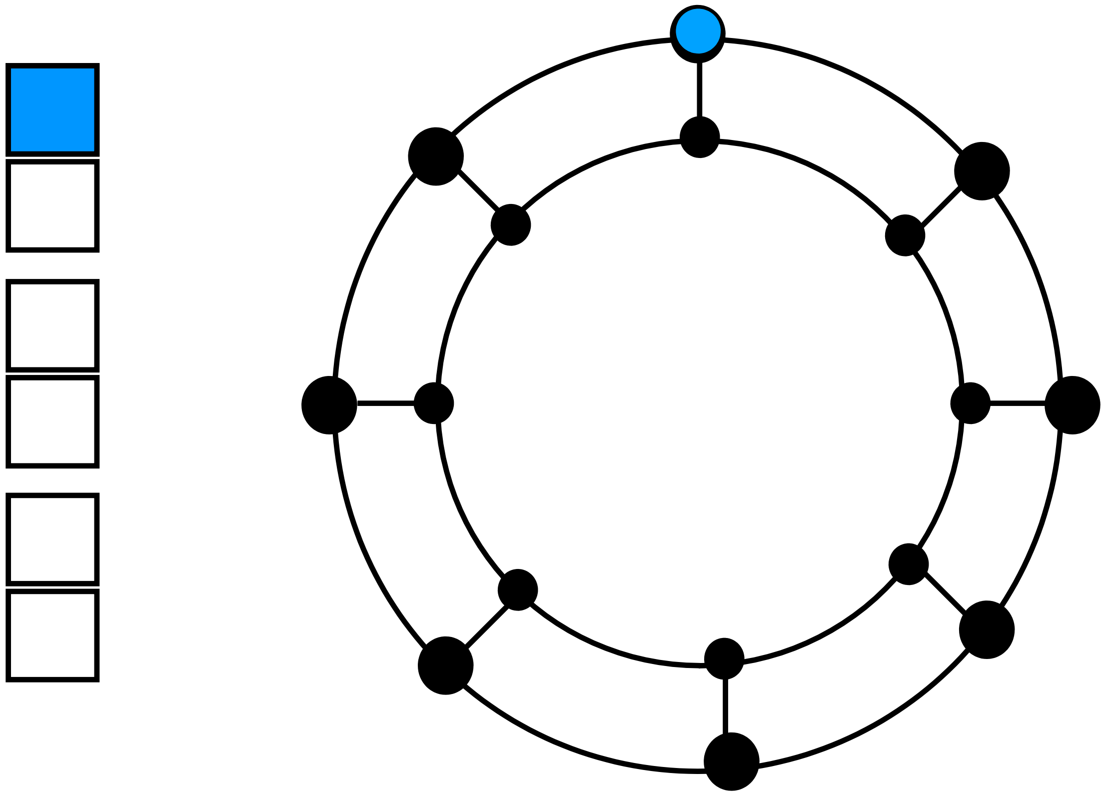
# Example: 1D N-ladder



How to construct basis of an irreducible representation?

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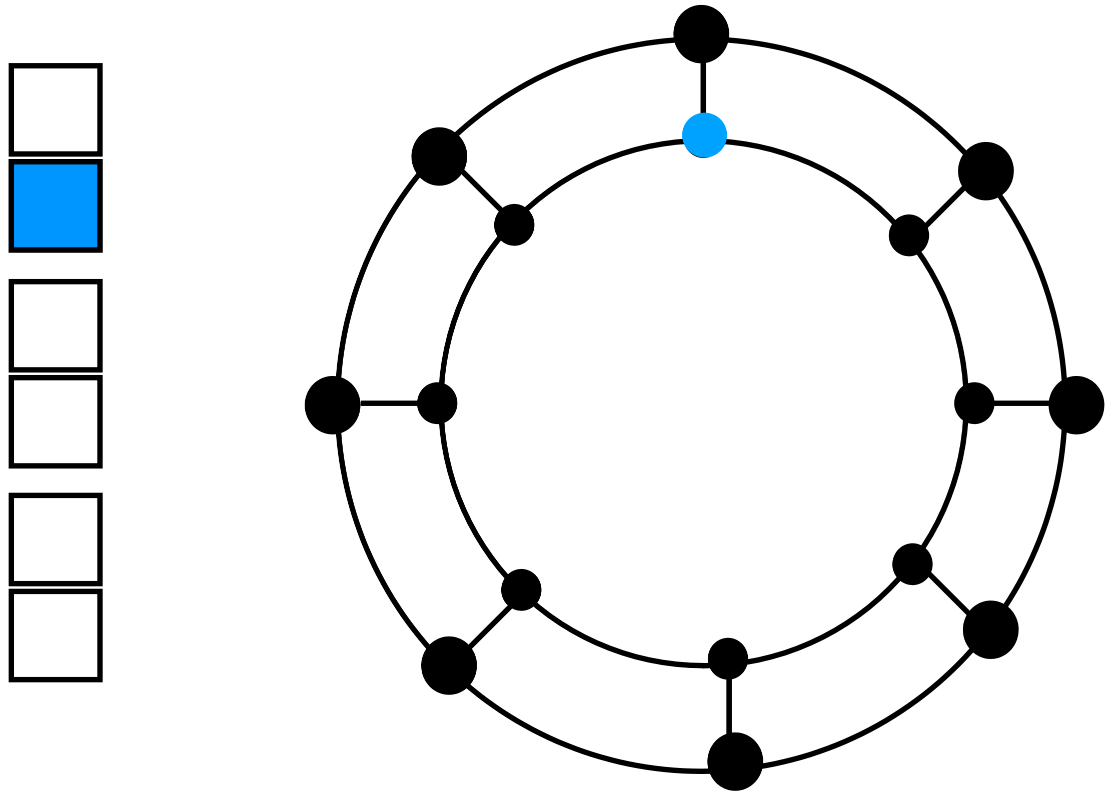

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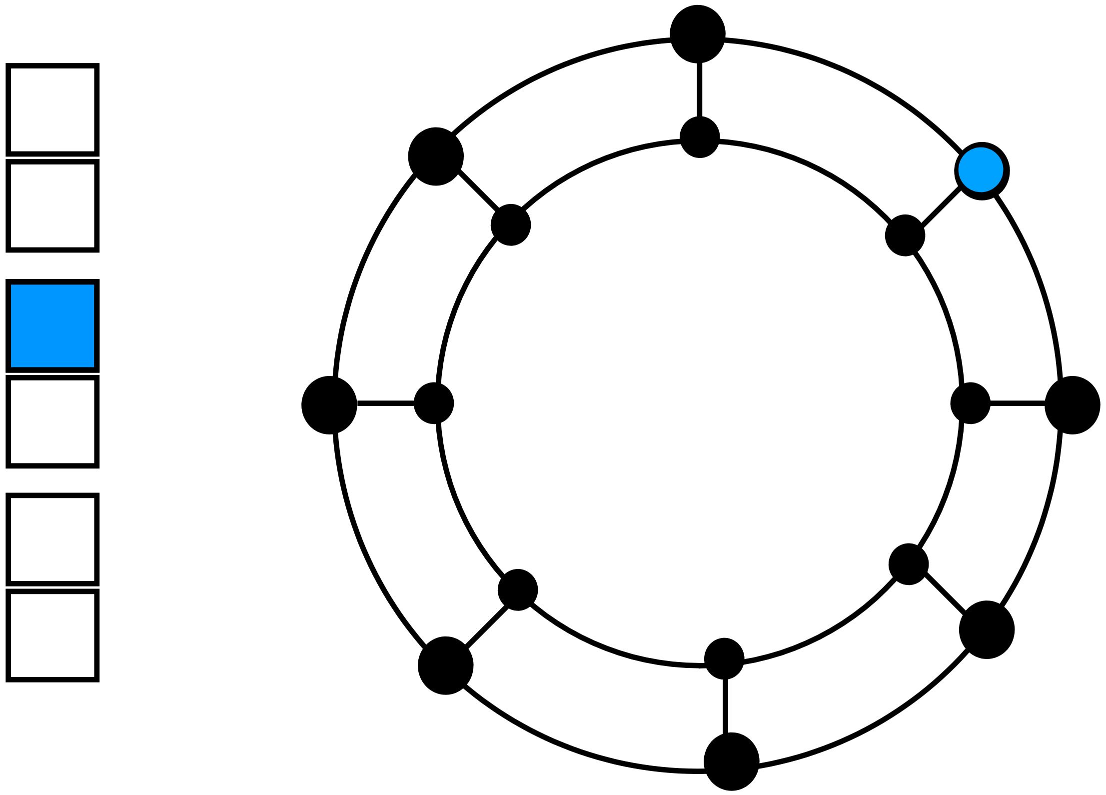

How to construct basis of an irreducible representation?

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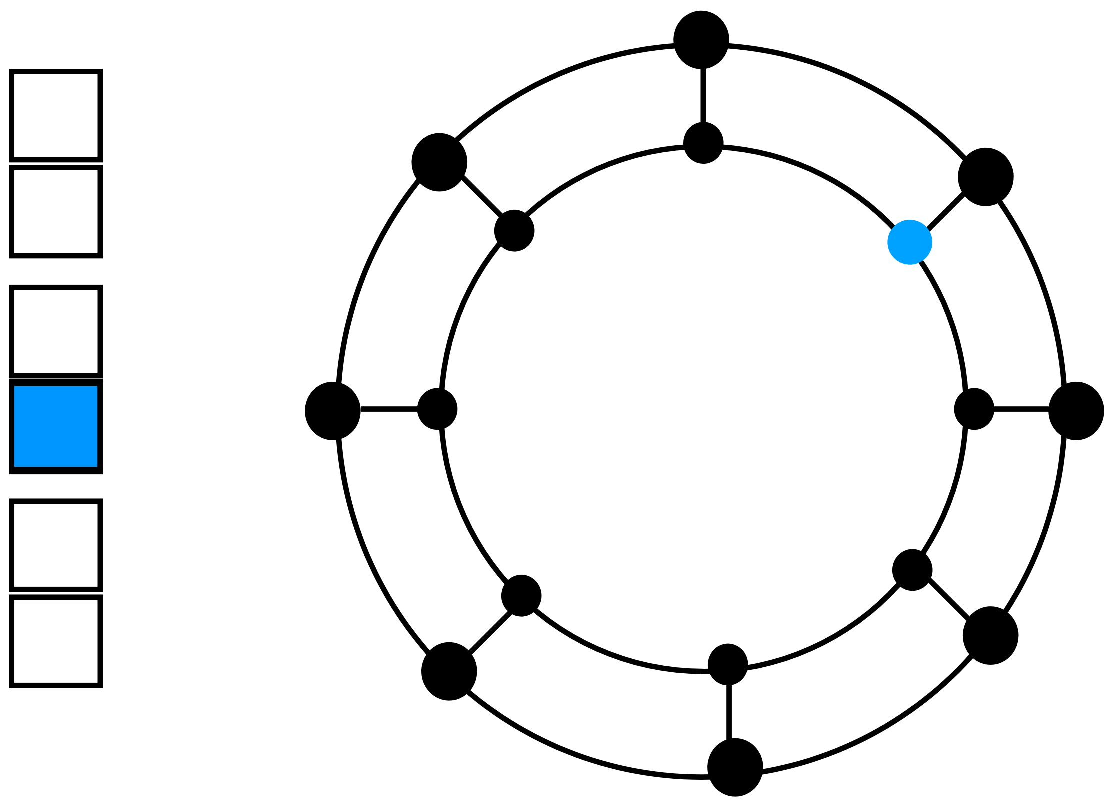

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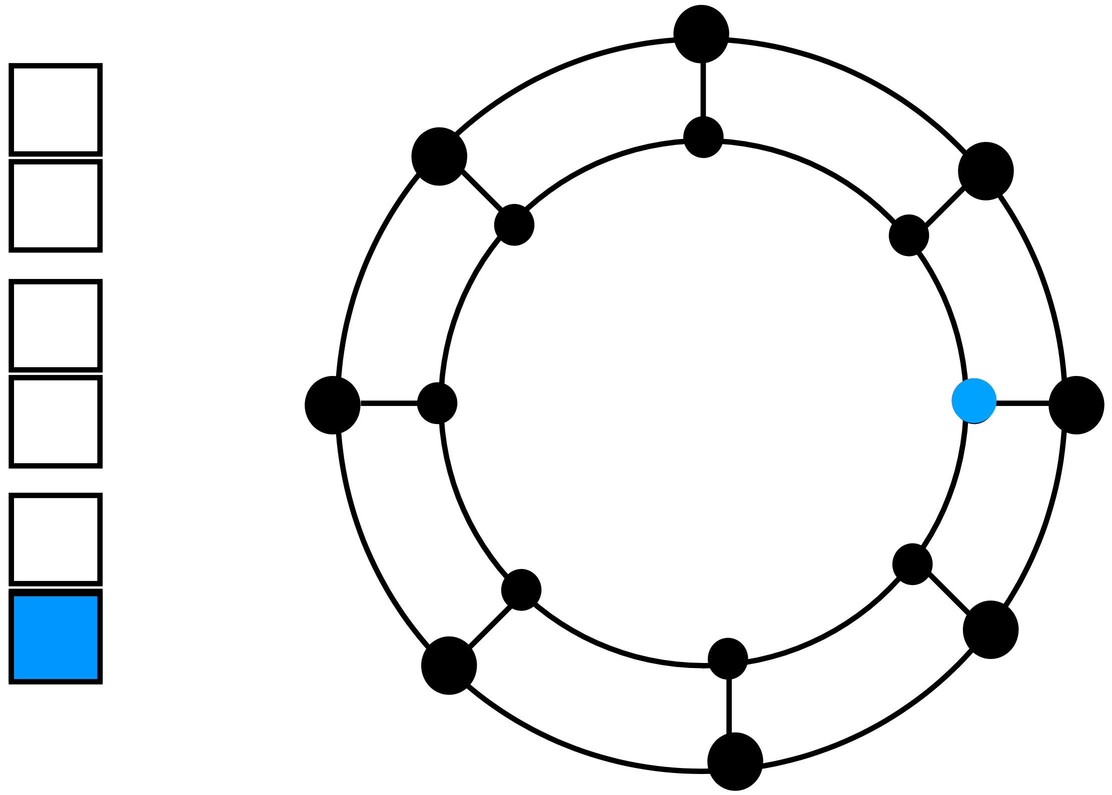

How to construct basis of an irreducible representation?

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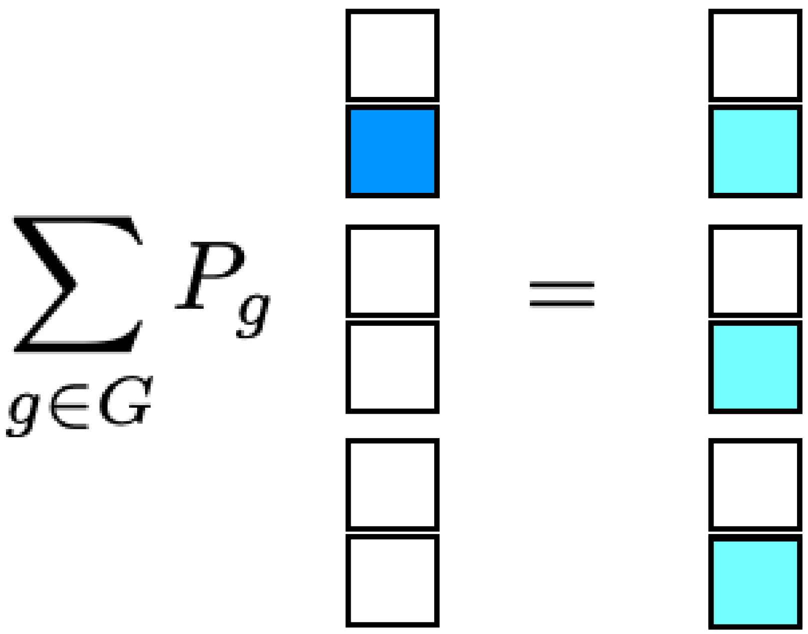
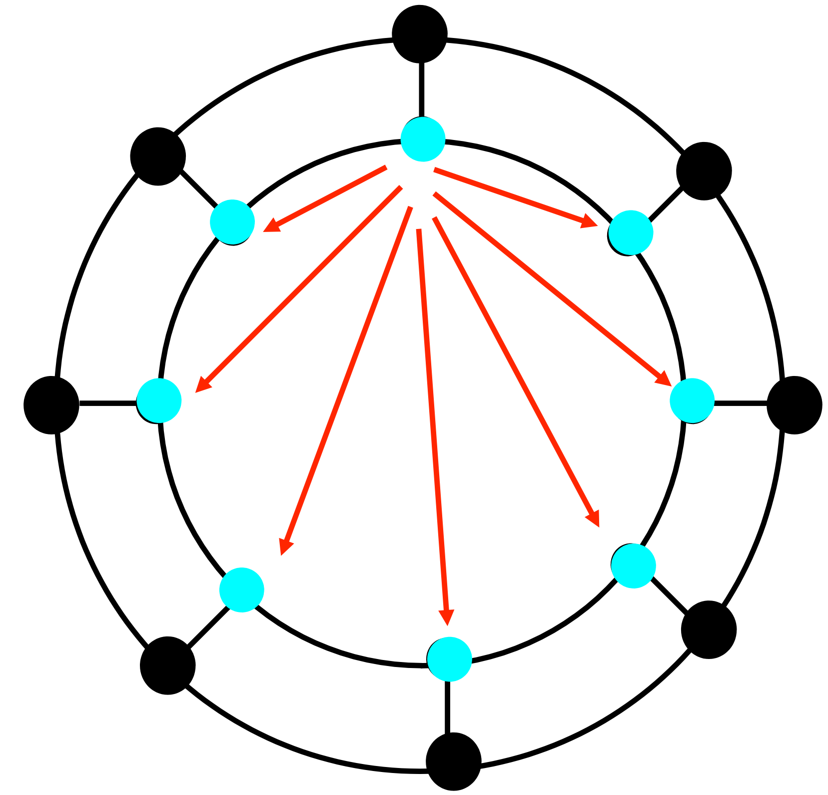


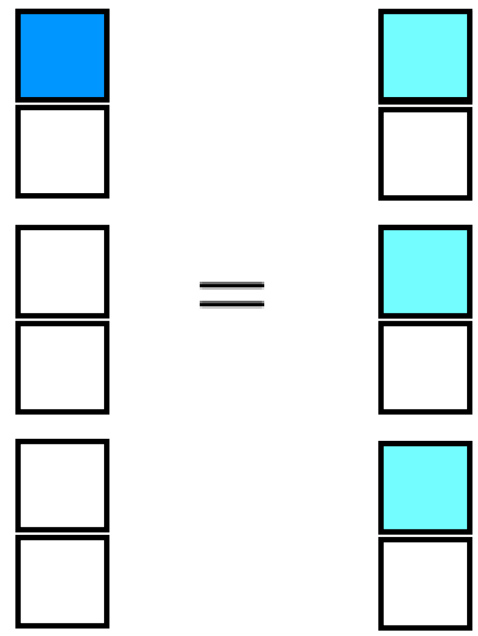



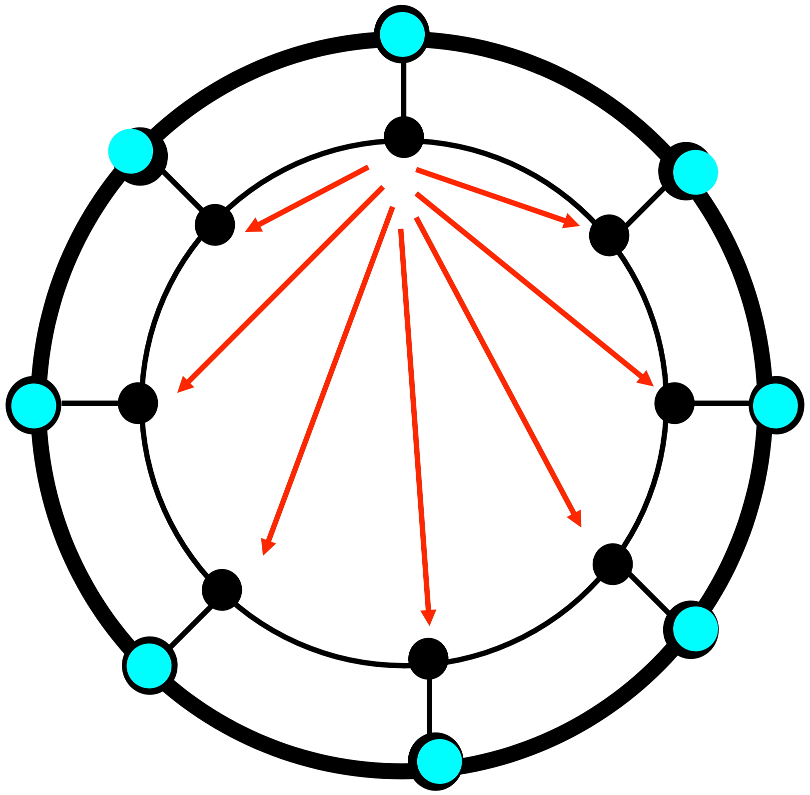
How to construct basis of an irreducible representation?

- Represent group elements (symmetry operations) by linear operators (matrices) in a given Hilbert space
- Select a random vector (seed)
- Apply all symmetry operations on the seed to obtain N vectors (not necessarily linearly independent)
- Form a linear combination with coefficients given by representation theory (tabulated)

# Example: 1D N-ladder

$$\sum_{g\in G} P_g \quad = $$





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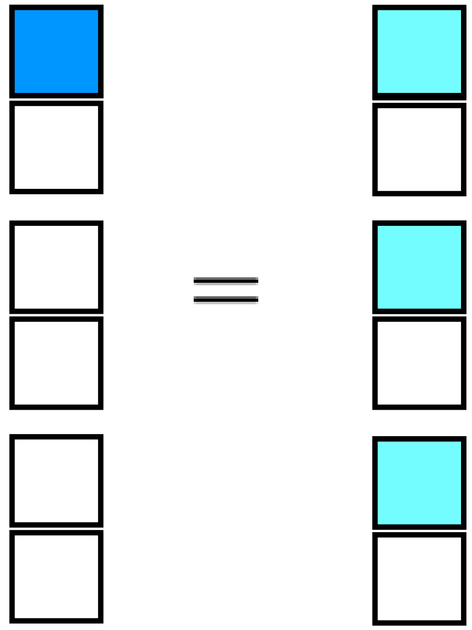
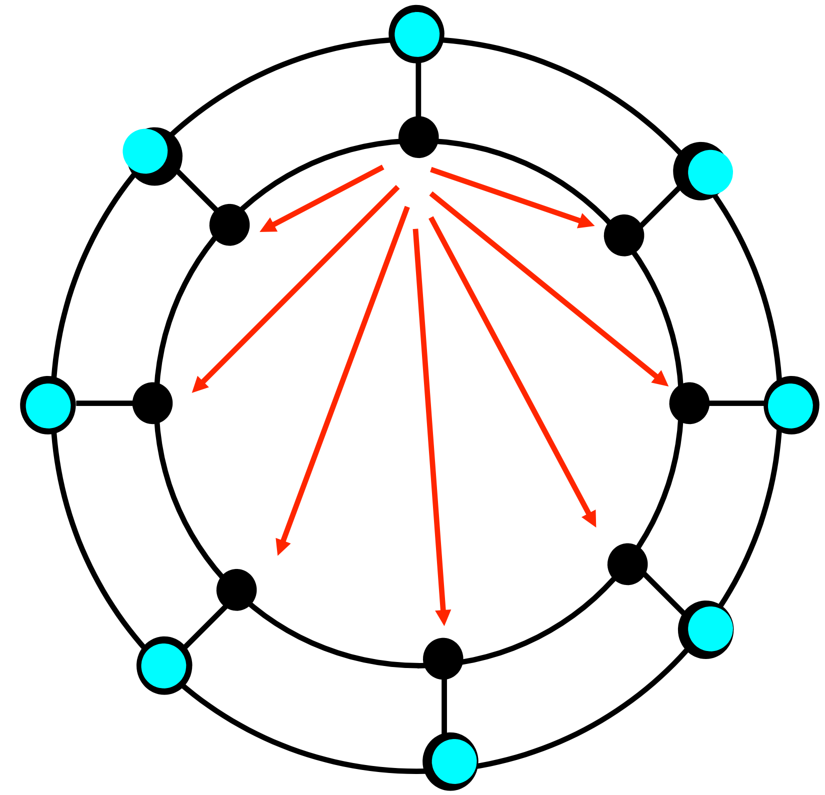
# Example: 1D N-ladder

$$\sum_{g \in G} P_g$$





$$|n\Gamma i\rangle = \sum_{g \in G} a_{\Gamma i}(g) \hat{P}_g |\mathrm{init}_n\rangle$$

General index (chain, principal quantum number)

Irreducible representation (k index, orbital quantum number l)

Column index - only for multi-dimensional representations (non-abelian groups) (magnetic quantum number m)

Symmetry group

Coefficients (do not depend on the studied system); tabulated

Operator representing group element g (rotation, translation)

Random seed vector (orthogonal to the space we have already covered)

# Bloch theorem for lattice models

$$H = \sum_{\mathbf{R}} \sum_{\mathbf{S}} t(\mathbf{S}) c^\dagger_{\mathbf{R}+\mathbf{S}} c_{\mathbf{R}} \qquad\qquad c_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{R}}$$

periodicity

lattice site coincides with the unit cell
(not the most general case)

Unitary transformation (very common trick for periodic systems):

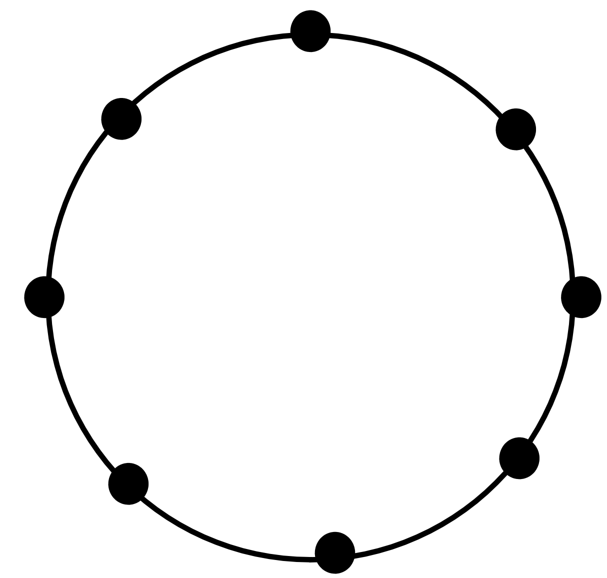
$$c_{\mathbf{R}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{k}}$$

$$H = \frac{1}{N} \sum_{\mathbf{R}} \sum_{\mathbf{S}} \sum_{\mathbf{k},\mathbf{k}'} t(\mathbf{S}) e^{-i\mathbf{k}\cdot(\mathbf{R}+\mathbf{S})} c^\dagger_{\mathbf{k}} e^{i\mathbf{k}'\cdot\mathbf{R}} c_{\mathbf{k}'}$$

$$= \sum_{\mathbf{k},\mathbf{k}'} \underbrace{\left( \frac{1}{N} \sum_{\mathbf{R}} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} \right)}_{\delta_{\mathbf{k}\mathbf{k}'}} \underbrace{\left( \sum_{\mathbf{S}} e^{-i\mathbf{k}\cdot\mathbf{S}} t(\mathbf{S}) \right)}_{t(\mathbf{k})} c^\dagger_{\mathbf{k}} c_{\mathbf{k}'} = \sum_{\mathbf{k}} t(\mathbf{k}) c^\dagger_{\mathbf{k}} c_{\mathbf{k}}$$

# Example: 1D chain with nn hopping

$$H = t\sum_{i=1}^{N-1}\left(c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}\right) + t\left(c_1^\dagger c_N + c_N^\dagger c_1\right)$$



Hopping matrix (Hamiltonian):

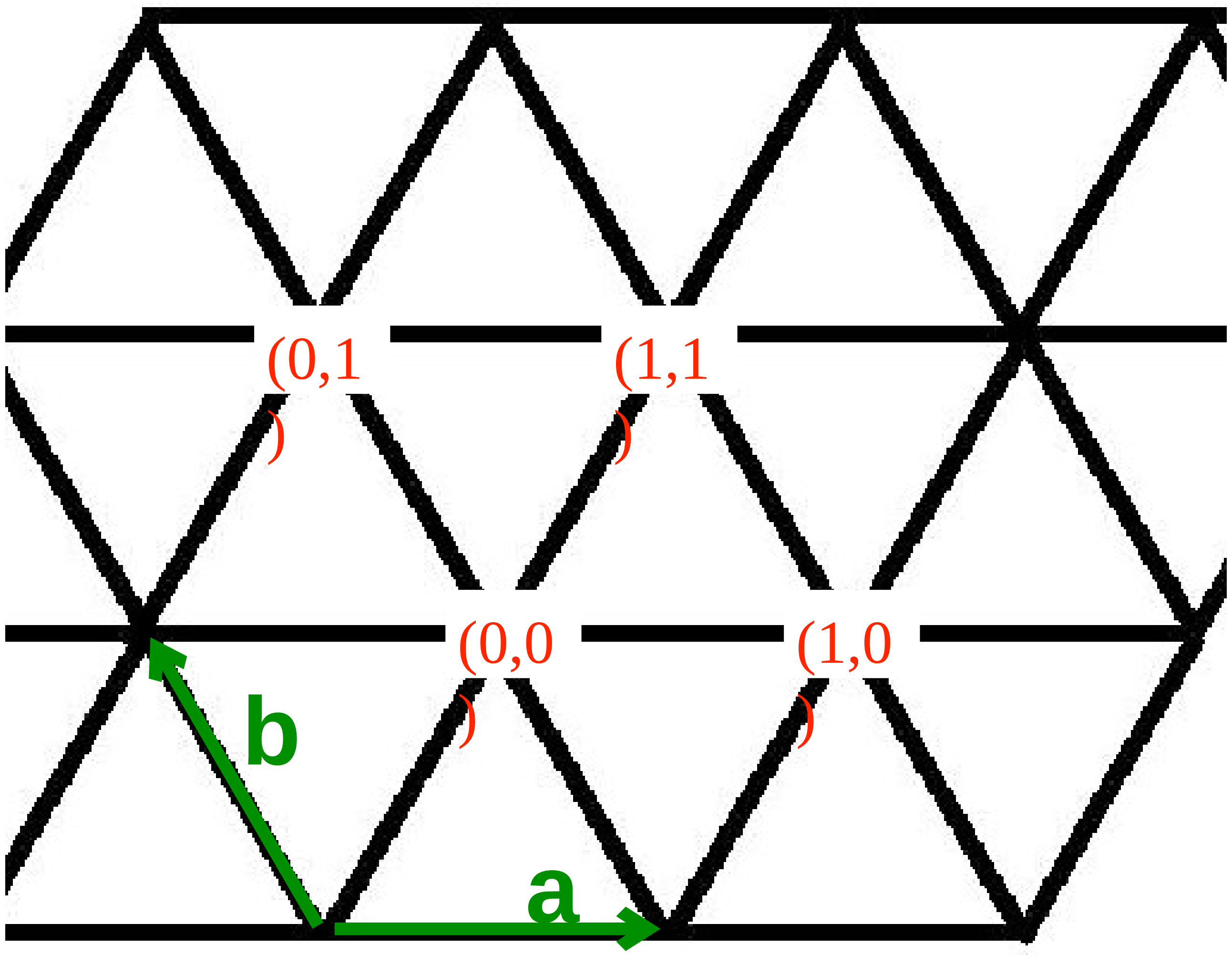
$$h = \begin{pmatrix} 0 & t & 0 & 0 & \dots & 0 & t \\ t & 0 & t & 0 & \dots & 0 & 0 \\ 0 & t & 0 & t & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & t \\ t & 0 & 0 & 0 & \dots & t & 0 \end{pmatrix}$$

Dispersion:

$$t(k) = 2t\cos(\frac{2\pi}{N}k), \quad k = 0, 1, \dots, N-1$$

*Diagonalize h directly for N=3. What eigenstates do you get?*
*Generalize the problem for square and cubic lattices.*

# Example: Triangular lattice

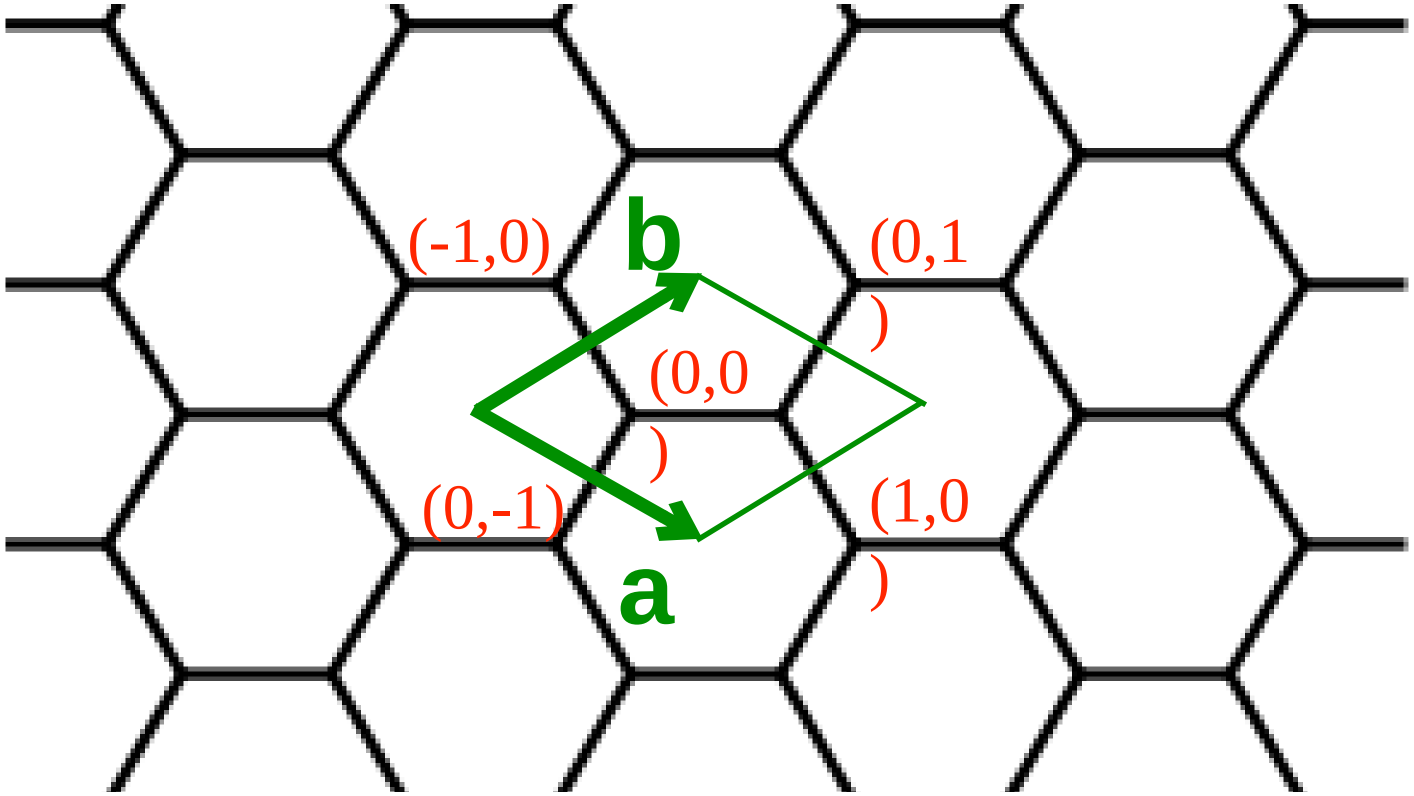



$$H = t\sum_{\mathbf{R}}\left(c^\dagger_{\mathbf{R}+(1,0)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,1)}c_{\mathbf{R}} + H.c.\right)$$

After FT:

$$t(k_a, k_b) = 2t\left(\cos(k_a) + \cos(k_b) + \cos(k_a + k_b)\right)\,, \quad k_{a[b]} \in \langle 0, 2\pi)$$

# Example: Honeycomb lattice




$$H = t\sum_{\mathbf{R}}\left(c^\dagger_{\mathbf{R}}d_{\mathbf{R}} + d^\dagger_{\mathbf{R}}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,0)}d_{\mathbf{R}} + d^\dagger_{\mathbf{R}+(-1,0)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)}d_{\mathbf{R}} + d^\dagger_{\mathbf{R}+(0,-1)}c_{\mathbf{R}}\right)$$

After FT:

$$H = t\sum_{k_a,k_b}(1 + e^{ik_a} + e^{ik_b})c^\dagger_{\mathbf{k}}d_{\mathbf{k}} + h.c.$$

# Example: Honeycomb lattice

$$H = t\sum_{\mathbf{R}} \left( c^\dagger_{\mathbf{R}} d_{\mathbf{R}} + d^\dagger_{\mathbf{R}} c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,0)} d_{\mathbf{R}} + d^\dagger_{\mathbf{R}+(-1,0)} c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)} d_{\mathbf{R}} + d^\dagger_{\mathbf{R}+(0,-1)} c_{\mathbf{R}} \right)$$

After FT:

$$H = t\sum_{k_a,k_b} (1 + e^{ik_a} + e^{ik_b}) c^\dagger_{\mathbf{k}} d_{\mathbf{k}} + h.c.$$

At each k-point $\mathbf{k}=(k_a,k_b)$ we have a 2x2 matrix to diagonalize:

$$h(k_a,k_b) = \begin{pmatrix} 0 & 1 + e^{ik_a} + e^{ik_b} \\ 1 + e^{-ik_a} + e^{-ik_b} & 0 \end{pmatrix}$$

Finally we get the dispersion relation:

$$\epsilon(\mathbf{k}) = \pm\sqrt{3 + 2\left(\cos(k_a) + \cos(k_b) + \cos(k_a + k_b)\right)}$$

# Example: Honeycomb lattice

$$H = t\sum_{\mathbf{R}} \left( c^\dagger_{\mathbf{R}} d_{\mathbf{R}} + d^\dagger_{\mathbf{R}} c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,0)} d_{\mathbf{R}} + d^\dagger_{\mathbf{R}+(-1,0)} c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)} d_{\mathbf{R}} + d^\dagger_{\mathbf{R}+(0,-1)} c_{\mathbf{R}} \right)$$

After FT:

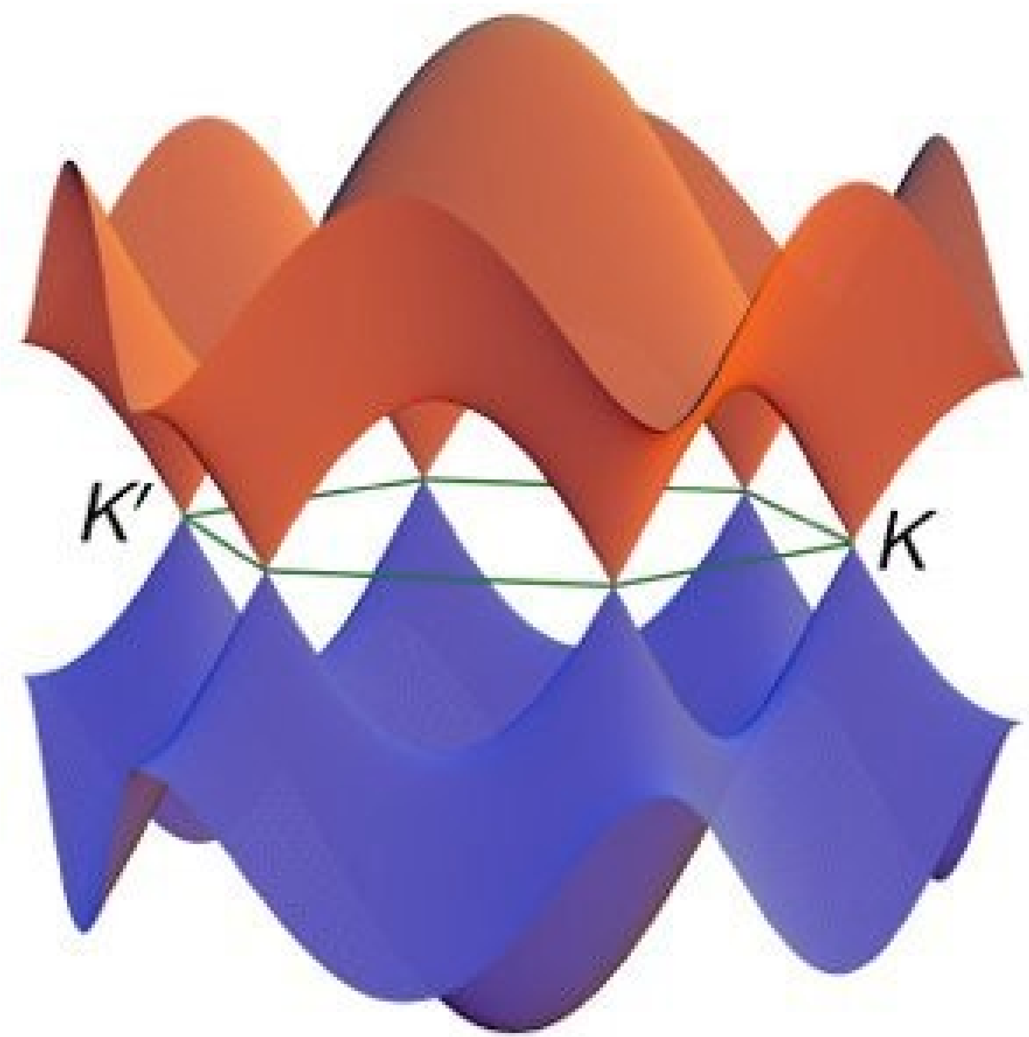
$H = t \sum_{k_a,k_b} ($

At each k-p

$h(k_a, k_b) =$

Finally we

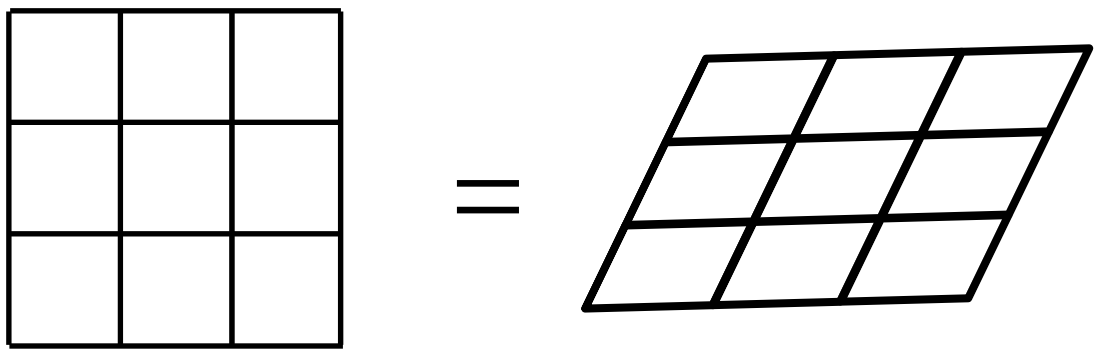
$\epsilon(\mathbf{k}) =$



# Geometrical meaning of k-vector

Observation:

The parameters **k**=($k_a$,$k_b$,…) look like a vector, **k**.**R** looks like a scalar product, but **we did not specify any angles**.



The relationship of k-space and R-space is that of duality.

The R-lattice defines a reciprocal G-lattice.
The k-vectors studied so far span a unit cell of the G-lattice.

Unit cell volume: $\Omega = |\mathbf{a}.(\mathbf{b}\times\mathbf{c})|$

G-basis vectors: $\mathbf{G}_a = 2\pi\frac{\mathbf{b}\times\mathbf{c}}{\Omega}$ $\quad \mathbf{G}_b = 2\pi\frac{\mathbf{c}\times\mathbf{a}}{\Omega}$ $\quad \mathbf{G}_c = 2\pi\frac{\mathbf{a}\times\mathbf{b}}{\Omega}$

Remarks:

- $\mathbf{G}_a$ is perpendicular to all basis vector except **a** and scales as 1/|**a**|
- For orthogonal basis $\mathbf{G}_a$ is parallel to **a** and has the length 2π/|**a**|

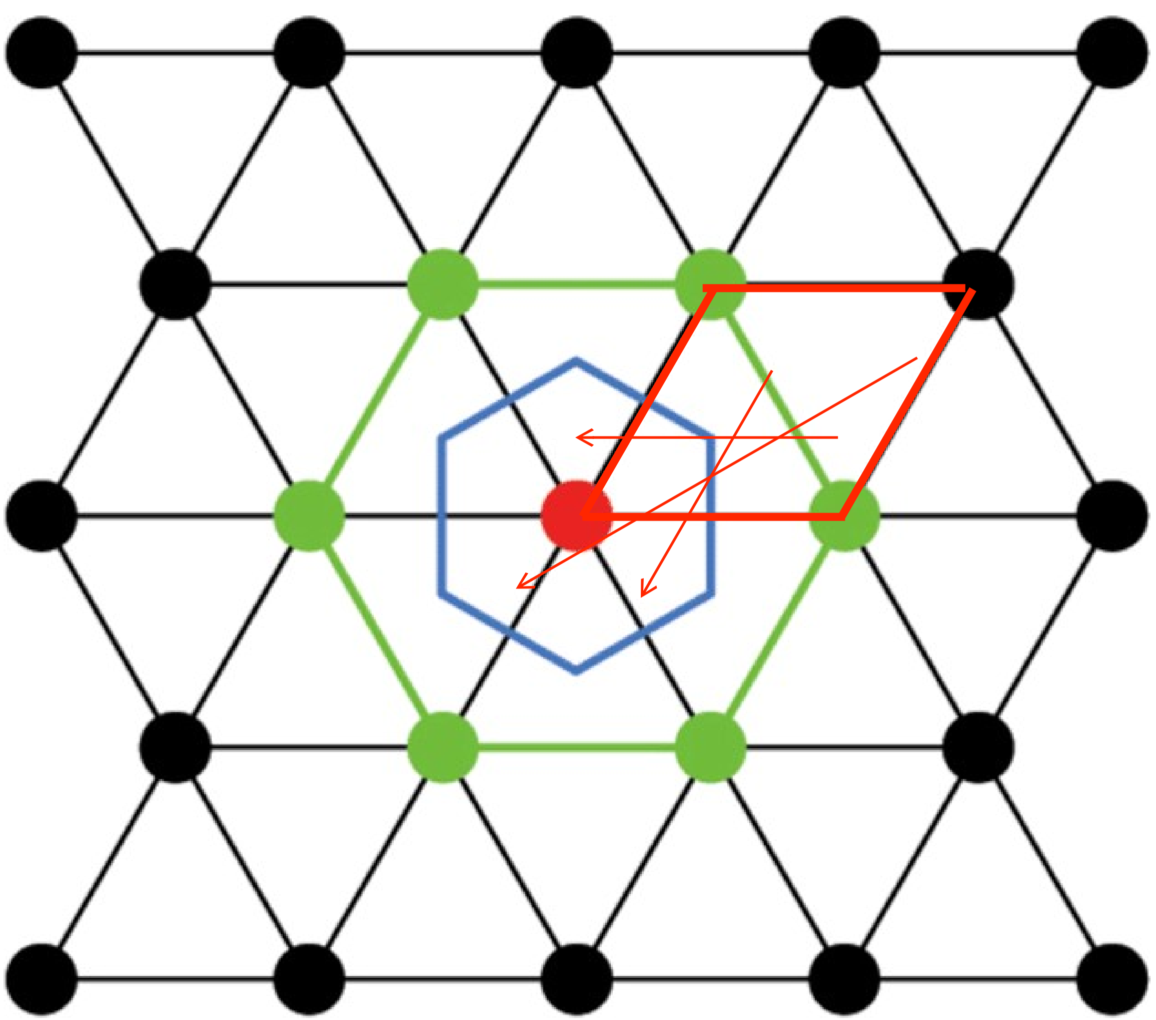
$\exp(i\mathbf{G}.\mathbf{R}) = 1$

# 1st Brillouin zone

Observation:

The vectors **k** and **k+G** are equivalent (give the same Bloch state)

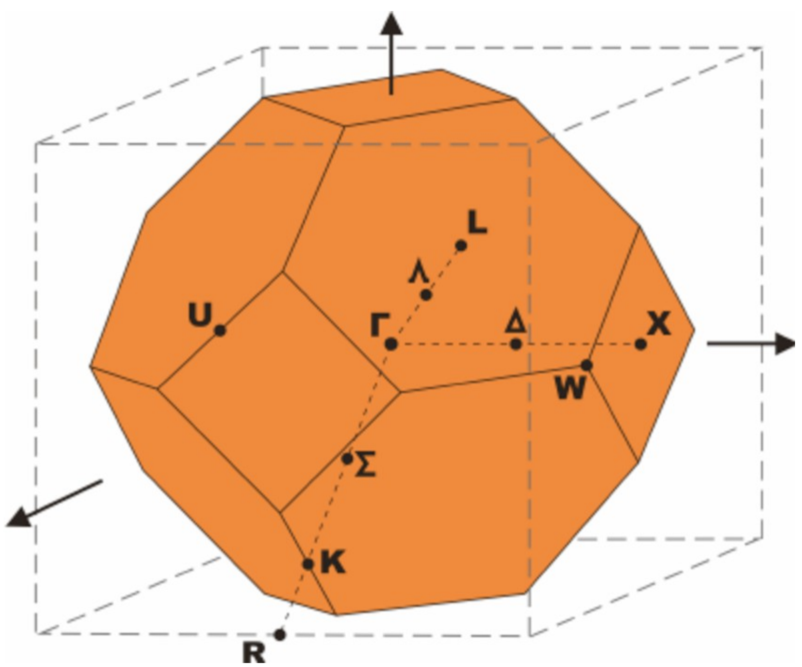
=> we do not have to use the primitive cell in the k-space (as long as we span the same set of inequivalent k-vectors)



- Woronoi cell of the G-lattice
- one-to-one mapping to primitive cell
- respects point symmetry of the lattice
- standard notation for special points

(solid state codes usually have automated routines, e.g. xcrysden)

Example:
fcc Brillouin zone



$$T_R : \mathbf{r} \rightarrow R\mathbf{r}$$
$$T_R f(\mathbf{r}) = f(R^{-1}\mathbf{r})$$