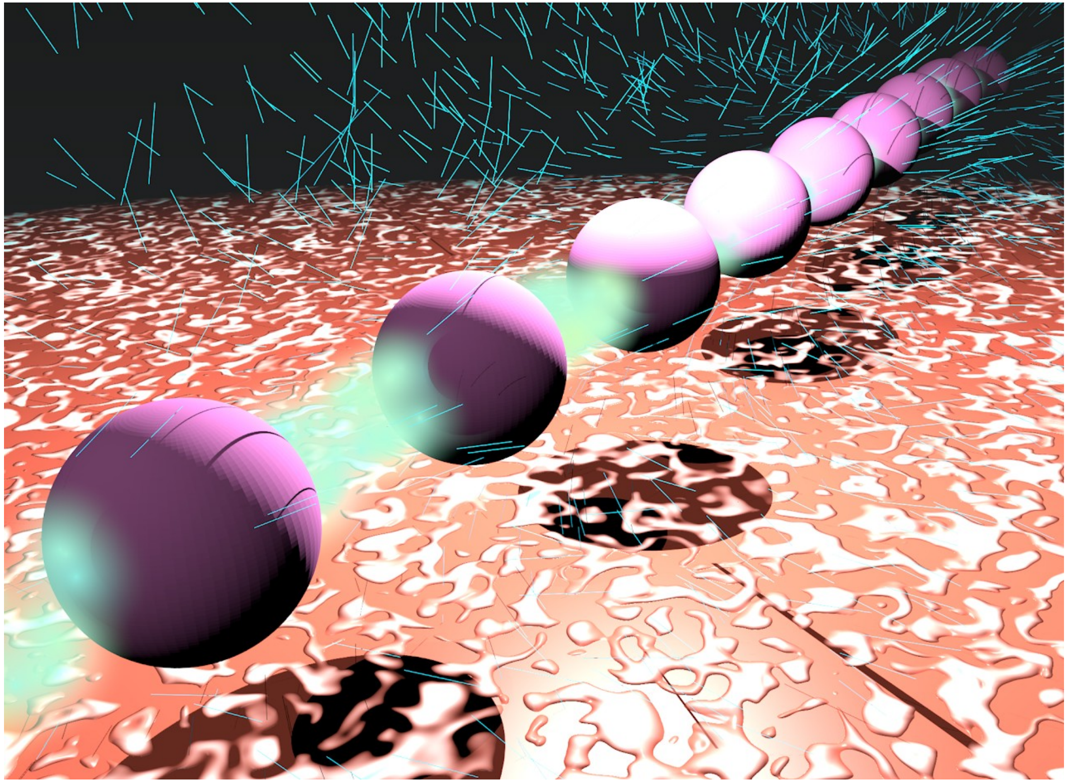
Symmetries, reciprocal space and Bloch's theorem



March 6th 2023

A reminder from session #1

Hamiltonians can be described in a second quantized formalism

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j$$

Creation operator

Annihilation operator

And can be diagonalized

$$H = \sum_n \epsilon_n \Psi_n^\dagger \Psi_n$$

$$\Psi_n^\dagger = \sum_i a_{n,i} c_i^\dagger$$

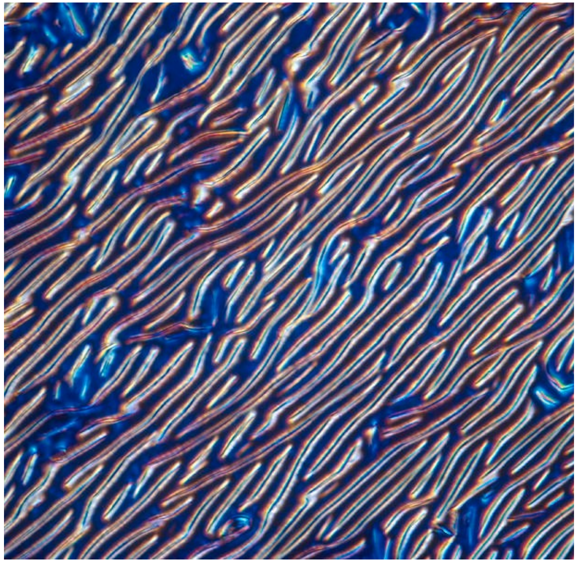
Eigenenergy

Today’s learning outcomes

- We can classify quantum matter according which symmetries it breaks
- Symmetry allows to simplify quantum problems
- Non-interacting systems with translational symmetry can be solved using Bloch’s theorem

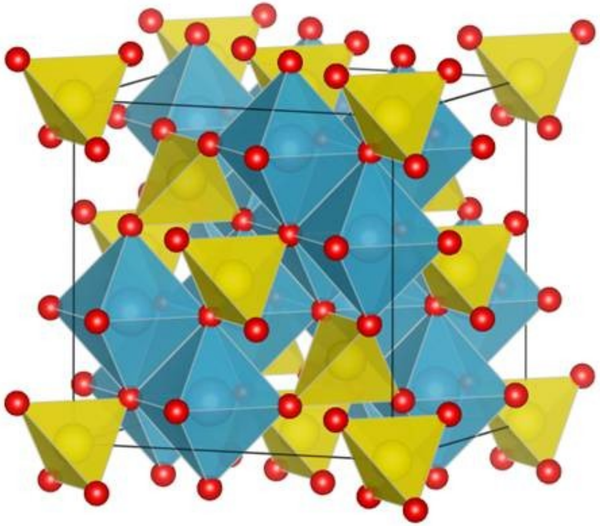
Complexity in nature

Liquid crystals



Galaxies

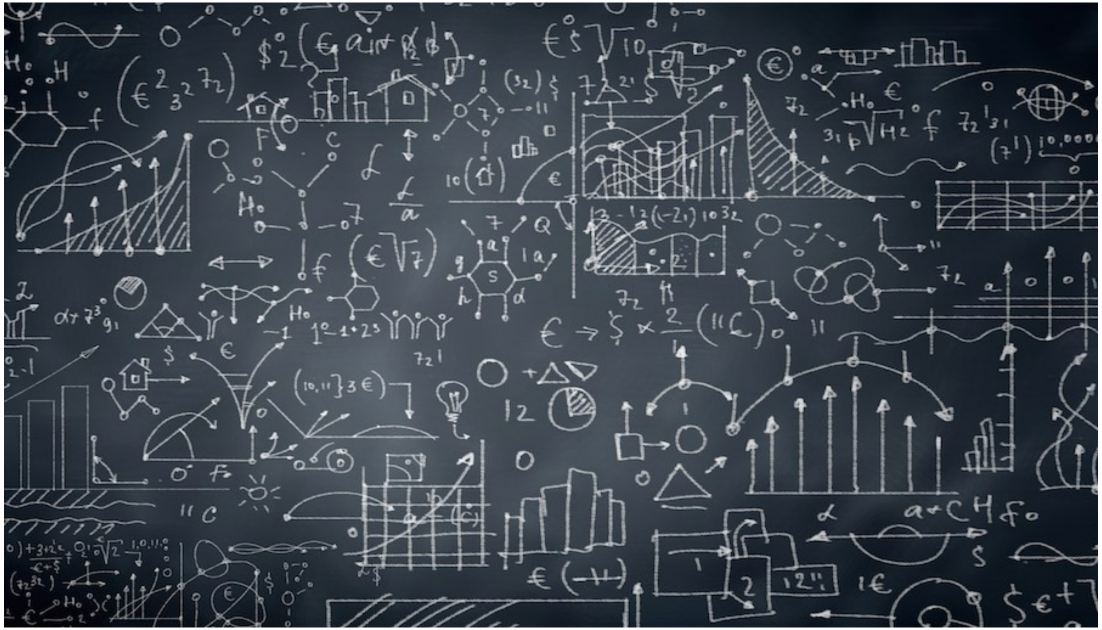
Complex materials



How can we extract robust conclusions from complex systems?

The key idea of symmetry

Symmetries allow to “guess” solutions without explicitly solving a problem



even without understanding the microscopic mechanism governing the system

The key idea of symmetry

The underlying laws of physics are symmetric
But the real system may or may not be symmetric

No symmetry

Spontaneous symmetry breaking

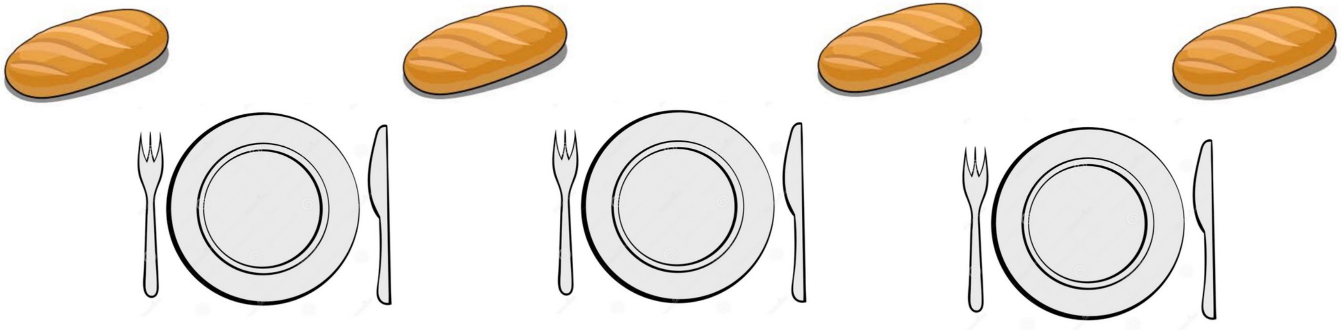
Symmetry

Mathematical constrained solution

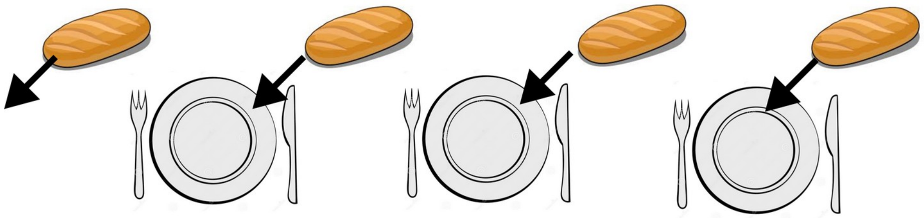
Symmetry breaking

An example of symmetry breaking

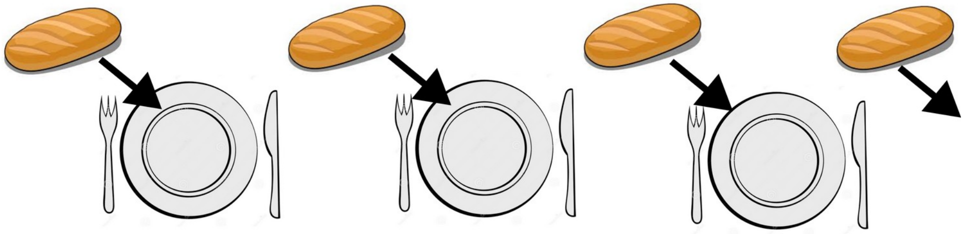
Pick your bread in a group meal



Solution #1



Solution #2



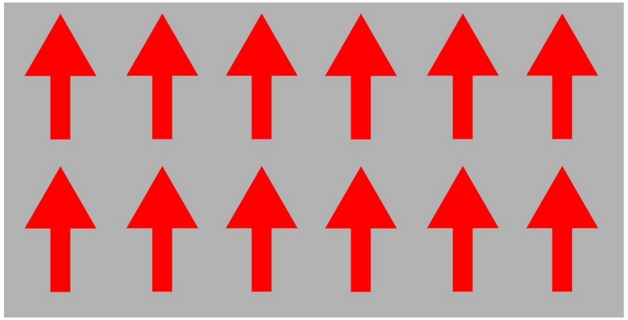
Spontaneous symmetry breaking

Central idea: a ground state can break the symmetry of a Hamiltonian

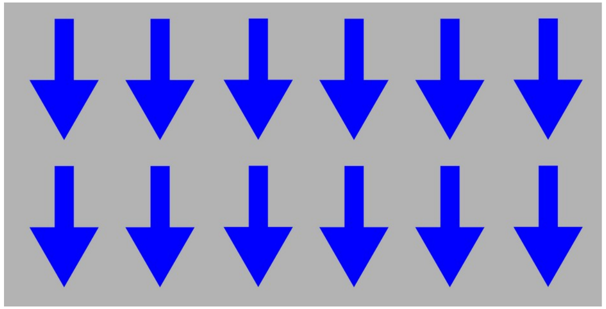
It can happen in the thermodynamic limit (infinite particles)

Hamiltonian for a ferromagnet $H = -\sum_{ij} \vec{S}_i \cdot \vec{S}_j$

Solution #1



Solution #2

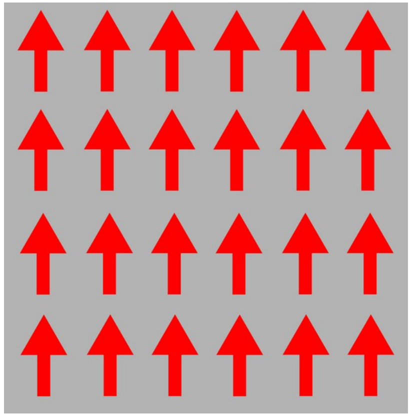


Nature (fluctuations) will choose one of the ground states as the macroscopic one

Classifying quantum matter according to symmetries

Broken
time-reversal symmetry

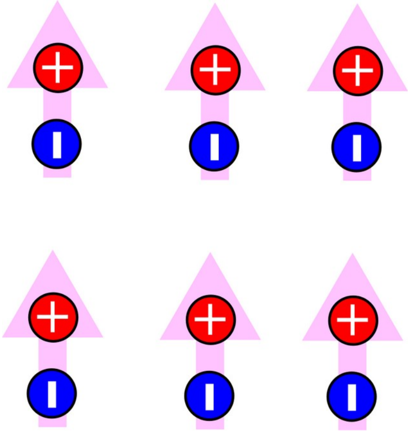
Classical magnets



$$\mathbf{M} \to -\mathbf{M}$$

Broken
rotational symmetry

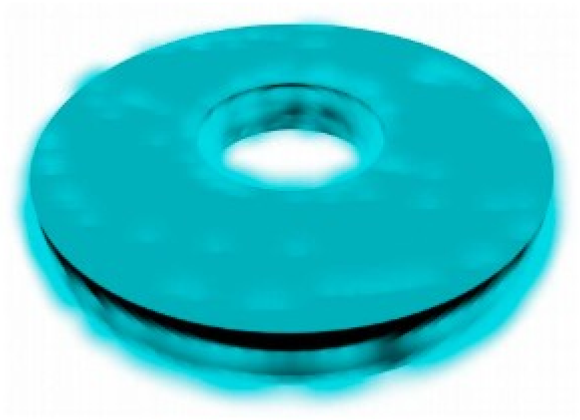
Ferroelectrics



$$\mathbf{r} \to R\mathbf{r}$$

Broken
gauge symmetry

Superconductors



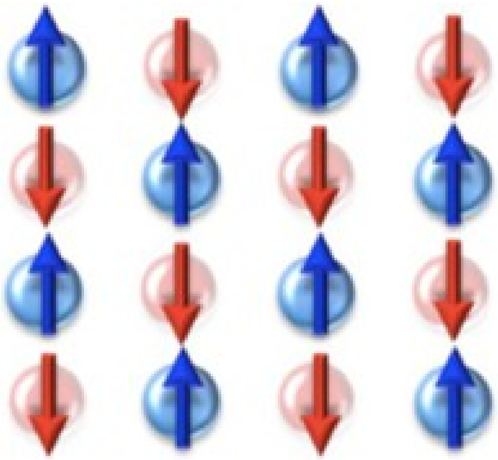
$$\langle c_\uparrow c_\downarrow \rangle \to e^{i\phi} \langle c_\uparrow c_\downarrow \rangle$$

How is symmetry related with quantum materials?

(Broken) symmetries allow to classify matter

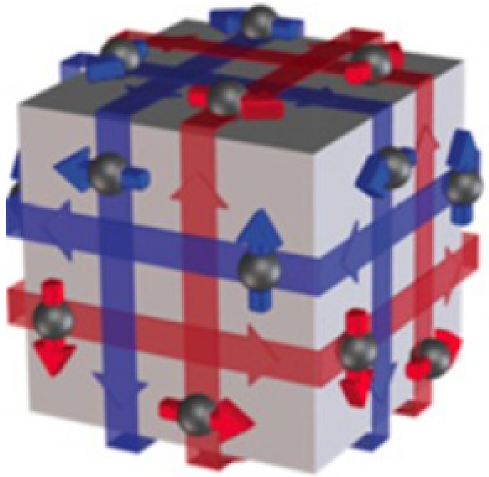
Symmetry classification

Ferromagnets
Superconductors
Ferroelectrics



Topological classification

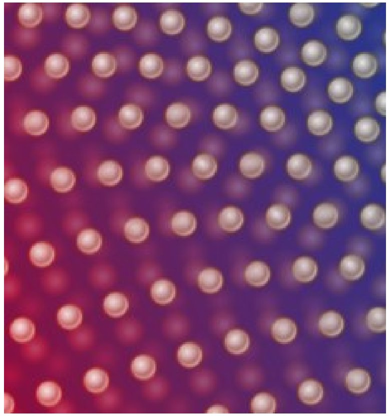
Trivial insulators
Topological insulators
Topologically ordered matter



Emergent excitations when symmetries get broken

Phonons

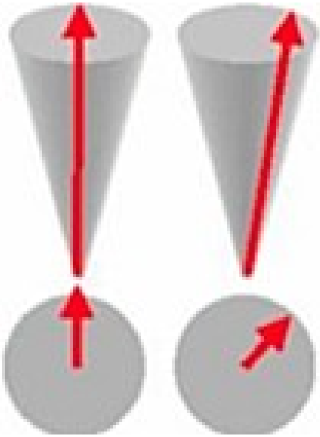
Crystals $\langle \vec{R} \rangle \neq 0$



Spin 0
Charge 0
Gapless

Magnons

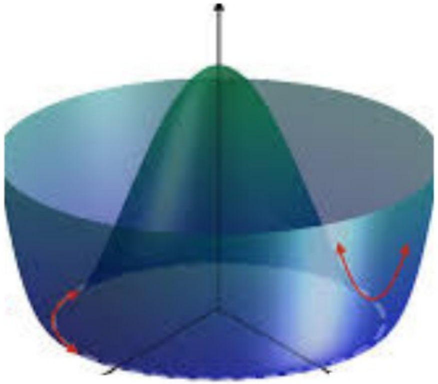
Magnets $\langle \vec{S} \rangle \neq 0$



Spin 1
Charge 0
Gapless/Gaped

Higgs mode

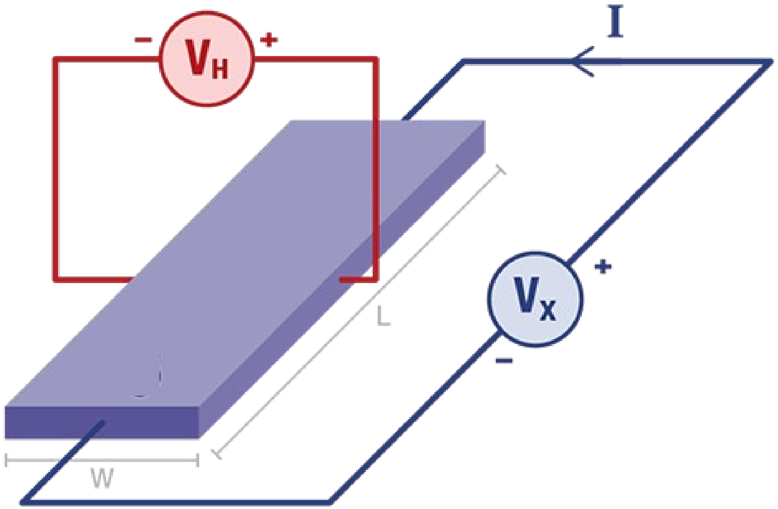
Superconductors $\langle c_\uparrow c_\downarrow \rangle \neq 0$



Spin 0
Charge 0
Gaped

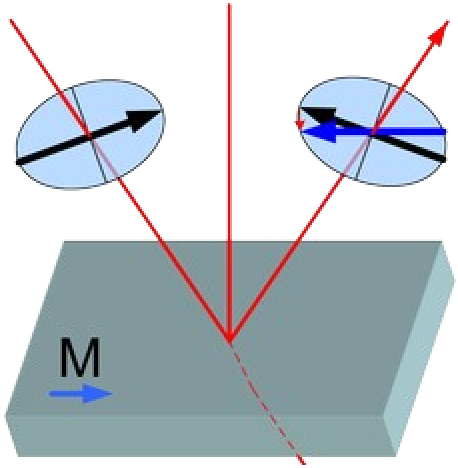
How to know if a material is magnetic?

Measure its Hall conductivity



Current generated perpendicular to a bias voltage

Measure its magneto-optical Kerr effect



Different reflection for left-handed and right-handed polarized light

What a material being “ferromagnetic” means?

An intuitive definition

“It sticks to your fridge”

A formal definition

$$\Theta|\Psi\rangle \neq |\Psi\rangle$$

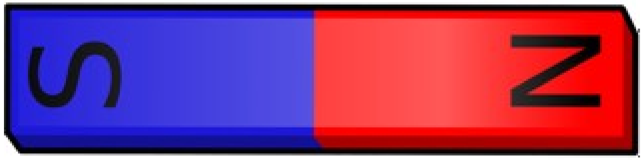
Time reversal operator

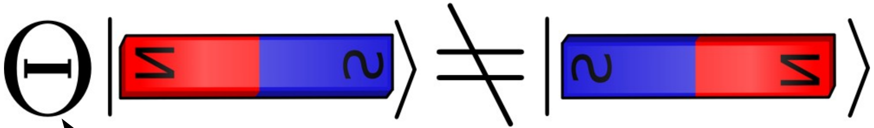
Wavefunction

It breaks time-reversal symmetry

A physical definition of a magnet

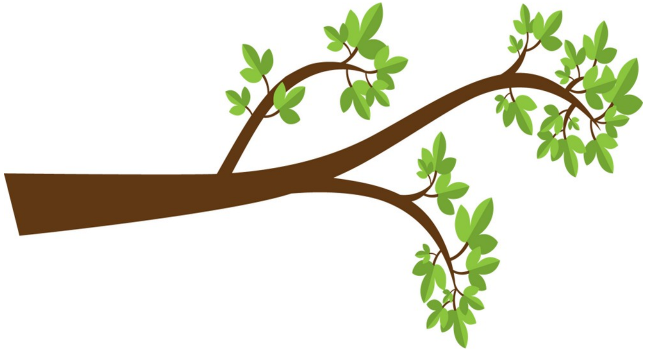
Magnet

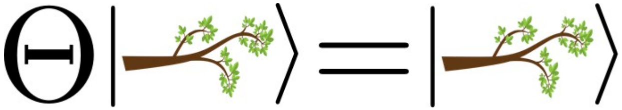




Time reversal operator

Not a magnet





Magnetic materials are not invariant under time reversal symmetry

The role of symmetry

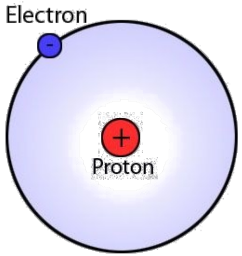
Symmetries enforce observables to vanish

$$\langle A \rangle = 0$$

Certain operator

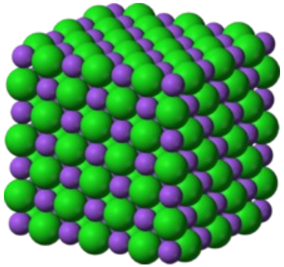
Magnetic moment
Electric dipole
Hall conductivity

Symmetries constrain the mathematical solution of a problem



Hydrogen atom

$$\Psi(r,\theta,\phi) = Y_{lm}(\theta,\phi)R(r)$$



Periodic crystals

$$\Psi(\mathbf{R}+\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}}\Psi(\mathbf{r})$$

Why is symmetry important?

Symmetries help to characterize complex problems capturing their physics

New quantum excitations when symmetries are broken (Goldstone modes)

$$H = -\sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \qquad \longrightarrow \qquad \mathcal{H} = \sum_k \epsilon_k b_k^\dagger b_k$$

Symmetry breaking (ferromagnetism)

Interacting local magnetic moments

Emergent bosonic excitations (magnons)

Symmetries allow to greatly simplify quantum problems

Infinite systems can be "folded" to small systems (Bloch's theorem)

$$H = \sum_k H_k$$

"Infinite system" Hamiltonian

(finite) Bloch's Hamiltonian

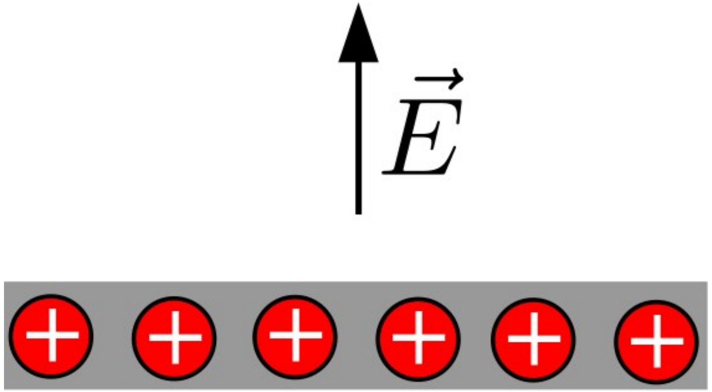
Simplifying problems using symmetries

A familiar example using symmetries

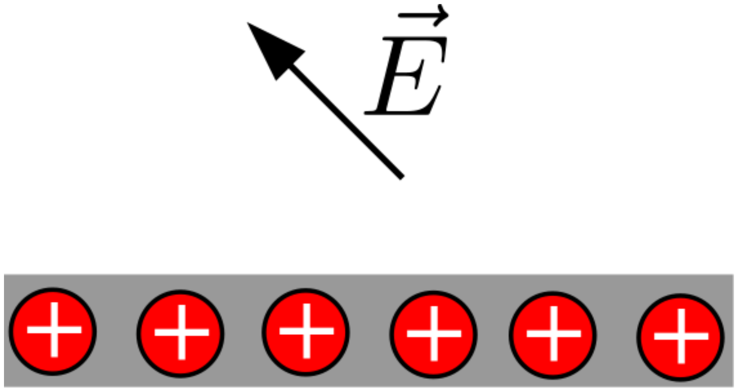
Back to electromagnetism

Imagine an infinite charged plane

Option #1



Option #2



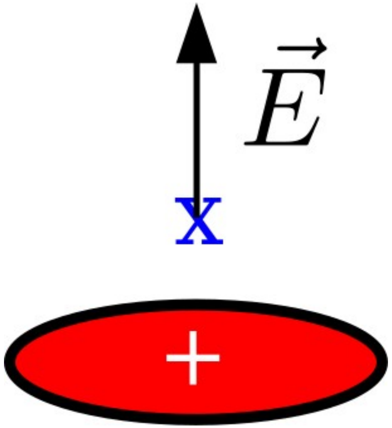
What is the direction of the electric field?

A familiar example using symmetries

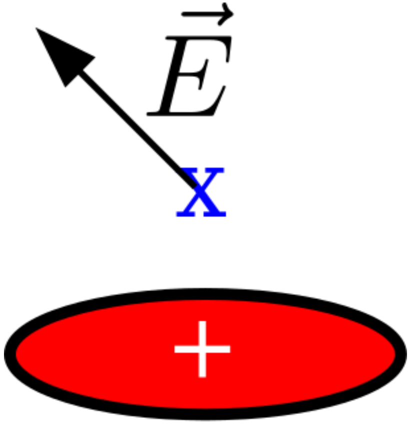
Back to electromagnetism

Imagine an egg-shaped charge

Option #1



Option #2

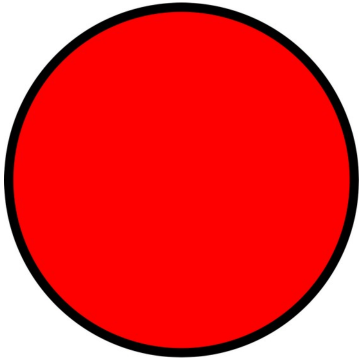


What is the direction of the electric field in position x?

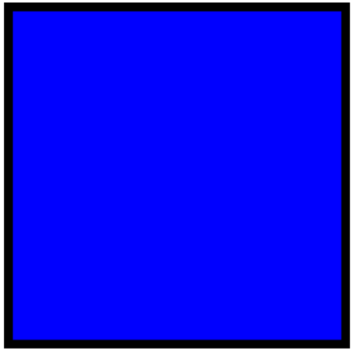
The intuitive notion of symmetry

Symmetry: Transformation performed in a system, that keeps it invariant

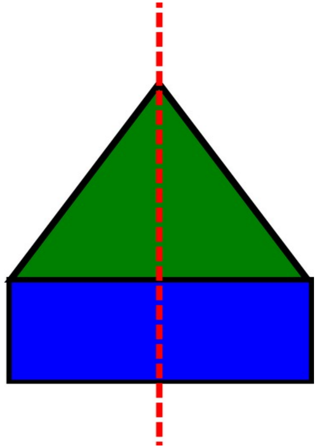
Arbitrary rotation



90 degrees rotation



Right-left reflection



(Symmetry) transformations in quantum physics

How does a transformation affect a wavefunction?

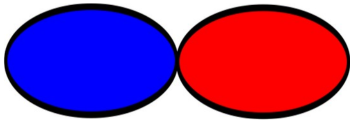
$$|\phi\rangle = S|\Psi\rangle$$

“New” wavefunction

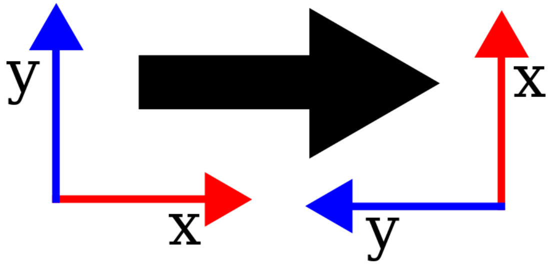
“Old” wavefunction

(Symmetry) transformation

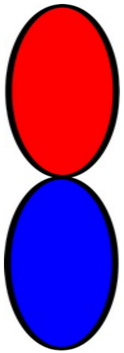
$$|\Psi\rangle$$



Rotate 90 degrees



$$|\phi\rangle$$



(Symmetry) transformations in quantum physics

A generic symmetry transformation

$$|\phi\rangle = S|\Psi\rangle$$

By definition, any symmetry transformation must leave any wavefunction normalized

$$\langle\phi|\phi\rangle = \langle\Psi|S^\dagger S|\Psi\rangle = \langle\Psi|\Psi\rangle \longrightarrow S^\dagger = S^{-1}$$

The Hermitian of a symmetry is its own inverse

Symmetry transformations

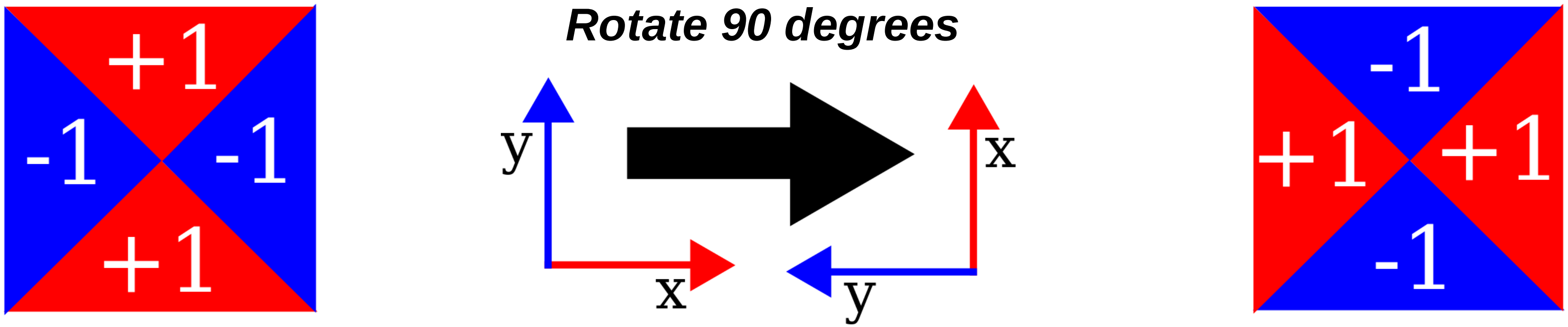
A wavefunction is symmetric under a transformation if $S|\Psi\rangle = \lambda|\Psi\rangle$

λ ***is the eigenvalue of the transformation***

What is the eigenvalue of this transformation?

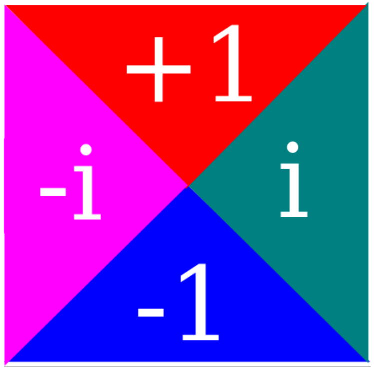
$|\phi\rangle$ $|\Psi\rangle$

Rotate 90 degrees

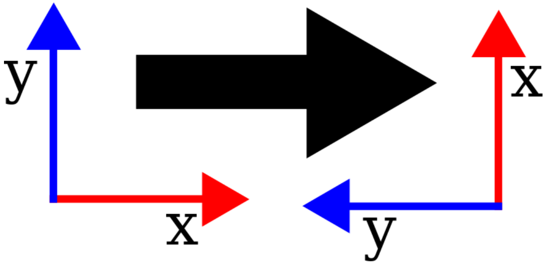


A symmetry transformation

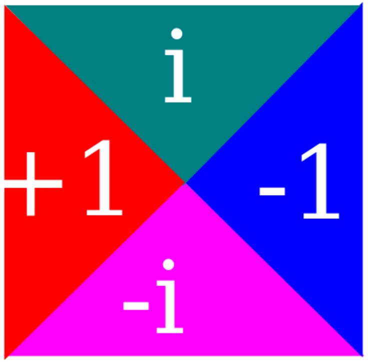
$|\Psi\rangle$



Rotate 90 degrees



$S|\Psi\rangle$

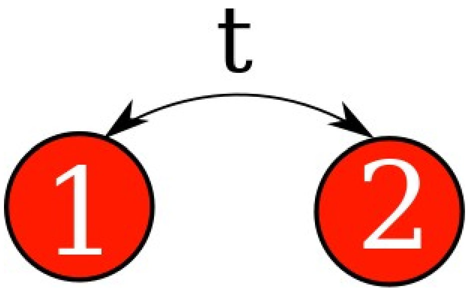


What is the eigenvalue λ **of this transformation?**

$$S|\Psi\rangle = \lambda|\Psi\rangle$$

Symmetry transformation in a wavefunction

Hamiltonian



$$H = t[c_1^\dagger c_2 + c_2^\dagger c_1]$$

Eigenfunctions $\quad H = t\Psi_\alpha^\dagger \Psi_\alpha - t\Psi_\beta^\dagger \Psi_\beta$

$$\Psi_\alpha^\dagger = \frac{1}{\sqrt{2}}[c_1^\dagger + c_2^\dagger] \qquad \Psi_\beta^\dagger = \frac{1}{\sqrt{2}}[c_1^\dagger - c_2^\dagger]$$

What are their eigenvalues λ_γ under mirror symmetry?

$$c_1 \rightarrow c_2$$
$$c_2 \rightarrow c_1$$

$$S|\Psi_\gamma\rangle = \lambda_\gamma |\Psi_\gamma\rangle$$

Symmetries in a Hamiltonian

A Hamiltonian is invariant under a transformation if

$$SHS^{-1} = H$$

$$[S, H] = SH - HS = 0$$

S Symmetry transformation

H Hamiltonian

A reminder from linear algebra

If two linear operators commute, there is a common basis of eigenstates

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$S|\Psi_n\rangle = \lambda_n|\Psi_n\rangle$$

Hamiltonian eigenvalue

Symmetry eigenvalue

Eigenvalues of symmetry operations

Recall the property of symmetry operations

$$S^{\dagger} = S^{-1}$$

All the eigenvalues of symmetry operations are complex numbers in unit circle

$$S|\Psi\rangle = \lambda|\Psi\rangle$$

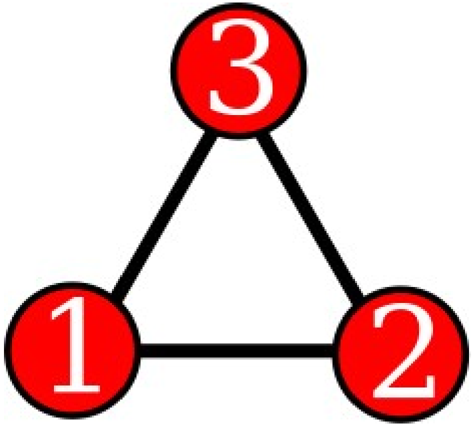
Complex eigenvalue

Real number

$$\lambda = e^{i\phi}$$

Guessing the form of wavefunctions

Take this Hamiltonian



$$H = c_1^\dagger c_2 + c_2^\dagger c_3 + c_3^\dagger c_1 + h.c.$$

We know that 120 degrees rotation leaves the Hamiltonian invariant

What are the eigenvalues under the rotation symmetry operation?

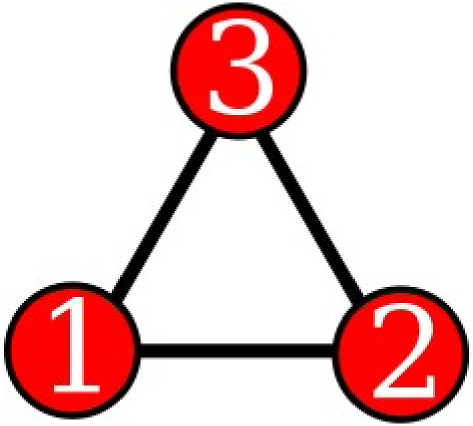
Rotation operator

Symmetry eigenvalue

$$R|\Psi\rangle = e^{i\phi}|\Psi\rangle$$

Guessing the form of wavefunctions

Take this Hamiltonian



$$R|\Psi\rangle = e^{i\phi}|\Psi\rangle$$

Rotating three times brings the system back to itself

$$R^3 = I$$

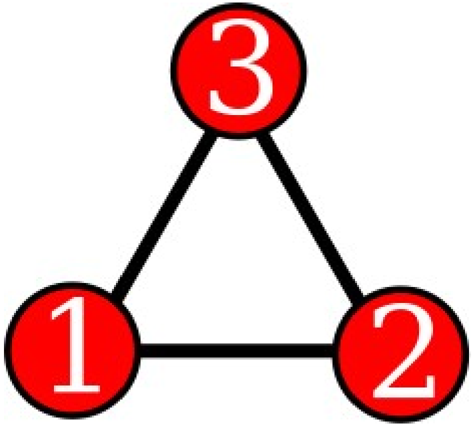
$$(e^{i\phi})^3 = 1$$

Possible phases

$$\phi = \frac{2n\pi}{3} \qquad n = 0, 1, 2$$

Guessing the form of wavefunctions

Take this Hamiltonian



$$\phi = \frac{2n\pi}{3} \quad n = 0, 1, 2$$

$$R|\Psi\rangle = e^{i\phi}|\Psi\rangle$$

The possible form of an eigenstate

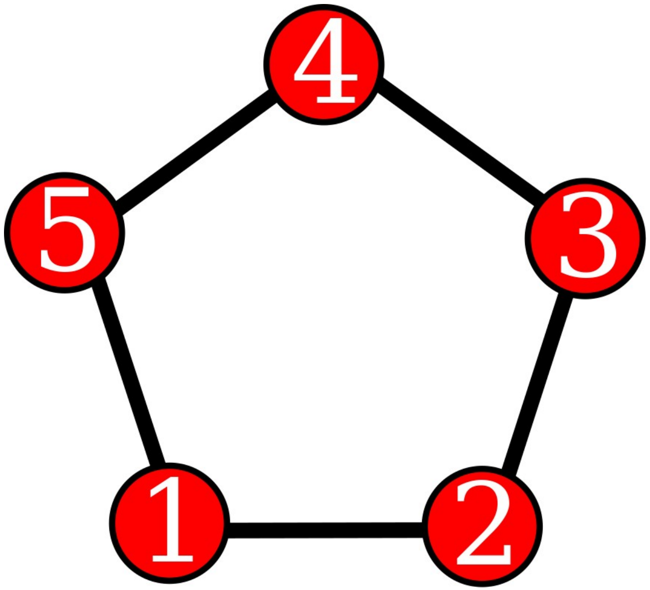
$$\Psi^\dagger = \alpha_1 c_1^\dagger + \alpha_2 c_2^\dagger + \alpha_3 c_3^\dagger$$

α_i Complex number

What are the exact coefficients of the wavefunction?

Guessing a harder wavefunction

Take this Hamiltonian



$$H = \sum_{\langle ij \rangle} c_i^\dagger c_j$$

What are the symmetry eigenvalues?

$$R|\Psi\rangle = e^{i\phi}|\Psi\rangle$$

For the ground state, what is the value of

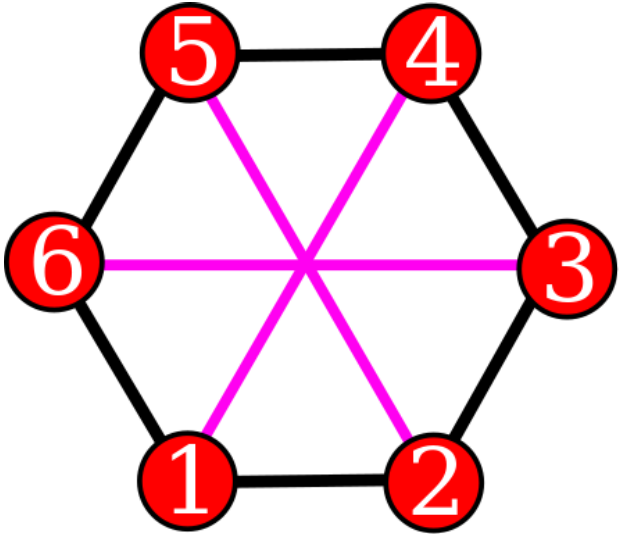
$$\left|\langle\Omega|c_1\Psi^\dagger_{GS}|\Omega\rangle\right|^2$$

vacuum

Ground state

Guessing a harder wavefunction

Take this Hamiltonian



$$H = \sum_{ij} t_{ij} c_i^\dagger c_j$$

What are the symmetry eigenvalues?

$$R|\Psi\rangle = e^{i\phi}|\Psi\rangle$$

For the ground state, what is the value of

$$|\langle\Omega|c_1 \Psi^\dagger_{GS}|\Omega\rangle|^2$$

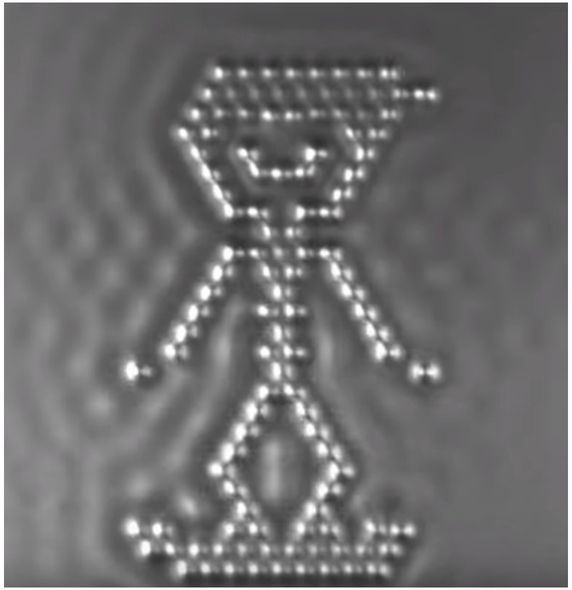
vacuum

Ground state

Lattice models in experiments

Manipulating individual atoms at the atomic scale

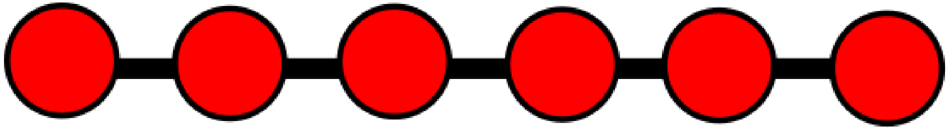
https://www.youtube.com/watch?v=oSCX78-8-q0



The smallest film created by humankind

Translational symmetry in chains

One dimensional tight binding chain



$$H = \sum_{n=-\infty}^{\infty} c_n^\dagger c_{n+1} + h.c.$$

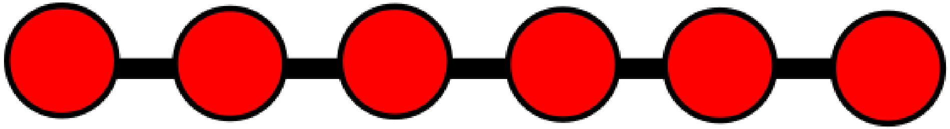
The Hamiltonian commutes with the translation operator → Bloch's theorem

$$T : c_n \to c_{n+1} \qquad [H, T] = 0 \qquad T|\Psi_\phi\rangle = e^{i\phi}|\Psi_\phi\rangle$$

$\phi \equiv$ Bloch phase of the wavefunction $\qquad \phi \in [0, 2\pi)$

Translational symmetry in chains

One dimensional tight binding chain



$$H = \sum_{n=-\infty}^{\infty} c_n^\dagger c_{n+1} + h.c.$$

$$[H, T] = 0$$

$$T|\Psi_\phi\rangle = e^{i\phi}|\Psi_\phi\rangle$$

$$H|\Psi_\phi\rangle = \epsilon_\phi|\Psi_\phi\rangle$$

The mapping between ϕ and ϵ_ϕ is what we call band structure

$e^{i\phi} \equiv$ Symmetry eigenvalue

$\epsilon_\phi \equiv$ Energy eigenvalue

Translational symmetry in chains

In the original (real-space) basis

$$H = \sum_{n=-\infty}^{\infty} c_n^\dagger c_{n+1} + h.c.$$

In the diagonal basis

$$H = \sum_\phi \epsilon_\phi \Psi_\phi^\dagger \Psi_\phi$$

From the symmetry eigenvalue, we can determine the expansion of $\Psi_\phi^\dagger$

$$T\Psi_\phi^\dagger T^{-1} = e^{i\phi}\Psi_\phi^\dagger \qquad \Psi_\phi^\dagger = \sum_n a_{n,\phi} c_n^\dagger \qquad a_{n,\phi} = e^{in\phi}$$

And by taking that eigenfunction, we get the eigenvalues of the Hamiltonian

$$\Psi_\phi^\dagger = \sum_n e^{in\phi} c_n^\dagger \qquad H|\Psi_\phi\rangle = \epsilon_\phi |\Psi_\phi\rangle \qquad \epsilon_\phi = 2\cos\phi$$

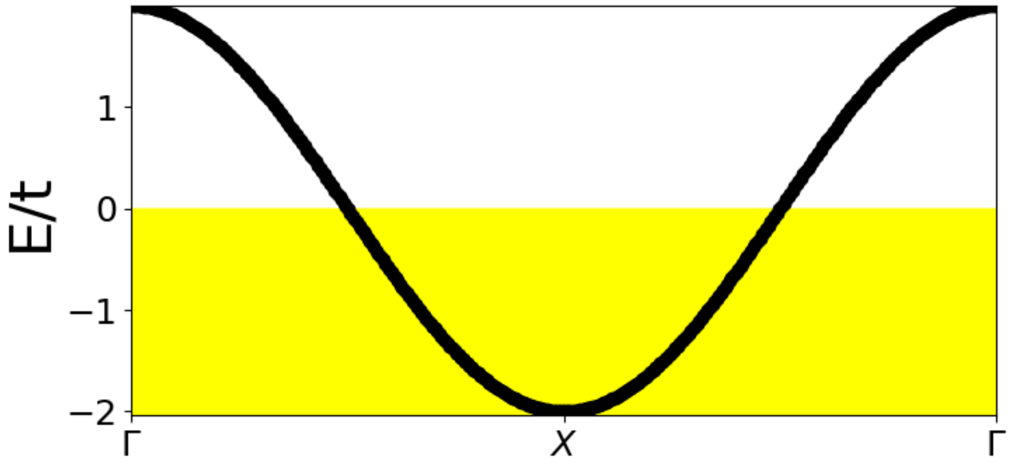
Computing electronic band structures with Python

pyqula Python library

Installation

```
pip install pyqula
```

Band structure

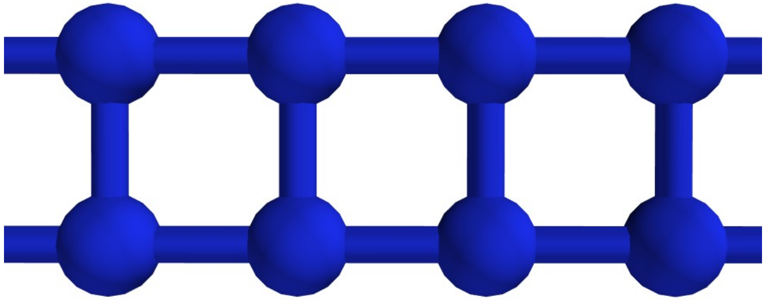


Example script for a 1D tight binding chain

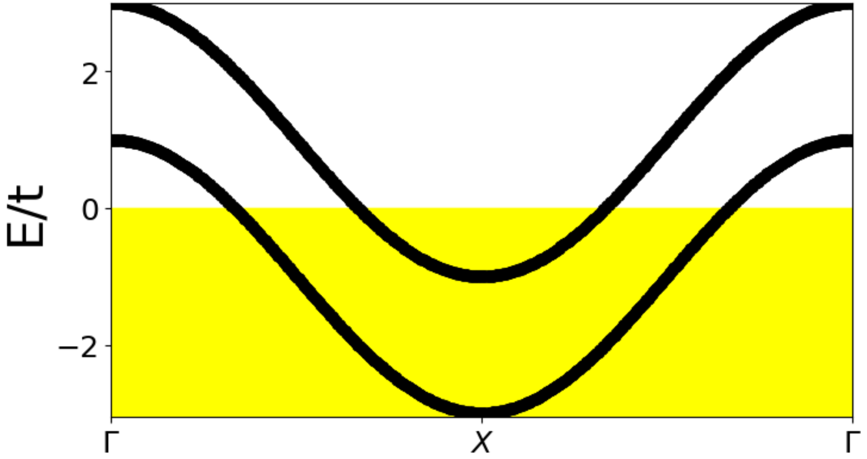
```
from pyqula import geometry
g = geometry.chain() # create a chain geometry
h = g.get_hamiltonian() # get the tight binding Hamiltonian
(k,e) = h.get_bands() # get the band structure
```

Computing electronic band structures with Python

Let us consider now a model in a 1D ladder



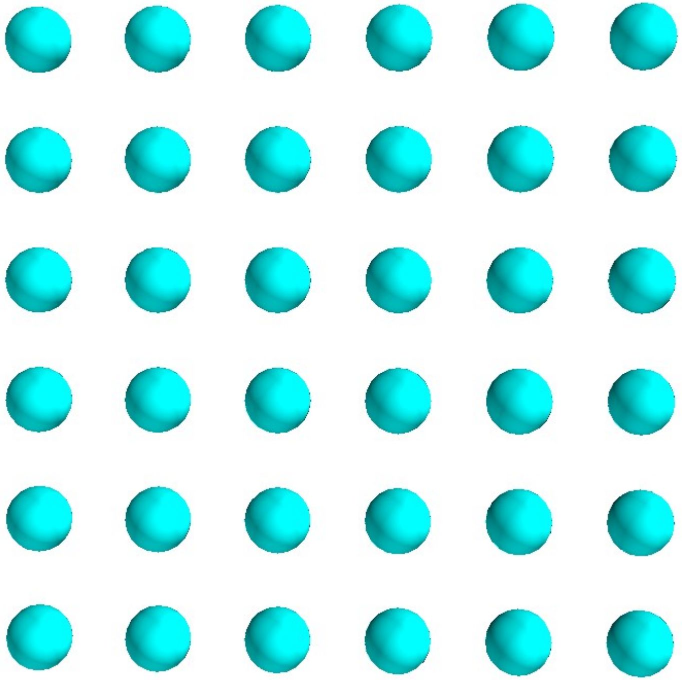
Band structure



Example script for a 1D tight binding ladder

```
from pyqula import geometry
g = geometry.ladder() # create a ladder geometry
h = g.get_hamiltonian() # get the tight binding Hamiltonian
(k,e) = h.get_bands() # get the band structure
```

Translational symmetry in lattices



Translation in y

T_y

T_x Translation in x

Two possible symmetry operations

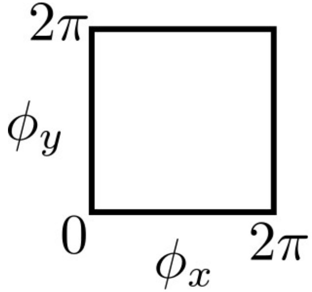
$$T_x|\Psi_{(\phi_x,\phi_y)}\rangle = e^{i\phi_x}|\Psi_{(\phi_x,\phi_y)}\rangle$$

$$T_y|\Psi_{(\phi_x,\phi_y)}\rangle = e^{i\phi_y}|\Psi_{(\phi_x,\phi_y)}\rangle$$

$$\phi_x \in [0,2\pi) \qquad \phi_y \in [0,2\pi)$$

The “phases” live in the reciprocal space

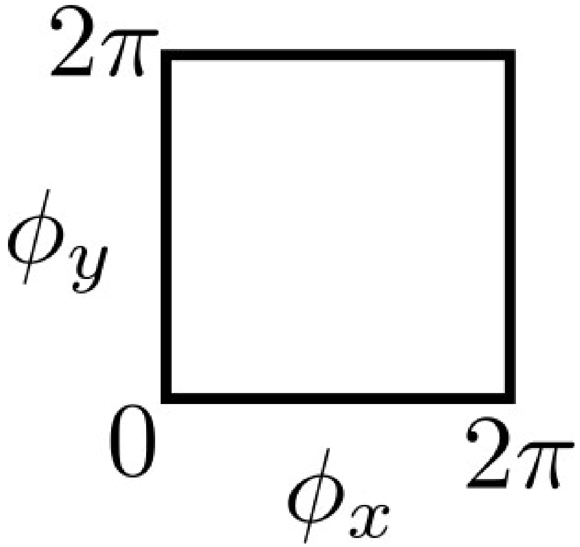
$$\vec{\phi} = (\phi_x, \phi_y) \in$$



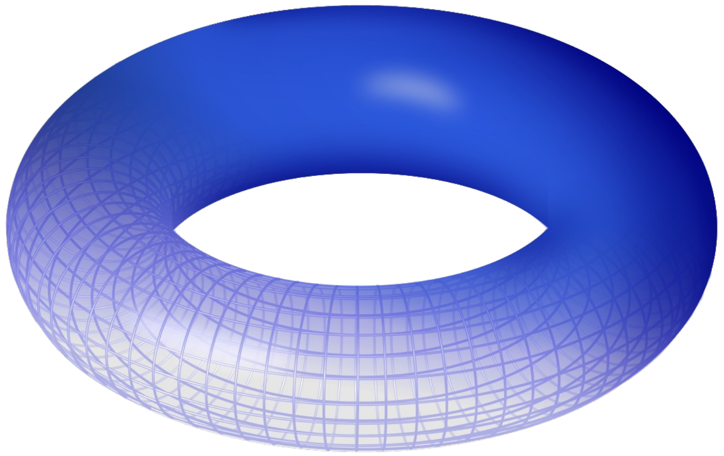
Reciprocal space

The symmetry eigenvalues live in the "reciprocal space"

$$T_x|\Psi_{(\phi_x,\phi_y)}\rangle = e^{i\phi_x}|\Psi_{(\phi_x,\phi_y)}\rangle$$
$$T_y|\Psi_{(\phi_x,\phi_y)}\rangle = e^{i\phi_y}|\Psi_{(\phi_x,\phi_y)}\rangle$$



Effectively, the 2D reciprocal space is a torus (periodic boundary conditions)



Take home

- Symmetries allow to
  - Classify quantum matter
  - Simplify quantum problems
    - Solve single-particle models with translational symmetry
- Remember to submit the exercise by Friday 23:59 in MyCourses

In the next session

- How to predict macroscopic properties of crystals from microscopic models