# Crystallography and lattice Wannier functions in ABINIT

# CRYSTALLOGRAPHY

mainly **pre-processing tools**

**Crystal structure** = **Unit cell** + **Symmetry** + **Atomic positions**

***check primitivity***

**all symmetries** ⇄ **all atoms**

**space group** **asymmetric atoms**

# space groups

"International tables for crystallography"

Space group number (*spgroup*) 1 .. 230

Bravais lattice (*brvltt*) P,F,I,A,B,C,R

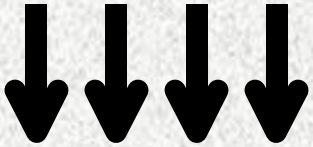
Axis orientation (spgaxor) → Hexagonal/Rhombohedral

→ abc-cab-bca-acb-bac-cba

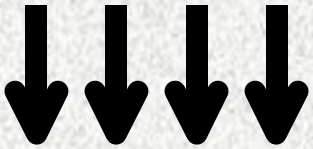
Axis origin (spgorig) 1/2

# symmetry recognition

**structural data: ALL atoms + lattice parameters**



**compute ALL Symmetries**



**space group**

**point group**

# magnetic space groups


**230 space groups**

**Shubnikov**

**I** 230 non-colored groups
**II** 230 gray groups
**III** **674 colored black/white groups**
**IV** **517 colored black/white groups**

**32 point groups**

32+32+**52** **point groups**

# magnetic space groups

1/2 symmetry operations B - B
1/2 symmetry operations B - W

**use the previous generators + magnetic generators**

$$\{R|t\}\ S = \left\{ \begin{array}{ccc|c} R_{11} & R_{12} & R_{13} & t_1 \\ R_{21} & R_{22} & R_{23} & t_2 \\ R_{31} & R_{32} & R_{33} & t_3 \end{array} \right\} \{B/W\}$$

# miscellaneous

Determination of the wave vector symmetry group

{R|t} leaving invariant q

symmetrize the dynamical matrix D

Symmetrization of the stresses (relaxations)

Check of the translation group

# future work

**non-magnetic space groups :**

improve generators

**magnetic space groups :**

further testing + improvements

automatic recognition

**CRYSTALLOGRAPHIC LIBRARY**

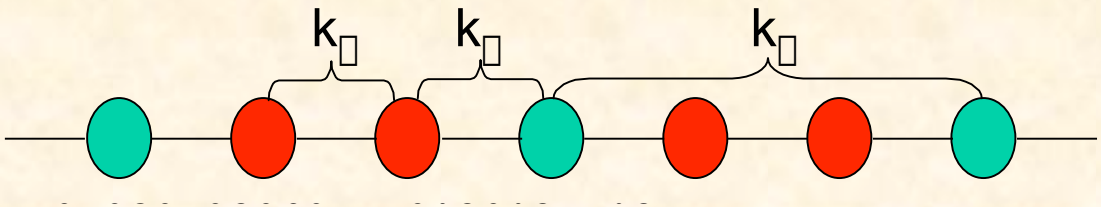
# LATTICE WANNIER FUNCTIONS

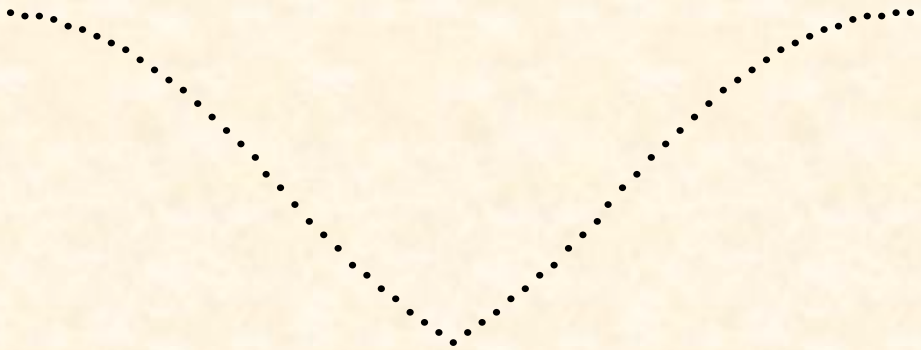
$$w_{nR}(r) = V \int_{BZ} e^{-iqR} \psi_{nq} dq$$

maximally localized LWF

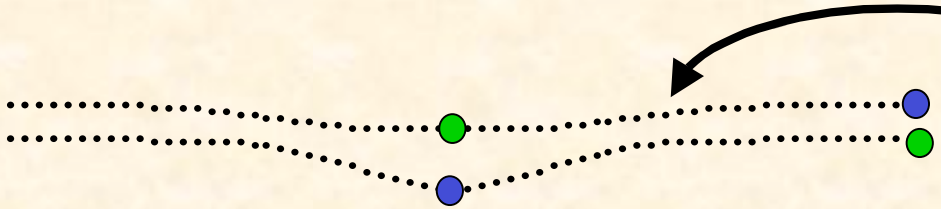
iterative procedure :
interpolation of a certain group of bands
by maximizing the overlap between neighbouring q points

strict symmetry constraints
atomic displacement pattern



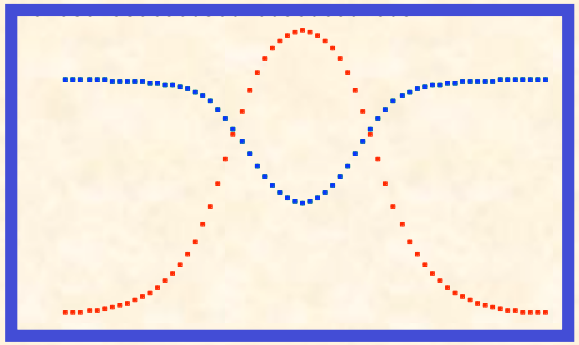



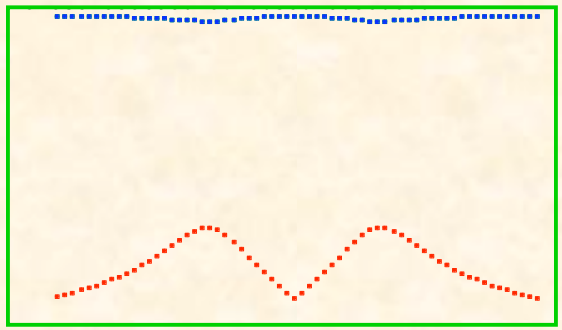
$k_{\square}$ = 0.4
$k_{\square}$ = 0.1
$k_{\square}$ = -1.0

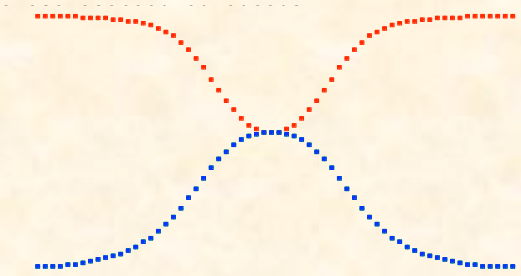


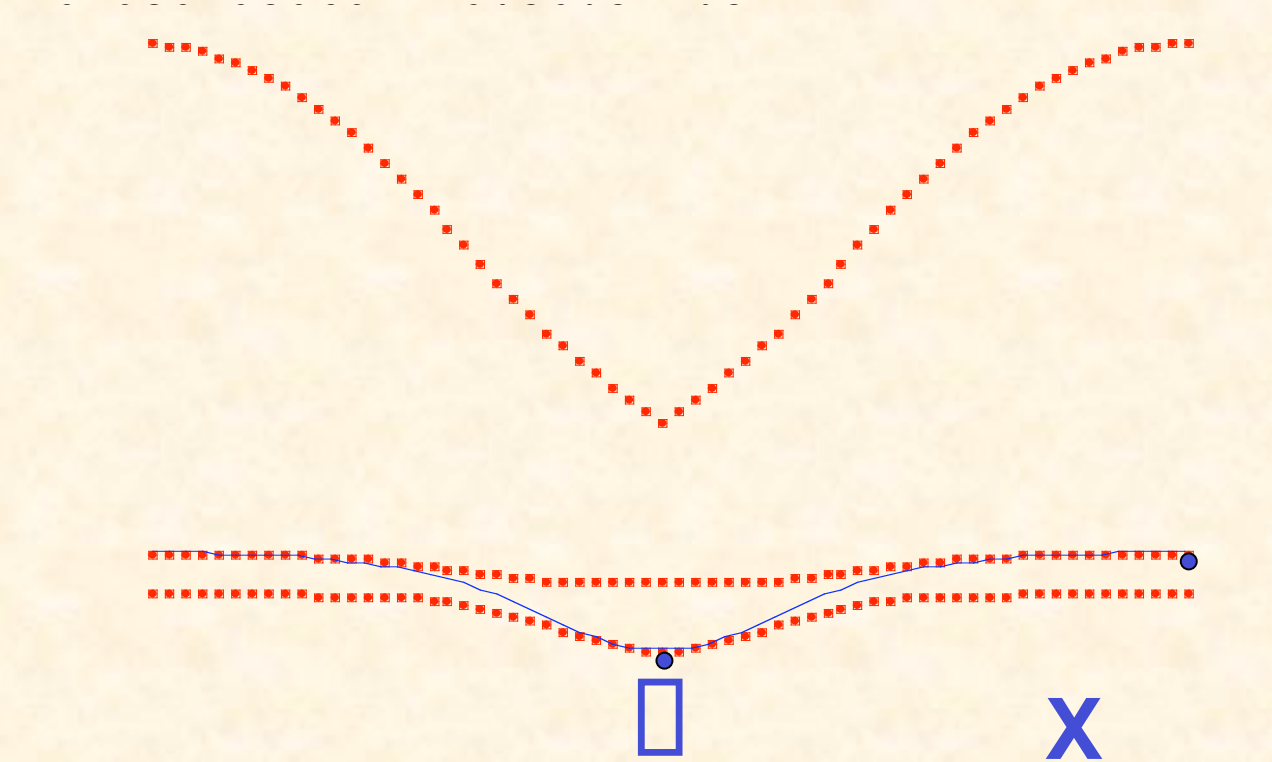
avoided crossing

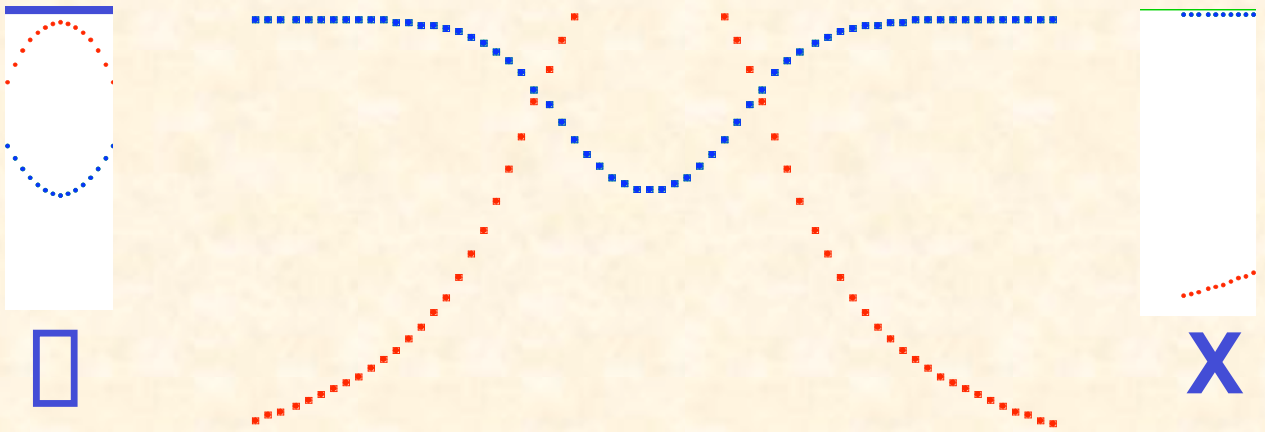
x □ x



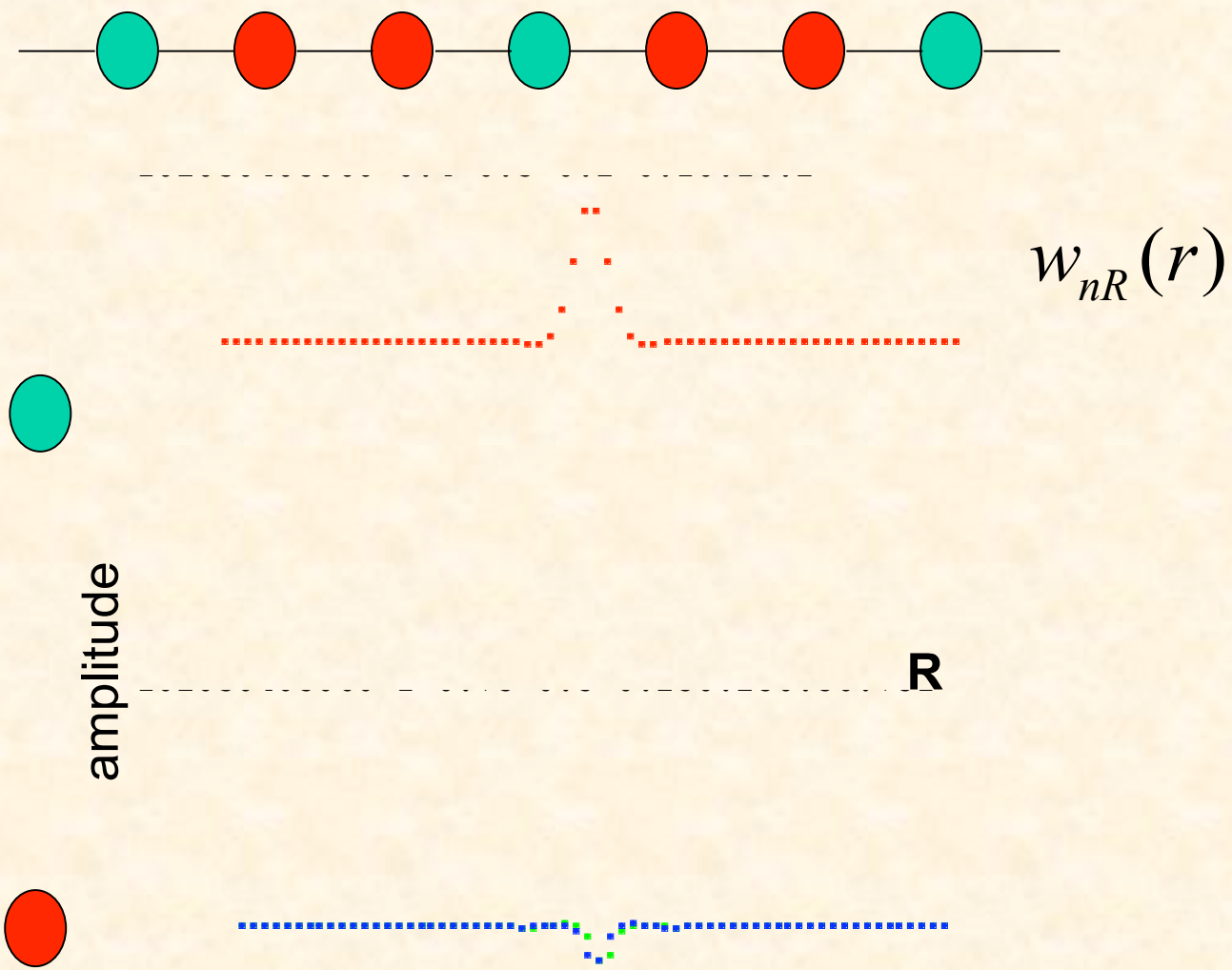








the lattice Wannier function:



# in ABINIT :

# lwf

## DEBUGGING stage

special features:

energy window of frozen states

future development

transformation to *regions* of frozen states of the BZ
*pinning* of the $\Omega_{nq}$ to general or high-symmetry points