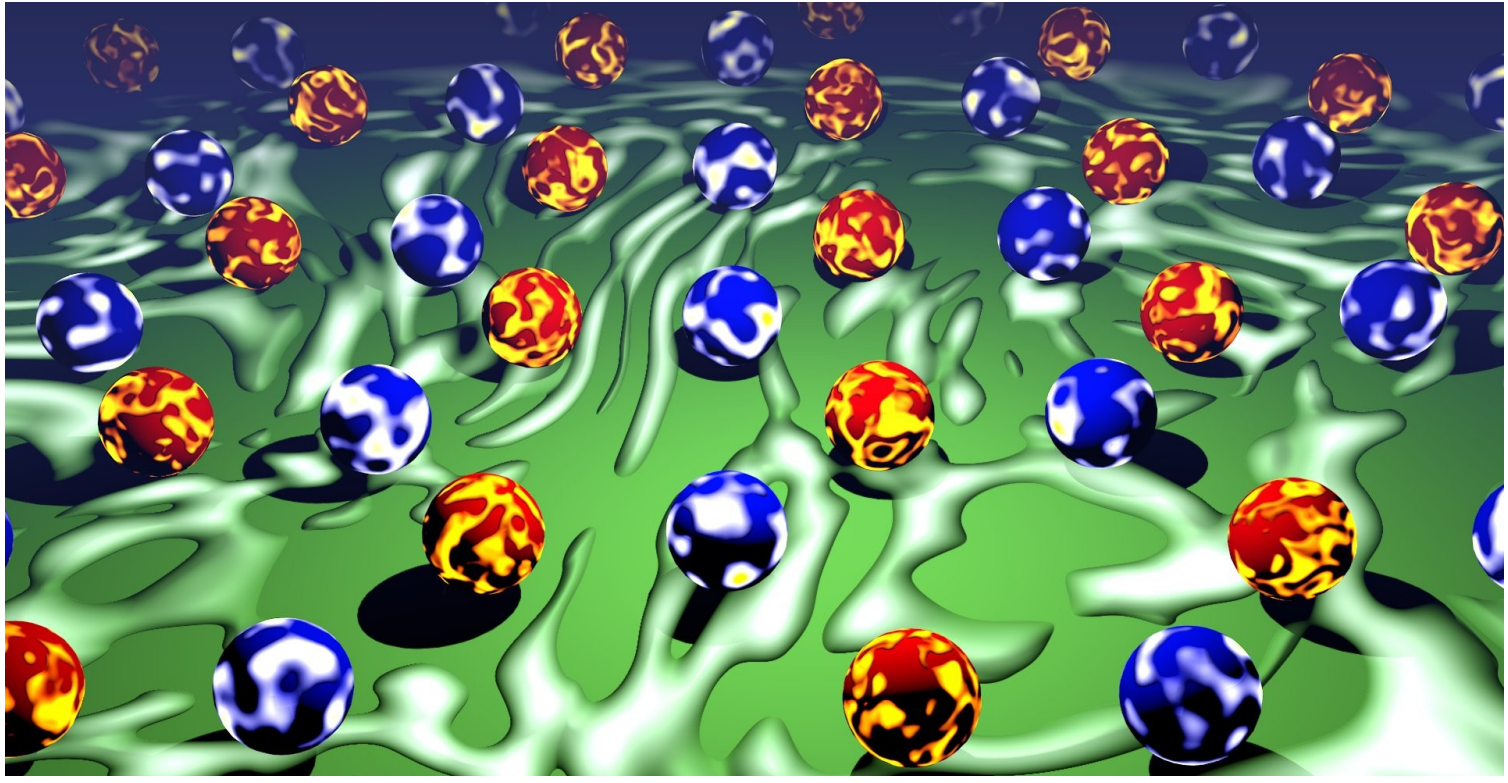
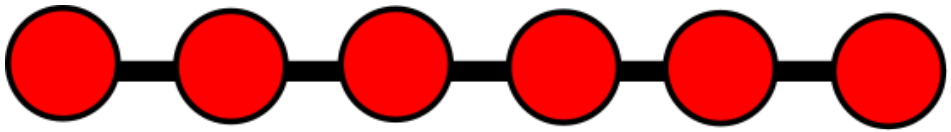
Band-structure theory



March 13th 2023

A reminder from session #2

One dimensional tight binding chain



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

The Hamiltonian commutes with the translation operator

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

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

Today's learning outcomes

The spectra of non-interacting infinite periodic systems can be folded to a collection of finite systems

$$H = \sum_k H_k$$

Full Hamiltonian

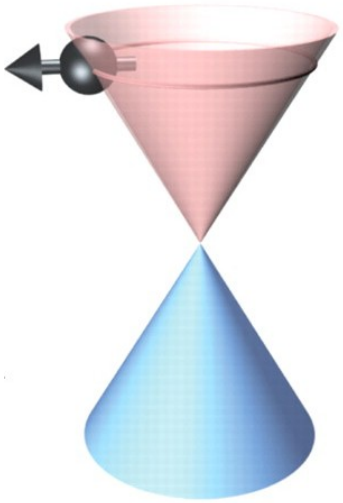
Bloch Hamiltonian

Today’s plan

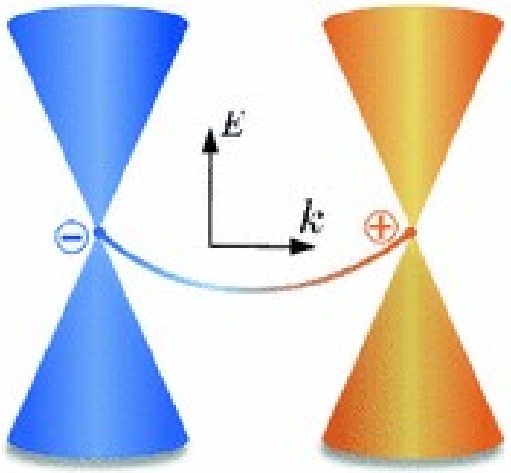
- Single band 1D band-structures
- Multi-band 1D band-structures
- Single band high dimensional band-structures
- Key properties of electronic dispersions
- ARPES

The physics of band-structures

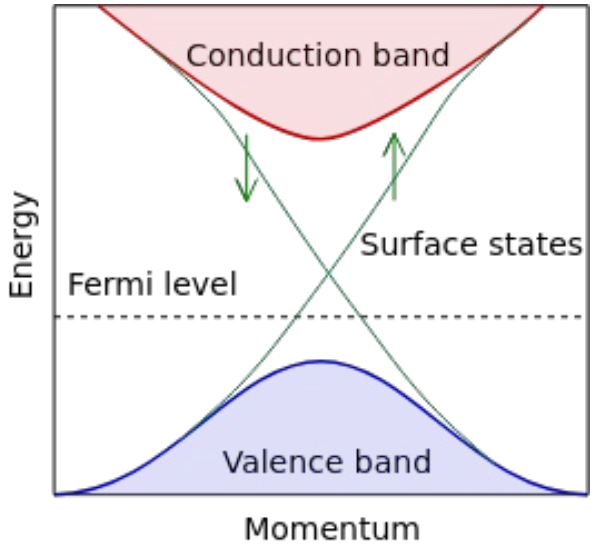
Dirac fermions



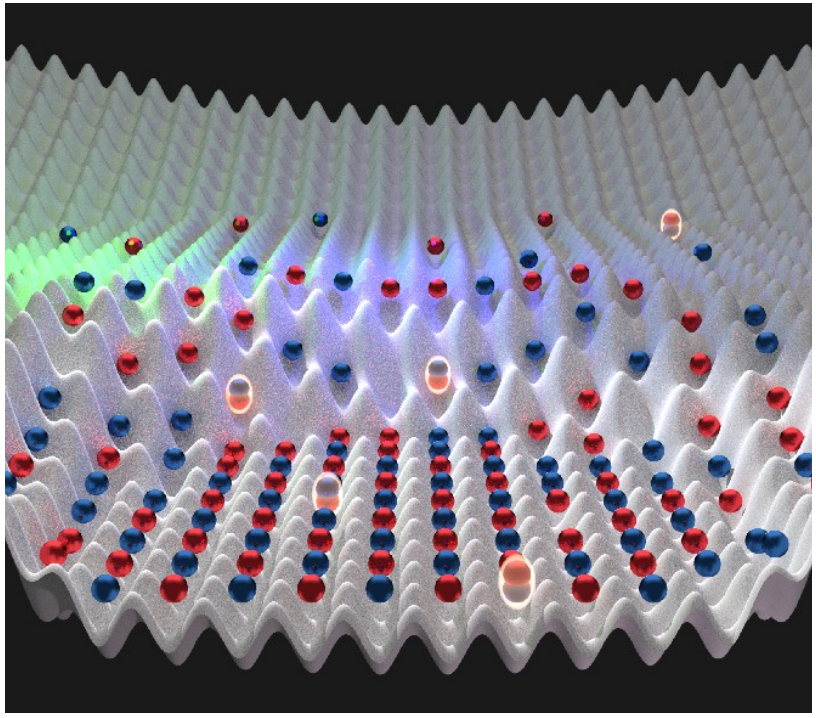
Weyl semimetals

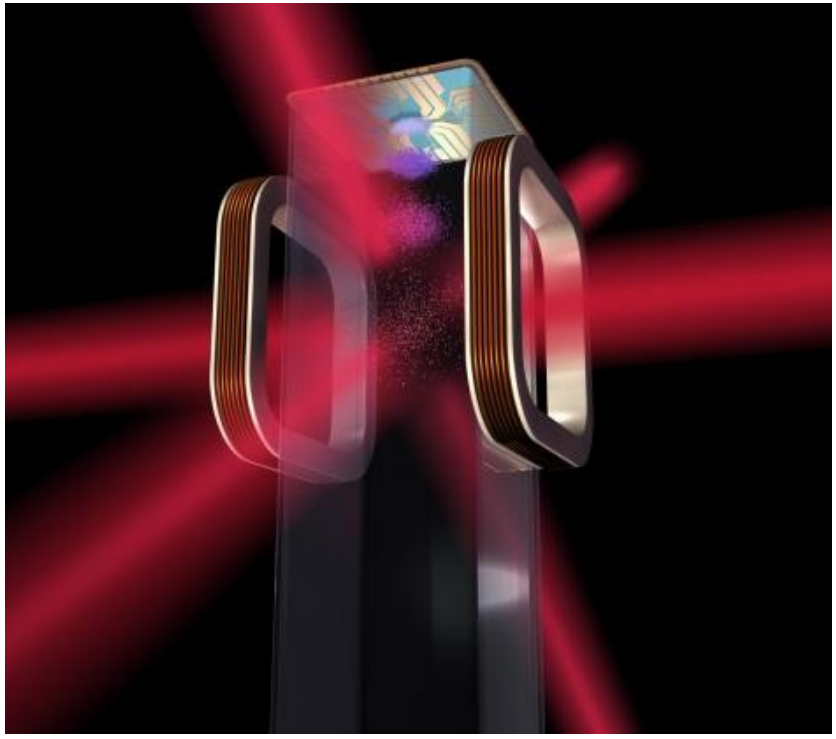


Topological insulators



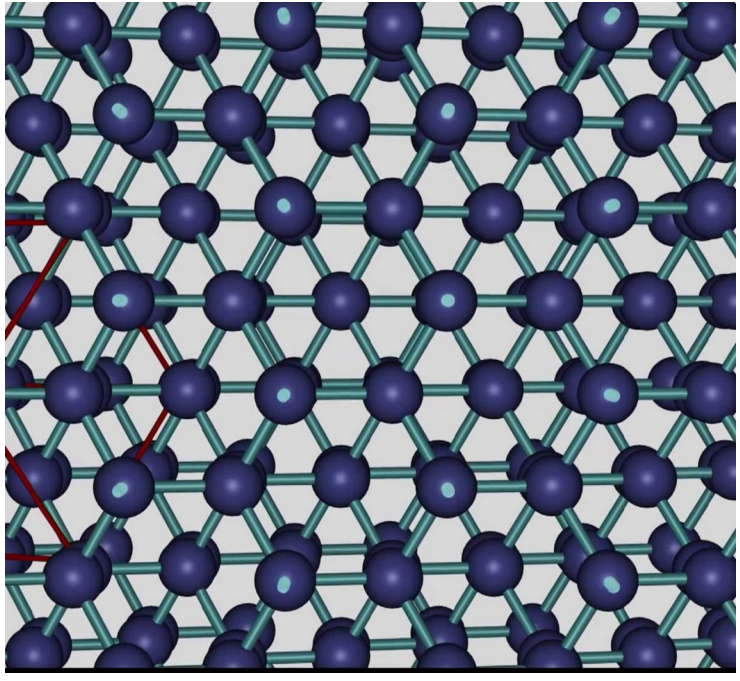
Artificial band-structures with cold-atoms

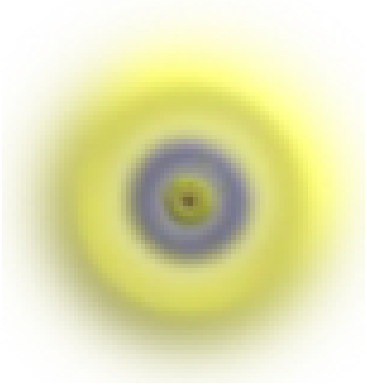




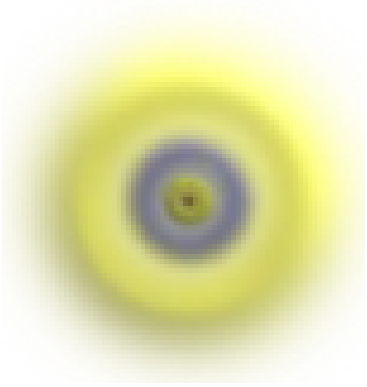
Atoms trapped with lasers allow to realize artificial band structures

Electronic band-structures





Atom #1

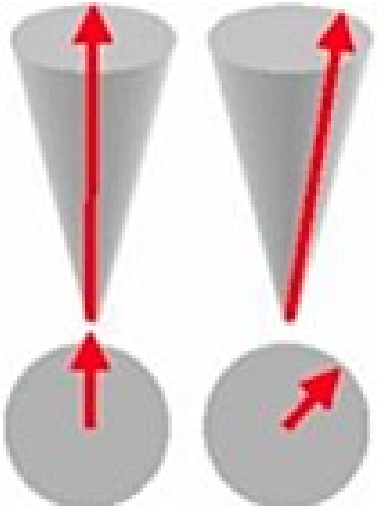


Atom #2

We will focus on the band-structures associated to electronic states

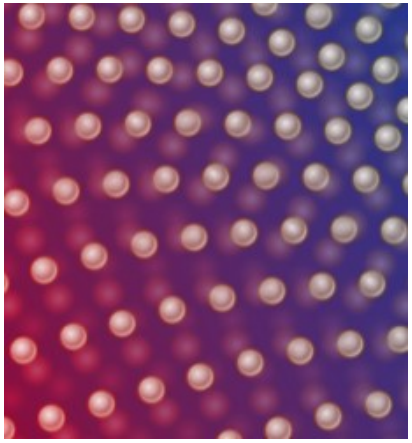
Band-structures in materials beyond electrons

Magnons



Magnets

Phonons



Any crystal

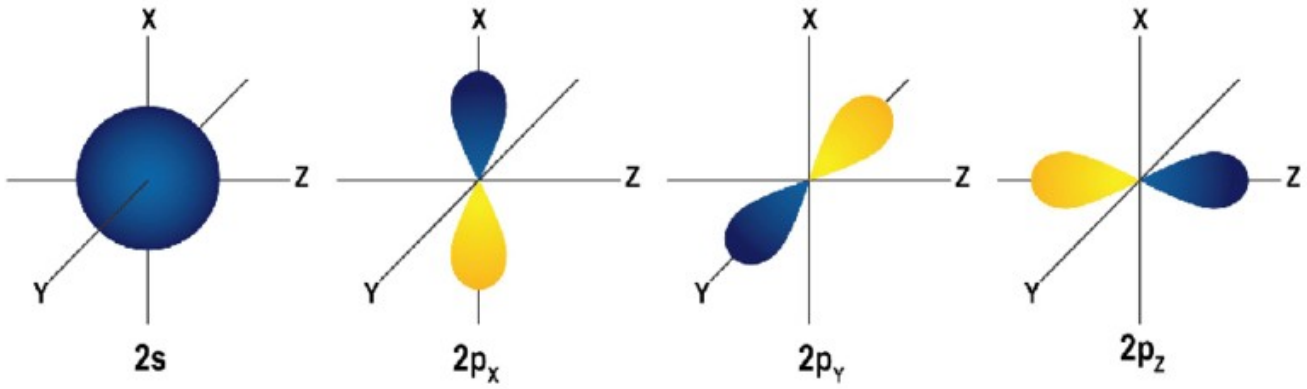
BdG quasiparticles

Superconductors

Single orbital band-structures

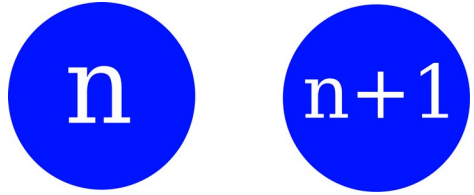
Basis of our Hamiltonian

Atomic orbital (non-orthogonal between different sites)



We will take as basis orthogonalized orbitals (Wannier states)

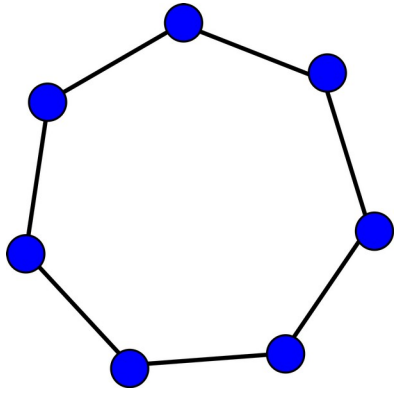
$$\langle n|n+1\rangle = 0 \qquad \int \Psi_n(\mathbf{r})\Psi^*_{n+1}(\mathbf{r})d^N\mathbf{r} = 0$$



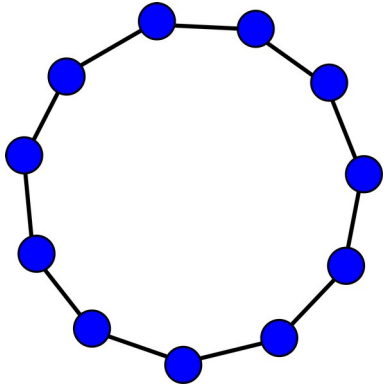
From the finite to the infinite limit

We take a periodic large system, and then the limit when the sites are infinite

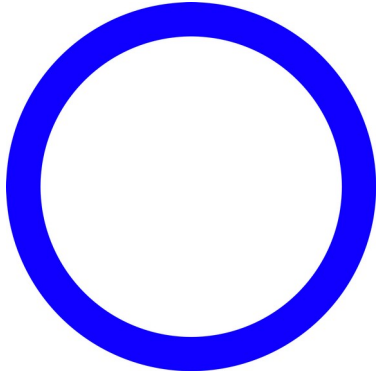
L= 7 sites



L= 11 sites



$L = \infty$ sites



$$\Psi_\phi^\dagger = \frac{1}{\sqrt{L}} \sum_{n=0}^{n=L} e^{in\phi} c_n^\dagger$$

We will take this notation

(for simplicity)

$$\Psi_\phi^\dagger = \sum_n e^{in\phi} c_n^\dagger$$

A note on translational symmetry

For any generic wavefunction

$$\phi(x+a) = e^{i\hat{p}a}\phi(x)$$

Taylor expansion

Momentum $\hat{p} = -i\partial_x$

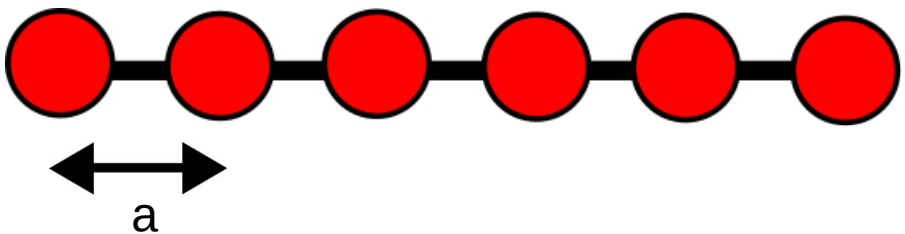
$e^{i\phi}$ symmetry eigenvalue

k Crystal momentum

a lattice constant

For a Bloch wavefunction

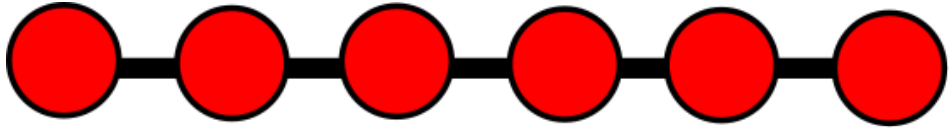
$$\Psi(x+a) = e^{i\phi}\Psi(x)$$



$$e^{i\phi} \equiv e^{ika}$$

One dimensional band structure

We know that for an infinite 1D periodic system



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

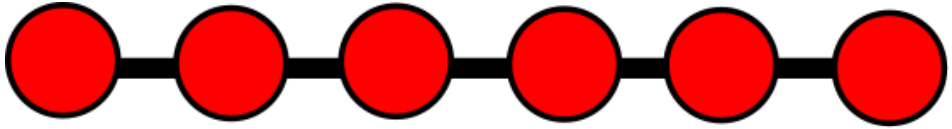
The Hamiltonian is diagonalized as

$$H = \sum_\phi \epsilon_\phi \Psi_\phi^\dagger \Psi_\phi \qquad \Psi_\phi^\dagger \sim \sum_n e^{i\phi n} c_n^\dagger \qquad \langle \Psi_\phi | \Psi_{\phi'} \rangle = \delta_{\phi,\phi'}$$

How do we compute the Hamiltonian eigenvalues ϵ_ϕ?

One dimensional band structure

Hamiltonian 1D periodic system



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

Direct and inverse transformation

$$\Psi_\phi^\dagger \sim \sum_n e^{i\phi n} c_n^\dagger$$

$$c_n^\dagger \sim \sum_\phi e^{-i\phi n} \Psi_\phi^\dagger$$

Plug it in the Hamiltonian

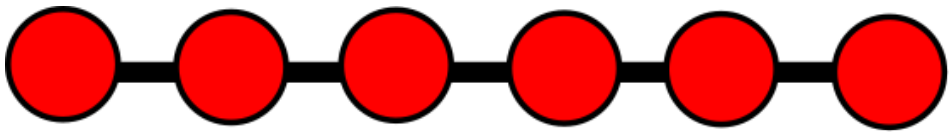
$$\sum_n e^{in(\phi'-\phi)} = \delta_{\phi,\phi'}$$

Orthogonality

$$H = \sum_{n,\phi,\phi'} e^{-i\phi n} \Psi_\phi^\dagger e^{i\phi'(n+1)} \Psi_{\phi'} + h.c. = \sum_\phi e^{i\phi} \Psi_\phi^\dagger \Psi_\phi + h.c. \equiv \sum_\phi H_\phi$$

One dimensional band structure

Hamiltonian 1D periodic system



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

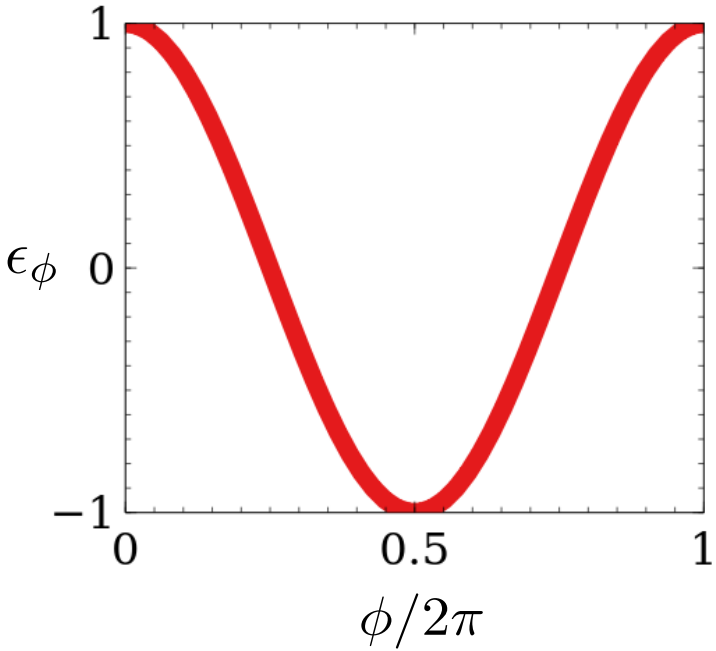
$$H = \sum_\phi \epsilon_\phi \Psi_\phi^\dagger \Psi_\phi$$

$\epsilon_\phi = 2\cos\phi$ ← Electronic dispersion

$$\phi \in [0, 2\pi)$$

Bloch wavefunctions

$$\Psi_\phi^\dagger \sim \sum_n e^{i\phi n} c_n^\dagger$$



Question: one dimensional band-structure

What is the band-structure of the following Hamiltonian?

$$H = \sum_{i=-\infty}^{\infty} c_i^\dagger c_{i+1} + \eta c_i^\dagger c_{i+2} + h.c.$$

Option A

$$\epsilon_\phi = 2\cos\phi + 2\eta\cos 2\phi$$

Option B

$$\epsilon_\phi = 2\cos\left(\phi + \eta\right)$$

Question: one dimensional band-structure

What is the band-structure of the following Hamiltonian?

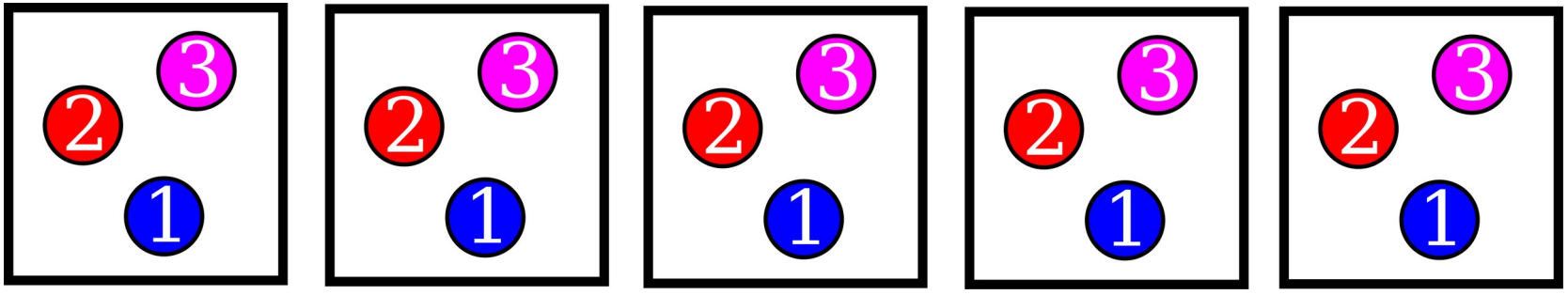
$$H = \sum_{i=-\infty}^{\infty} c_i^\dagger c_{i+1} + \eta c_i^\dagger c_{i+2} + h.c.$$

Solution: **Option A**

$$\epsilon_\phi = 2\cos\phi + 2\eta\cos 2\phi$$

Multi-orbital band-structures

Multi-orbital band-structures

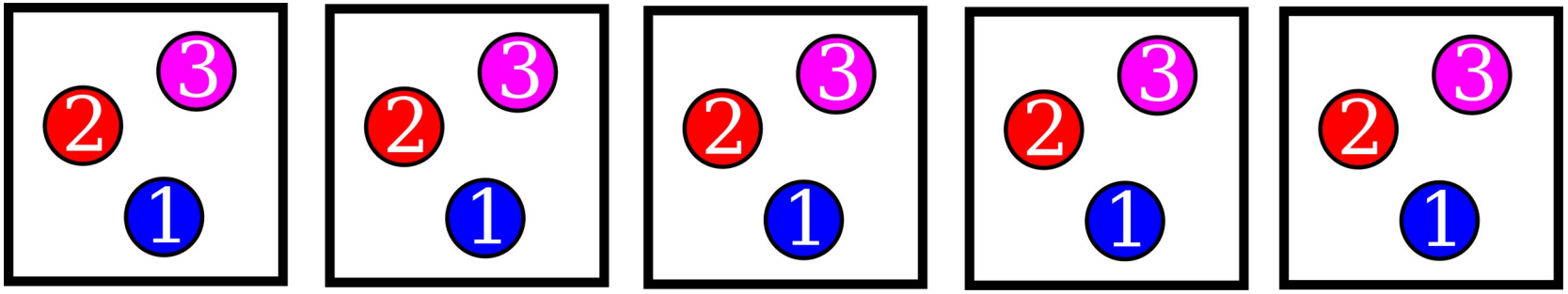


$$c^{\dagger}_{\alpha,n}$$

index of the orbital in the unit cell

Index of the unit cell

Multi-orbital band-structures



$$H = \sum_{n,\alpha,\beta} t_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n} + \sum_{n,\alpha,\beta} \gamma_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n+1} + h.c.$$

Intra-cell hoppings

Inter-cell hoppings

Multi-orbital band-structures

$$H = \sum_{n,\alpha,\beta} t_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n} + \sum_{n,\alpha,\beta} \gamma_{\alpha\beta} c^{\dagger}_{\alpha,n} c_{\beta,n+1} + h.c.$$

Unitary transformation

$$\Psi^{\dagger}_{\phi,\alpha} \sim \sum_{n,\beta} e^{i\phi n} U_{\alpha\beta} c^{\dagger}_{n,\beta} \qquad H = \sum_{\phi,\alpha} \epsilon_{\phi,\alpha} \Psi^{\dagger}_{\phi,\alpha} \Psi_{\phi,\alpha}$$

$\epsilon_{\phi,\alpha}$ **are the eigenvalues of the matrix**

$$h(\phi) = t_{\mu\nu} + \gamma_{\mu\nu} e^{i\phi} + h.c.$$

Question: one dimensional multi-orbital band-structure

What is the band-structure of the following Hamiltonian?

$$H = \sum_{i=-\infty}^{\infty} c^{\dagger}_{A,i} c_{B,i} + \eta c^{\dagger}_{B,i} c_{A,i+1} + h.c.$$

Option A

$$\epsilon_{\phi} = \pm |1 + \eta e^{-i\phi}|$$

Option B

$$\epsilon_{\phi} = 2\cos\phi + 2\eta\cos\phi$$

Question: one dimensional multi-orbital band-structure

What is the band-structure of the following Hamiltonian?

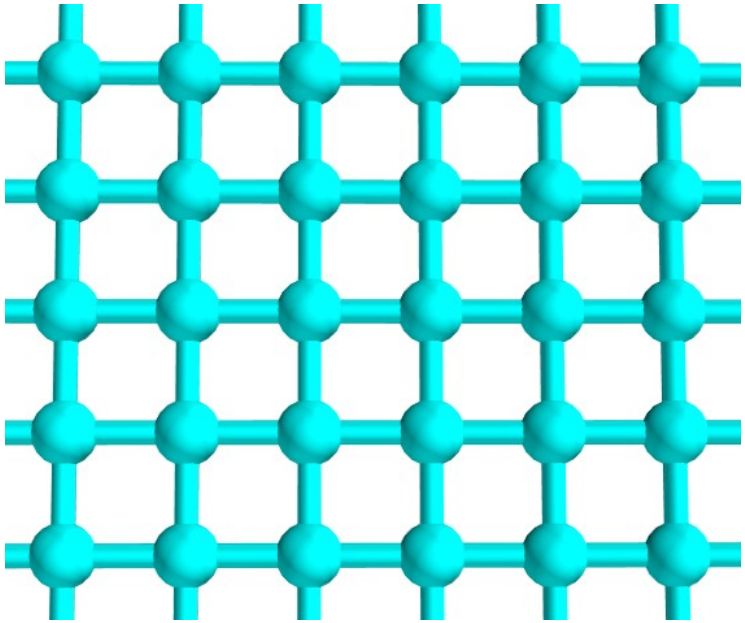
$$H = \sum_{i=-\infty}^{\infty} c^{\dagger}_{A,i} c_{B,i} + \eta c^{\dagger}_{B,i} c_{A,i+1} + h.c.$$

Solution: $h(\phi) = \begin{pmatrix} 0 & 1+\eta e^{-i\phi} \\ 1+\eta e^{i\phi} & 0 \end{pmatrix}$

Option A $\epsilon_{\phi} = \pm|1+\eta e^{-i\phi}|$

Higher dimensional band-structures

Higher dimensional band-structures



T_y Translation in y

T_x Translation in x

Two possible symmetry operations

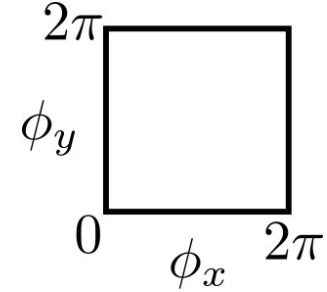
$$T_x|\Psi_{(\phi_x,\phi_y)}\rangle = e^{i\phi_x}|\Psi_{(\phi_x,\phi_y)}\rangle$$

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

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

The "phases" live in the reciprocal space

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



Reciprocal space

The phase is associated to the Bloch wavevector $\vec{k}$

$$\phi_x \equiv \vec{a}_1 \cdot \vec{k}$$

$$\phi_y \equiv \vec{a}_2 \cdot \vec{k}$$

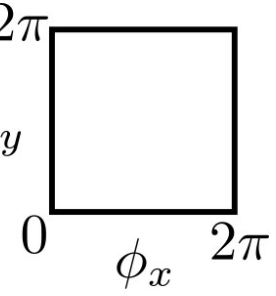
$\vec{k}$ Is a vector in the Brillouin zone

Two possible symmetry operations

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

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

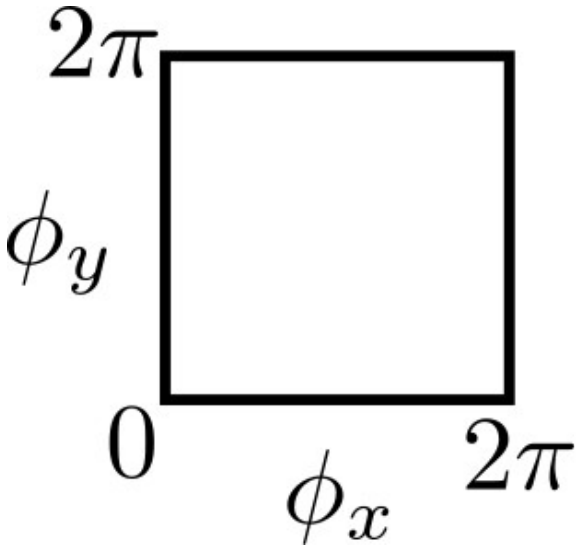
$$\vec{\phi} = (\phi_x, \phi_y) \in$$



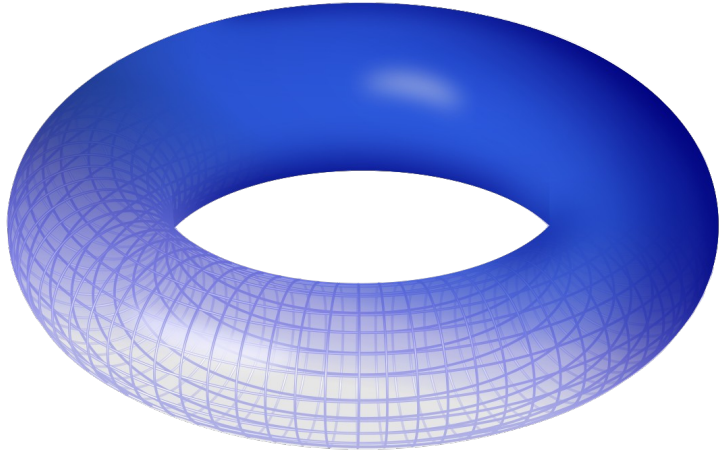
Reciprocal space

The symmetry eigenvalues live in the “reciprocal space”

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

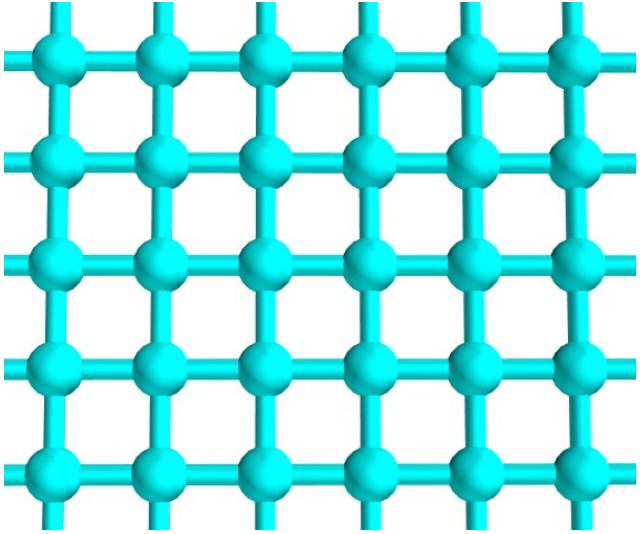


Effectively, the 2D reciprocal space is a torus (periodic boundary conditions)



Exercise: two-dimensional band-structure

What is the band-structure of a single orbital in a square lattice?

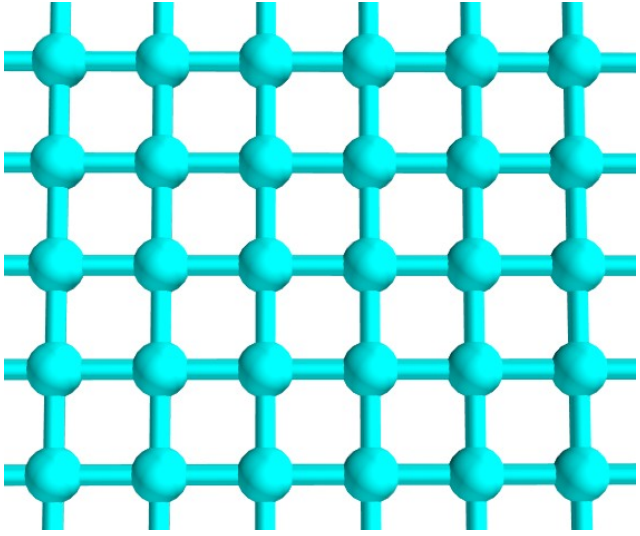


$$H = \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Sum over first neighbors

Exercise: two-dimensional band-structure

What is the band-structure of a single orbital in a square lattice?

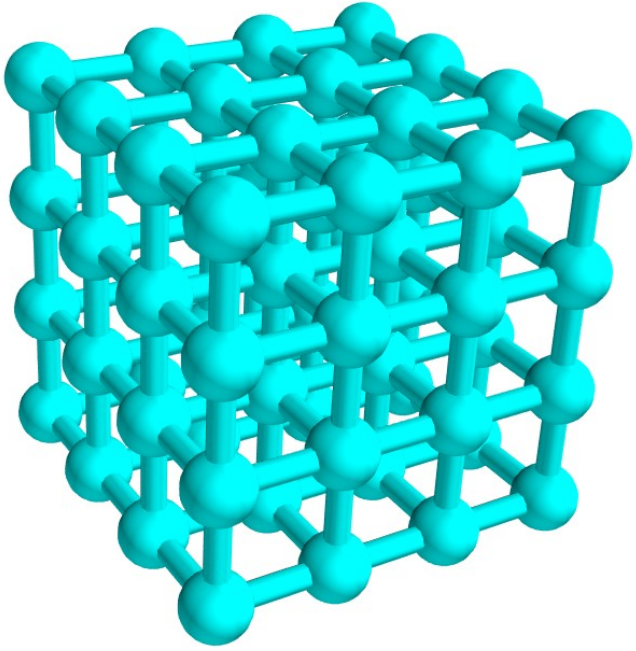


$$H = \sum_{\langle ij \rangle} c_i^\dagger c_j$$

$$\epsilon(k) = 2\cos k_x + 2\cos k_y$$

Exercise: three-dimensional band-structure

What is the band-structure of a single orbital in a cubic lattice?

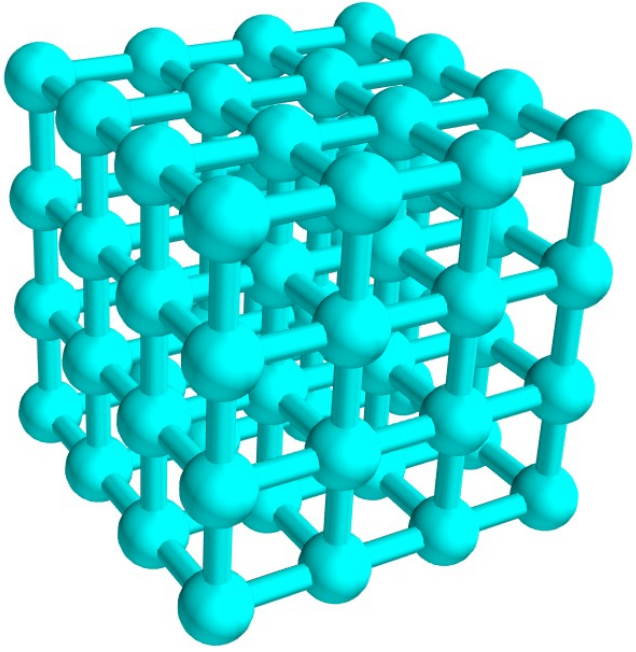


$$H = \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Sum over first neighbors

Exercise: three-dimensional band-structure

What is the band-structure of a single orbital in a cubic lattice?



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

$$\epsilon(k) = 2\cos k_x + 2\cos k_y + 2\cos k_z$$

Macroscopic properties

Properties of the electronic dispersion

From now on, lets work with a specific electronic dispersion $\epsilon_{\vec{k}}$

Density of states $$D(\omega) \sim \int \delta(\omega - \epsilon_{\vec{k}}) d^N \vec{k}$$

Group velocity

$$v_F = \frac{\partial \epsilon_{\vec{k}}}{\partial k_\alpha}$$

Effective mass

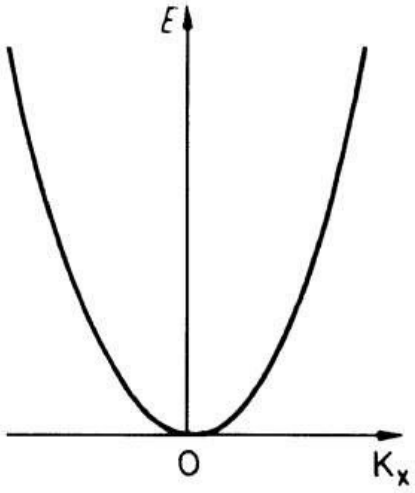
$$\frac{1}{m_{\alpha\beta}} = \frac{\partial^2 \epsilon_{\vec{k}}}{\partial k_\alpha \partial k_\beta}$$

Fermi surface

$$\{\vec{k}\} \text{ with } \epsilon_{\vec{k}} = \epsilon_F$$

Three important electronic dispersions

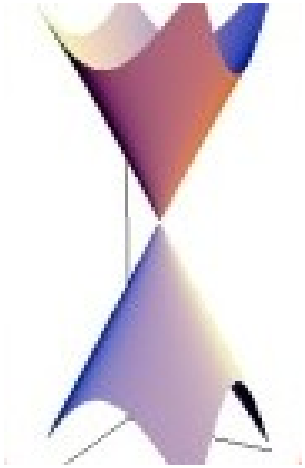
Parabolic bands



Semiconductors, metals

Effective free-electrons

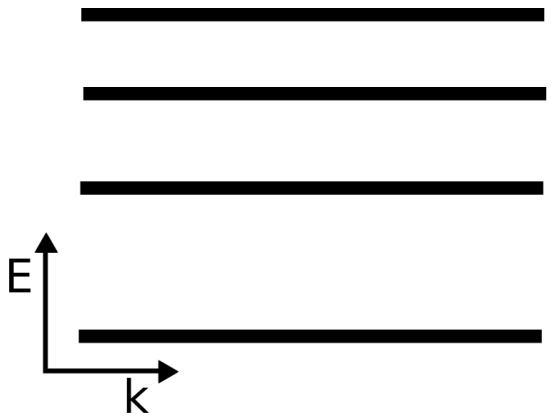
Dirac dispersion



graphene

Topology & relativistic physics

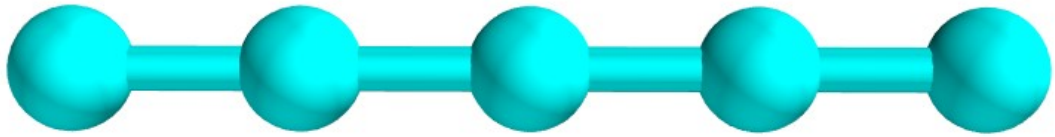
Flat bands



Quantum Hall

Topology & correlations

Parabolic dispersion



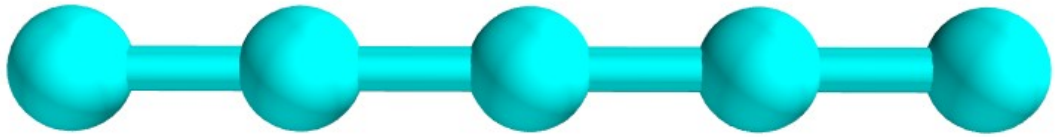
Small k expansion

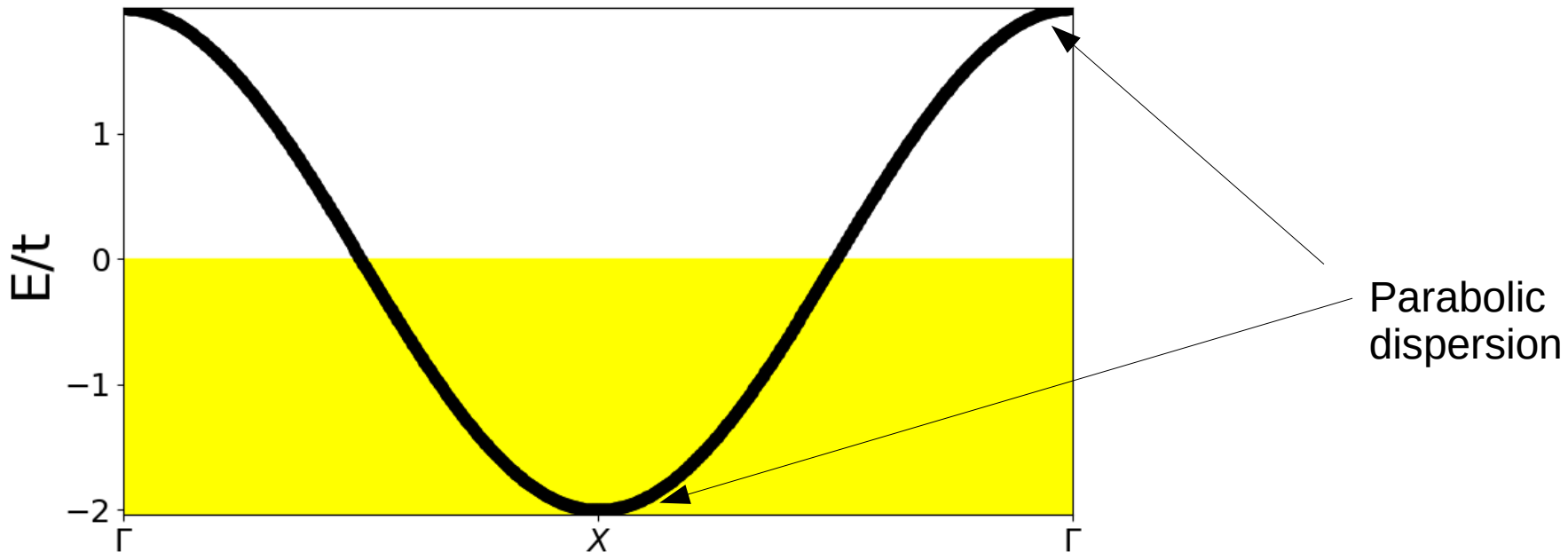
$$\epsilon(k) = 2t\cos ka \approx 2t\left[1 - \frac{k^2a^2}{2}\right]$$

$$\epsilon(k) \sim k^2$$

Conventional parabolic dispersion

Parabolic dispersion





Solving tight binding models

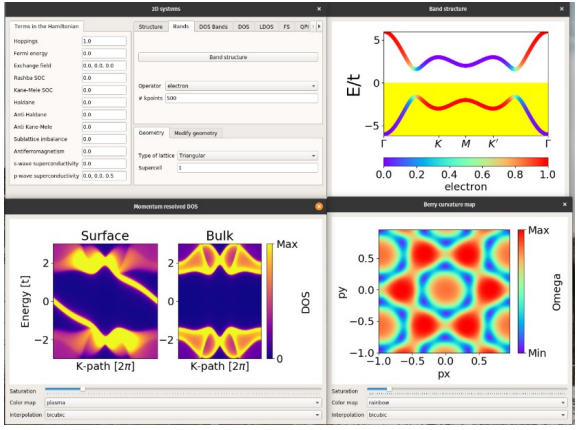
pyqula

```
from pyqula import geometry
g = geometry.honeycomb_lattice()
h = g.get_hamiltonian()
h.add_rashba(0.2) # Rashba spin-orbit coupling
h.add_zeeman([0.,0.,0.6]) # Zeeman field
from pyqula import topology
(kx,ky,omega) = h.get_berry_curvature() # compute Berry curvature
c = h.get_chern() # compute the Chern number
```

- Python library
- Ideal for complex models/calculations
- For writing in Python

https://github.com/joselado/pyqula

Quantum-lattice

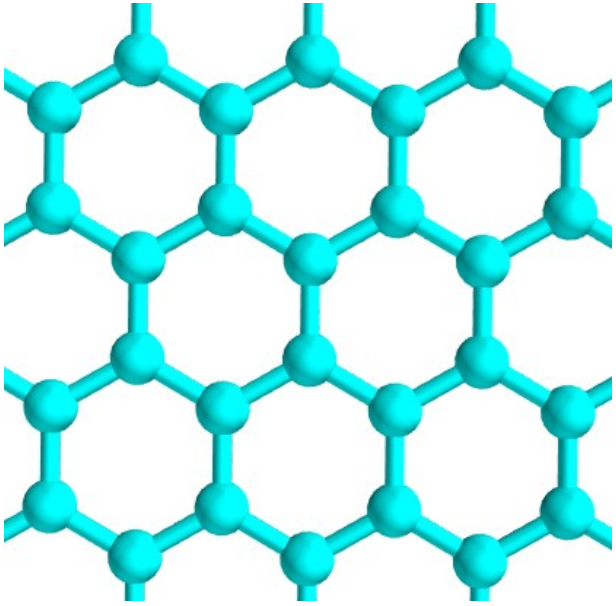


- User-friendly interface for tight binding models
- Ideal for simple models and quick checks
- Fully interface-based, no scripting

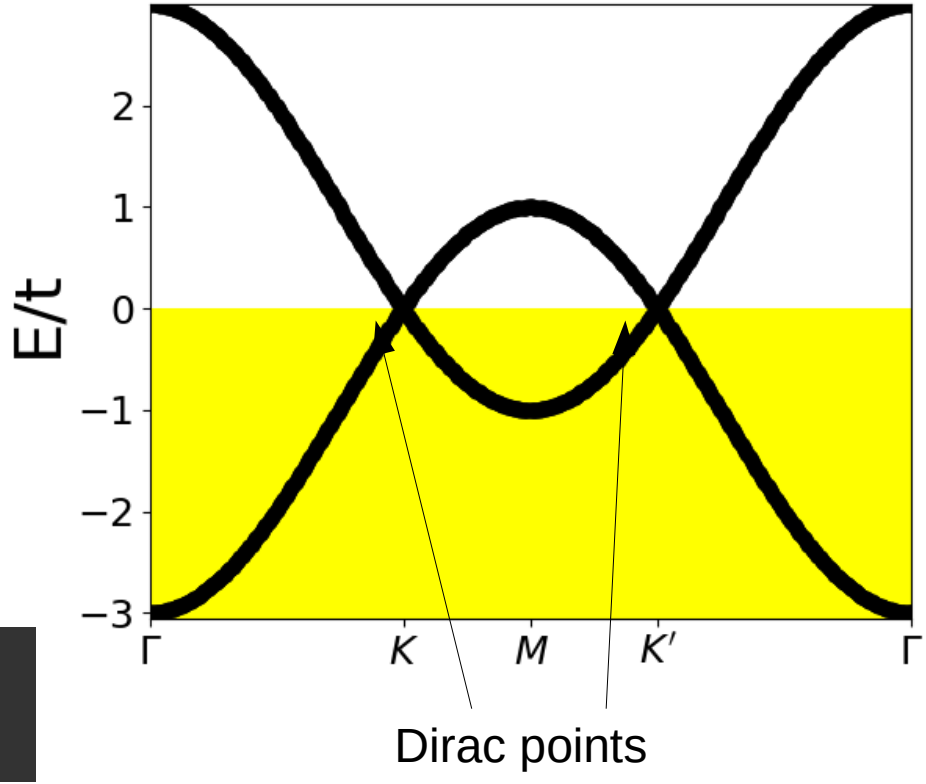
https://github.com/joselado/quantum-lattice

Dirac dispersion

Honeycomb lattice



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



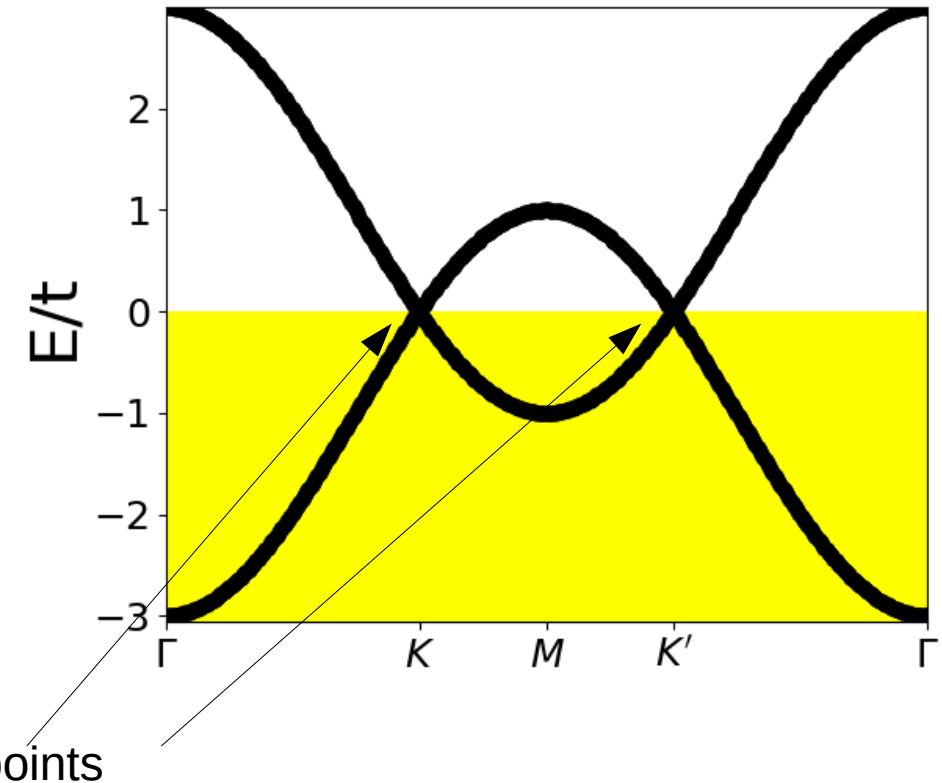
Dirac dispersion

Low energy Hamiltonian at K-points

$$H(k) = \begin{pmatrix} 0 & k_x + ik_y \\ k_x - ik_y & 0 \end{pmatrix}$$

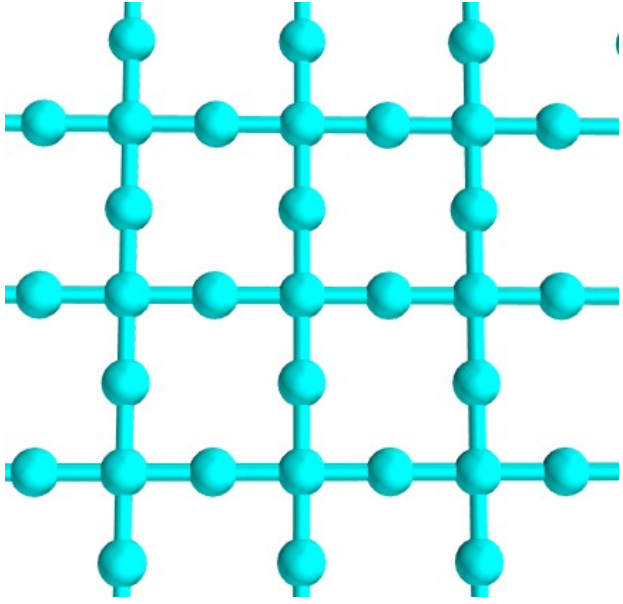
Two-dimensional Dirac equation

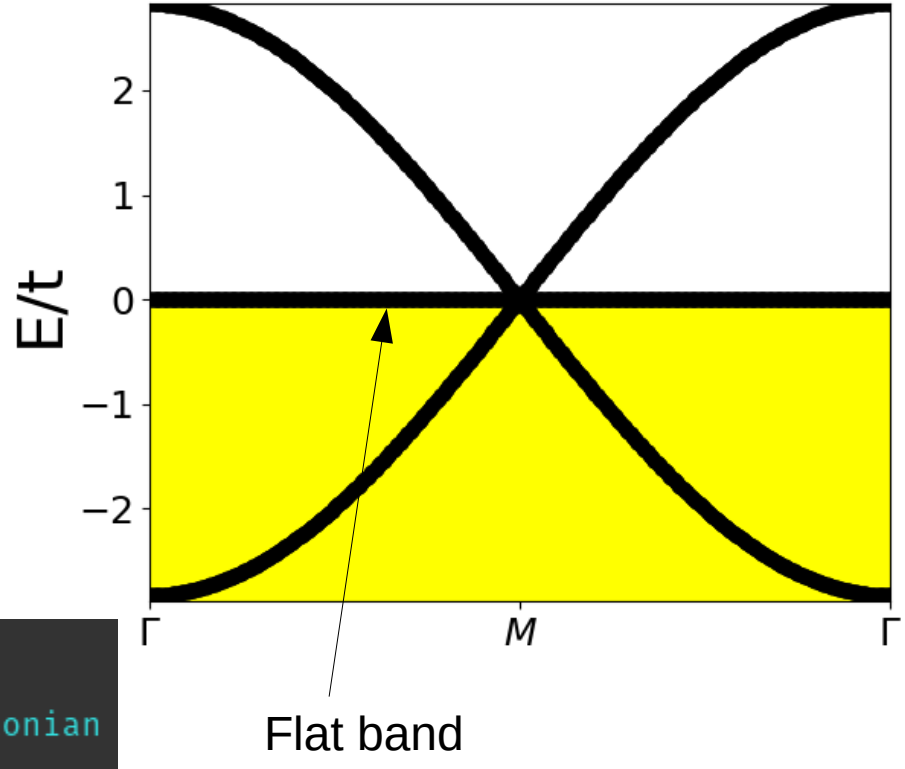
$$\epsilon(k) = \pm\sqrt{k_x^2 + k_y^2}$$



Flat bands

Lieb lattice

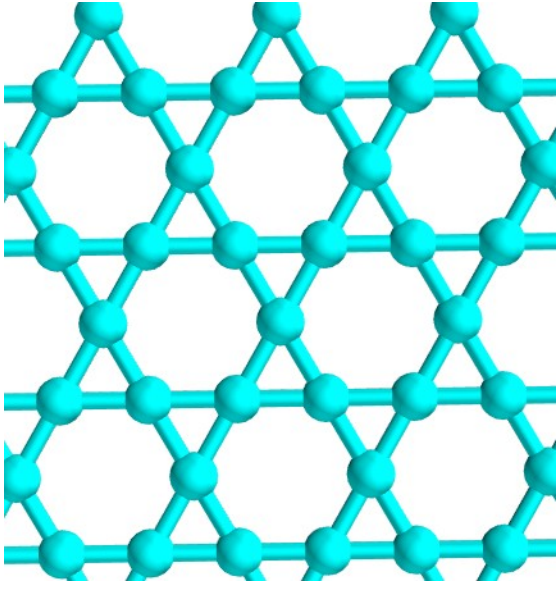




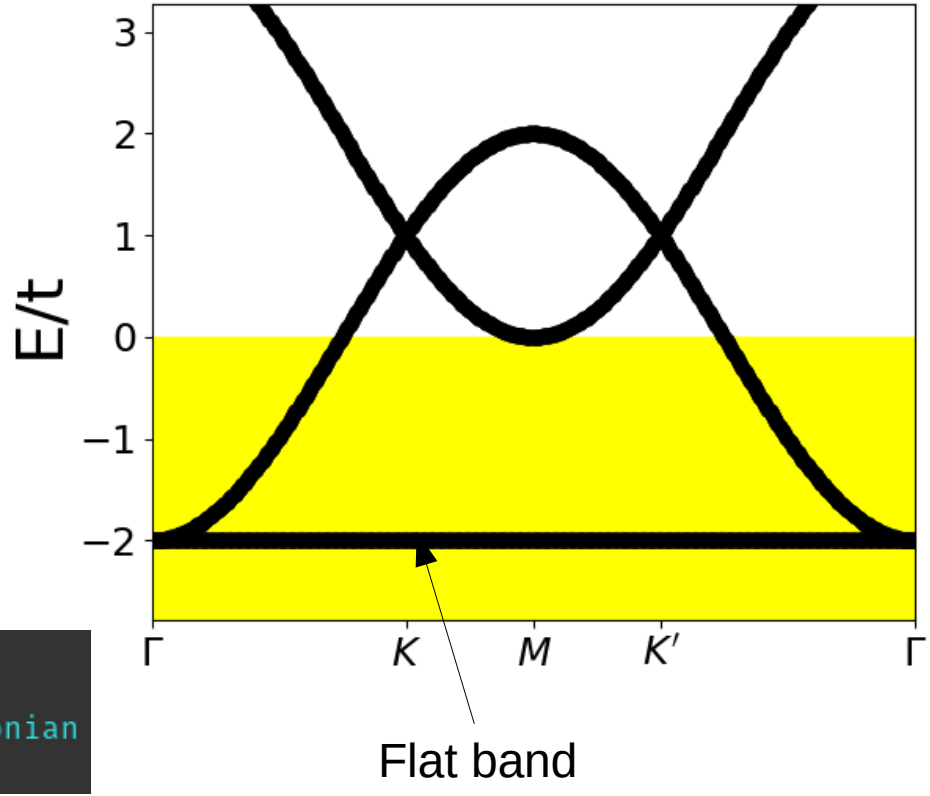

```
from pyqula import geometry
g = geometry.lieb_lattice() # create the lattice
h = g.get_hamiltonian() # get the tight binding Hamiltonian
(k,e) = h.get_bands() # get the band structure
```

Flat bands

Kagome lattice

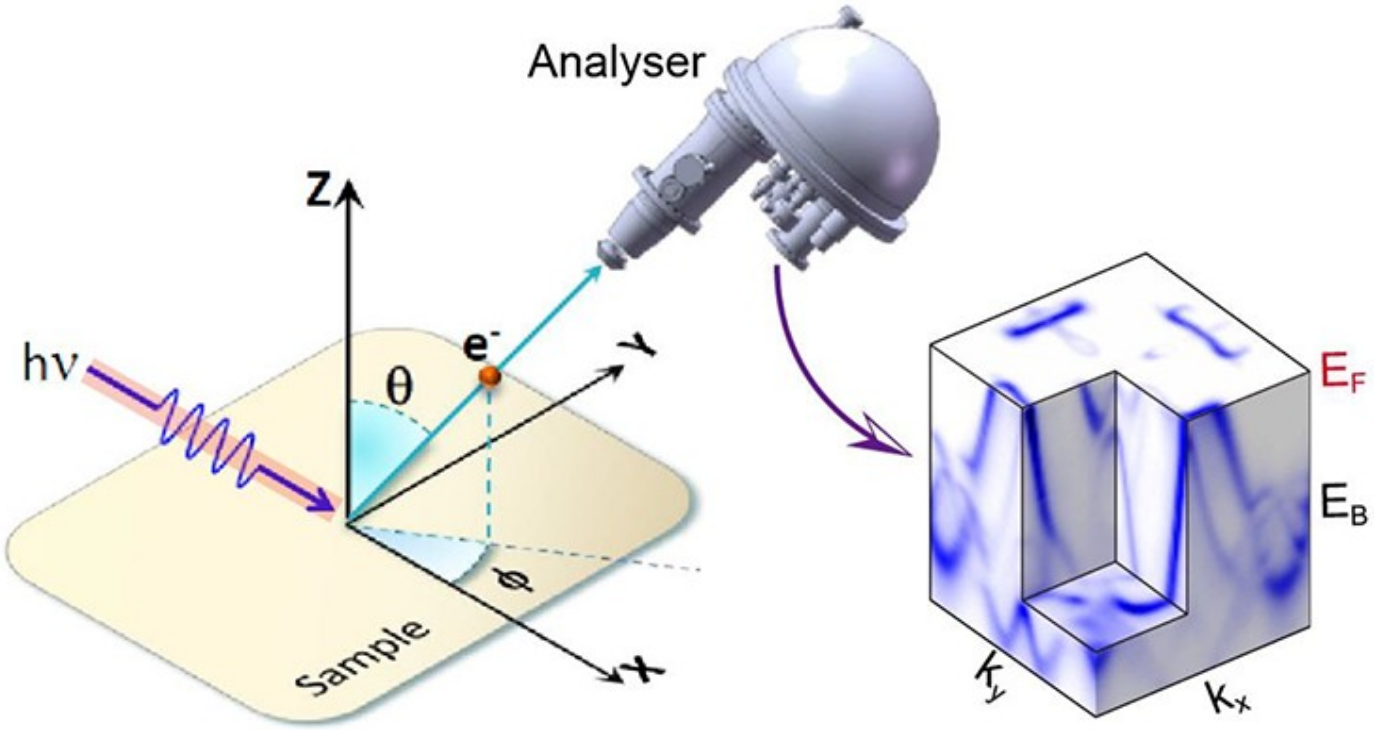


```
from pyqula import geometry
g = geometry.kagome_lattice() # create the lattice
h = g.get_hamiltonian() # get the tight binding Hamiltonian
(k,e) = h.get_bands() # get the band structure
```



Measuring band structures

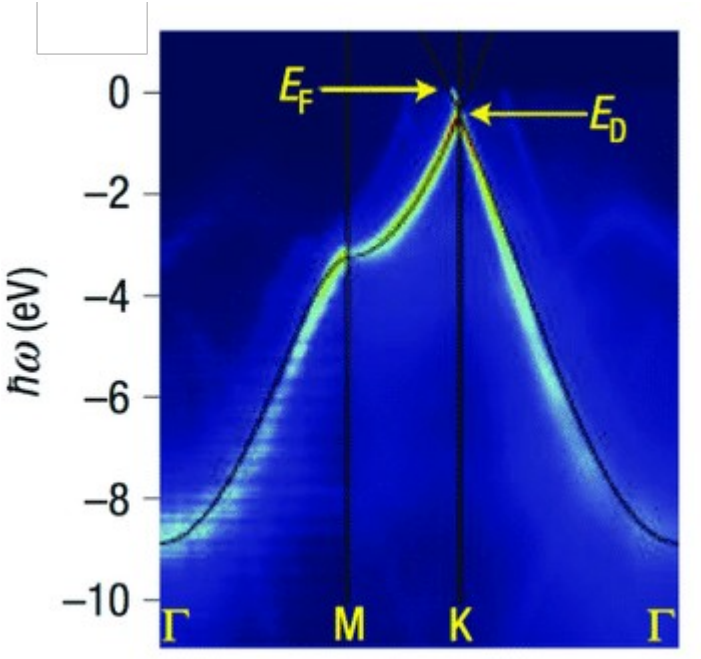
Angle-resolved photoemission spectroscopy



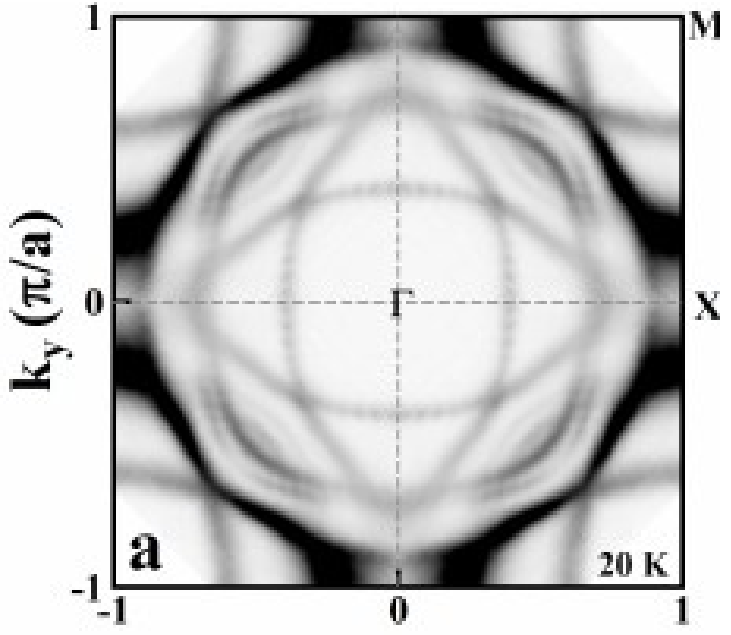
Angle-resolved photoemission spectroscopy (ARPES)

Angle-resolved photoemission spectroscopy

Measuring band-structures with ARPES



Measuring Fermi surfaces with ARPES



Take home

- The spectra of periodic system can be computed with band-structure theory
- The electronic dispersion determines the electronic properties of a compound
- For the next session
  - Submit the exercise of this session by Friday 23:59