



Center for Molecular Modeling

Computational Materials Physics



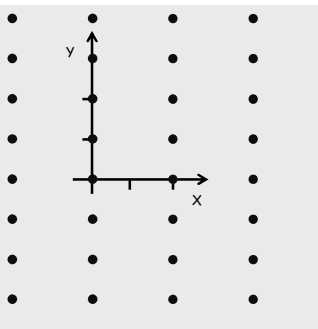
Department of Materials Science and Engineering

plane waves and the reciprocal lattice

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<http://molmod.ugent.be>
<http://www.ugent.be/ea/dmse/en>
my talks on Youtube: <http://goo.gl/P2b1Hs>

Plane waves



Define a function

$$f(\vec{r}) = \text{Re}(e^{i\vec{k}\cdot\vec{r}})$$

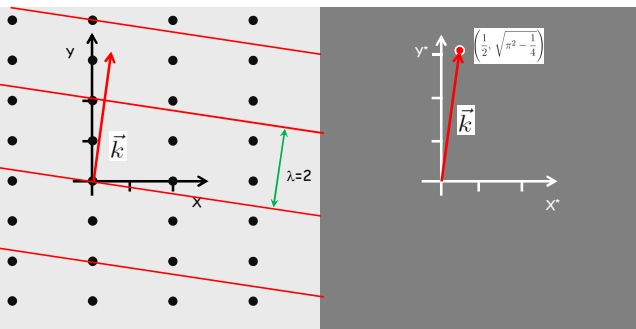
with \vec{k} some given vector

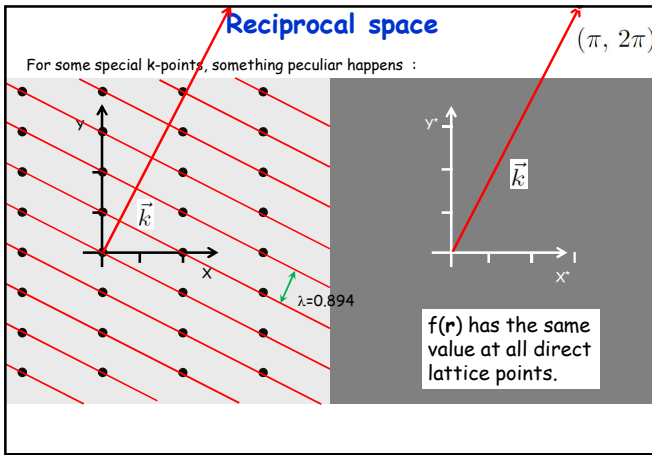
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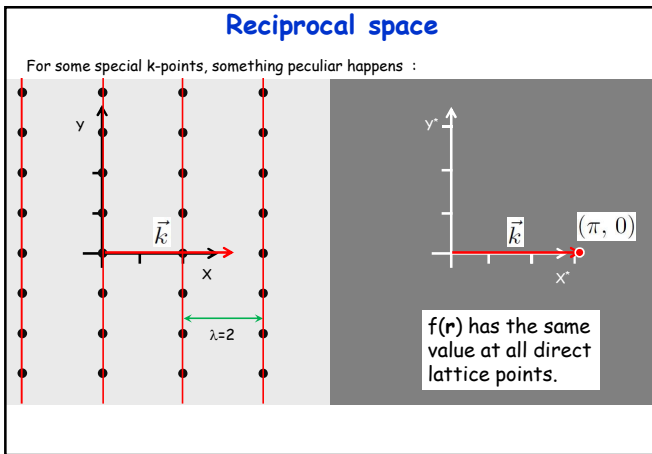
- Same function value in any plane perpendicular to \vec{k} .
- Periodic, with period $\lambda = 2\pi/k$

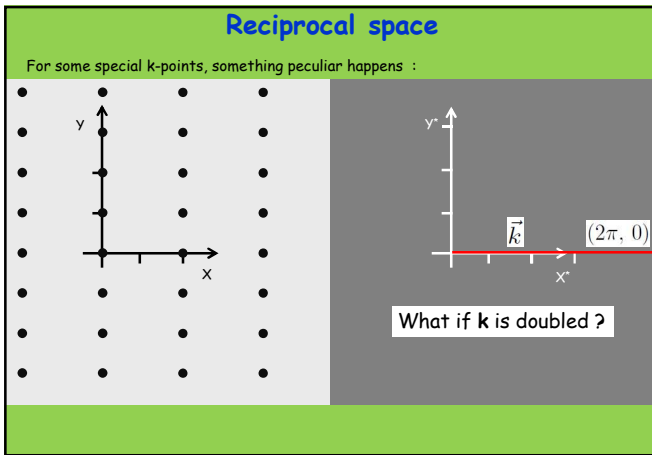
Units of \vec{k} : 1/distance.
Hence, \vec{k} is a point in reciprocal space.

Reciprocal space





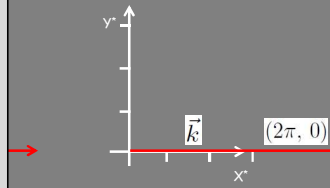




Reciprocal space

For some special k-points, something peculiar happens :

spoiler prevention

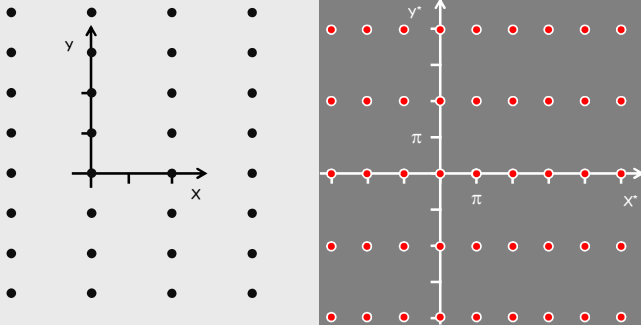


What if k is doubled ?

→ f(r) keeps having the same value at every lattice point.

Reciprocal lattice

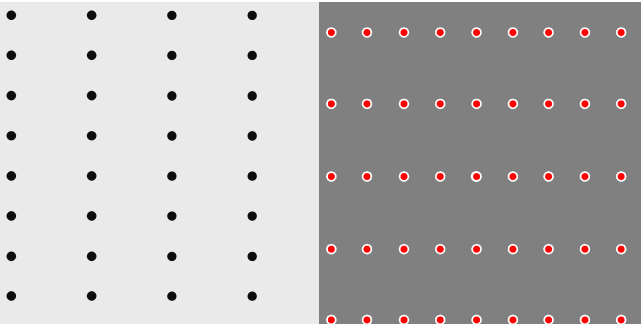
The set of all points in reciprocal space that fulfill this condition form a lattice :

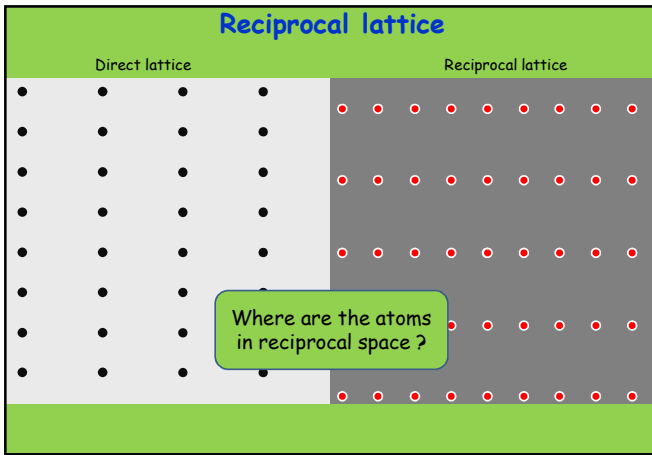


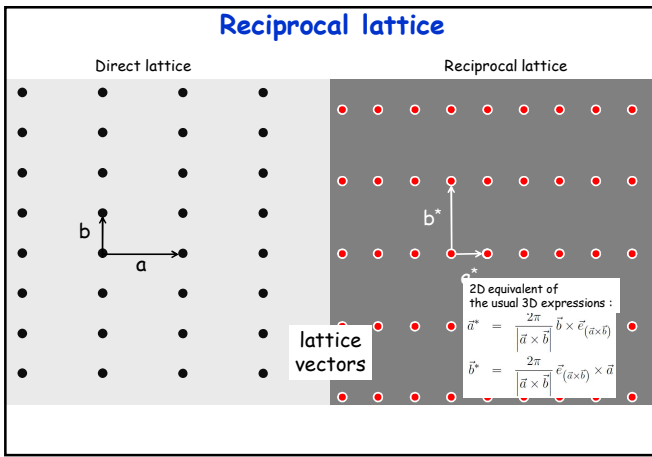
Reciprocal lattice

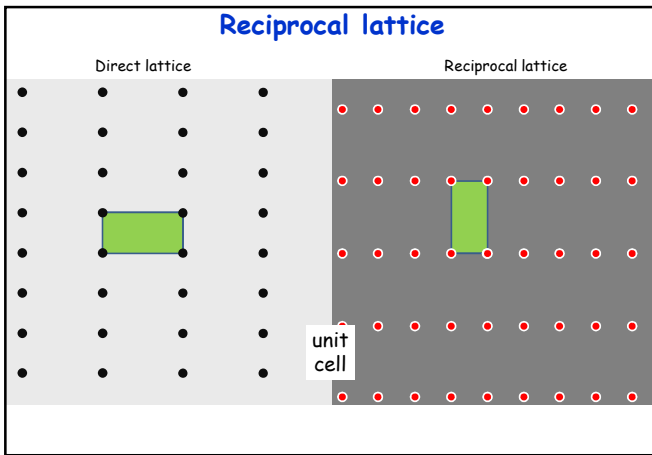
Direct lattice

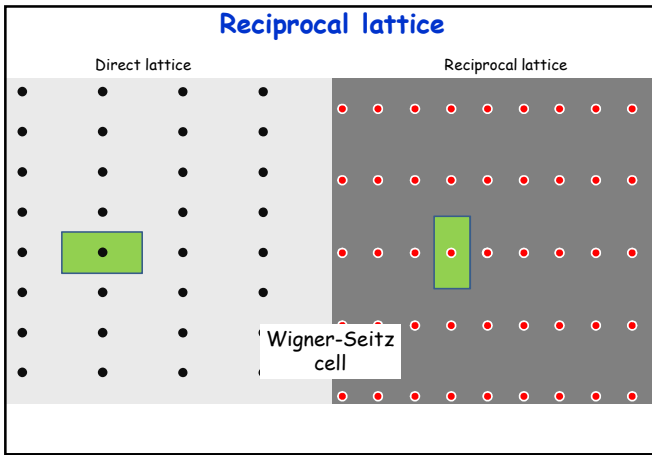
Reciprocal lattice

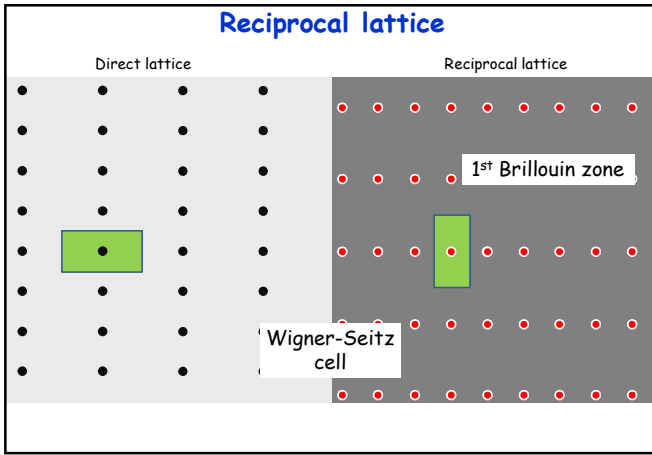












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[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Fricke Groups] [Magnetic Space Groups]

Space Groups Retrieval Tools	
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

2014: International Year of Crystallography

ICr2014

Sections

Retrieval Tools

Magnetic Symmetry and Applications

Group-Subgroup Representations

Solid State

Structure Utilities

Retrieval Tools

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The k-vector types of space group $P4/mmm$ (123)

(Table for arithmetic crystal class $4/mmmP$)

$P4/mmm-D_{4h}^1$ (123) to $P4_2/nm-D_{4h}^{19}$ (138)

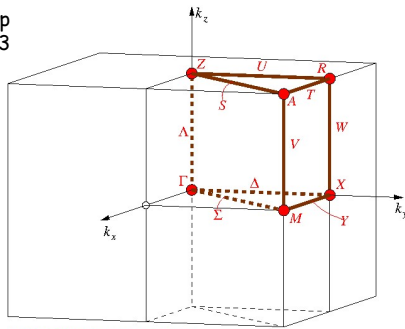
Reciprocal space group ($P4/mmm$), No.123



k-vector description		ITA description			
CDML ¹		Wyckoff Position		Coordinates	
Label	Coefficients				
GM	0,0,0	1	a	4/mmm	0,0,0
Z	0,0,1/2	1	b	4/mmm	0,0,1/2
M	1/2,1/2,0	1	c	4/mmm	1/2,1/2,0
A	1/2,1/2,1/2	1	d	4/mmm	1/2,1/2,1/2
R	0,1/2,1/2	2	e	m/m	0,1/2,1/2
X	0,1/2,0	2	f	m/m	0,1/2,0
LD	0,0,u	2	g	4/m	0,0,z : 0 < z < 1/2
V	1/2,1/2,u	2	h	4/m	1/2,1/2,z : 0 < z < 1/2

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for space group
nr. 123

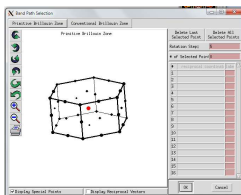


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<http://www.cryst.ehu.es>

Brillouin zone by Xcrysden

- Get any cif from a database (choose)
- `cif2struct <any-name>.cif` to convert to wien2k input
- `cp <any-name>.struct case.struct`
- `x sgroup`
- `cp case.struct_sgroup case.struct`
- `xcrysden --wien_struct case.struct`

Example: CdSe



Reciprocal lattice

What is this good for ?

The electron density $\rho(\mathbf{r})$ of the crystal has the periodicity of the Bravais lattice.

All reciprocal lattice vectors correspond to plane waves with the periodicity of the Bravais lattice.

the electron density can be expressed as a sum over the reciprocal lattice (Fourier transform)

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DFT: everything can be expressed by the electron density.

Everything can be expressed as a sum over the reciprocal lattice... !
