

# Geometric considerations

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## 1 Real space

\* The three primitive translation vectors are  $\mathbf{R}_{1p}$ ,  $\mathbf{R}_{2p}$ ,  $\mathbf{R}_{3p}$ .  
Representation in Cartesian coordinates (atomic units):

$$\mathbf{R}_{1p} \rightarrow \text{rprimd}(1 : 3, 1)$$

$$\mathbf{R}_{2p} \rightarrow \text{rprimd}(1 : 3, 2)$$

$$\mathbf{R}_{3p} \rightarrow \text{rprimd}(1 : 3, 3)$$

Related input variables : `acell,rprim,angdeg`

\* Atomic positions are specified by the coordinates  $\mathbf{x}_\tau$  for  $\tau = 1 \dots N_{atom}$   
where  $N_{atom}$  is the number of atoms.

Representation in reduced coordinates

$$\mathbf{x}_\tau = x_{1\tau}^{red} \cdot \mathbf{R}_{1p} + x_{2\tau}^{red} \cdot \mathbf{R}_{2p} + x_{3\tau}^{red} \cdot \mathbf{R}_{3p}$$

$$\tau \rightarrow \text{iatom}$$

$$N_{atom} \rightarrow \text{natom}$$

$$x_{1\tau}^{red} \rightarrow \text{xred}(1, \text{iatom})$$

$$x_{2\tau}^{red} \rightarrow \text{xred}(2, \text{iatom})$$

$$x_{3\tau}^{red} \rightarrow \text{xred}(3, \text{iatom})$$

Related input variables : `xangst,xcart,xred`

\* The volume of the primitive unit cell is

$$\Omega_{Or} = \mathbf{R}_1 \cdot (\mathbf{R}_2 \times \mathbf{R}_3)$$

$$\Omega_{Or} \rightarrow \text{ucvol (unit cell volume)}$$

Computed in `metric.f`

\* The scalar products in the reduced representation are valuated thanks to

$$\mathbf{r} \cdot \mathbf{r}' = \begin{pmatrix} r_1^{red} & r_2^{red} & r_3^{red} \end{pmatrix} \begin{pmatrix} \mathbf{R}_{1p} \cdot \mathbf{R}_{1p} & \mathbf{R}_{1p} \cdot \mathbf{R}_{2p} & \mathbf{R}_{1p} \cdot \mathbf{R}_{3p} \\ \mathbf{R}_{2p} \cdot \mathbf{R}_{1p} & \mathbf{R}_{2p} \cdot \mathbf{R}_{2p} & \mathbf{R}_{2p} \cdot \mathbf{R}_{3p} \\ \mathbf{R}_{3p} \cdot \mathbf{R}_{1p} & \mathbf{R}_{3p} \cdot \mathbf{R}_{2p} & \mathbf{R}_{3p} \cdot \mathbf{R}_{3p} \end{pmatrix} \begin{pmatrix} r_1^{red'} \\ r_2^{red'} \\ r_3^{red'} \end{pmatrix}$$

that is  $\mathbf{r} \cdot \mathbf{r}' = \sum_{ij} r_i^{red} \mathbf{R}_{ij}^{met} r_j^{red'}$

where  $\mathbf{R}_{ij}^{met}$  is the metric tensor in real space :

$$\mathbf{R}_{ij}^{met} \rightarrow \mathbf{rmet}(i, j)$$

Computed in `metric.f`.

## 2 Reciprocal space

\* The three primitive translation vectors in reciprocal space are  $\mathbf{G}_{1p}, \mathbf{G}_{2p}, \mathbf{G}_{3p}$  (computed in `metric.f`)

$$\begin{aligned} \mathbf{G}_{1p} &= \frac{1}{\Omega_{Or}} (\mathbf{R}_{2p} \times \mathbf{R}_{3p}) \rightarrow \mathbf{gprimd}(1 : 3, 1) \\ \mathbf{G}_{2p} &= \frac{1}{\Omega_{Or}} (\mathbf{R}_{3p} \times \mathbf{R}_{1p}) \rightarrow \mathbf{gprimd}(1 : 3, 2) \\ \mathbf{G}_{3p} &= \frac{1}{\Omega_{Or}} (\mathbf{R}_{1p} \times \mathbf{R}_{2p}) \rightarrow \mathbf{gprimd}(1 : 3, 3) \end{aligned}$$

This definition is such that  $\mathbf{G}_{ip} \cdot \mathbf{R}_{jp} = \delta_{ij}$

[WARNING: often, a factor of  $2\pi$  is present in definition of  $\mathbf{G}_{ip}$ , but not here, for historical reasons.]

\* Reduced representation of vectors ( $\mathbf{K}$ ) in reciprocal space

$$\mathbf{K} = K_1^{red} \mathbf{G}_{1p} + K_2^{red} \mathbf{G}_{2p} + K_3^{red} \mathbf{G}_{3p} \rightarrow (K_1^{red}, K_2^{red}, K_3^{red})$$

e.g. the reduced representation of  $\mathbf{G}_{1p}$  is (1,0,0).

\* The reduced representation of the vectors of the reciprocal space lattice is made of triplets of integers.

\*The scalar products in the reduced representation are evaluated thanks to

$$\mathbf{K} \cdot \mathbf{K}' = \begin{pmatrix} K_1^{red} & K_2^{red} & K_3^{red} \end{pmatrix} \begin{pmatrix} \mathbf{G}_{1p} \cdot \mathbf{G}_{1p} & \mathbf{G}_{1p} \cdot \mathbf{G}_{2p} & \mathbf{G}_{1p} \cdot \mathbf{G}_{3p} \\ \mathbf{G}_{2p} \cdot \mathbf{G}_{1p} & \mathbf{G}_{2p} \cdot \mathbf{G}_{2p} & \mathbf{G}_{2p} \cdot \mathbf{G}_{3p} \\ \mathbf{G}_{3p} \cdot \mathbf{G}_{1p} & \mathbf{G}_{3p} \cdot \mathbf{G}_{2p} & \mathbf{G}_{3p} \cdot \mathbf{G}_{3p} \end{pmatrix} \begin{pmatrix} K_1^{red'} \\ K_2^{red'} \\ K_3^{red'} \end{pmatrix}$$

that is  $\mathbf{K} \cdot \mathbf{K}' = \sum_{ij} K_i^{red} \mathbf{G}_{ij}^{met} K_j^{red'}$

where  $\mathbf{G}_{ij}^{met}$  is the metric tensor in reciprocal space :

$$\mathbf{G}_{ij}^{met} \rightarrow \mathbf{gmet}(i, j)$$

(computed in `metric.f`).

### 3 Symmetries

\* A symmetry operation in real space sends the point  $\mathbf{r}$  to the point  $\mathbf{r}' = \mathbf{S}_t\{\mathbf{r}\}$  whose coordinates are  $(\mathbf{r}')_\alpha = \sum_\beta S_{\alpha\beta} r_\beta + t_\alpha$  (Cartesian coordinates).

\* The symmetry operations that preserves the crystalline structure are those that send every atom location on an atom location with the same atomic type.

\* The application of a symmetry operation to a function of spatial coordinates  $\mathbf{V}$  is such that :

$$(\mathbf{S}_t \mathbf{V})(\mathbf{r}) = \mathbf{V}((\mathbf{S}_t)^{-1}\{\mathbf{r}\})$$

$$(\mathbf{S}_t)^{-1}\{\mathbf{r}\} = \sum_\beta S_{\alpha\beta}^{-1}(r_\beta - t_\beta)$$

\* For each symmetry operation,  $isym = 1 \dots nsym$ , the  $3 \times 3$   $\mathbf{S}^{red}$  matrix is stored in `symrel(:, :, isym)`.

[in reduced coordinates :  $r_\alpha^{red} = \sum_\beta S_{\alpha\beta}^{red} r_\beta^{red} + t_\beta^{red}$  ]

and the vector  $\mathbf{t}^{red}$  is stored in `tnons(:, isym)`.

\* The conversion between reduced coordinates and Cartesian coordinates is  $r'_\gamma = \sum_{\alpha\beta} (R_{\alpha p})_\gamma [S_{\alpha\beta}^{red} r_\beta^{red} + t_\alpha^{red}]$   
with [as  $G_{ip} \cdot R_{jp} = \delta_{ij}$ ]

$$r_\delta = \sum_\alpha (R_{\alpha p})_\delta r_\alpha^{red} \rightarrow \sum_\beta (G_{\beta p})_\delta r_\delta = r_\beta^{red}$$

So

$$S_{\gamma\delta} = \sum_{\alpha\beta} (R_{\alpha p})_\gamma S_{\alpha\beta}^{red} (G_{\beta p})_\delta$$