

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}_τ 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 2π 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 3×3 \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

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