystalline topology

What is an atomic band



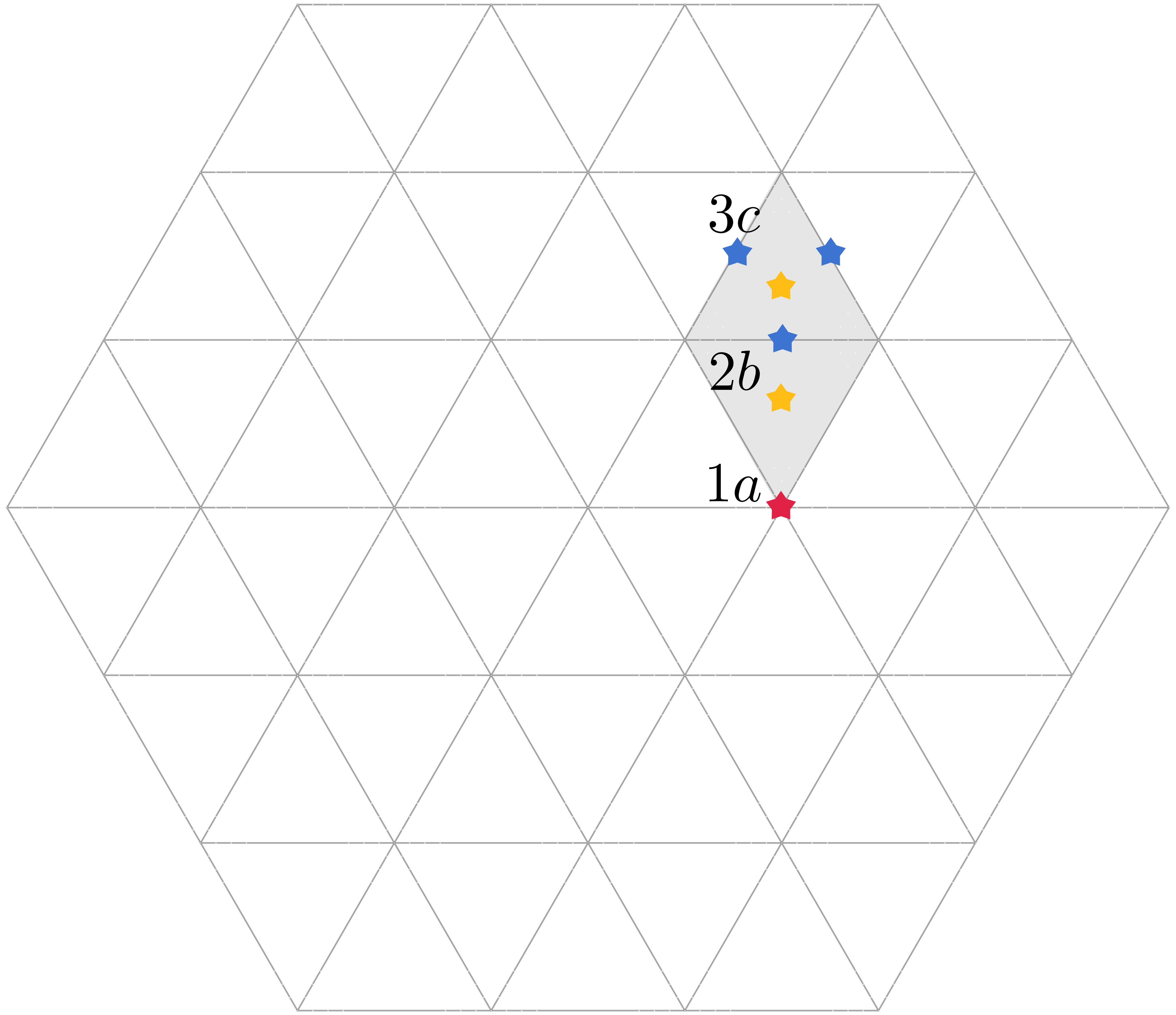
→ Atomic band are those constructed from the hybridisation of atomic orbitals on symmetric sites.

→ Start with a lattice on a space group G.

→ Example: triangular lattice in $p6mm$

→ Symmetries C_2, C_3, mirror M_{11}, inversion I and translations along lattice vectors $\boldsymbol{a}_1 = \sqrt{3}\boldsymbol{x}/2 + \boldsymbol{y}/2$, and $\boldsymbol{a}_2 = \sqrt{3}\boldsymbol{x}/2 - \boldsymbol{y}/2$

What is an atomic band



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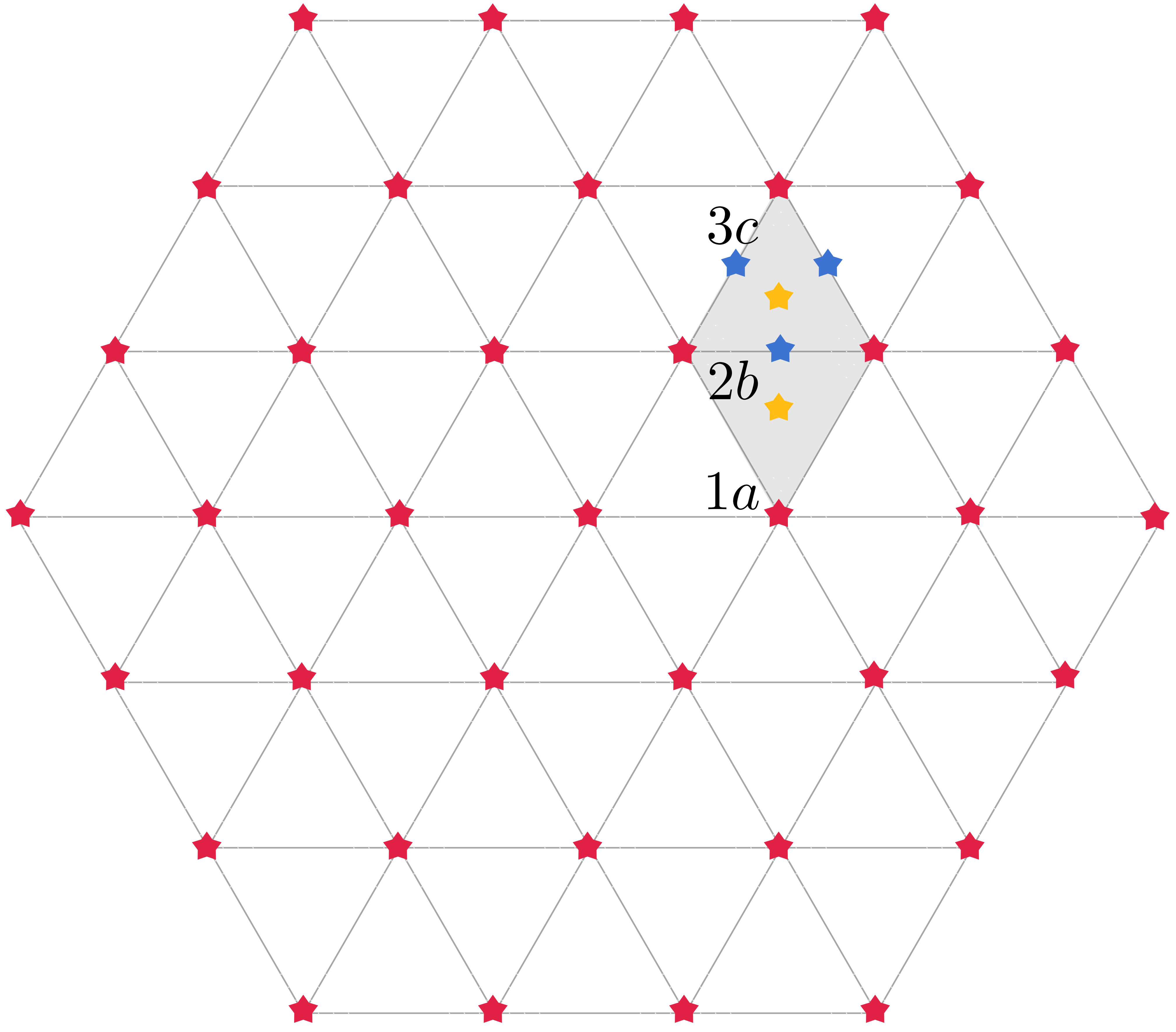
→ Positions in the lattice, called Wyckoff positions w with different multiplicities (how many times appear in the unit cell)

→ All sites in w is equivalent to each other: they have the same site symmetry group G_w

What is an atomic band



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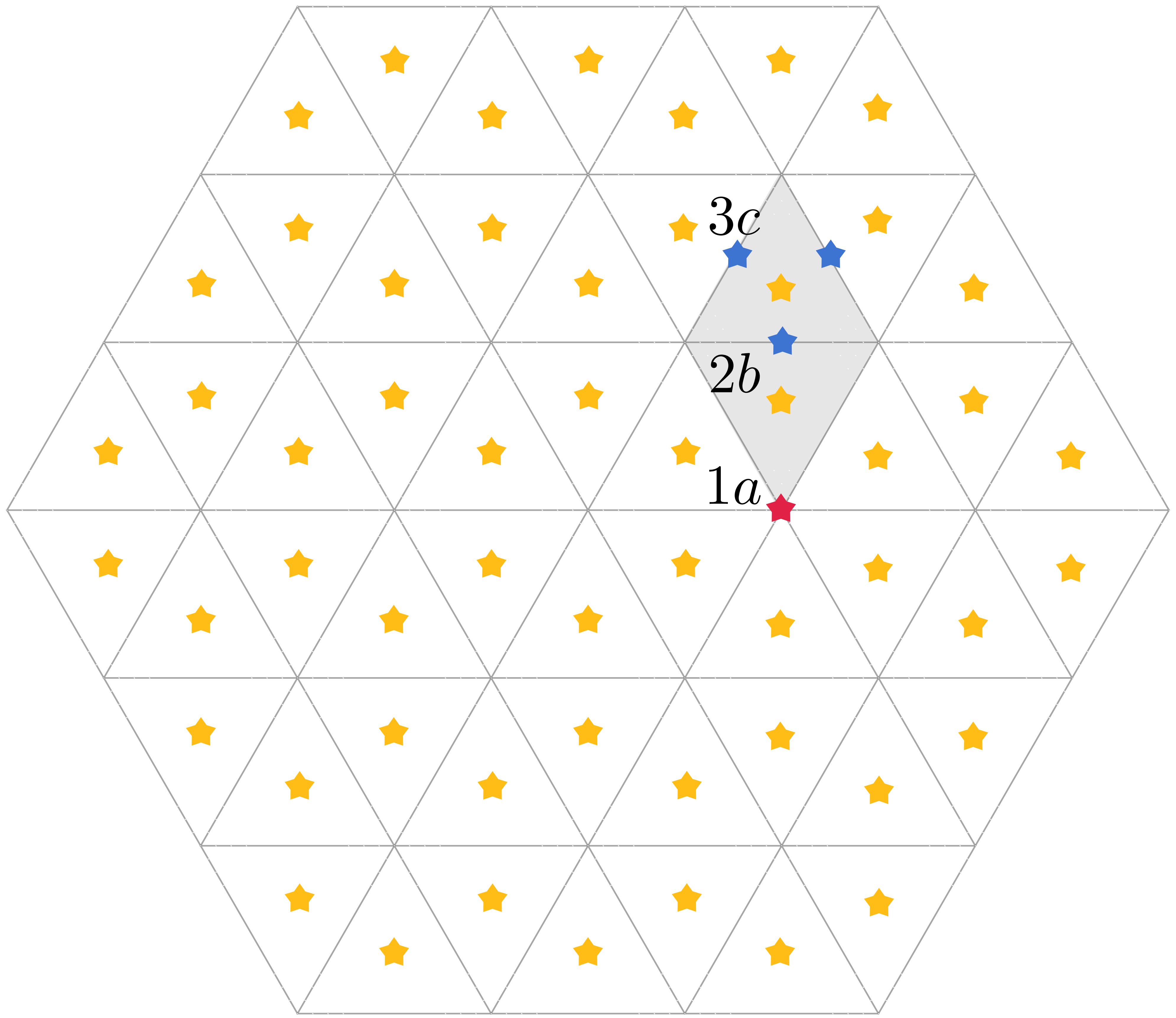

hexagonal lattice

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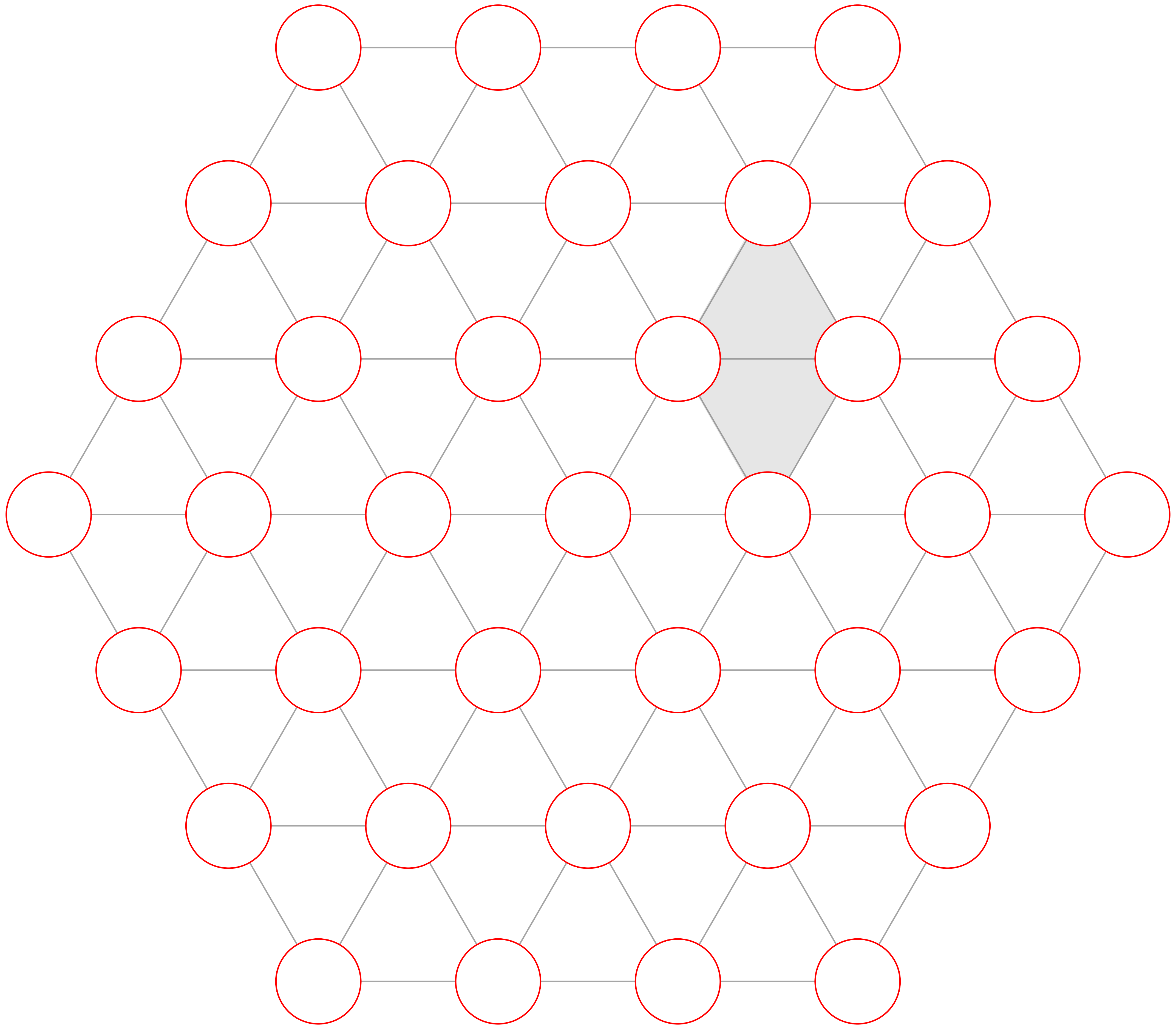
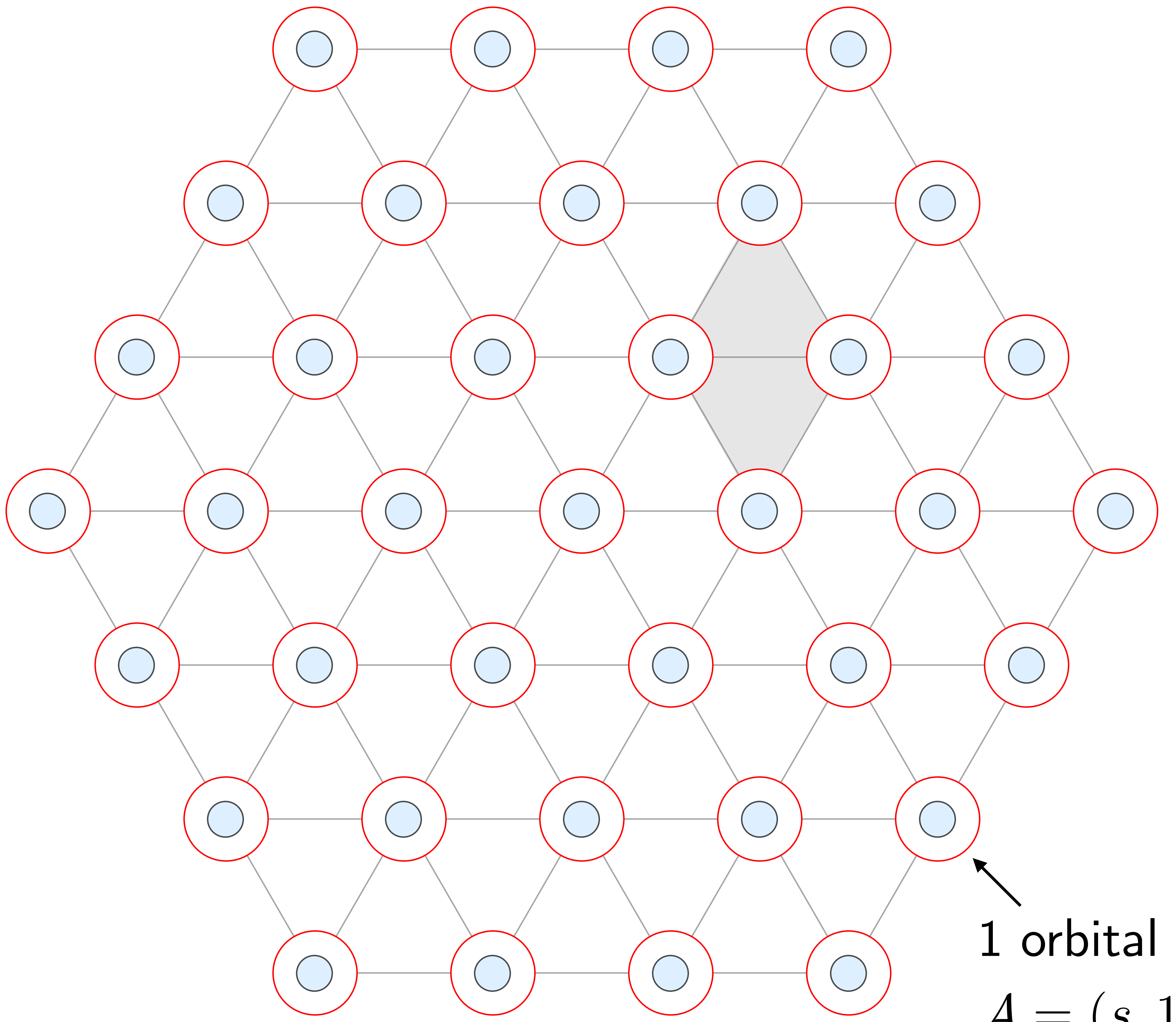


Choose lattice $w = 1a$ as a frame of reference.

Now we ask: where are the electrons?

Putting electrons on the lattice



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$\rightarrow$ Trivial atomic limit $\mathcal{A} = (\rho, w)$:

- $\rightarrow$ Same w as lattice
- $\rightarrow$ Transforms under rep ρ of G_w

Putting the Wannier centers away from the lattice sites

→ Chemically electrons in crystals form hybridized orbitals to achieve geometric configurations that maximize bonding.

→ The center of each orbital ★ then is shifted to a different site in the site in the unit cell

→ New orbitals transform in a new way under the lattice symmetry: Note the sp^2 orbitals gain a phase $e^{2\pi i/3}$ under C_3

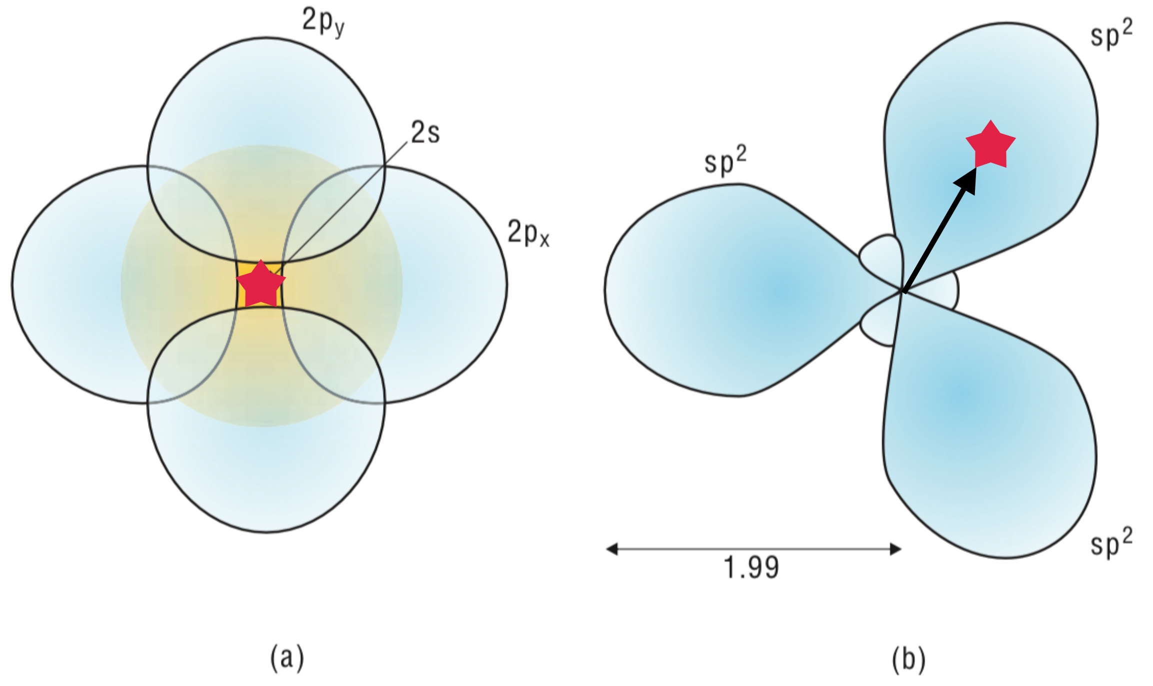


Figure 2.7 (a) The 2s, $2p_x$ and $2p_y$ orbitals on an atom. (b) Three sp^2 hybrid orbitals formed by combining the three original orbitals. The orbitals are arranged at an angle of 120° to each other and point towards the vertices of an equilateral triangle.

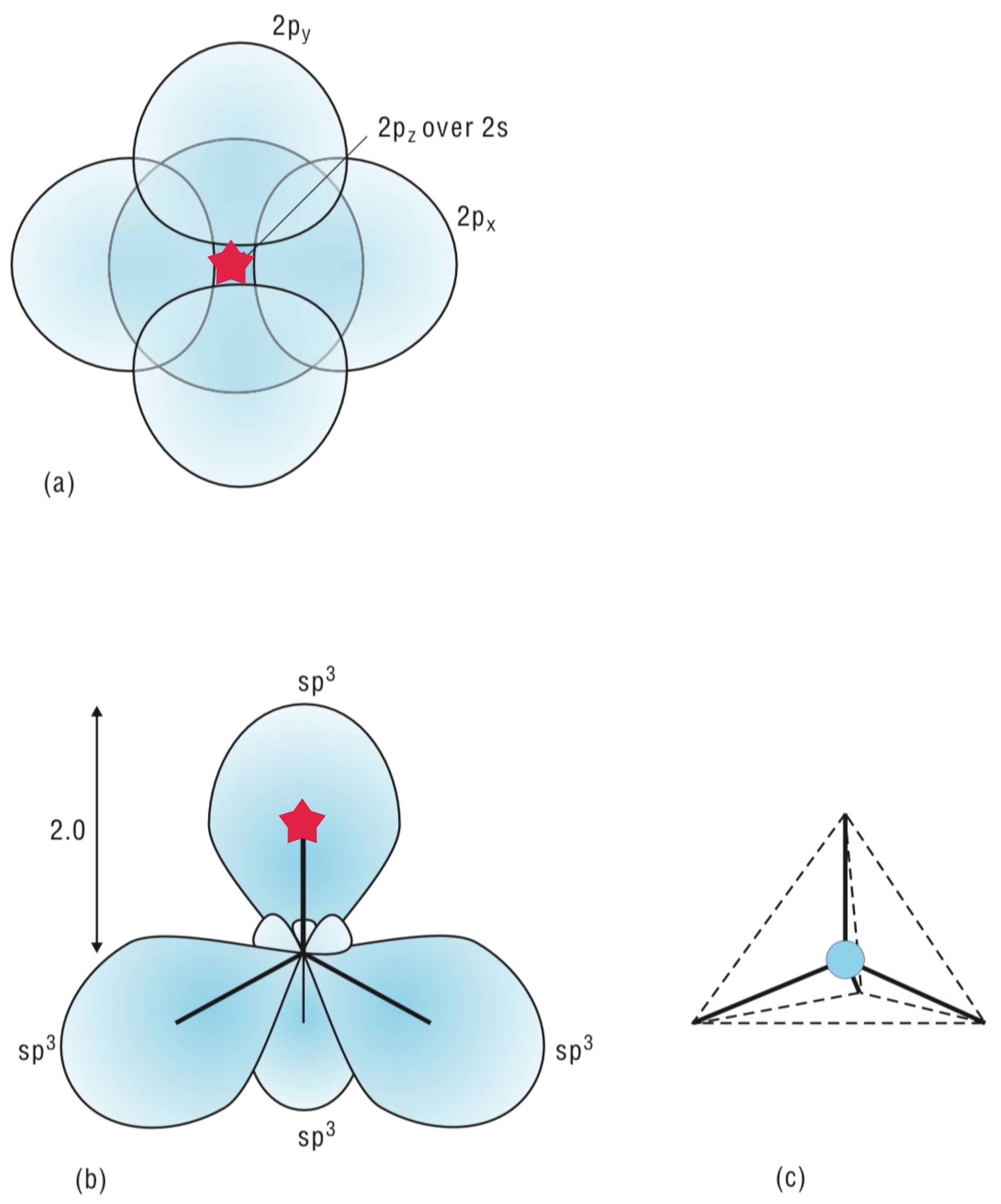
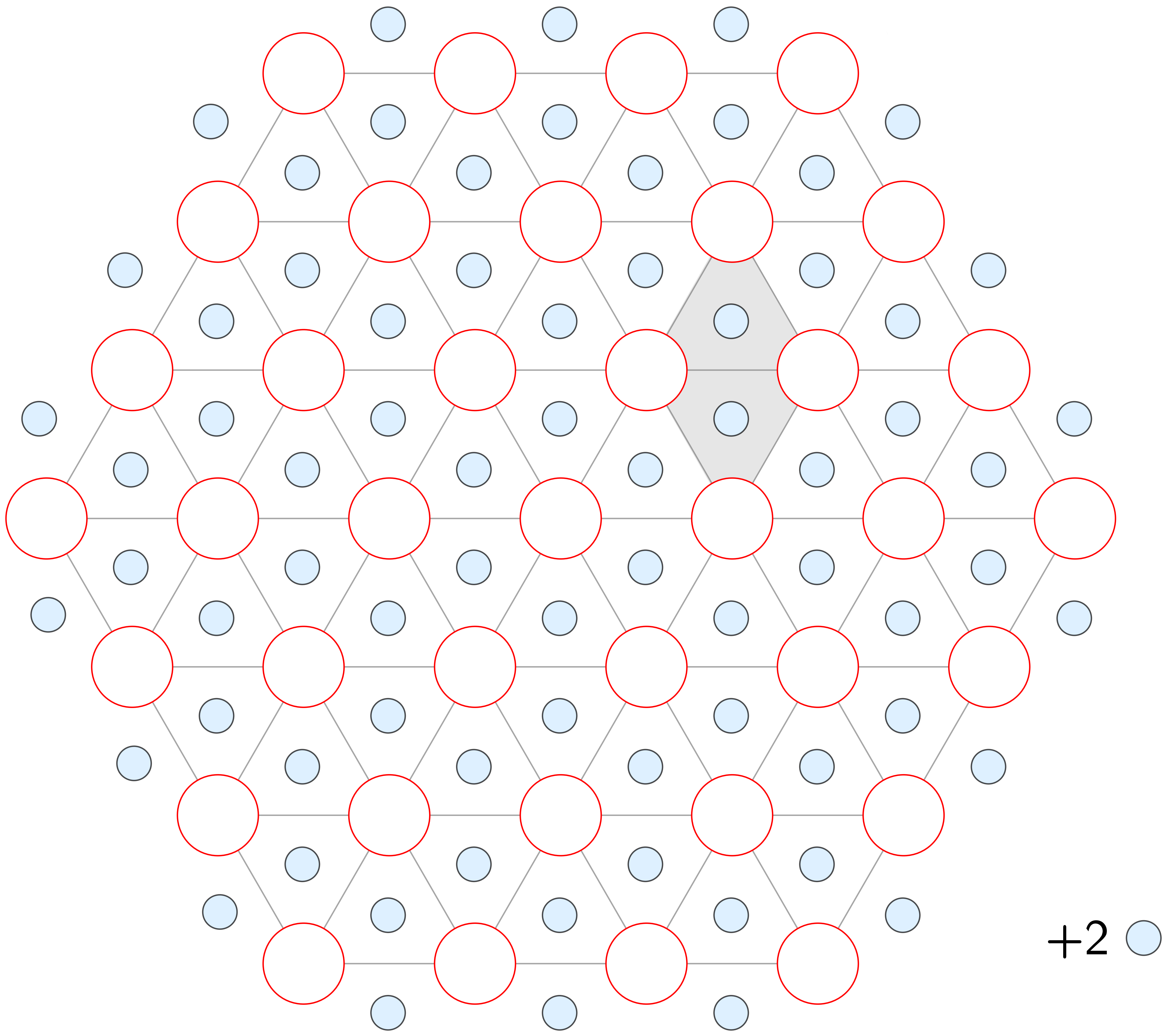


Figure 2.8 (a) The 2s, $2p_x$, $2p_y$ and $2p_z$ orbitals on an atom. (b) Four sp^3 hybrid orbitals formed by combining the four original orbitals. The orbitals are at an angle of 109.5° to each other and point towards the vertices of a tetrahedron.

figures: Tilley *Understanding Solids* 2013

Putting electrons on the lattice



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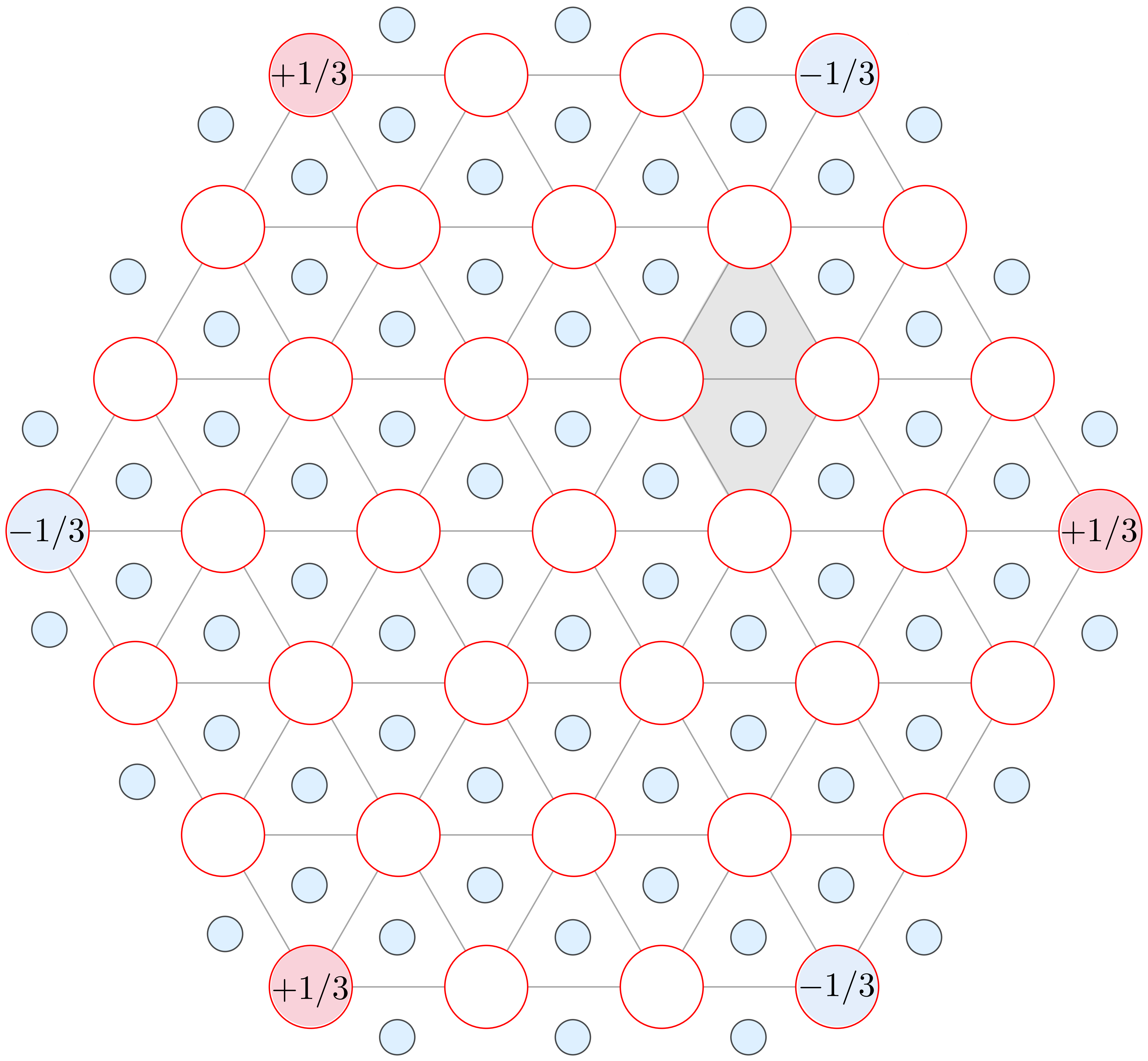
- $\rightarrow$ Different w that lattice.
- $\rightarrow$ Transforms under rep ρ of $G_{w'}$
- $\rightarrow$ Filling anomalies: maybe we need to break the symmetry to fill in all states
- $\rightarrow$ Boundary signatures of quantized charge moments such as dipole or quadrupole moment

Putting electrons on the lattice



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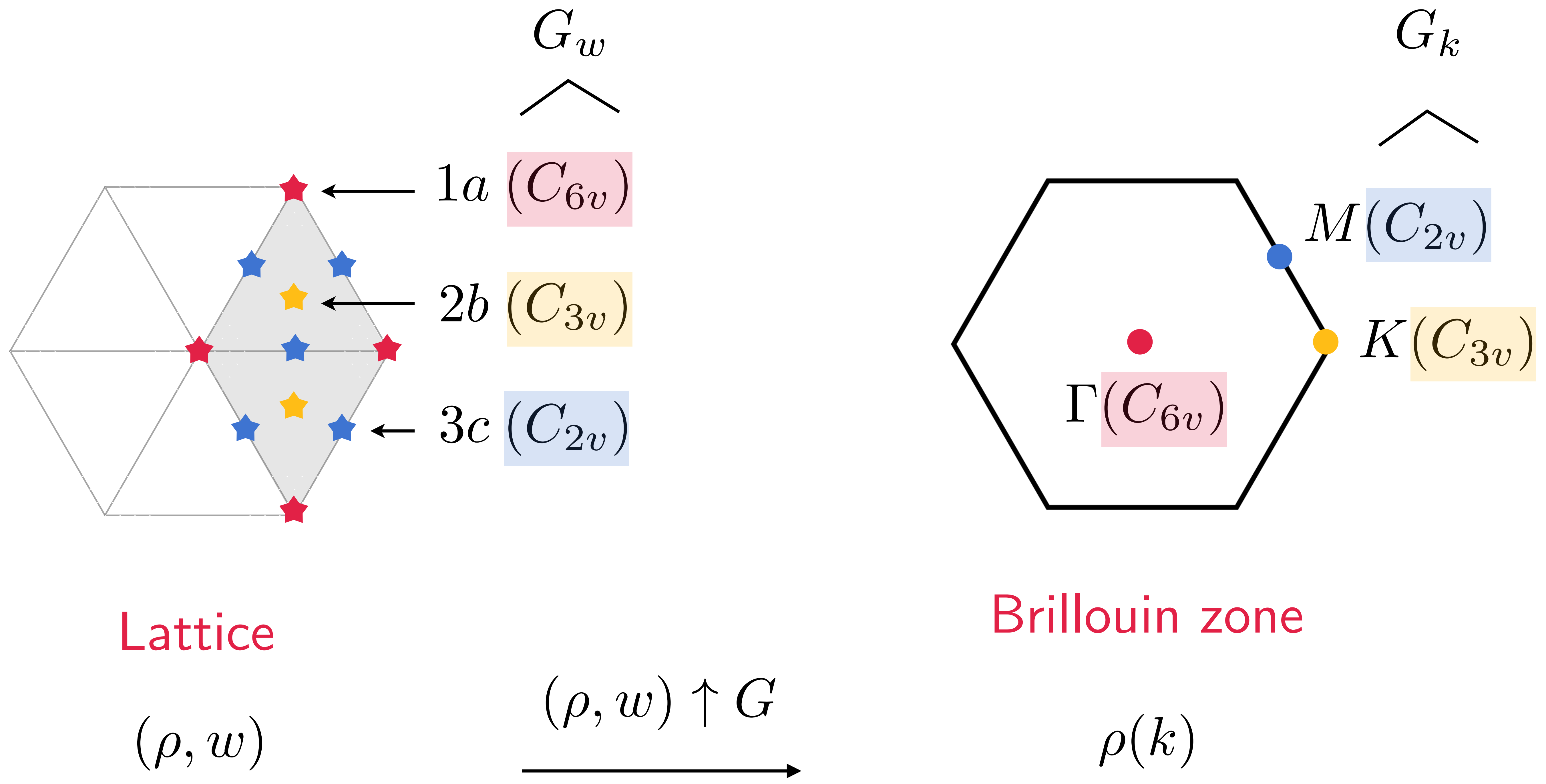
  → Boundary signatures of quantized charge moments such as dipole or quadrupole moment

Every distinct atomic limit has distinct symmetry labels

All atomic bands $\mathcal{A} = (\rho, w)$ transform under a representation of G. This representation can be found by looking at a single orbital ρ at one site of the Wyckoff position w, which is a representation of G_w: It uniquely determines the representation at a momenta k with group G_k.

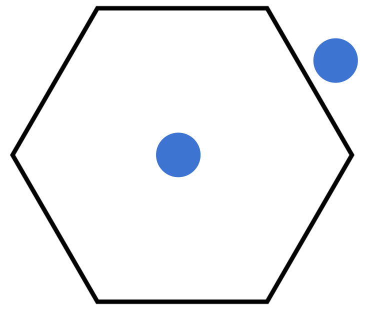
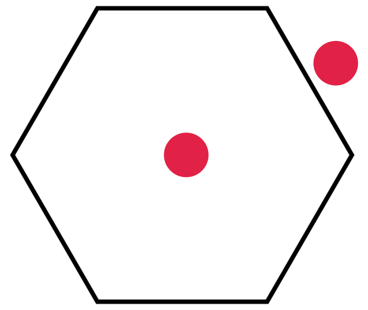
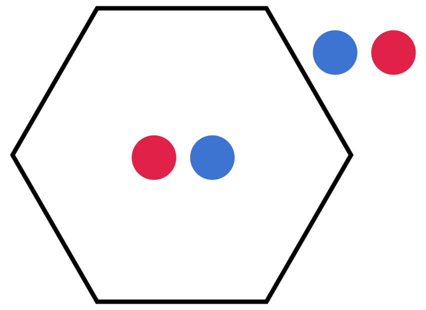
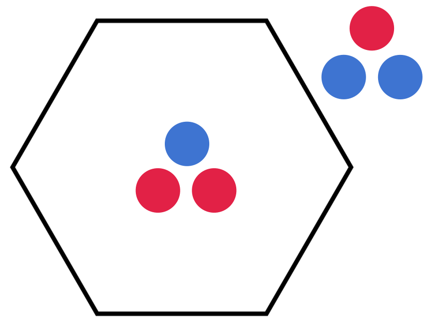


Some elementary band representations in $p6mm$

$\rightarrow$ Any atomic insulator can be obtained out of mixing an irreducible (or elementary) set of band representations.

$\rightarrow$ Lattice with C_3 and C_2 and inversion symmetry only two inversion symmetric momenta: Γ and M which we label with positive (blue) and negative (red) coloring.

$\mathcal{A}$	$(s, 1a)$	$(p_z, 1a)$	$(s, 2b)$	$(\{p_x, p_y\}, 2b)$	$(s, 3c)$	$(p_x, 2c)$	$(p_y, 3c)$
$\rho(\Gamma)$	Γ_1	Γ_2	$\Gamma_1 \oplus \Gamma_4$	$\Gamma_5 \oplus \Gamma_6$	$\Gamma_1 \oplus \Gamma_5$	$\Gamma_3 \oplus \Gamma_6$	$\Gamma_4 \oplus \Gamma_6$
$\rho(K)$	K_1	K_2	K_3	$K_1 \oplus K_2 \oplus K_3$	$K_1 \oplus K_3$	$K_1 \oplus K_3$	$K_2 \oplus K_3$
$\rho(M)$	M_1	M_2	$M_1 \oplus M_4$	$M_1 \oplus M_2 \oplus M_3 \oplus M_4$	$M_1 \oplus M_3 \oplus M_4$	$M_1 \oplus M_2 \oplus M_3$	$M_1 \oplus M_2 \oplus M_4$

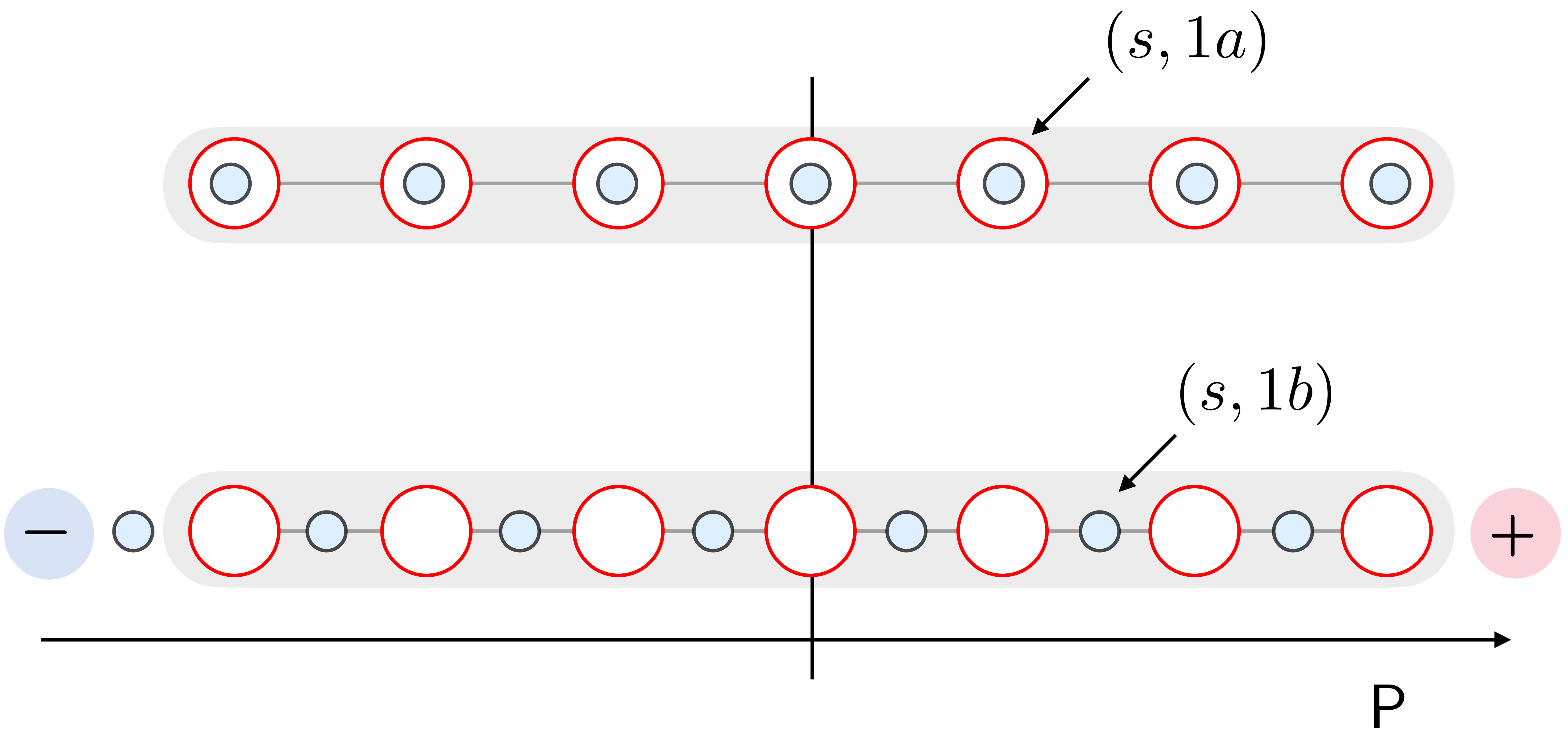
SSH chain with inversion symmetry

VOLUME 42, NUMBER 25 PHYSICAL REVIEW LETTERS 18 JUNE 1979

Solitons in Polyacetylene

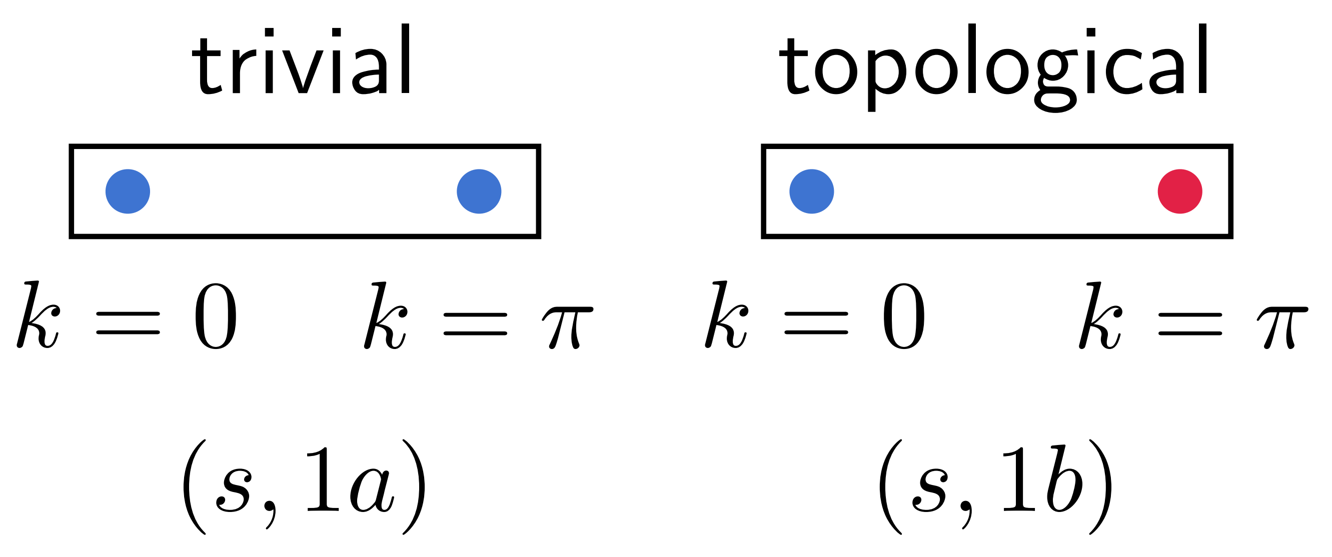
W. P. Su, J. R. Schrieffer, and A. J. Heeger
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104
(Received 15 March 1979)

We present a theoretical study of soliton formation in long-chain polyenes, including the energy of formation, length, mass, and activation energy for motion. The results provide an explanation of the mobile neutral defect observed in undoped $(CH)_x$. Since the soliton formation energy is less than that needed to create band excitation, solitons play a fundamental role in the charge-transfer doping mechanism.



One dimensional obstructed atomic band protected by inversion:

Topological invariant obtained by product of inversion eigenvalues in the Brillouin zone



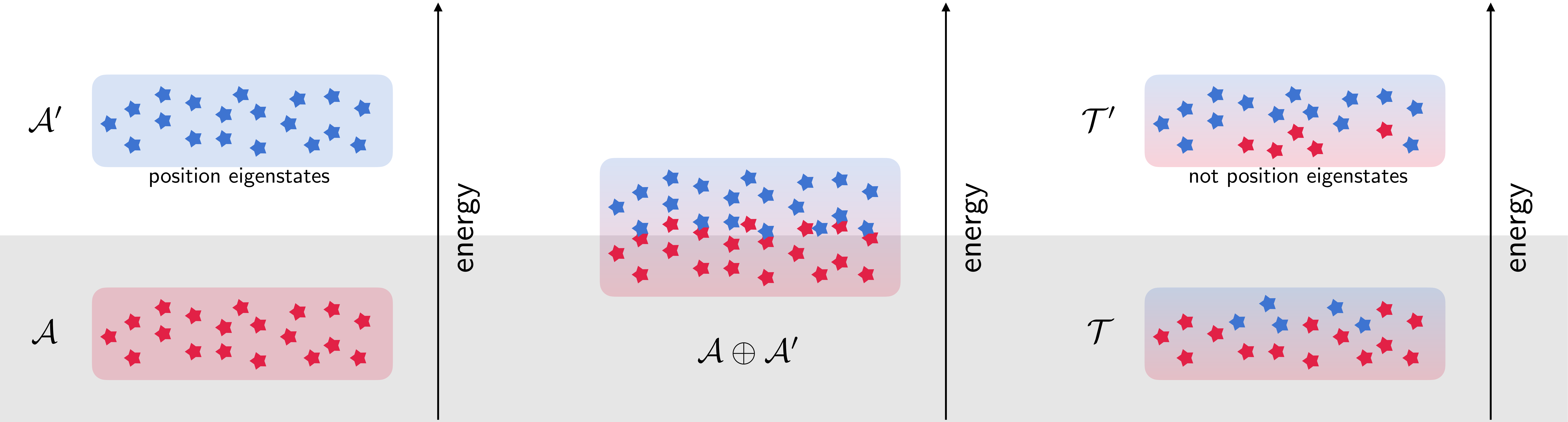
Topological response: Quantized polarization

Position and Berry phase: Modern theory of Polarization Resta King-Smith and Vanderbilt

$$p_x \sim P\hat{x}P \sim \phi$$

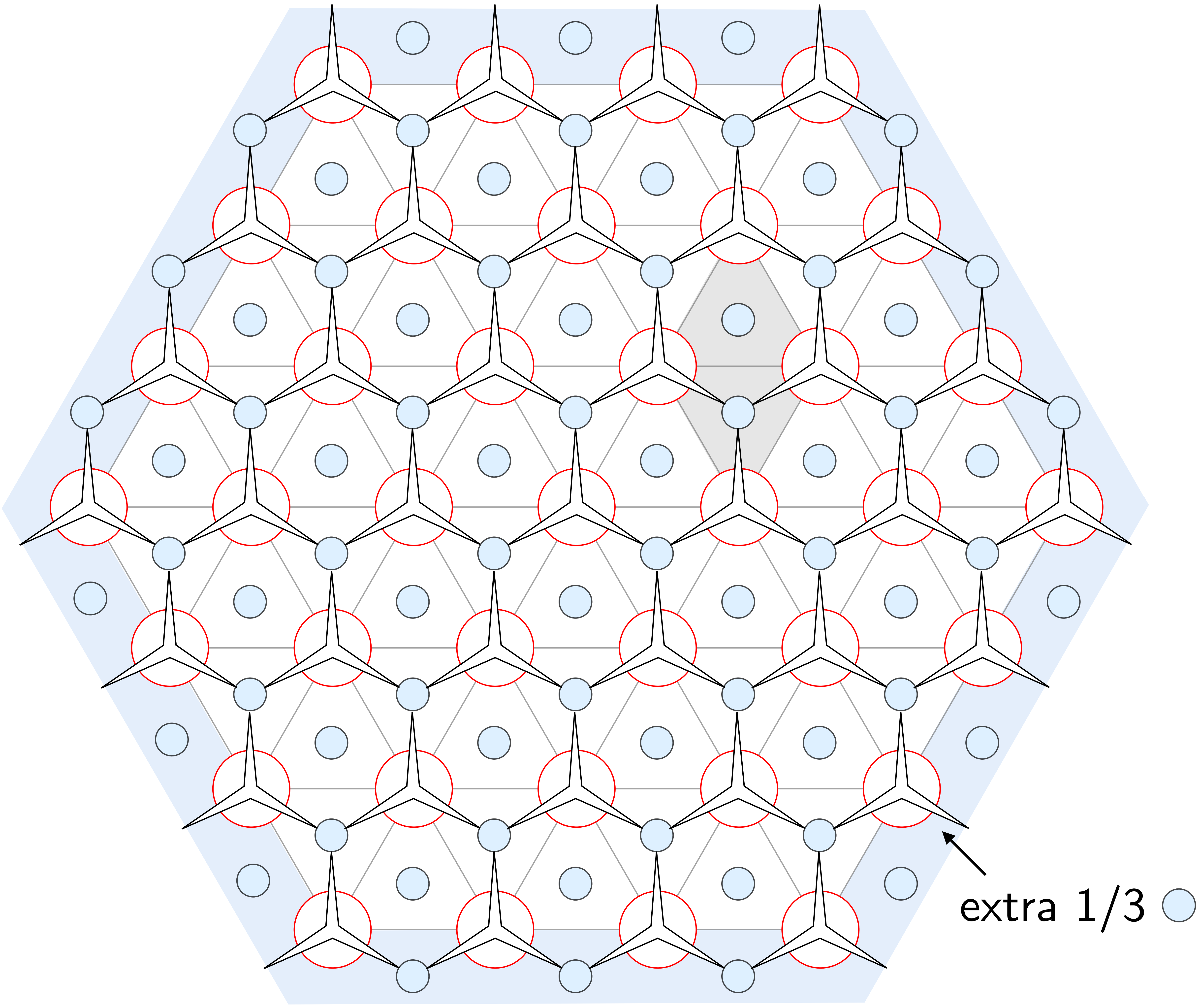
Band inversion: How to make a band topological?

Forget about energy details except that there is an Hamiltonian $\mathcal{H}$ that defines the bands



atomic insulator | semimetal | topological insulator

Topological bands without atomic description



→ Impossible to represent as localized states inside the unit cell

→ Short range entanglement between neighboring unit cells

→ Edge modes do not have a stand alone lattice realization: they are anomalous

→ Only stable topological bands have irremovable boundary modes

→ Obtained by mixing atomic bands,

$$\mathcal{T} \oplus \mathcal{T}' = \mathcal{A} \oplus \mathcal{A}'$$

→ Incompatible eigenvalues with an atomic band

on the horizon

Topological phases of systems with boundary:
Find different topologies than those with periodic boundaries

Motivation

An intriguing model:

→ Quantized topological response

→ Corner modes

→ No adiabatically disconnected parts of the bulk phase diagram

→ Topological or Trivial?

→ Subtle notion of topology

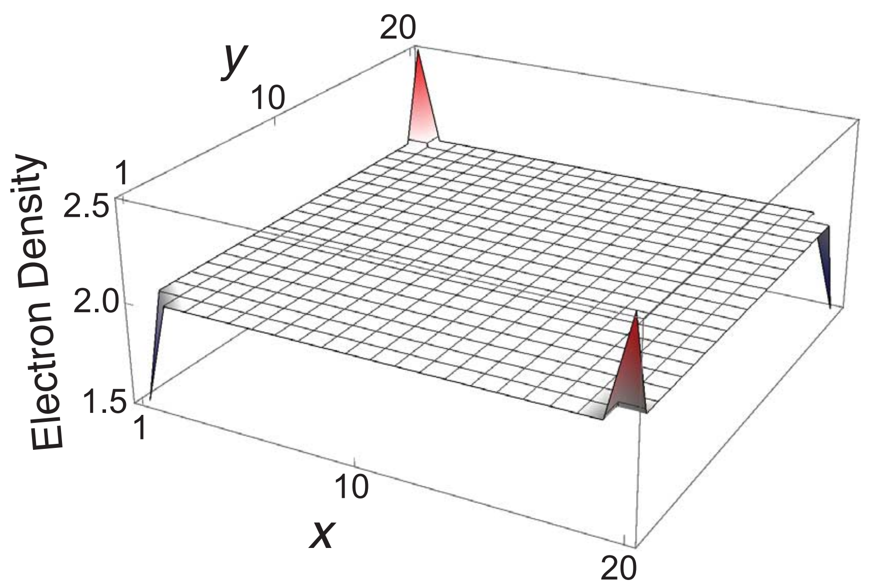
First model of higher order topology!

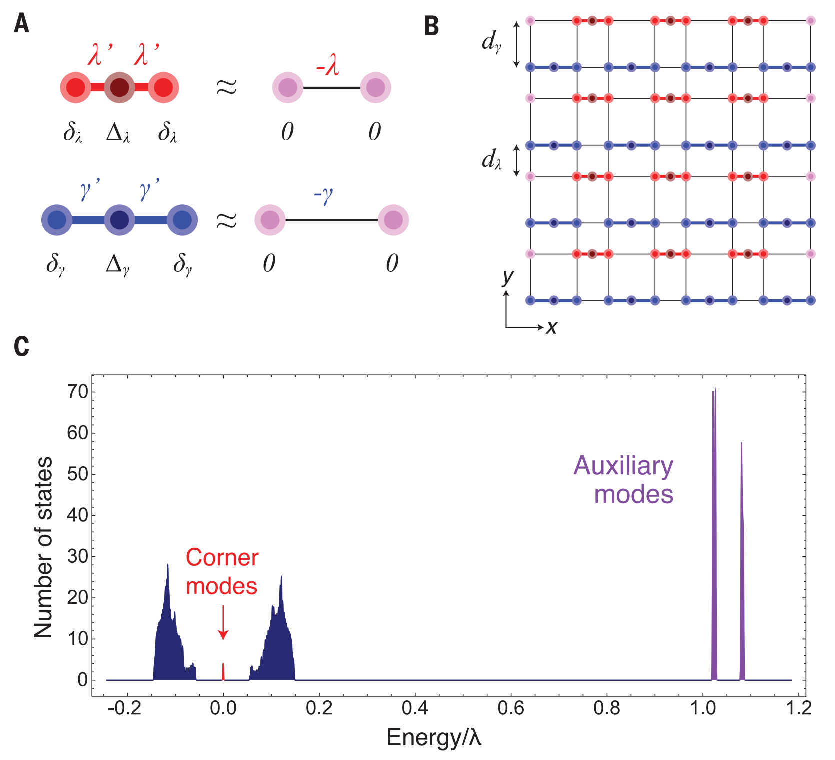
TOPOLOGICAL MATTER

Quantized electric multipole insulators

Wladimir A. Benalcazar,[1] B. Andrei Bernevig,[2] Taylor L. Hughes[1]*

The Berry phase provides a modern formulation of electric polarization in crystals. We extend this concept to higher electric multipole moments and determine the necessary conditions and minimal models for which the quadrupole and octupole moments are topologically quantized electromagnetic observables. Such systems exhibit gapped boundaries that are themselves lower-dimensional topological phases. Furthermore, they host topologically protected corner states carrying fractional charge, exhibiting fractionalization at the boundary of the boundary. To characterize these insulating phases of matter, we introduce a paradigm in which "nested" Wilson loops give rise to topological invariants that have been overlooked. We propose three realistic experimental implementations of this topological behavior that can be immediately tested. Our work opens a venue for the expansion of the classification of topological phases of matter.





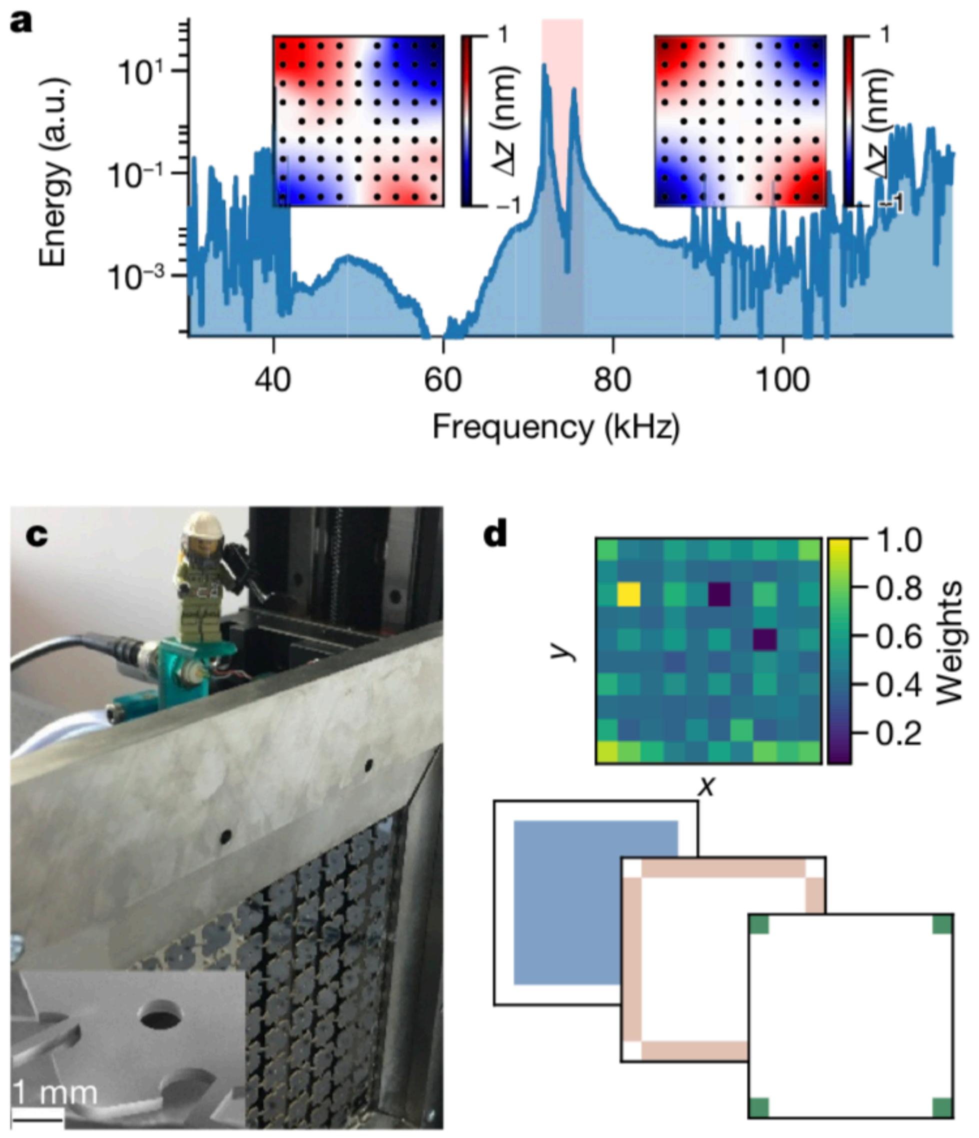
Experimental realizations

LETTER

doi:10.1038/nature25156

Observation of a phononic quadrupole topological insulator

Marc Serra-Garcia[1]*, Valerio Peri[1]*, Roman Süsstrunk[1], Osama R. Bilal[1,2], Tom Larsen[3], Luis Guillermo Villanueva[3] & Sebastian D. Huber[1]

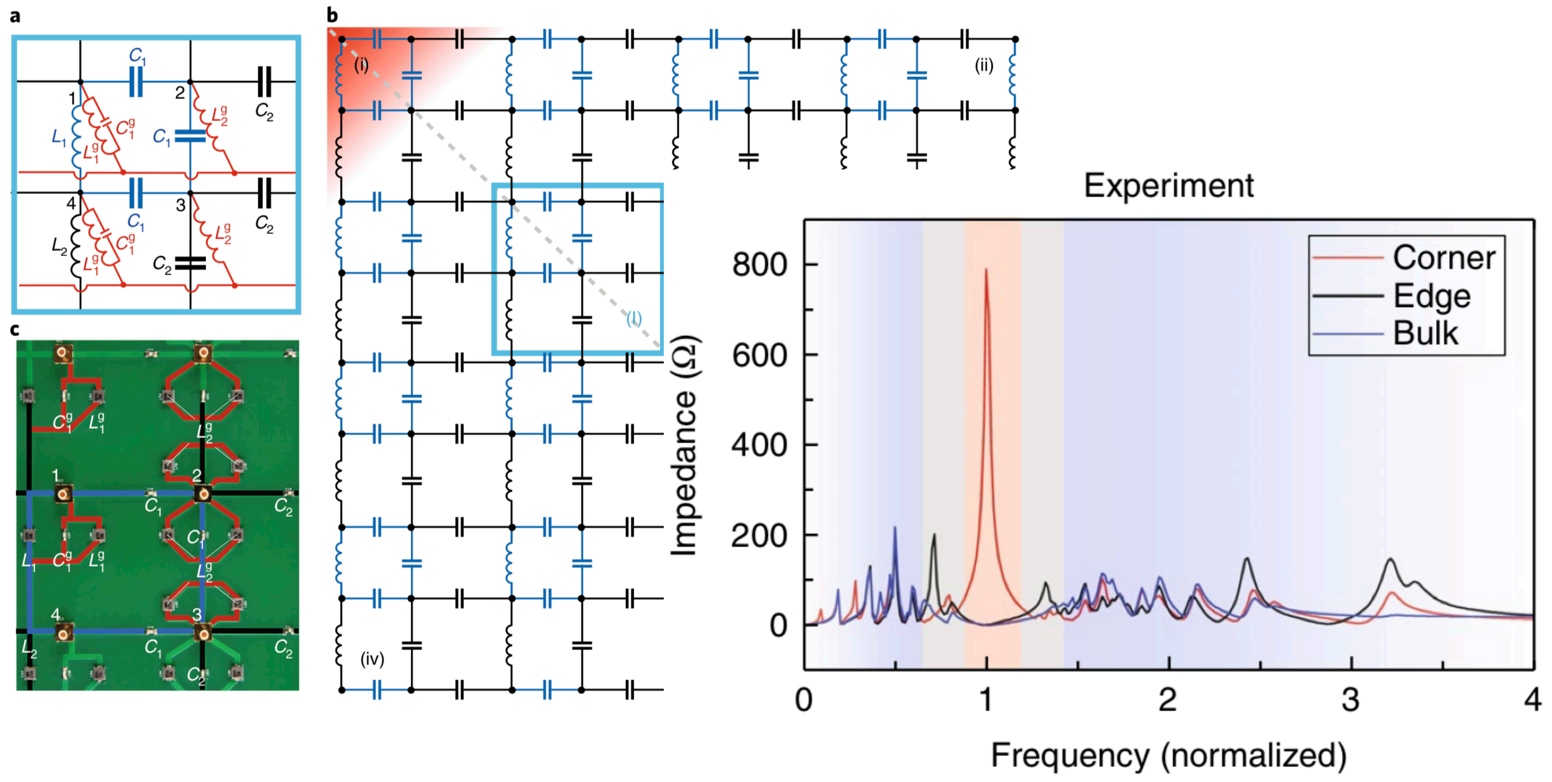


C_4 symmetry (at least weakly) broken

nature physics
ARTICLES
https://doi.org/10.1038/s41567-018-0246-1

Topolectrical-circuit realization of topological corner modes

Stefan Imhof[1], Christian Berger[1], Florian Bayer[1], Johannes Brehm[1], Laurens W. Molenkamp[1], Tobias Kiessling[1], Frank Schindler[2], Ching Hua Lee[3,4], Martin Greiter[5], Titus Neupert[2] and Ronny Thomale[5]*

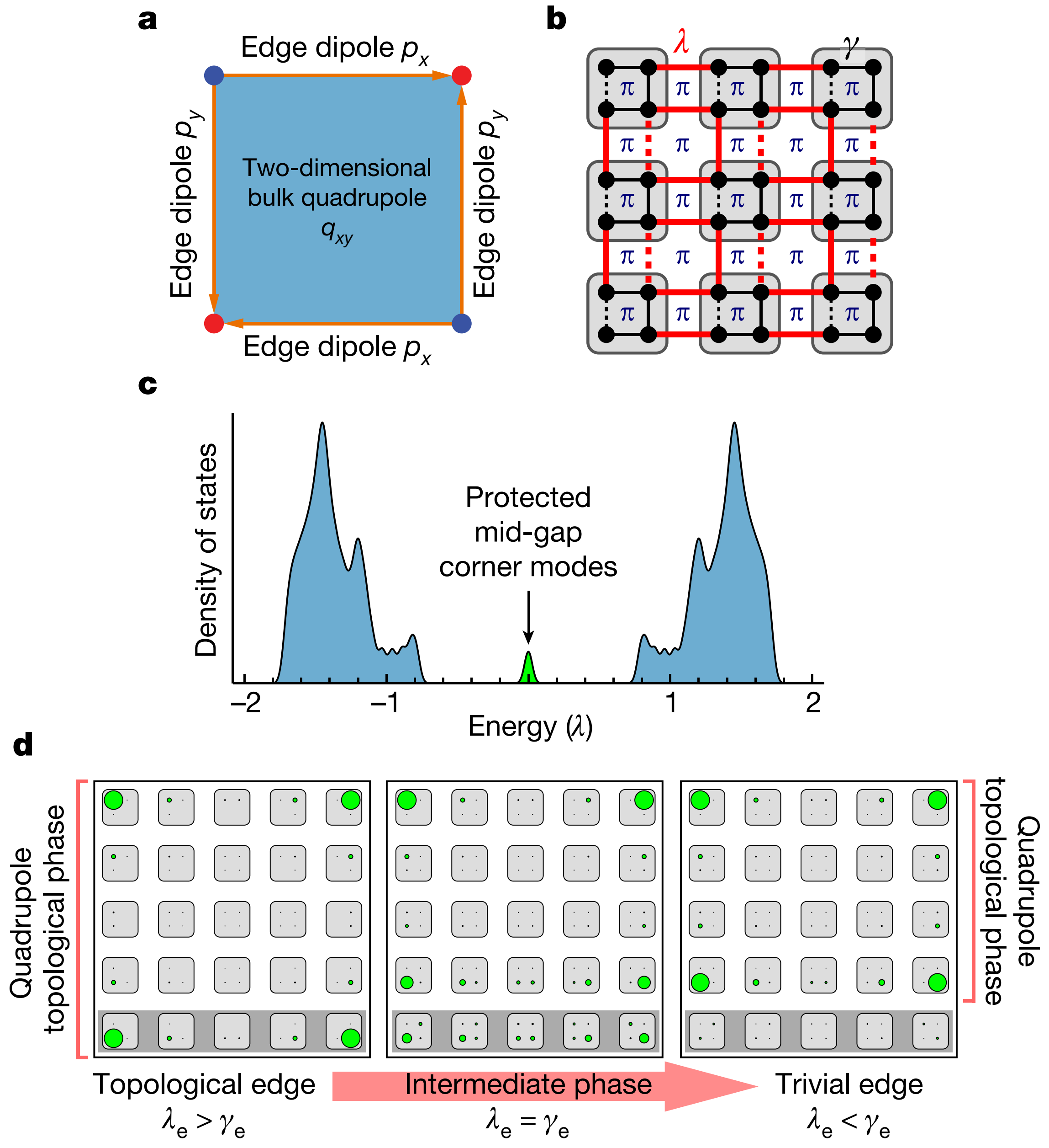


LETTER

doi:10.1038/nature25777

A quantized microwave quadrupole insulator with topologically protected corner states

Christopher W. Peterson[1], Wladimir A. Benalcazar[2], Taylor L. Hughes[2] & Gaurav Bahl[3]

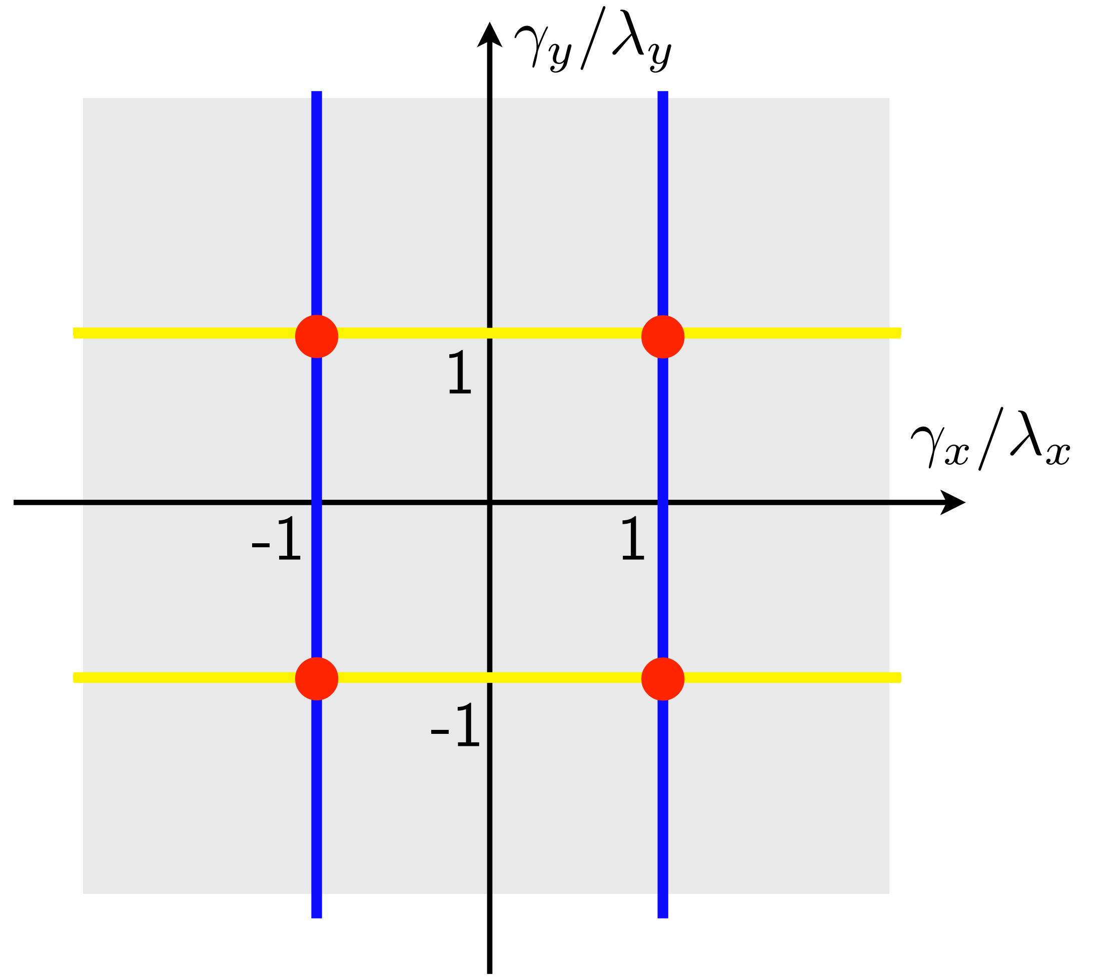


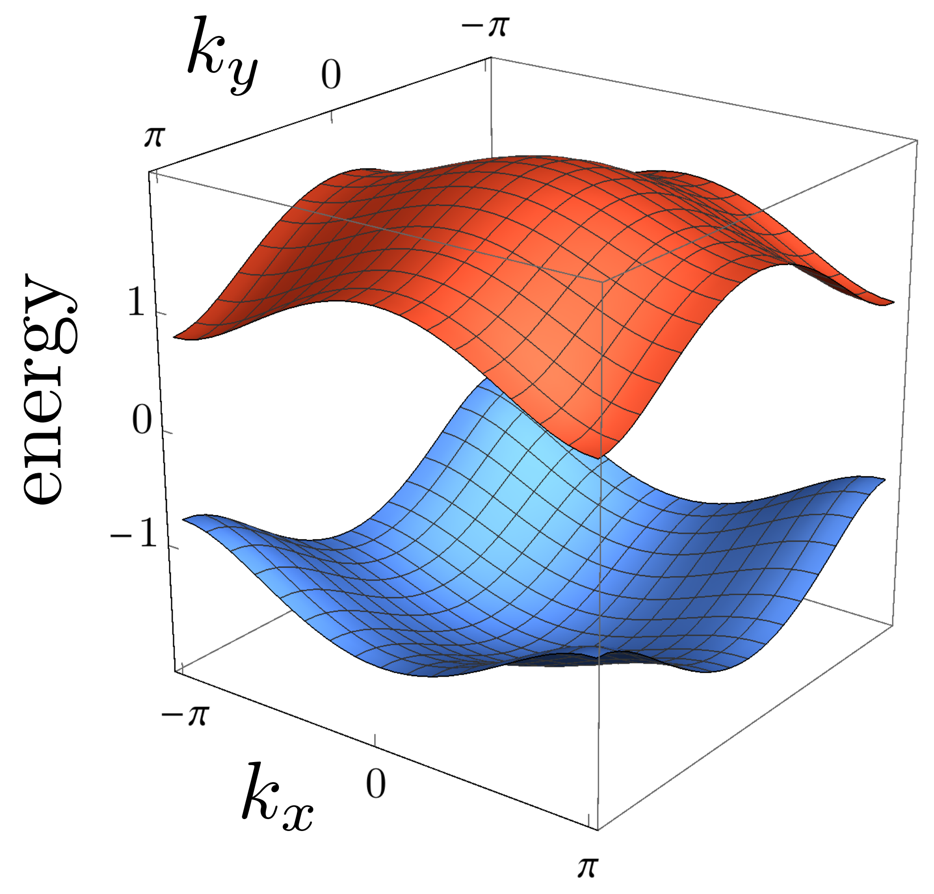
2D Quadrupolar insulator with anticommuting mirrors

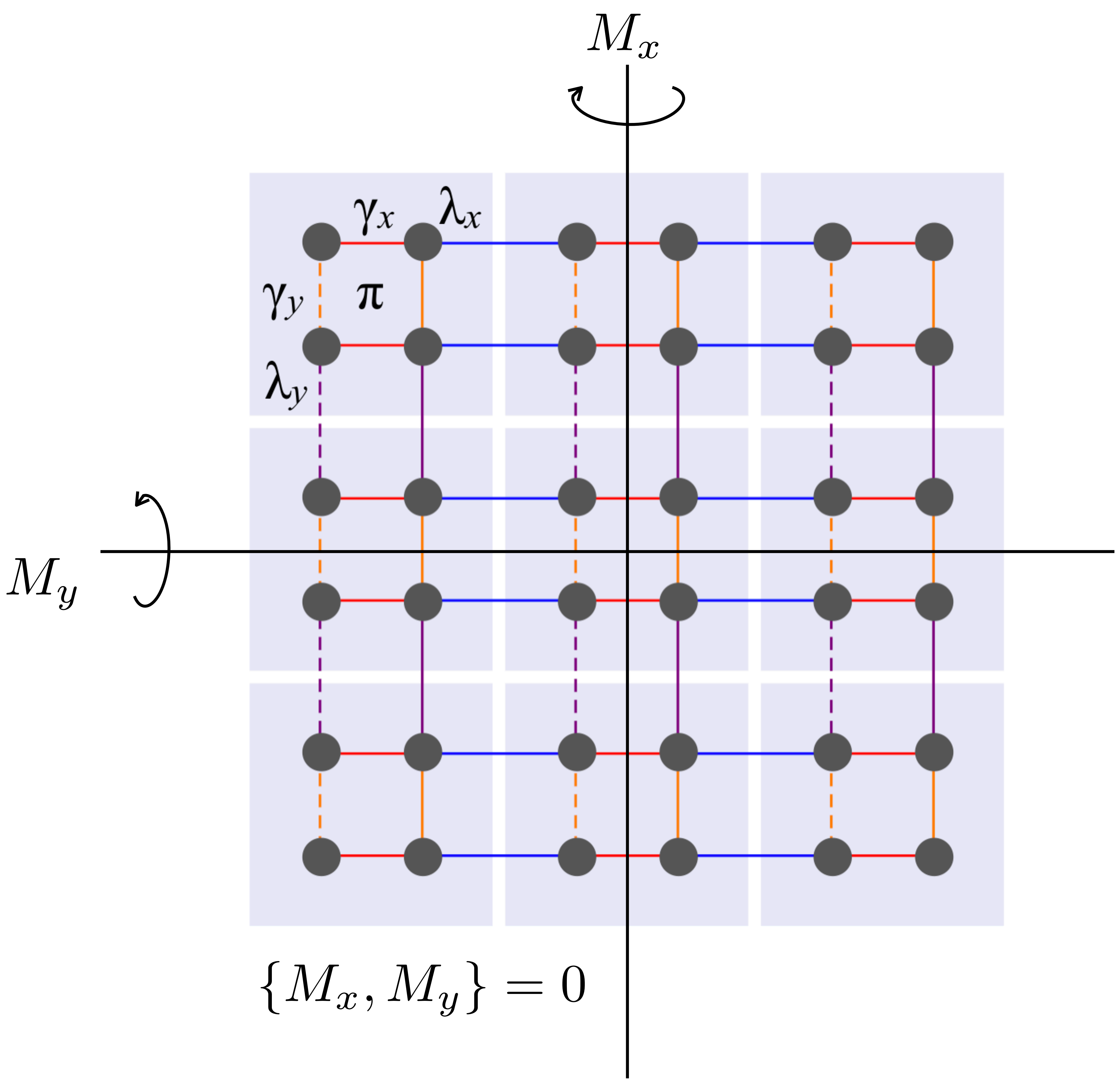
→ Lattice of spinless electrons with nearest neighbour hopping pierced by π fluxes

→ Symmetries M_x and M_y and translations T_x and T_y.

→ Electrons transform under a nonconventional representation for the crystallographic point group, $(M_x M_y)^2 = -1$, due to the π flux.



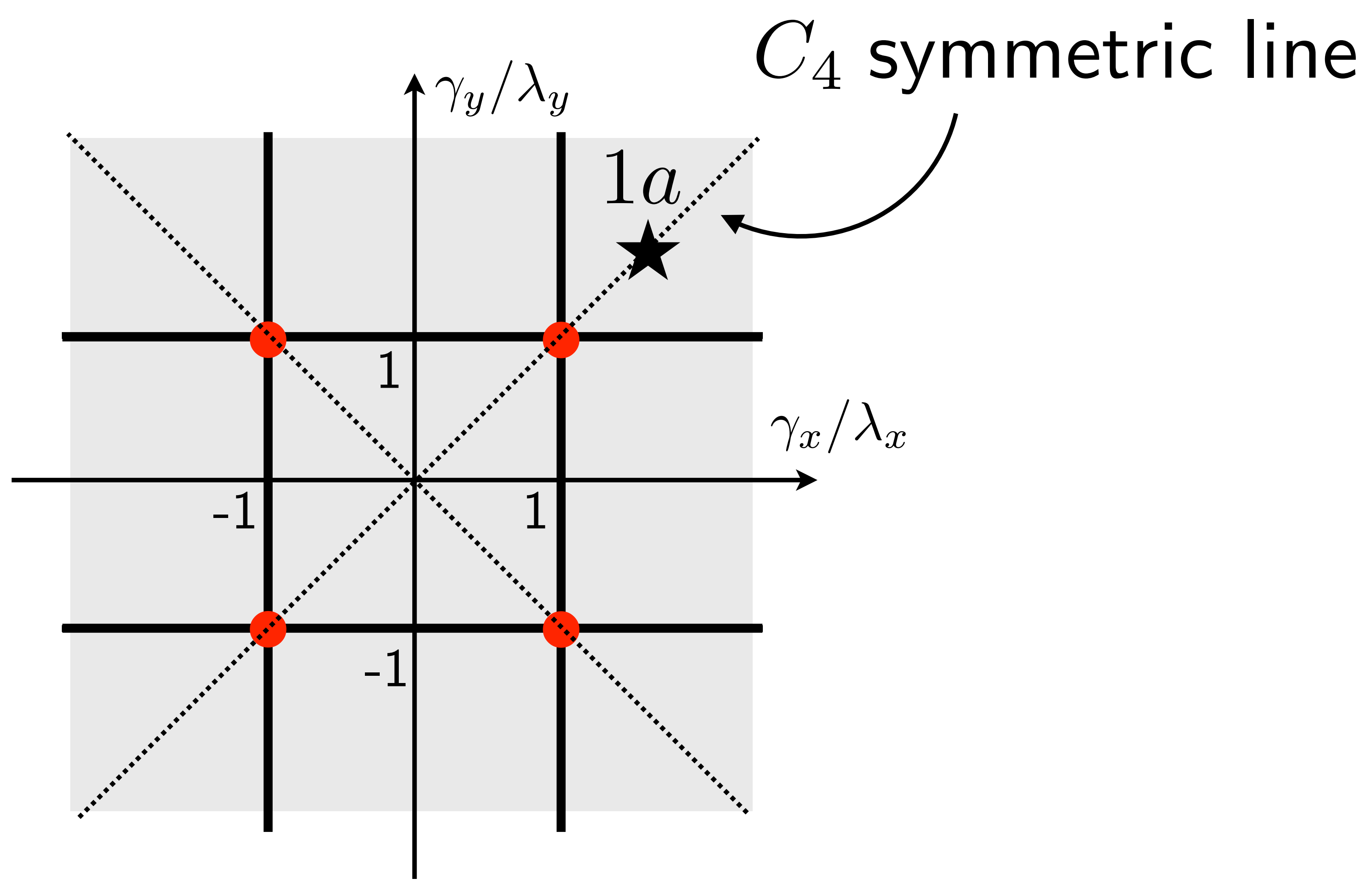


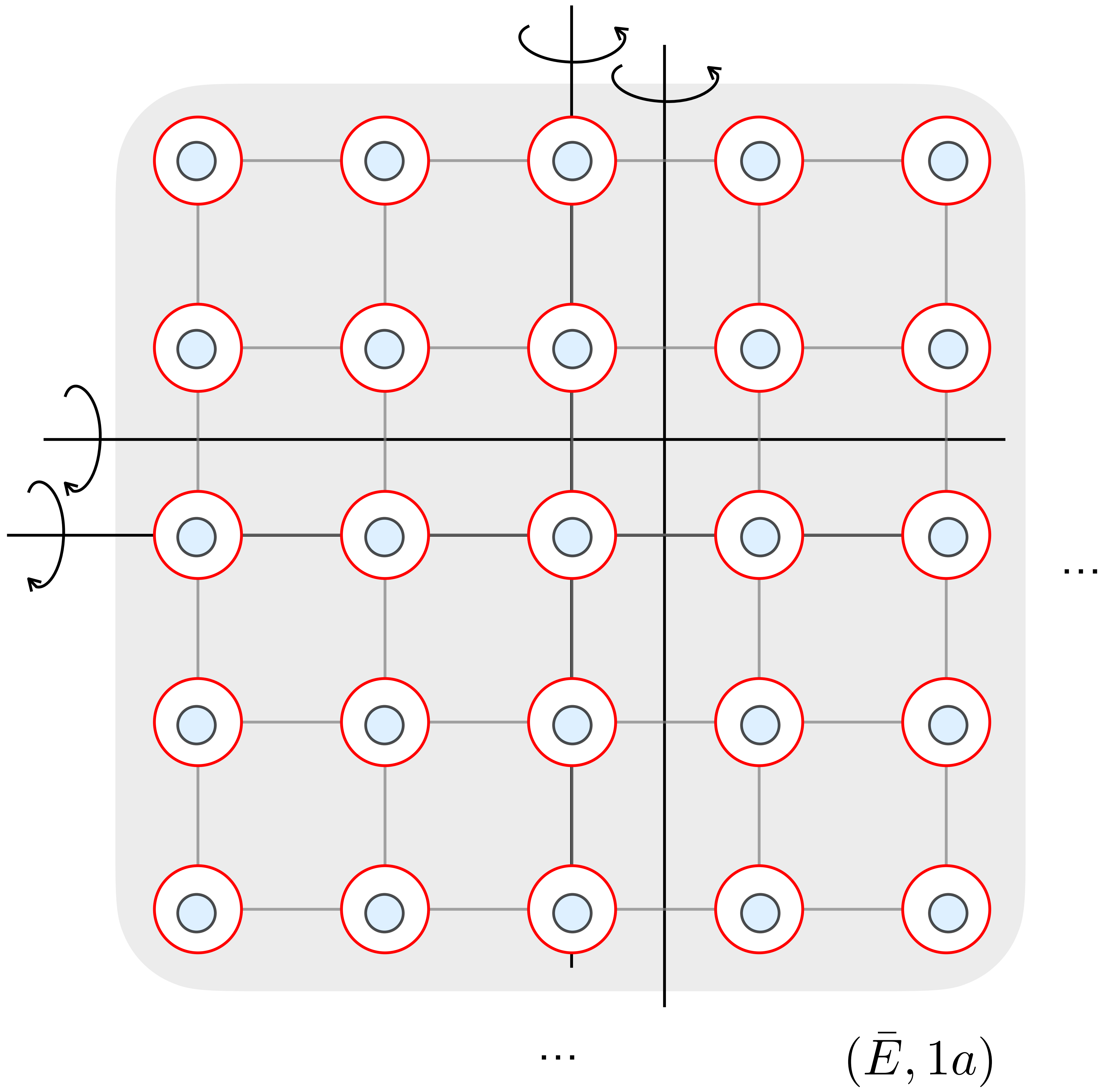


Fixed Wyckoff position: Adding C4 symmetry

→ Enforcing C_4 fixes the spatial position of the electron charges

→ Obstructed atomic limit protected by a bulk gap closing transition





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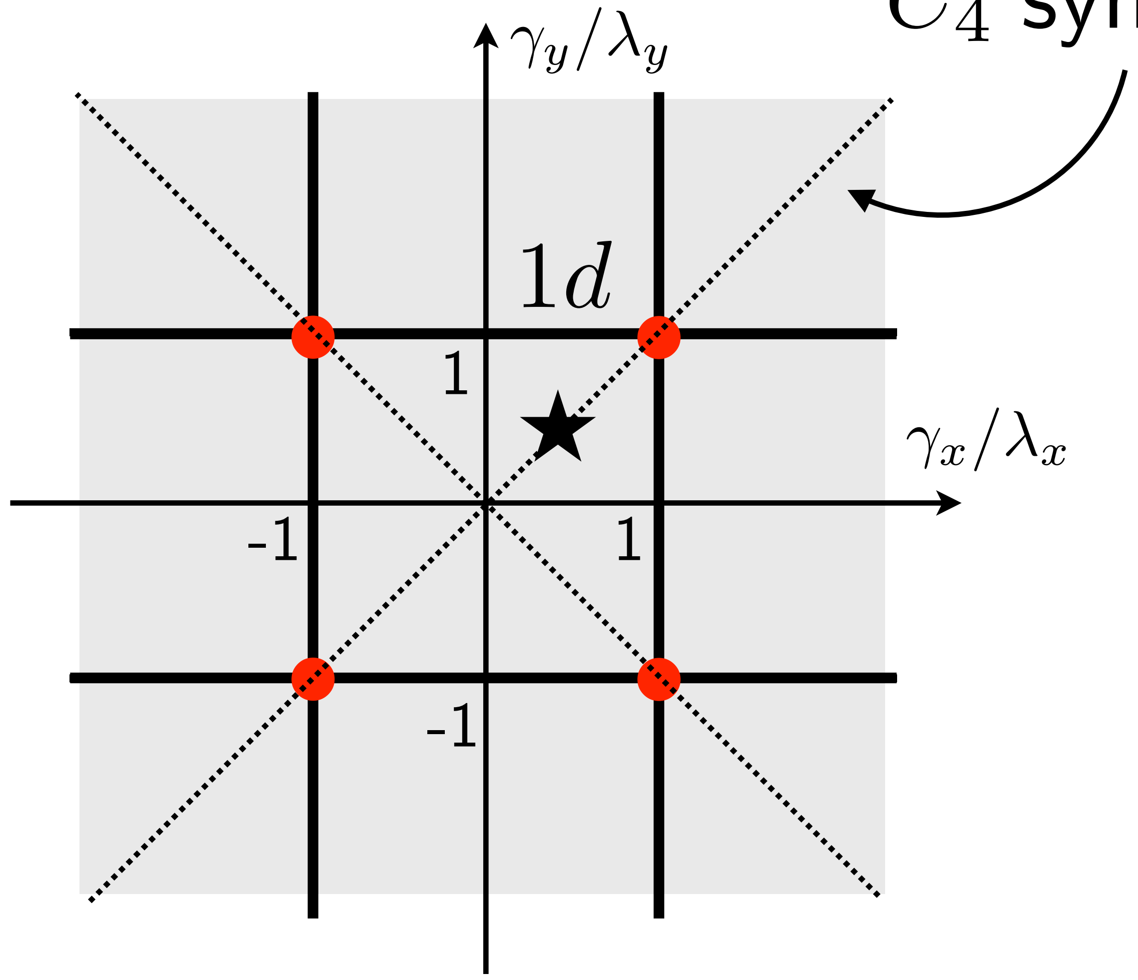
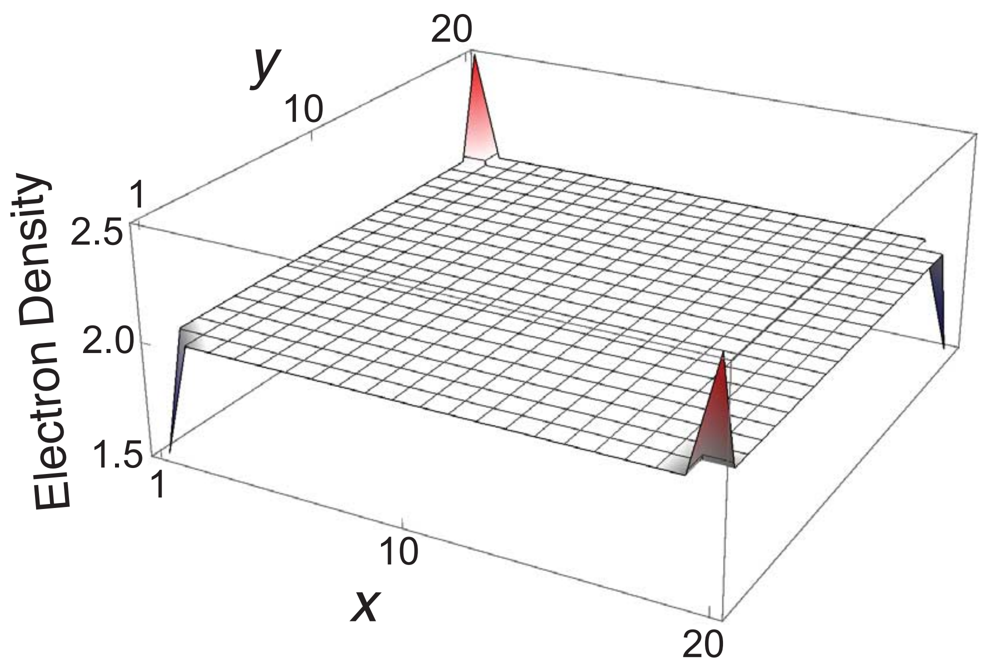
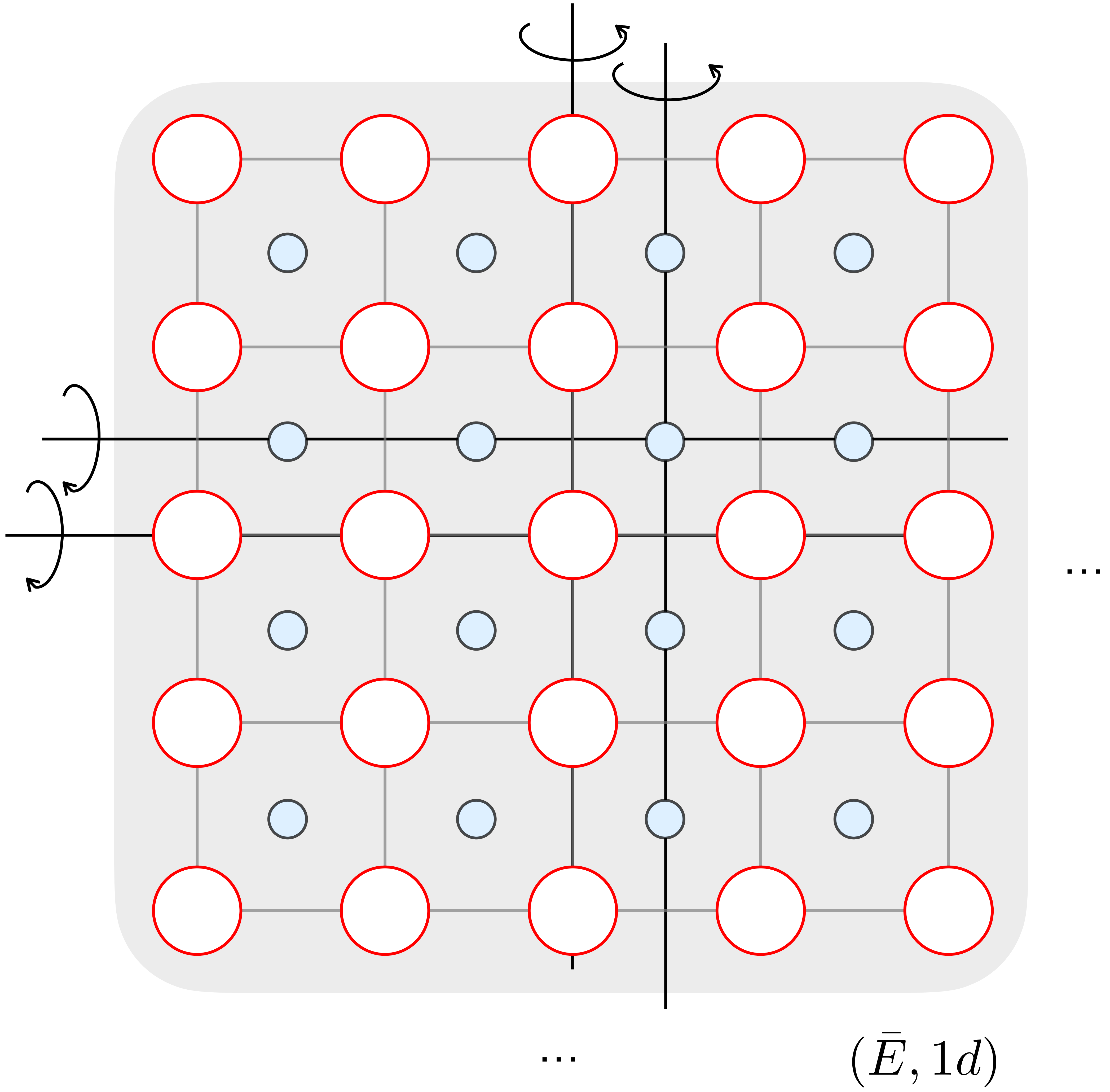
C_4 symmetric line



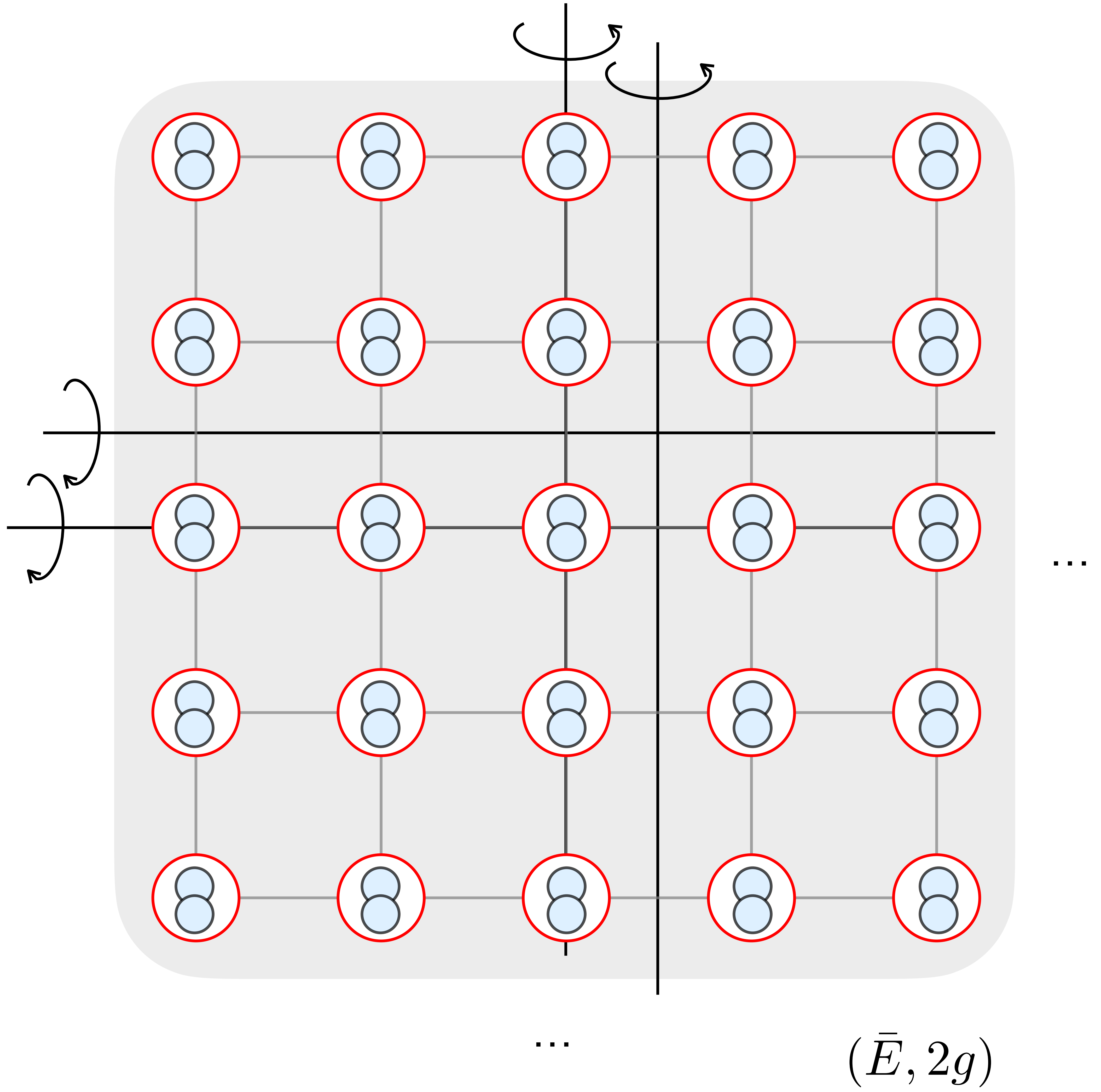




Movable Wyckoff position

The system transforms under an $\bar{E}$ representation of the point group:

Rep. / class	$\{1\}$	$\{\bar{1}\}$	$\{M_x M_y\}$	$\{M_y\}$	$\{M_x\}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
$\bar{E}$	2	-2	0	0	0



Admits distinct bases:

M_x diagonal: $M_x = \sigma_z$ and $M_y = \sigma_x$

M_y diagonal: $M_x = \sigma_x$ and $M_y = \sigma_z$

Adiabatic deformation between all $\mathcal{H}$ along the path

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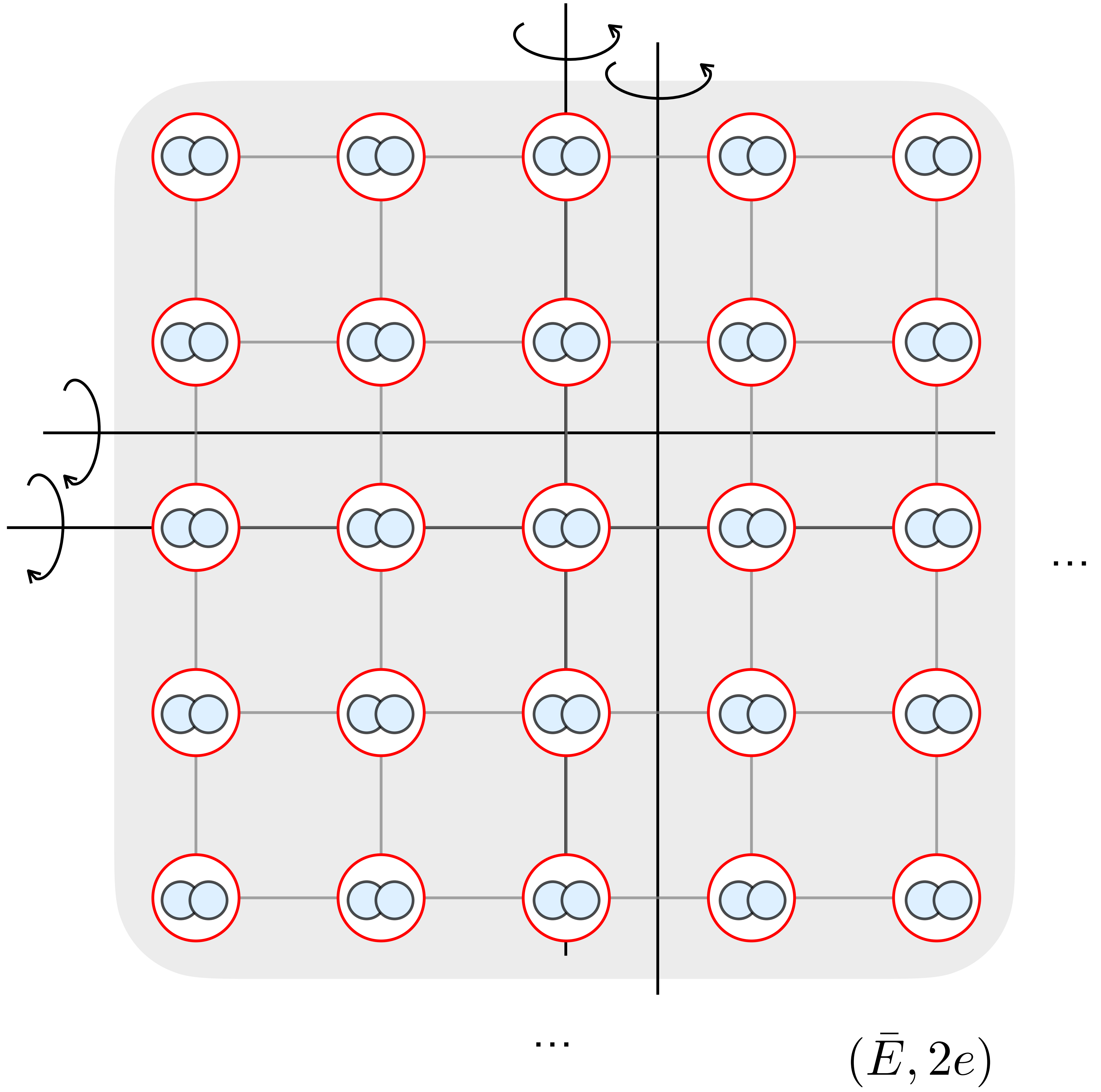

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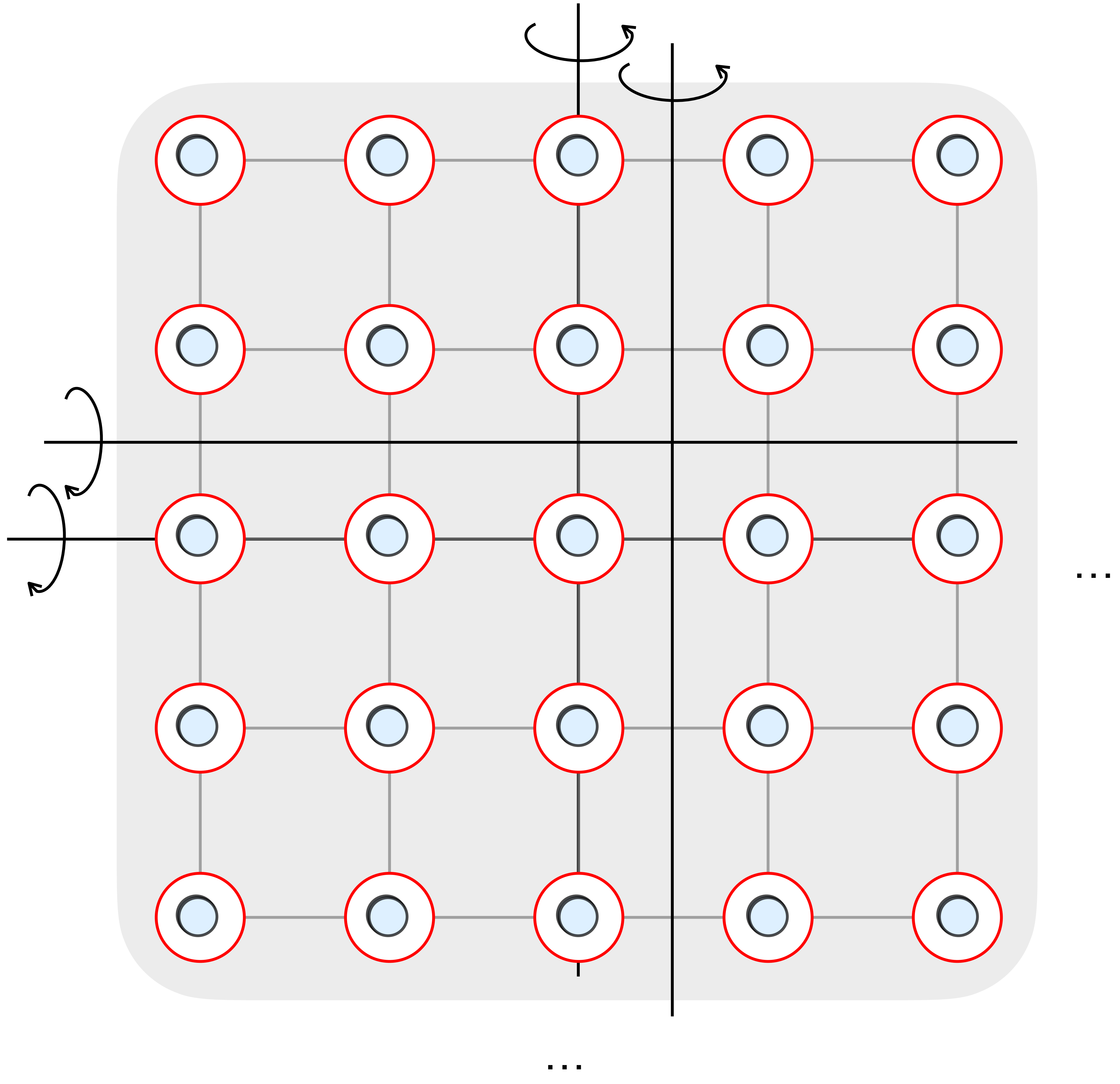
B_2	1	1	-1	-1	1
$\bar{E}$	2	-2	0	0	0



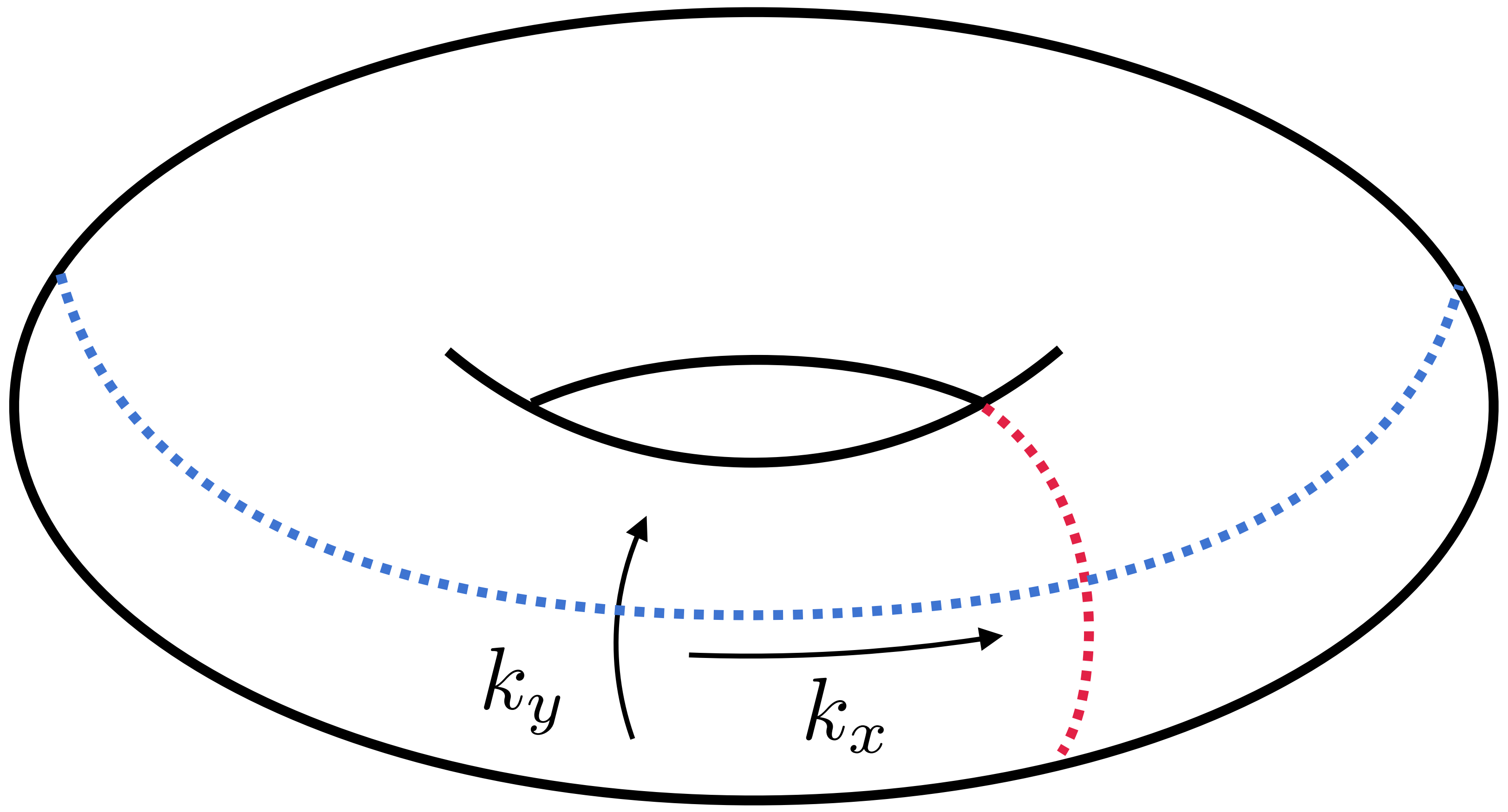
Admits distinct bases:

M_x diagonal: $M_x = \sigma_z$ and $M_y = \sigma_x$

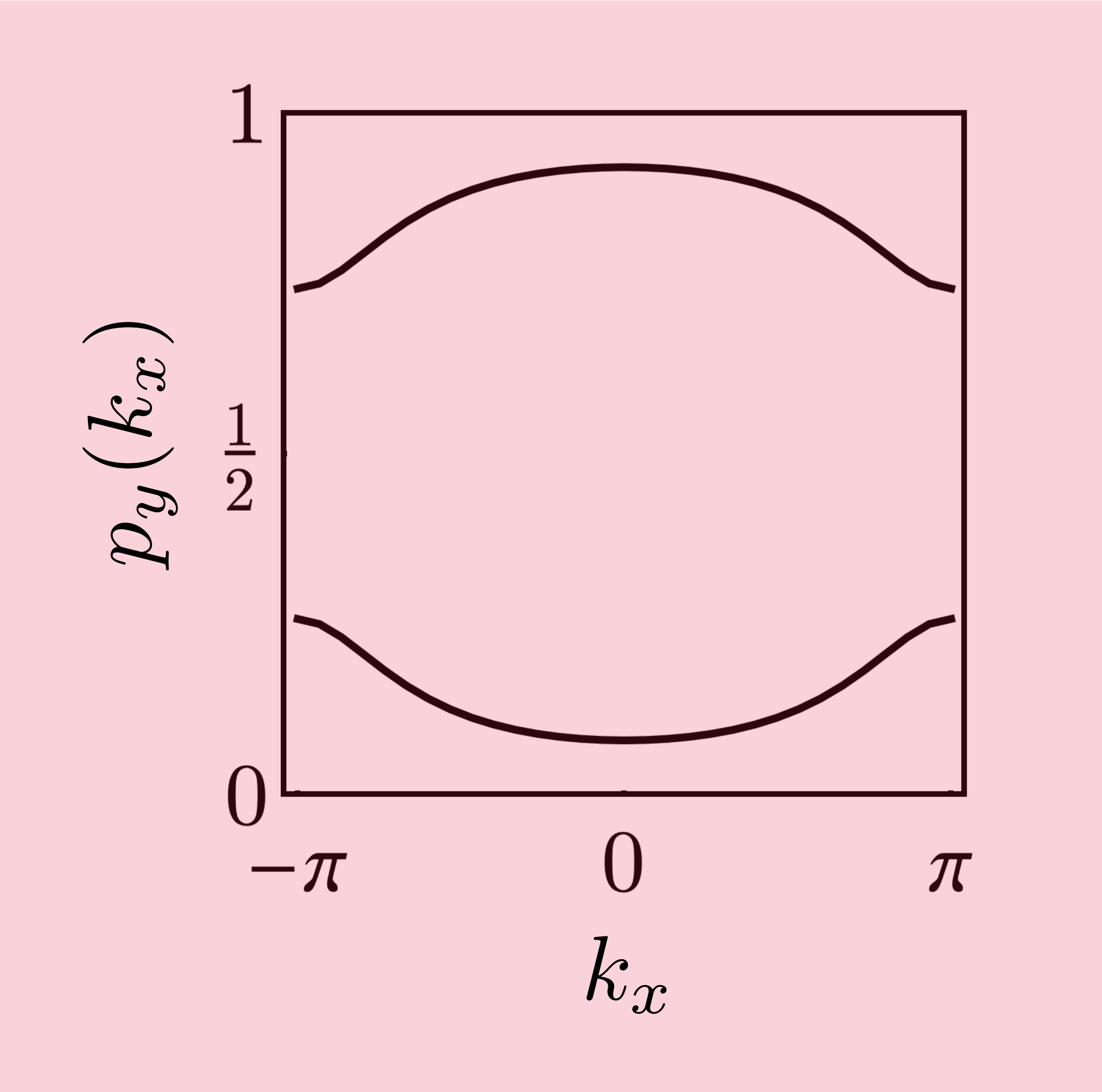
M_y diagonal: $M_x = \sigma_x$ and $M_y = \sigma_z$

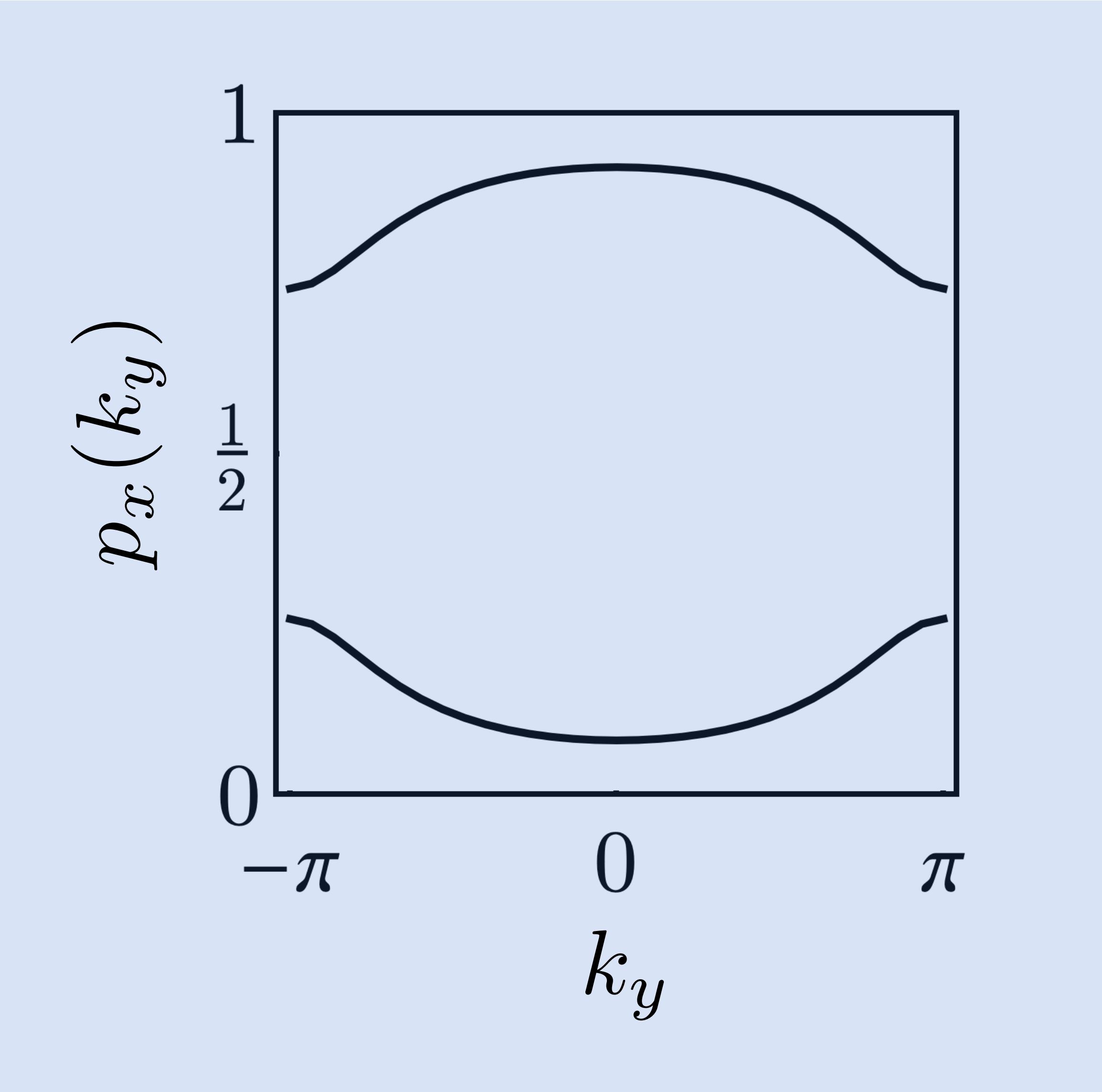
Adiabatic deformation between all $\mathcal{H}$ along the path

Positions in torus given by the Wannier spectrum



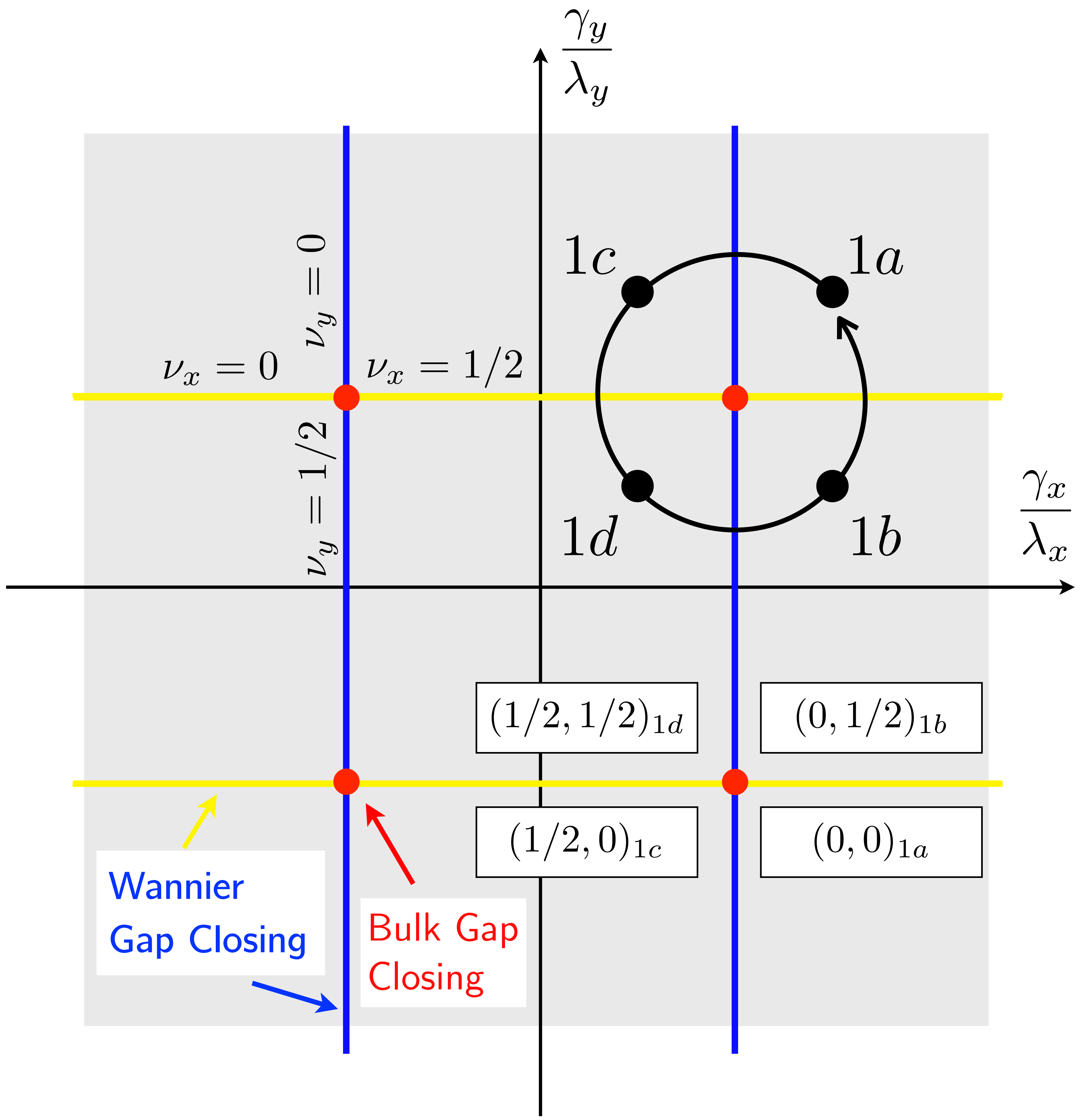
generically non quantized if the charge centers are movable

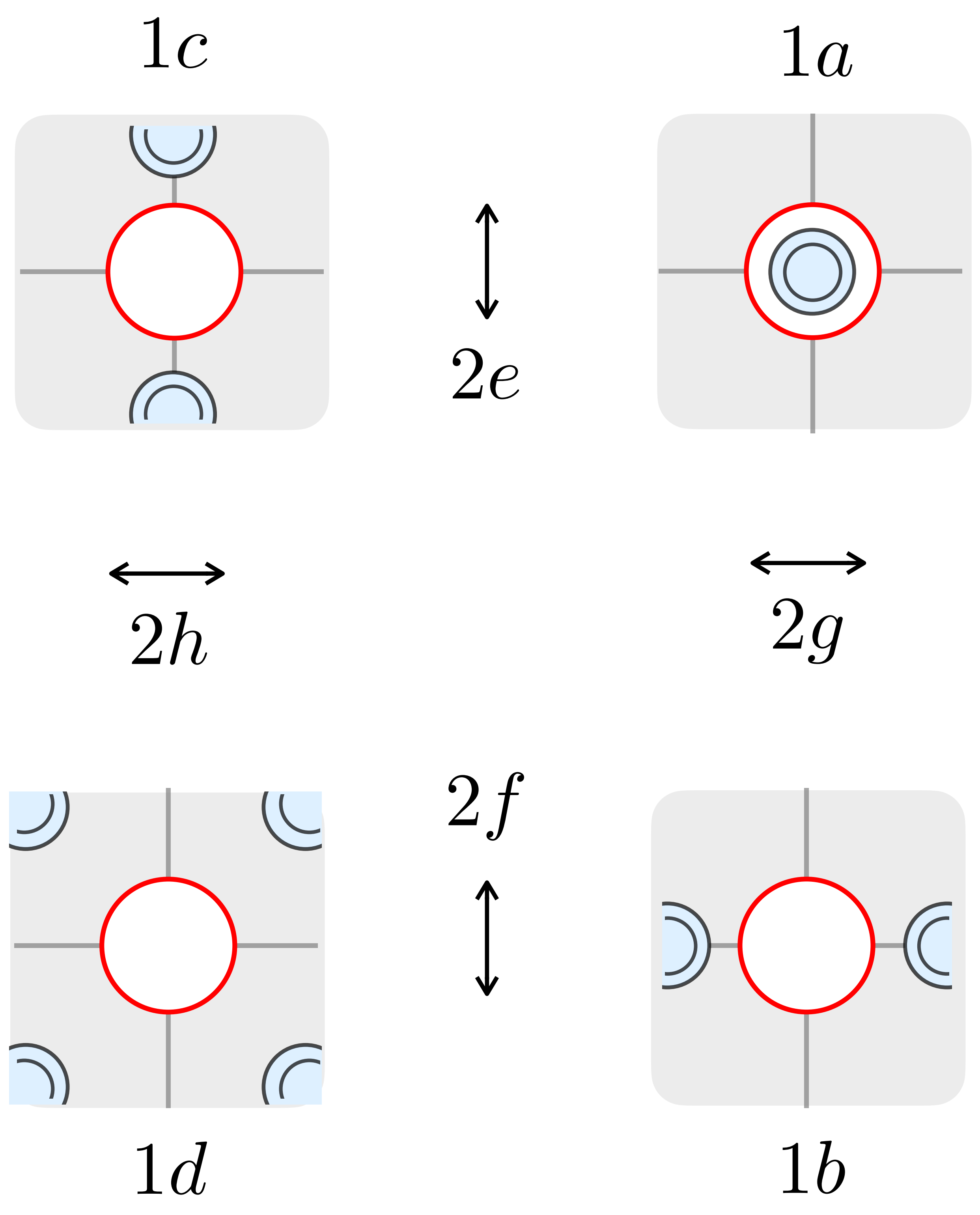




$p_r(k)$ are the eigenvalues of projected position operator $P_{occ}\hat{r}P_{occ}$ otherwise known as Berry phase

Phase diagram with periodic boundaries

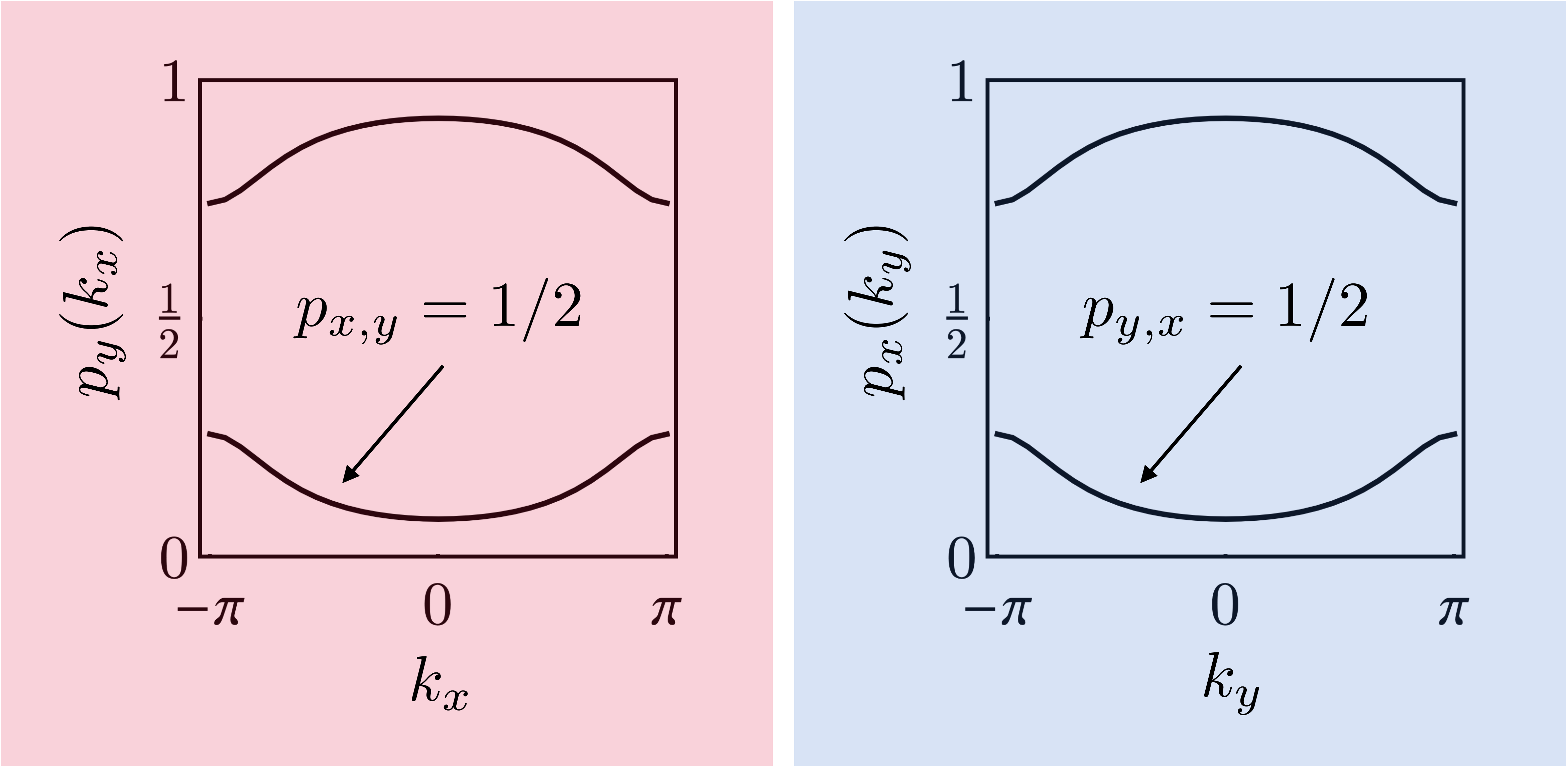


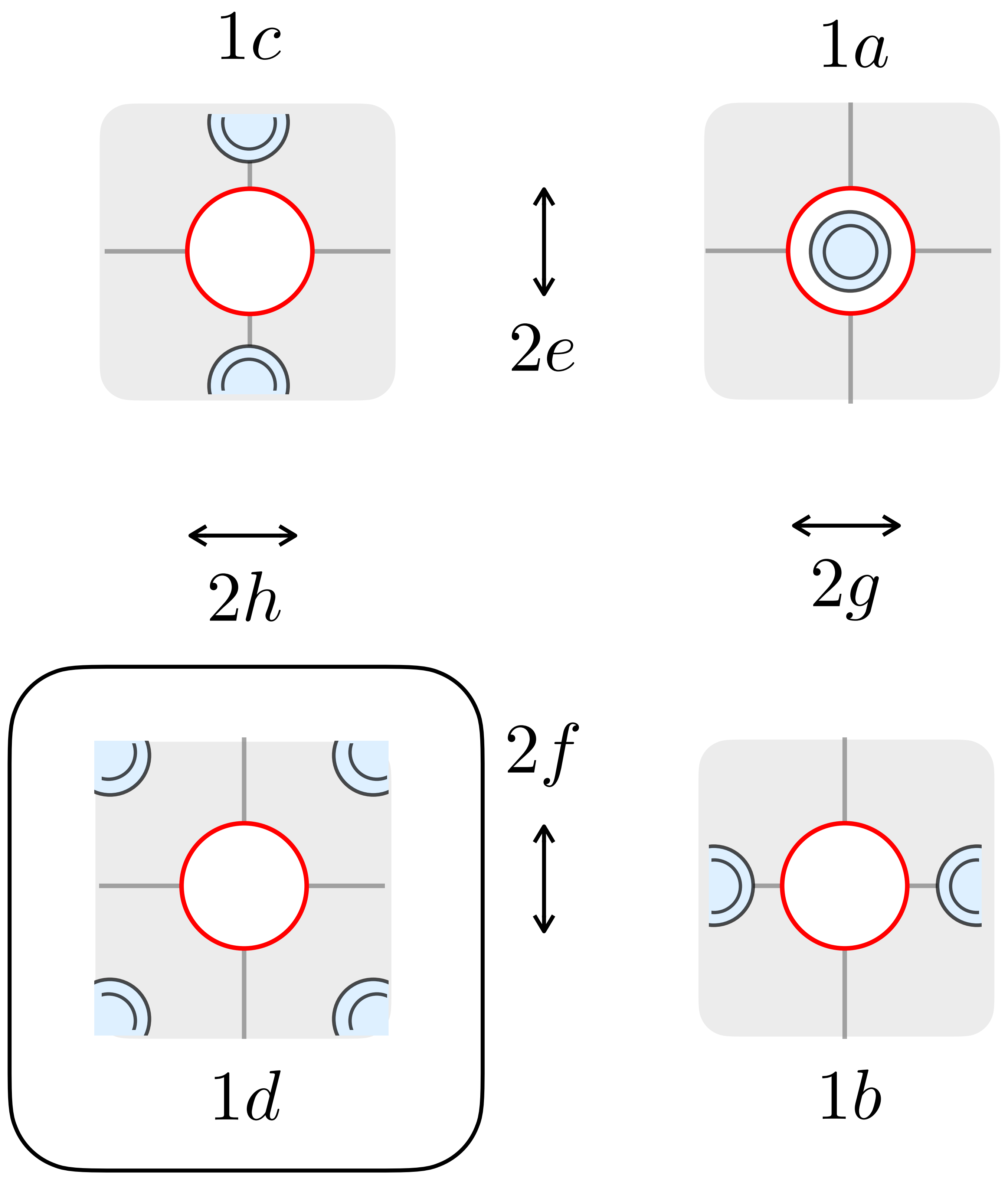


→ No topological phases on the torus, gapped path

→ Distinct charge moments but no quantization

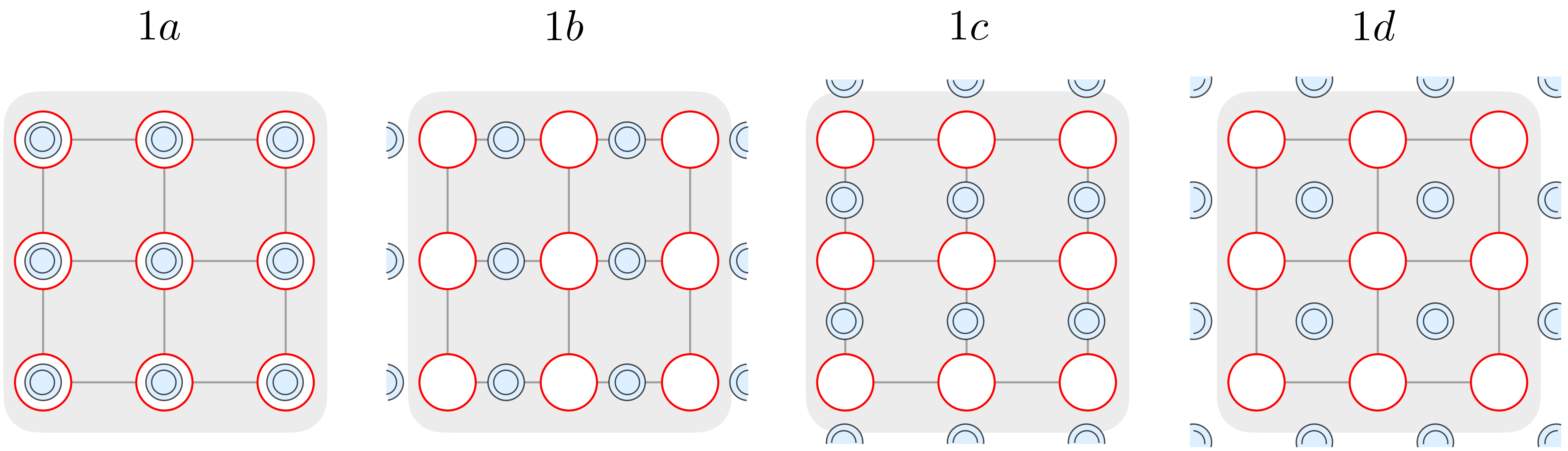
Berry phases of Berry phases





→ Distinct nested polarizations

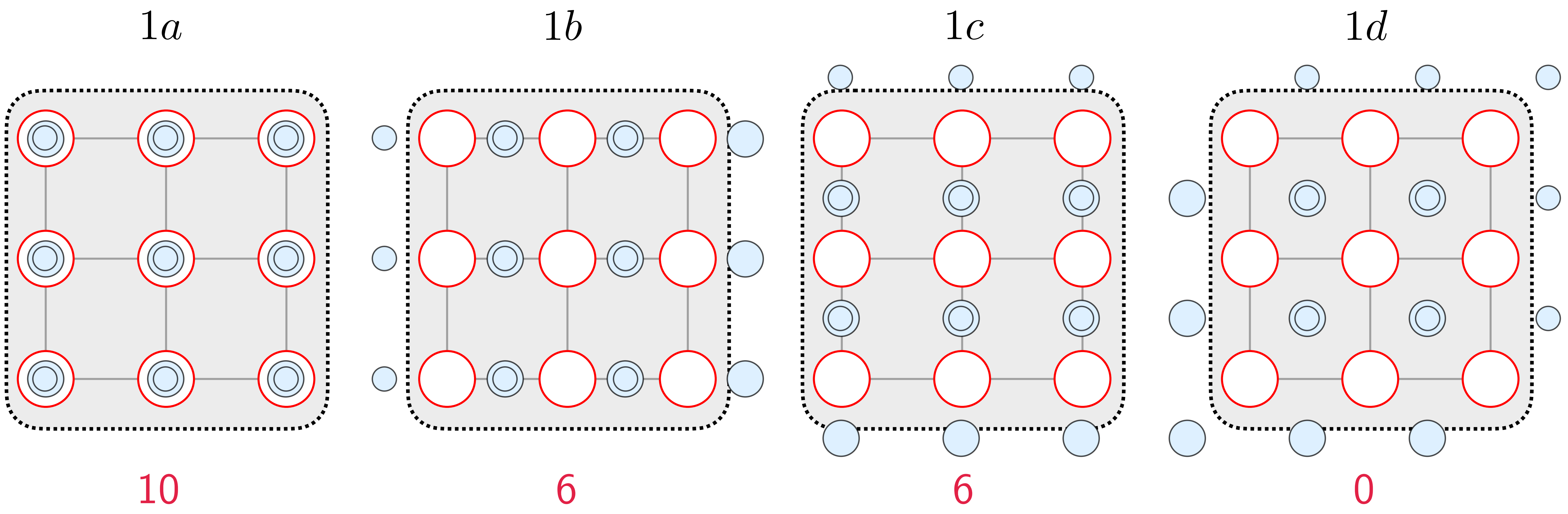
Anomaly with open boundaries



Filling at high symmetry lines on the torus: 18

$$G_{\text{torus}} = \{M_x, M_y, T_x, T_y\}$$

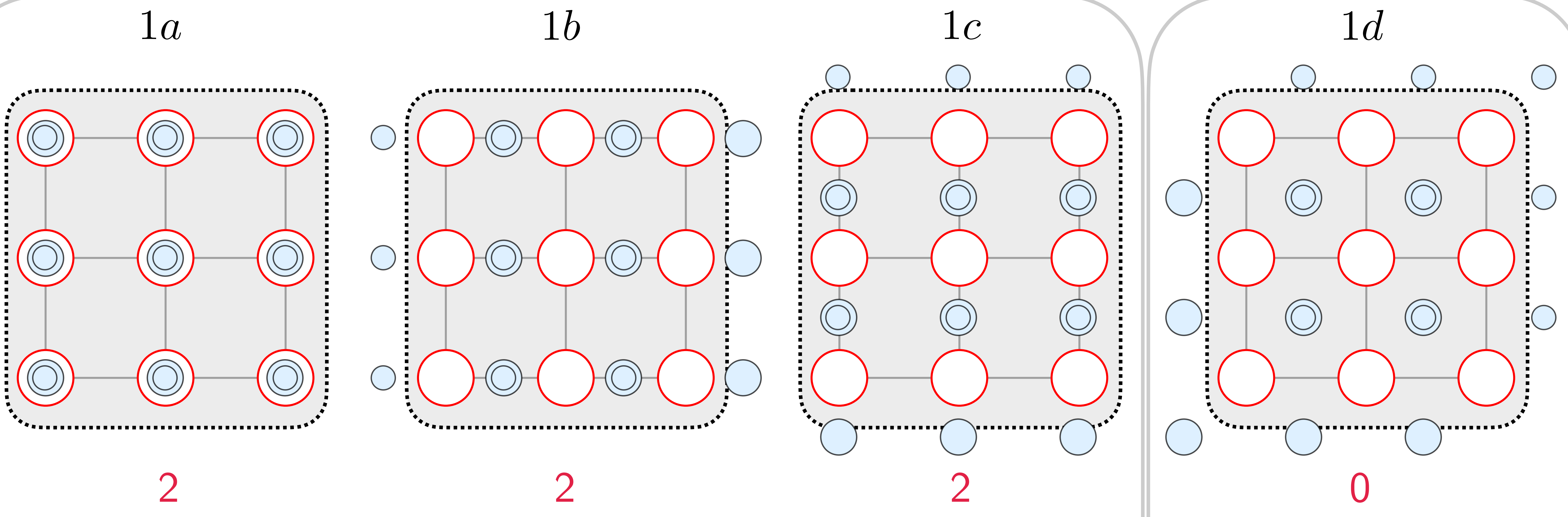
Anomaly with open boundaries



Filling modulo 4 is a topological invariant

$$G_{\text{open}} = \{M_x, M_y\}$$

Anomaly with open boundaries



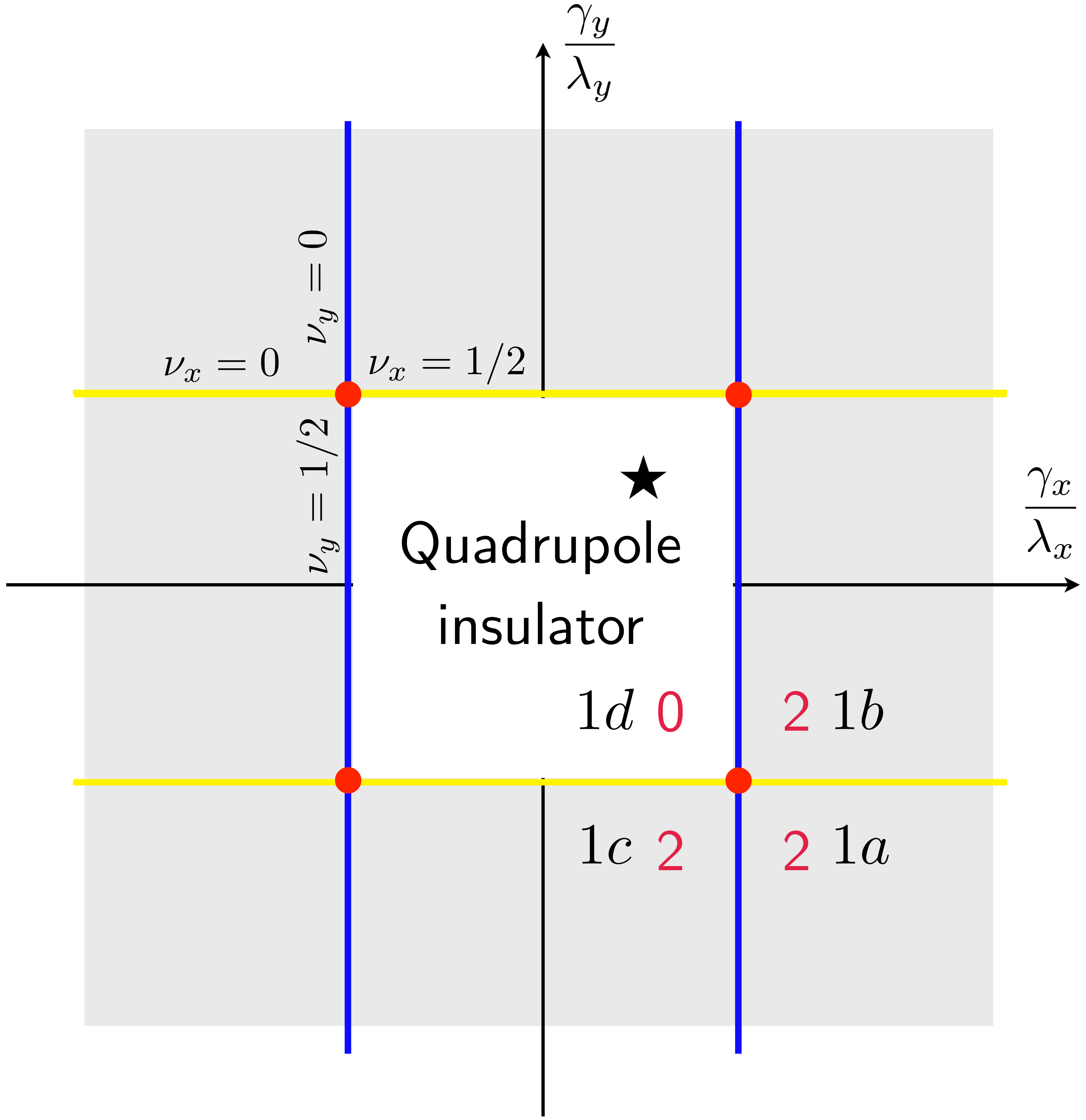
→ Can be filled symmetric

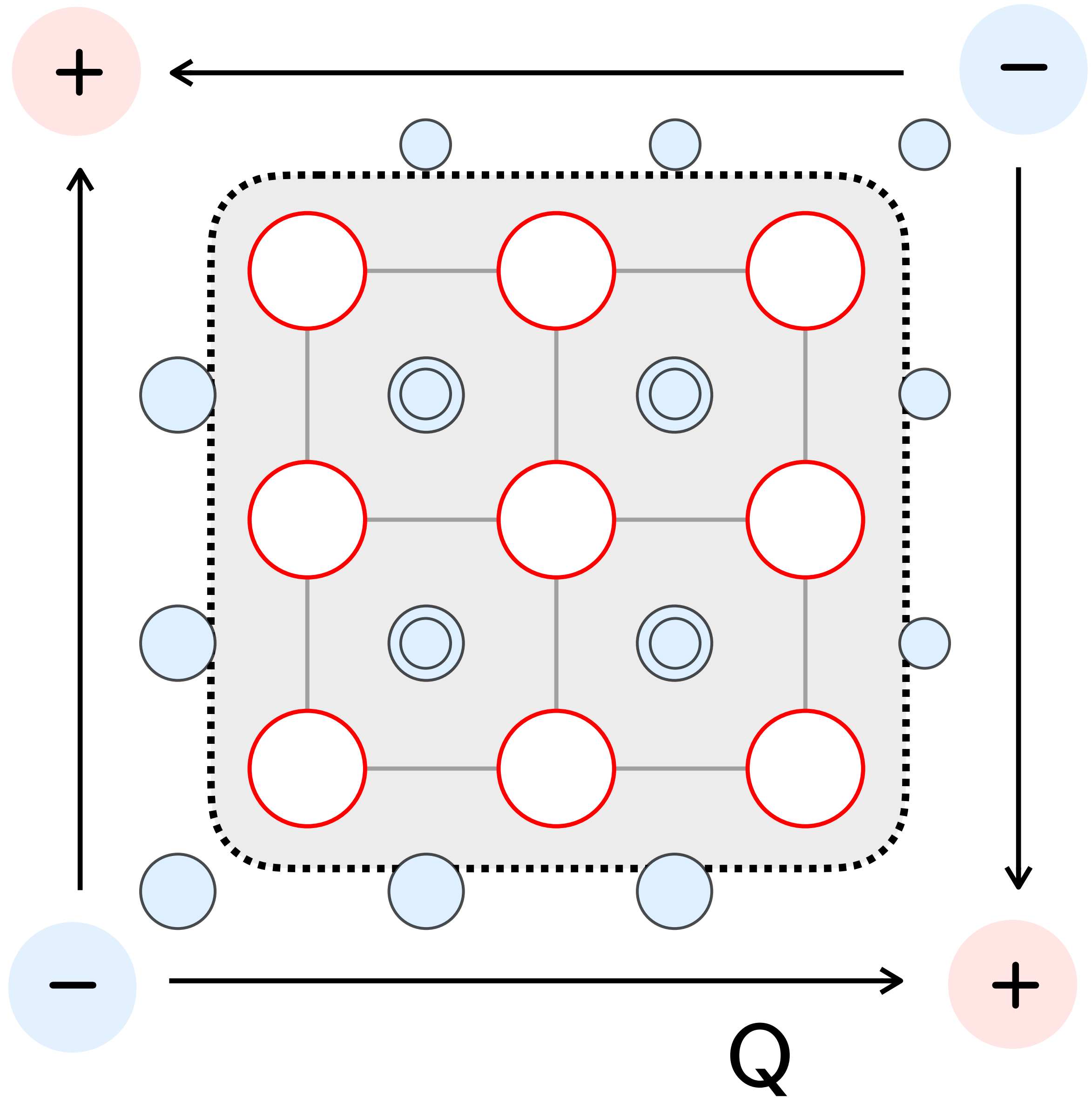
→ No corner modes

→ Cannot be filled symmetrically

→ Corner modes

Topological Phase diagram



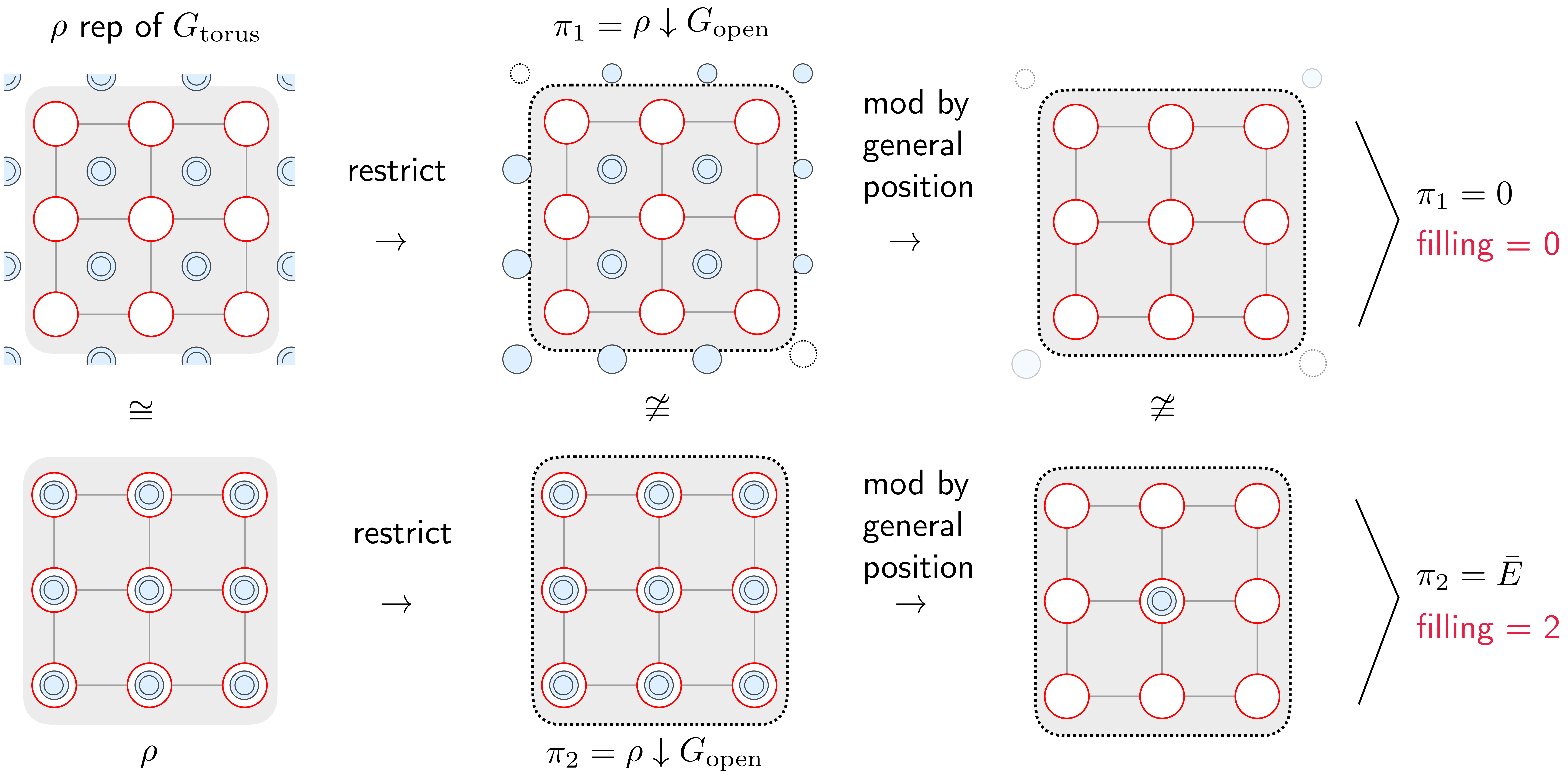


Response:

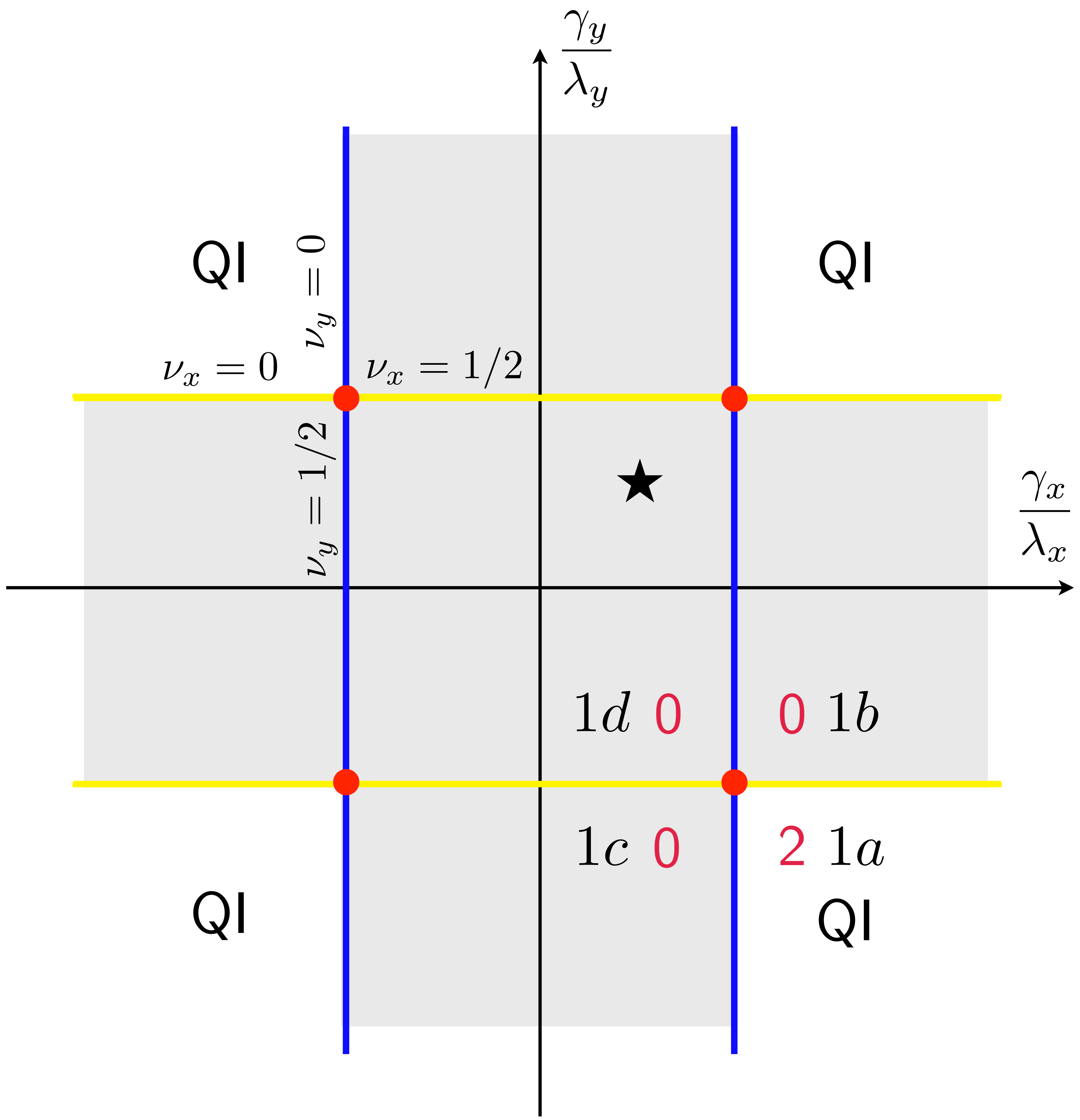
Corner modes and quantized quadrupole moment

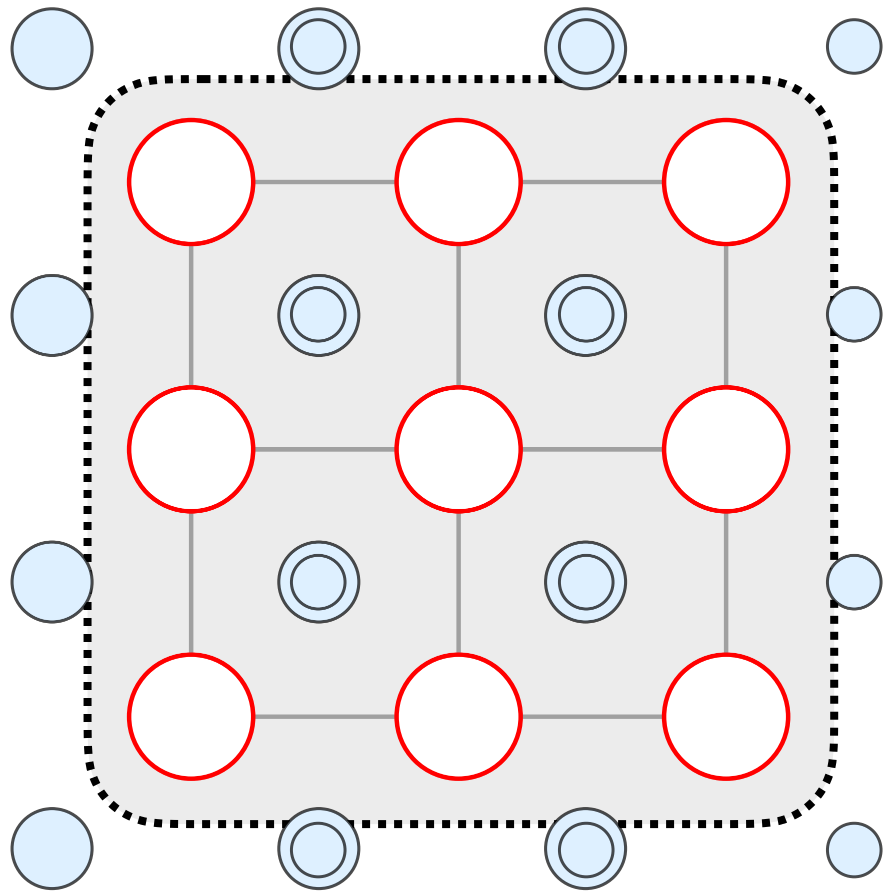
Filling modulo 4 is a topological invariant

Captured in symmetry representations



Different choice of boundary conditions





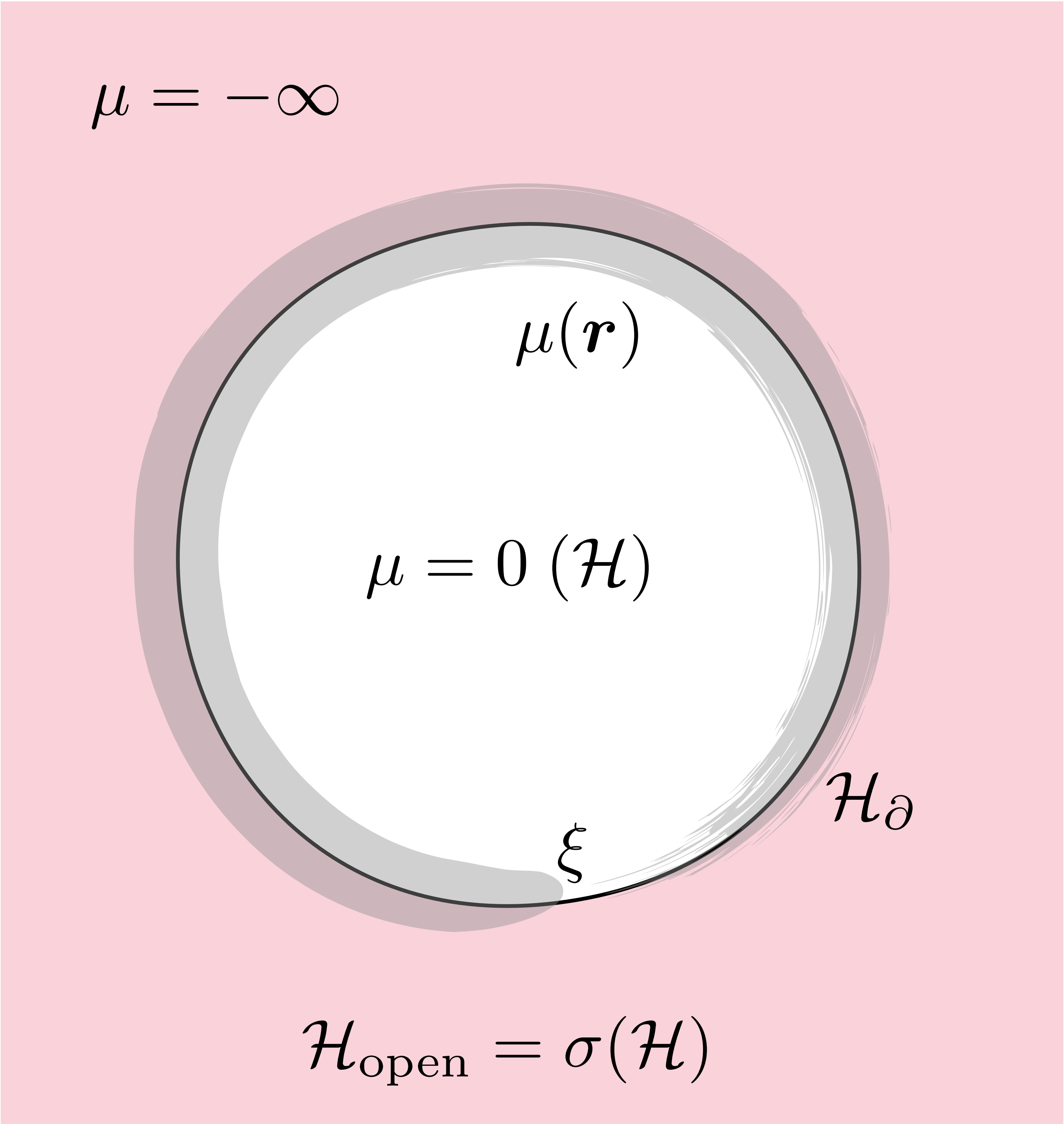
Response:

Remove corner modes by filling 6 more electrons on the top and bottom edges

For every choice of boundary there is a section of the phase diagram which becomes adiabatically disconnected from the others.

General definition and physical motivation

Definition of a boundary



→ The open boundary Hamiltonian $\mathcal{H}_{\text{open}} = \sigma(\mathcal{H})$ can be understood as a continuous map from the translationally invariant Hamiltonian $\mathcal{H}$

→ The map σ is parametrized by a chemical potential $\mu(\boldsymbol{r})$ that changes continuously from $\mu = 0$ (inside the gap) to $\mu = -\infty$ outside the boundary region ξ:

$$\sigma_0(\mathcal{H}) = \sum_n |\psi_n\rangle\langle\psi_n|\theta(\epsilon_n - \mu(\boldsymbol{r}))|\psi_n\rangle\langle\psi_n|$$

with $\mathcal{H}|\psi_n\rangle = \epsilon_n|\psi_n\rangle$.

→ A boundary Hamiltonian allows for additional boundary degrees of freedom that vanish outside the ξ region:

$$\mathcal{H}_\partial \equiv \sigma(\mathcal{H}) - \sigma_0(\mathcal{H})$$

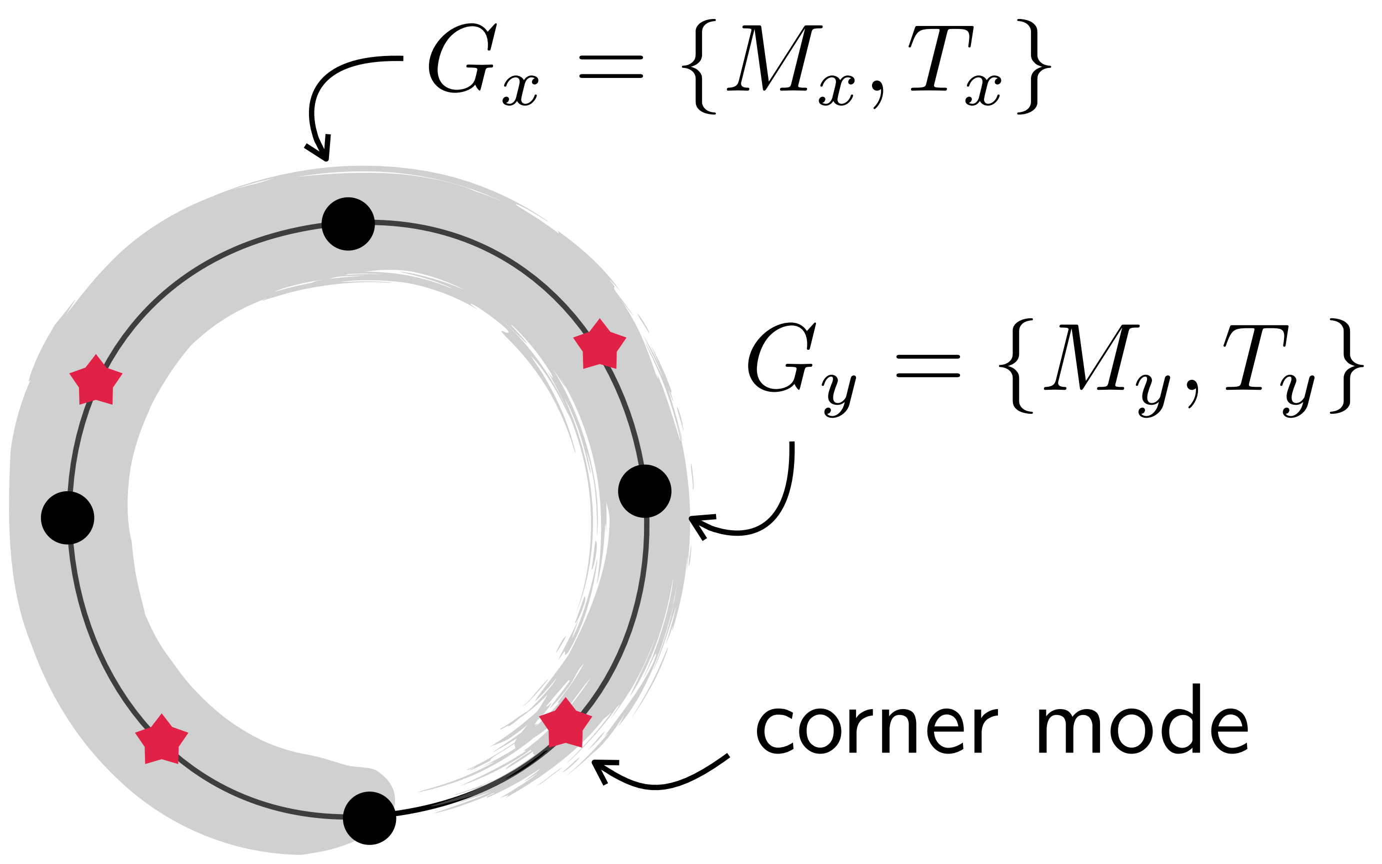
→ Open system $\sigma(\mathcal{H})$ is trivial if $\mathcal{H}_\partial$ is gapped for all $\mathcal{H}$.

Definition of boundary obstruction

Given a boundary σ, and two gapped translationally invariant Hamiltonians $\mathcal{H}_1$ and $\mathcal{H}_2$:

- $\rightarrow$ There is a smooth and symmetric trajectory in the space of gapped Hamiltonians $\mathcal{H}(t)$ where $\mathcal{H}(0) = \mathcal{H}_1$ and $\mathcal{H}(1) = \mathcal{H}_2$
- $\rightarrow$ The trajectory induced by the boundary $\sigma(\mathcal{H}(t))$ necessarily has an energy gap closing transition at a high symmetry boundary.

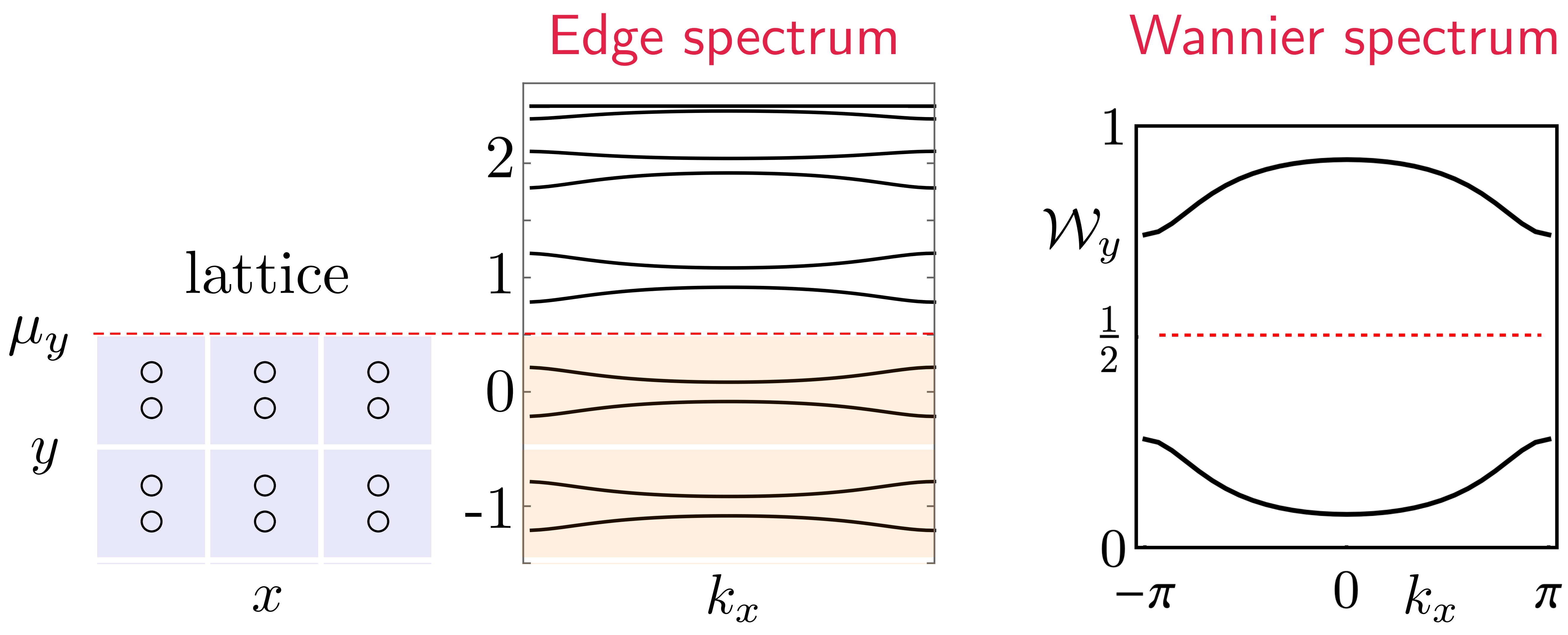
- $\rightarrow$ High symmetry surfaces in the Quadrupole insulator:
- $\rightarrow$ Bulk symmetry $G = \{M_x, M_y, T_x, T_y\}$
- $\rightarrow$ Globally stable
- $\rightarrow$ Reduced symmetry group allows for distinct topological phases akin to the SSH model.

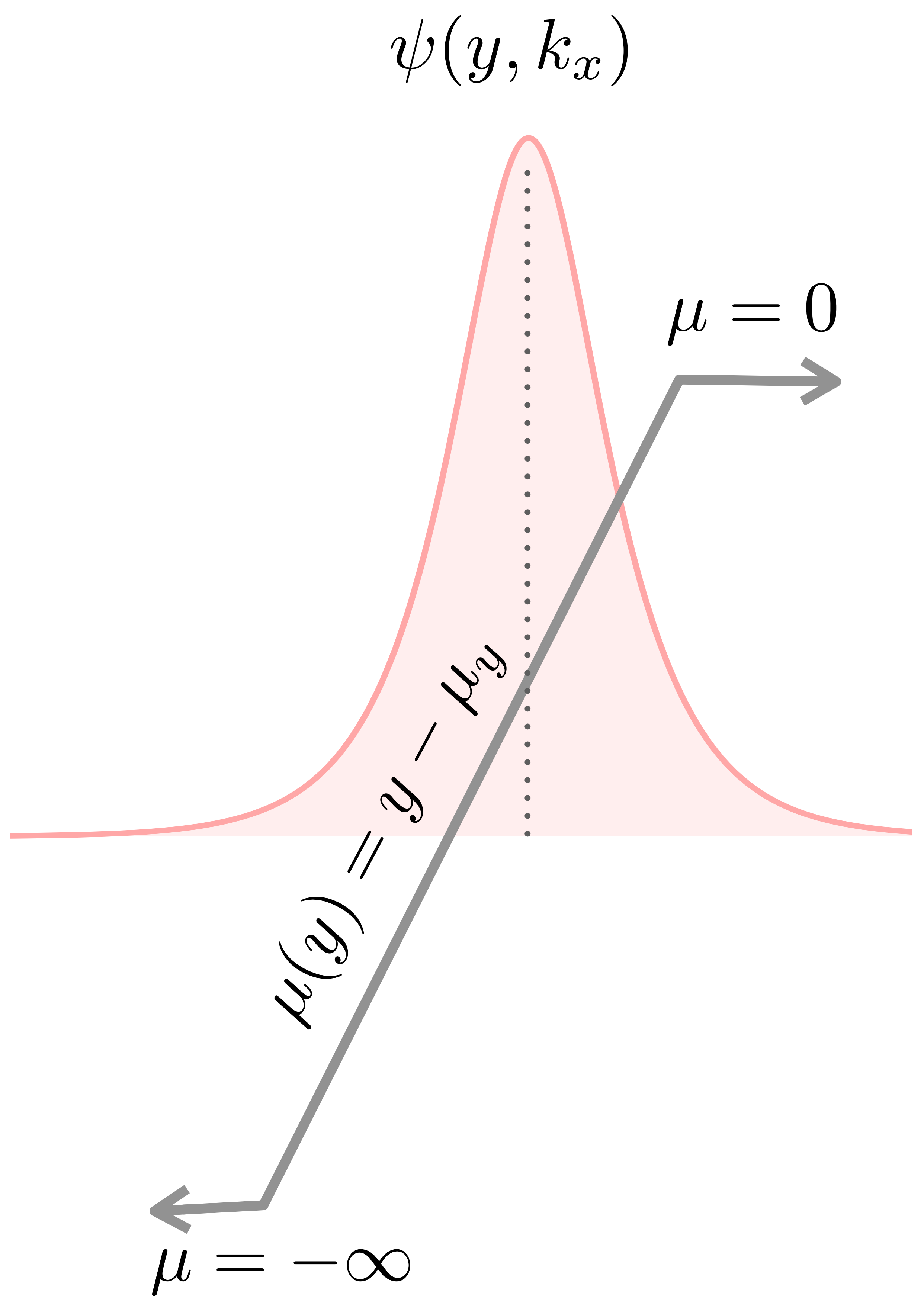


The connection between boundary and Wannier spectrum

→ When the chemical potential changes linearly across the boundary, the boundary spectrum coincides with the Wannier spectrum [Klich et al 10]

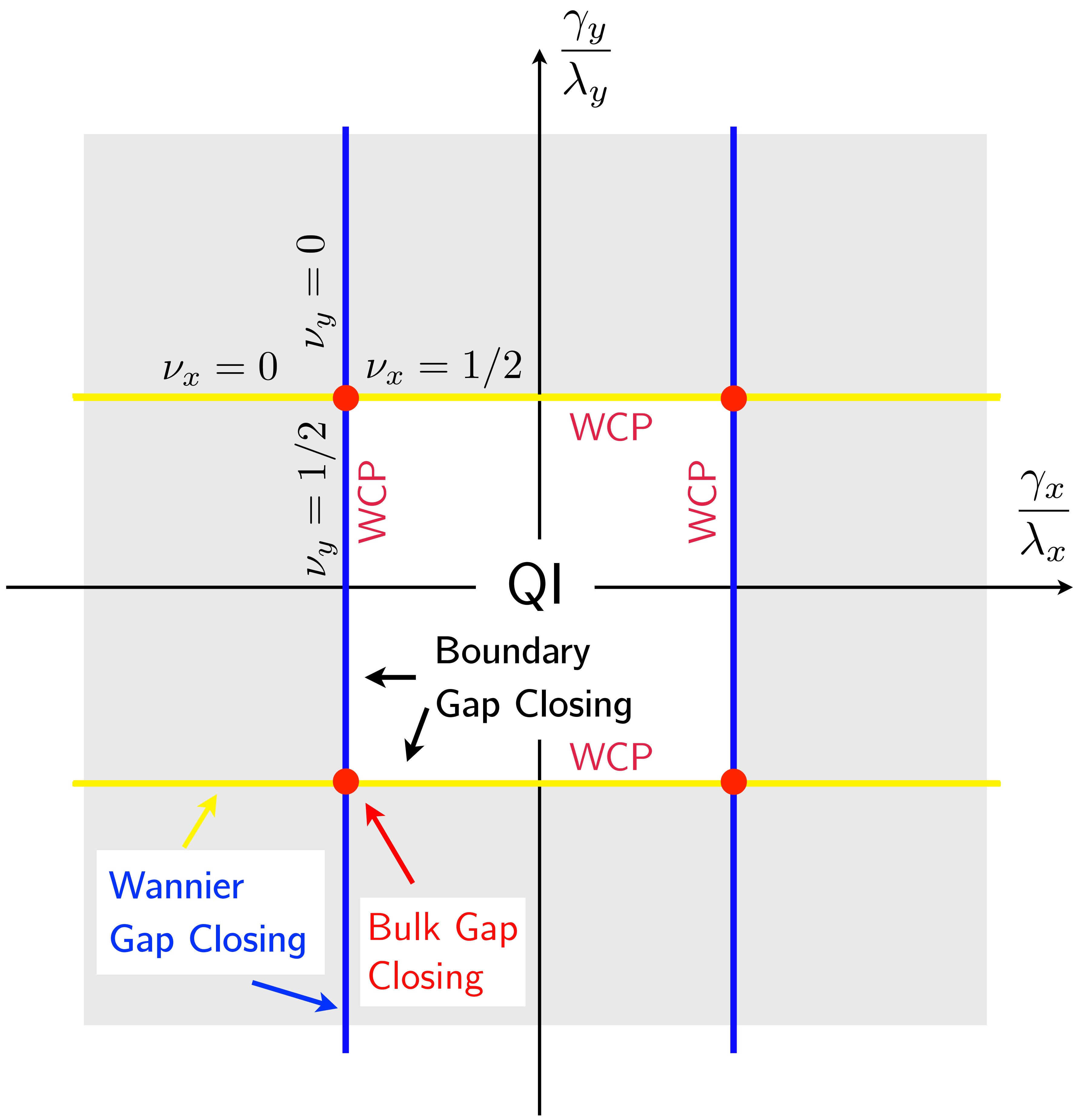
→ Wannier spectrum is periodic: We can define a Wannier chemical potential μ_b that coincides with the edge of the system.

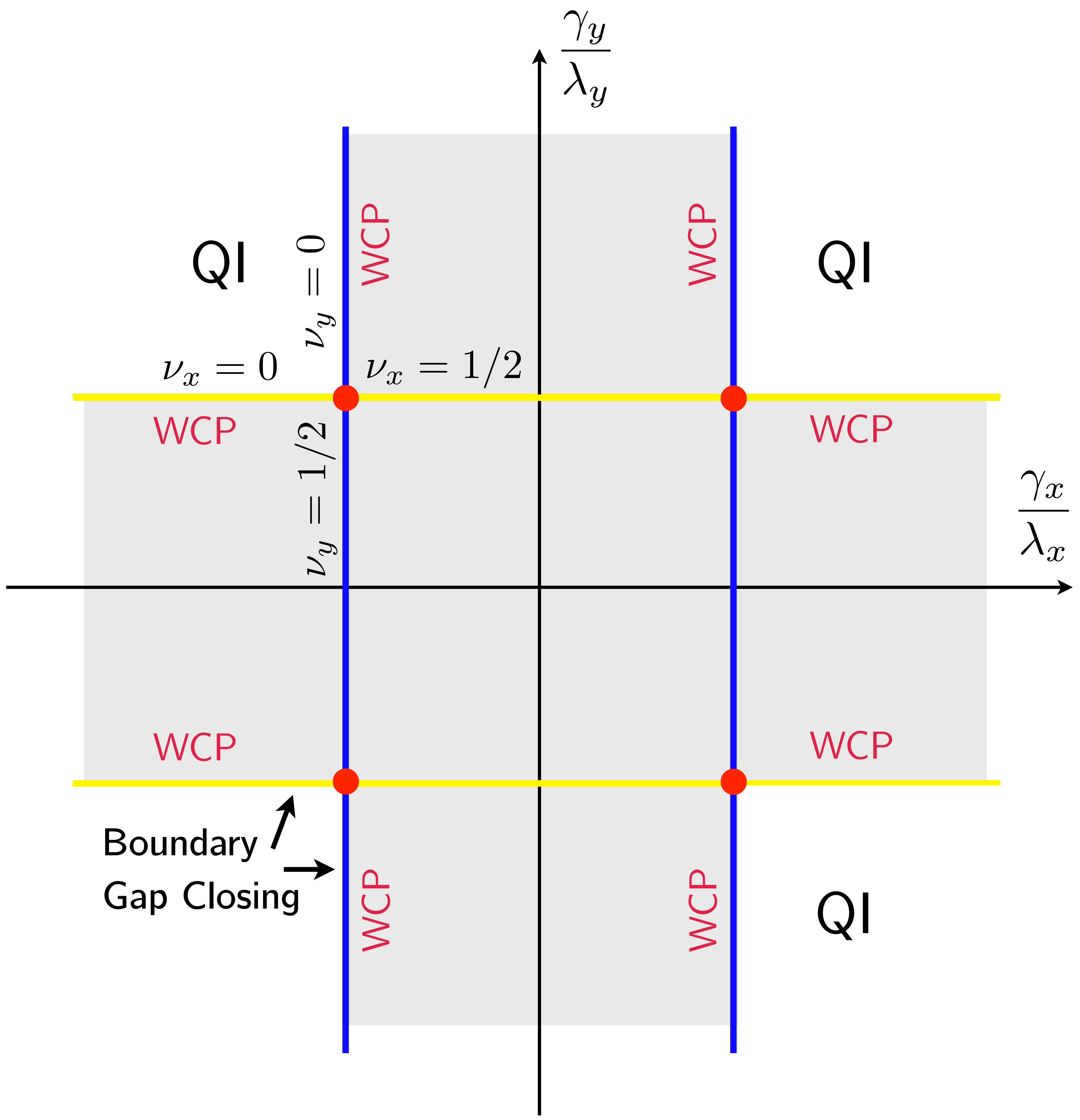




→ Not all Wannier gap closing phase transitions correspond to boundary closing phase transitions: Must fix the ambiguities

The connection between boundary and Wannier spectrum





Two choices of boundary / Wannier chemical potential: $\mathbb{Z}_2 \times \mathbb{Z}_2 \rightarrow \mathbb{Z}_2$ topological distinction

Boundary obstruction is not unique to atomic limits: Another example

A dimerized Chern insulator

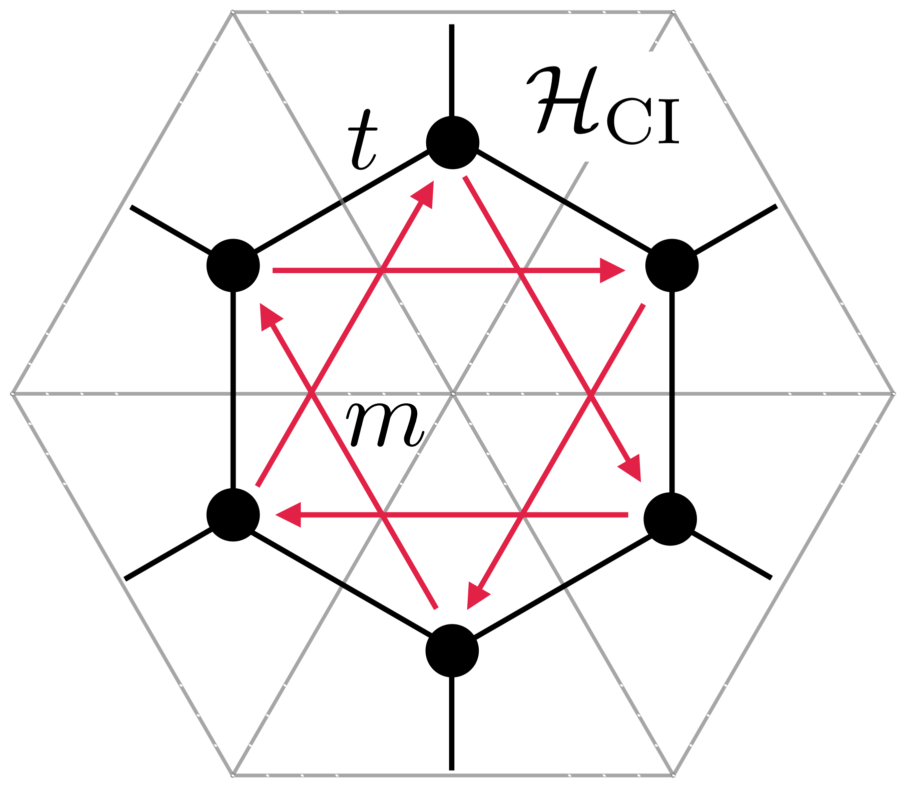
→ Consider the Haldane model $\mathcal{H}_{\mathrm{CI}}$ with Chern number $\mathrm{sgn}(m)$

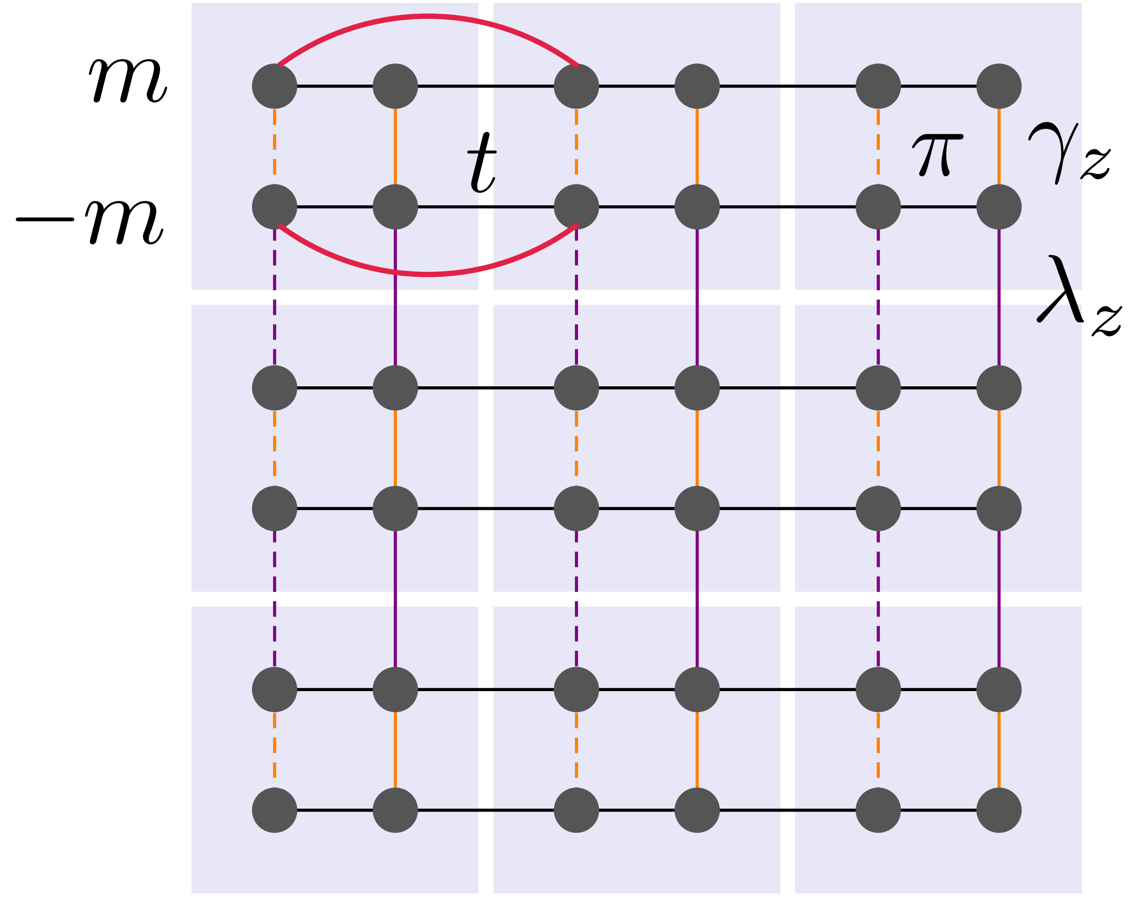
→ Stack alternating $\mathcal{H}_{\mathrm{CI}}$ with π fluxes through each layer:

$$\mathcal{H}_{CI}\tau_z + (\lambda_z \sin k_z)\tau_y + (\gamma_z + \lambda_z \cos k_z)\tau_x$$

→ Symmetries C_{2z} and $M_z\mathcal{T}$ satisfying $\{C_{2z}, M_z\mathcal{T}\} = 0$

→ Globally irremovable chiral boundary modes protected by the gap at high symmetry surfaces:





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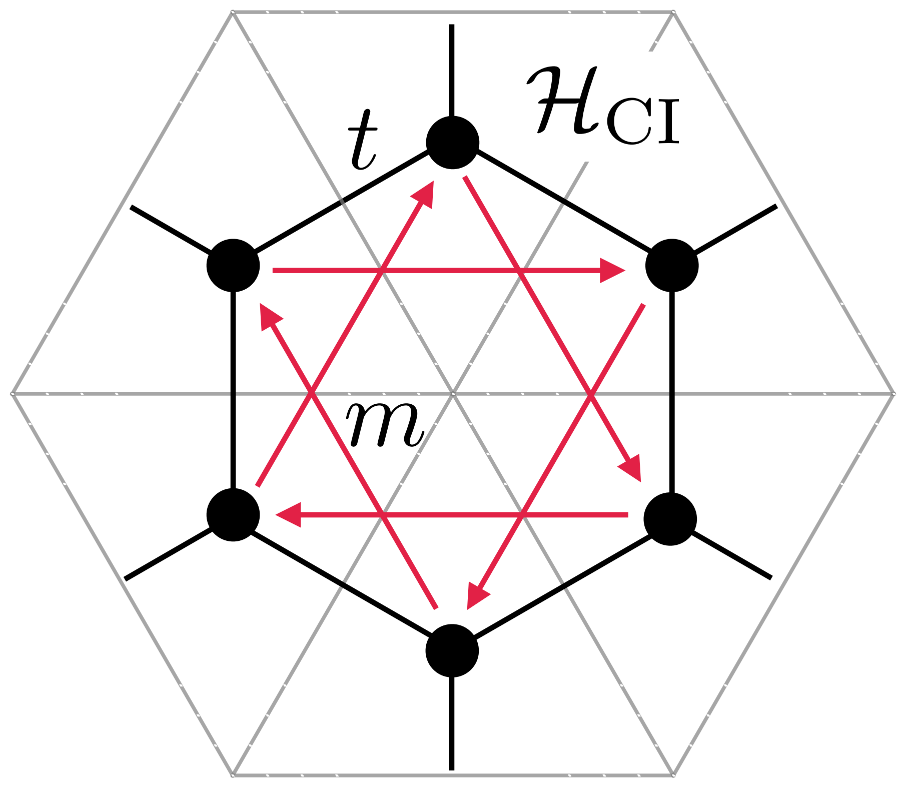
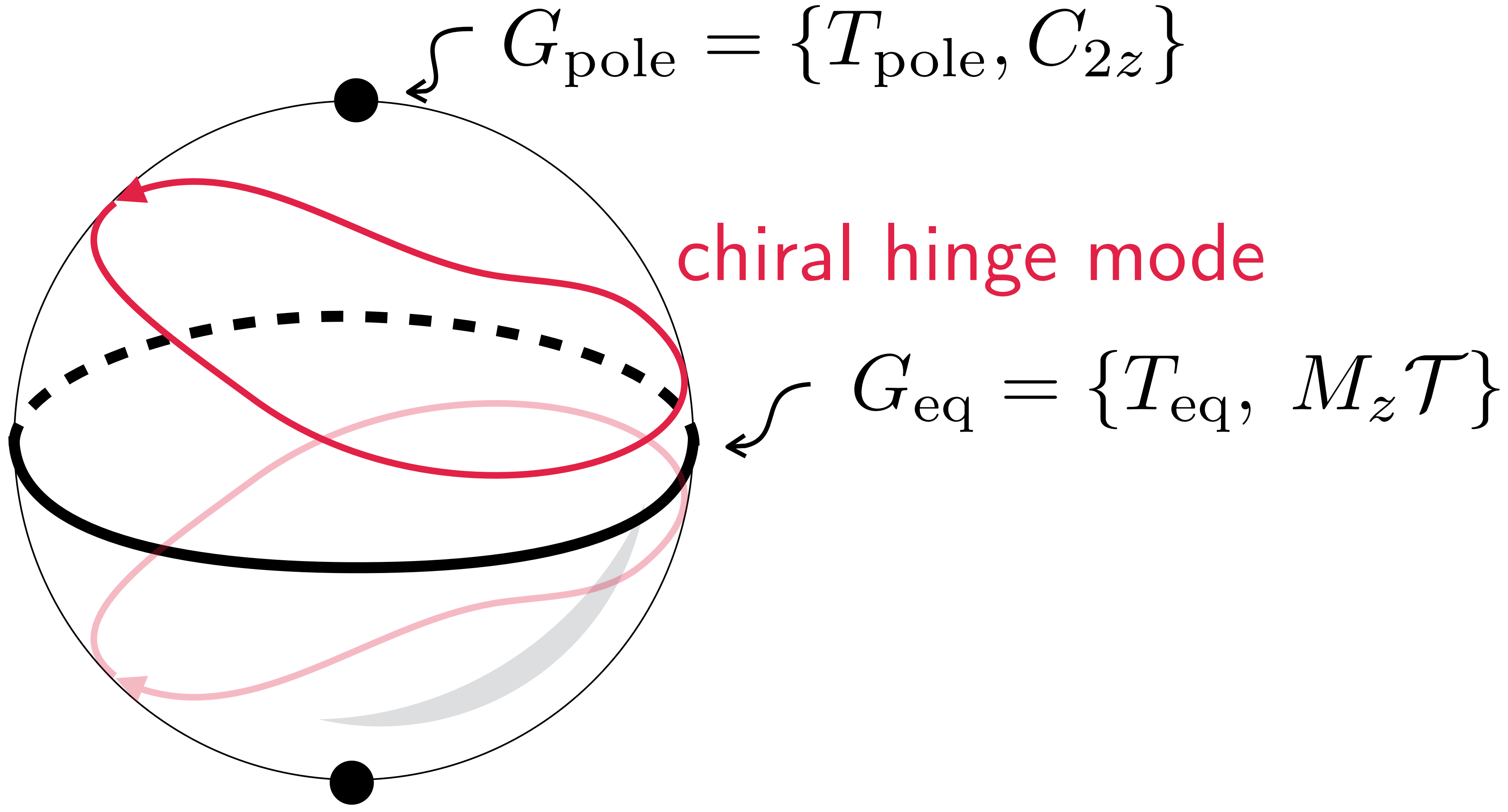
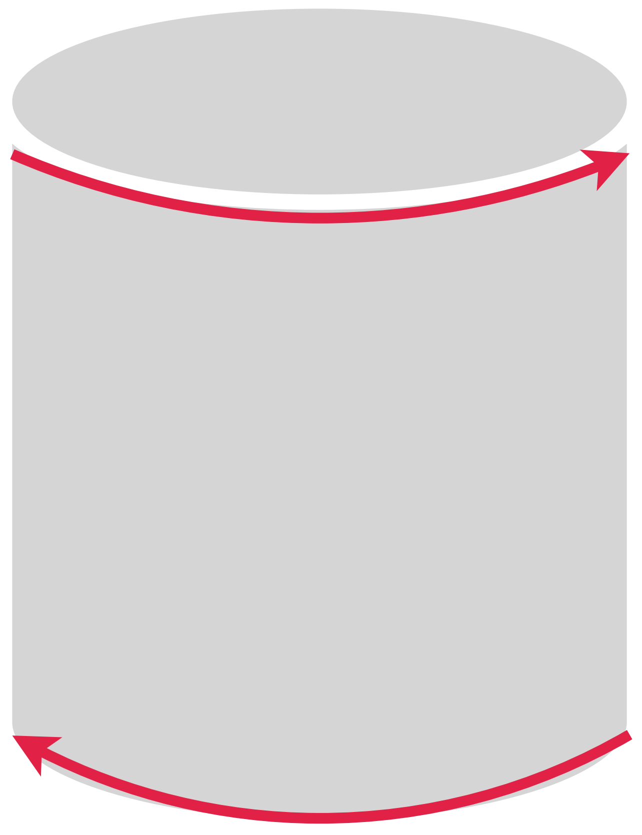
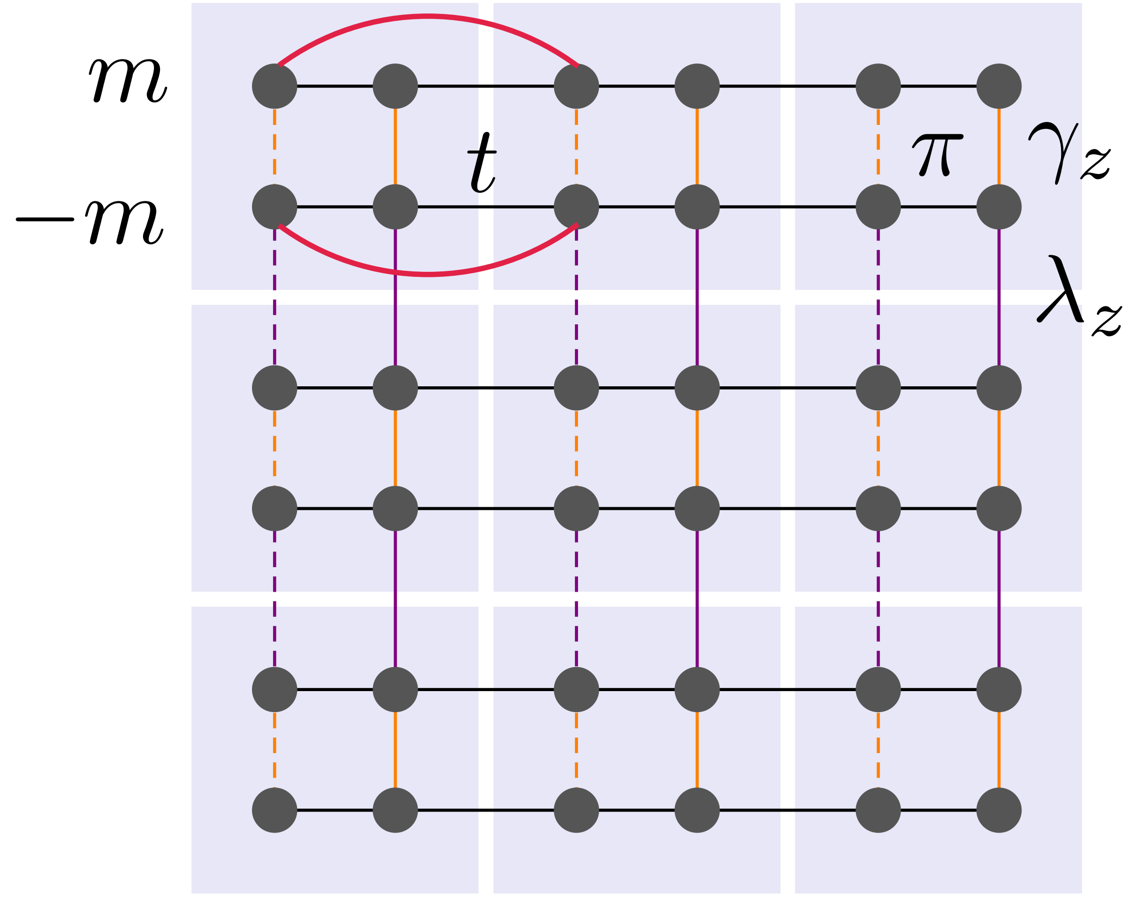








Overview

→ Introduced boundary obstructed topological phases:

  → Topology of an Hamiltonian with an open boundary $\sigma(\mathcal{H})$

  → Differentiate spurious and essential boundary features derived from the bulk

  → Globally irremovable boundary modes

  → Can induce a phase transition by tuning bulk parameters or changing the boundary

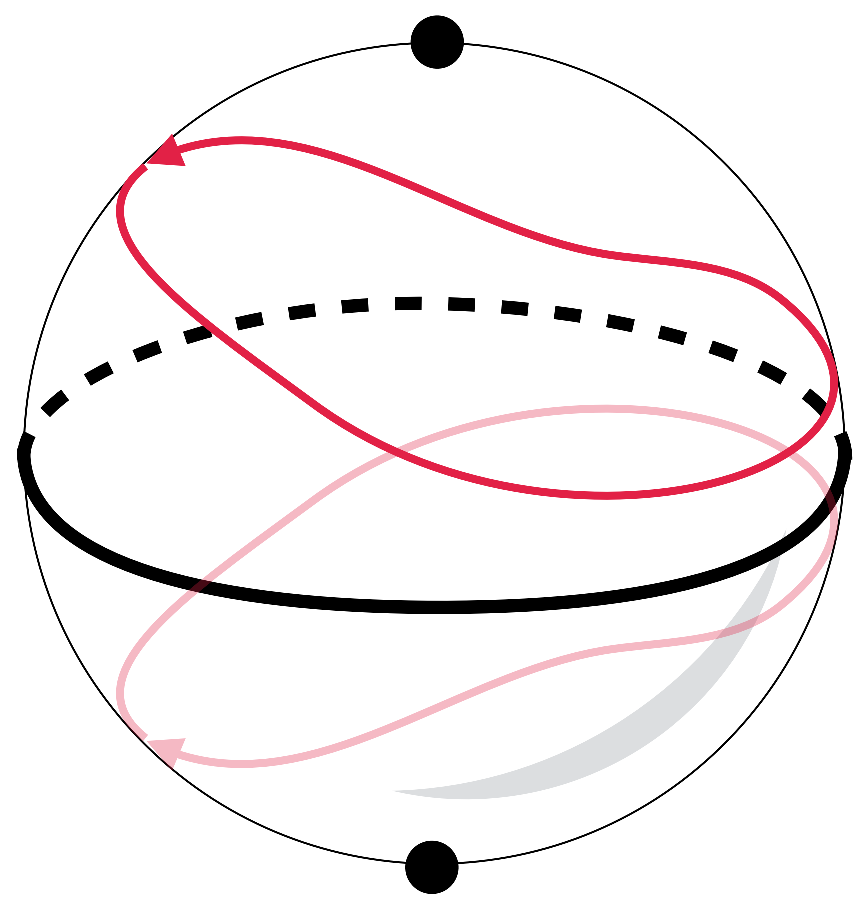
→ Diagnosed by symmetry eigenvalues in the open system
(to the extent topological phases can be captured by symmetry)

→ Diagnosed by Wannier spectrum by defining a Wannier chemical potential

→ Examples of BOTPs:

  → Double Mirror Quadrupole Insulator

  → Dimerized Chern insulator



Thank You!