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):

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

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

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

Related input variables : `acell,rprim,angdeg`

* Atomic positions are specified by the coordinates $\mathbf{x}_\tau$ for $\tau = 1 \ldots N_{atom}$ where N_{atom} is the member of atoms.
Representation in reduced coordinates

$$\begin{aligned}
\mathbf{x}_\tau &= x_{1\tau}^{red} \cdot \mathbf{R}_{1p} + x_{2\tau}^{red} \cdot \mathbf{R}_{2p} + x_{3\tau}^{red} \cdot \mathbf{R}_{3p} \\
\tau &\rightarrow \texttt{iatom} \\
N_{atom} &\rightarrow \texttt{natom} \\
x_{1\tau}^{red} &\rightarrow \texttt{xred}(1,\texttt{iatom}) \\
x_{2\tau}^{red} &\rightarrow \texttt{xred}(2,\texttt{iatom}) \\
x_{3\tau}^{red} &\rightarrow \texttt{xred}(3,\texttt{iatom})
\end{aligned}$$

Related input variables : `xangst,xcart,xred`

* The volume of the primitive unit cell is

$$\begin{aligned}
\Omega_{O\mathbf{r}} &= \mathbf{R}_1 \cdot (\mathbf{R}_2 \times \mathbf{R}_3) \\
\Omega_{O\mathbf{r}} &\rightarrow \texttt{ucvol}\,\text{(unit cell volume)}
\end{aligned}$$

Computed in `metric.f`

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

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

that is $\mathbf{r}\cdot\mathbf{r}' = \sum_{ij} r_i^{red}\mathbf{R}_{ij}^{met} r_j^{red\prime}$
where $\mathbf{R}_{ij}^{met}$ is the metric tensor in real space :

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

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`)

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

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

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

that is $\mathbf{K}\cdot\mathbf{K}' = \sum_{ij} K_i^{red}\mathbf{G}_{ij}^{met} K_j^{red\prime}$
where $\mathbf{G}_{ij}^{met}$ is the metric tensor in reciprocal space :

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

(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 :

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

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

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

[in reduced coordinates : $r'^{red}_\alpha = \sum_\beta S^{red}_{\alpha\beta} r^{red}_\beta + t^{red}_\beta$]

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

* The conversion between reduced coordinates and Cartesian coordinates is $r'_\gamma = \sum_{\alpha\beta}(R_{\alpha p})_\gamma [S^{red}_{\alpha\beta} r^{red}_\beta + t^{red}_\alpha]$

with [as $G_{ip} \cdot R_{jp} = \delta_{ij}$]

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

.

So

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