Geometric considerations

(X. Gonze, Y. Suzukawa, M. Mikami)

June 9, 2017

1 Real space

* The three primitive translation vectors are $\mathbf{R}_{1p}$, $\mathbf{R}_{2p}$, $\mathbf{R}_{3p}$.

Representation in Cartesian coordinates (atomic units):

\[
\begin{align*}
\mathbf{R}_{1p} & \rightarrow \mathbf{r}_{\text{prim}}(1:3,1) \\
\mathbf{R}_{2p} & \rightarrow \mathbf{r}_{\text{prim}}(1:3,2) \\
\mathbf{R}_{3p} & \rightarrow \mathbf{r}_{\text{prim}}(1:3,3) 
\end{align*}
\]

Related input variables: $a_{\text{cell}}, r_{\text{prim}}, a_{\text{deg}}$

* Atomic positions are specified by the coordinates $x_{\tau}$ for $\tau = 1 \ldots N_{\text{atom}}$, where $N_{\text{atom}}$ is the member of atoms.

Representation in reduced coordinates

\[
\begin{align*}
x_{\tau} & = x_{1\tau}^{\text{red}} \cdot \mathbf{R}_{1p} + x_{2\tau}^{\text{red}} \cdot \mathbf{R}_{2p} + x_{3\tau}^{\text{red}} \cdot \mathbf{R}_{3p} \\
\tau & \rightarrow \text{iatom} \\
N_{\text{atom}} & \rightarrow \text{natom} \\
x_{1\tau}^{\text{red}} & \rightarrow \text{xred}(1, \text{iatom}) \\
x_{2\tau}^{\text{red}} & \rightarrow \text{xred}(2, \text{iatom}) \\
x_{3\tau}^{\text{red}} & \rightarrow \text{xred}(3, \text{iatom}) 
\end{align*}
\]

Related input variables: $x_{\text{angst}}, x_{\text{cart}}, x_{\text{red}}$

* The volume of the primitive unit cell is

\[
\Omega_{\text{Or}} = \mathbf{R}_{1} \cdot (\mathbf{R}_{2} \times \mathbf{R}_{3}) \\
\Omega_{\text{Or}} \rightarrow \text{ucvol}(\text{unit cell volume})
\]

Computed in $\text{metric.f}$
* The scalar products in the reduced representation are evaluated thanks to
\[
\mathbf{r} \cdot \mathbf{r}' = \begin{pmatrix} \mathbf{r}_{1}^{\text{red}} & \mathbf{r}_{2}^{\text{red}} & \mathbf{r}_{3}^{\text{red}} \end{pmatrix} \begin{pmatrix} \mathbf{R}_{1p} \cdot \mathbf{R}_{1p} & \mathbf{R}_{1p} \cdot \mathbf{R}_{2p} & \mathbf{R}_{1p} \cdot \mathbf{R}_{3p} \\
\mathbf{R}_{2p} \cdot \mathbf{R}_{1p} & \mathbf{R}_{2p} \cdot \mathbf{R}_{2p} & \mathbf{R}_{2p} \cdot \mathbf{R}_{3p} \\
\mathbf{R}_{3p} \cdot \mathbf{R}_{1p} & \mathbf{R}_{3p} \cdot \mathbf{R}_{2p} & \mathbf{R}_{3p} \cdot \mathbf{R}_{3p} \end{pmatrix} \begin{pmatrix} \mathbf{r}_{1}^{\text{red}} \\
\mathbf{r}_{2}^{\text{red}} \\
\mathbf{r}_{3}^{\text{red}} \end{pmatrix}
\]
that is \(\mathbf{r} \cdot \mathbf{r}' = \sum_{ij} r_{i}^{\text{red}} R_{ij}^{\text{met}} r_{j}^{\text{red}}\)
where \(R_{ij}^{\text{met}}\) is the metric tensor in real space:
\[
R_{ij}^{\text{met}} \rightarrow r_{\text{met}}(i,j)
\]
Computed in \textit{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 \textit{metric.f})
\[
\mathbf{G}_{1p} = \frac{1}{\Omega_O}(\mathbf{R}_{2p} \times \mathbf{R}_{3p}) \rightarrow \text{gprimd}(1:3,1)
\]
\[
\mathbf{G}_{2p} = \frac{1}{\Omega_O}(\mathbf{R}_{3p} \times \mathbf{R}_{1p}) \rightarrow \text{gprimd}(1:3,2)
\]
\[
\mathbf{G}_{3p} = \frac{1}{\Omega_O}(\mathbf{R}_{1p} \times \mathbf{R}_{2p}) \rightarrow \text{gprimd}(1:3,3)
\]
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 (\(K\)) in reciprocal space
\(\mathbf{K} = K_{1}^{\text{red}} \mathbf{G}_{1p} + K_{2}^{\text{red}} \mathbf{G}_{2p} + K_{3}^{\text{red}} \mathbf{G}_{3p} \rightarrow (K_{1}^{\text{red}}, K_{2}^{\text{red}}, K_{3}^{\text{red}})\)
 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
\[
\mathbf{K} \cdot \mathbf{K}' = \begin{pmatrix} K_{1}^{\text{red}} & K_{2}^{\text{red}} & K_{3}^{\text{red}} \end{pmatrix} \begin{pmatrix} \mathbf{G}_{1p} \cdot \mathbf{G}_{1p} & \mathbf{G}_{1p} \cdot \mathbf{G}_{2p} & \mathbf{G}_{1p} \cdot \mathbf{G}_{3p} \\
\mathbf{G}_{2p} \cdot \mathbf{G}_{1p} & \mathbf{G}_{2p} \cdot \mathbf{G}_{2p} & \mathbf{G}_{2p} \cdot \mathbf{G}_{3p} \\
\mathbf{G}_{3p} \cdot \mathbf{G}_{1p} & \mathbf{G}_{3p} \cdot \mathbf{G}_{2p} & \mathbf{G}_{3p} \cdot \mathbf{G}_{3p} \end{pmatrix} \begin{pmatrix} K_{1}^{\text{red}} \\
K_{2}^{\text{red}} \\
K_{3}^{\text{red}} \end{pmatrix}
\]
that is \(\mathbf{K} \cdot \mathbf{K}' = \sum_{ij} K_{ij}^{\text{red}} \mathbf{G}_{ij}^{\text{met}} \mathbf{G}_{ij}^{\text{red}}\)
where \(G_{ij}^{\text{met}}\) is the metric tensor in reciprocal space:
\[
G_{ij}^{\text{met}} \rightarrow g_{\text{met}}(i,j)
\]
(computed in \textit{metric.f}).
3 Symmetries

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

* The symmetry operations that preserve 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 \( V \) is such that:

\[
(S_t V)(r) = V((S_t)^{-1}\{ r \})
\]

\[
(S_t)^{-1}\{ r \} = \sum_\beta S_{\alpha \beta}^{-1}(r_\beta - t_\beta)
\]

* For each symmetry operation, \( isym = 1 \ldots nsym \), the \( 3 \times 3 \) \( S_{\text{red}} \) matrix is stored in \( \text{symrel}(::, isym) \).

  [in reduced coordinates : \( r'_{\alpha} = \sum_\beta S_{\alpha \beta}^{\text{red}} r_\beta^{\text{red}} + t_\beta^{\text{red}} \)]

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

* The conversion between reduced coordinates and Cartesian coordinates is

\[
r_{\gamma} = \sum_\alpha (R_{\alpha p})_{\gamma} [S_{\alpha \beta}^{\text{red}} r_\beta^{\text{red}} + t_\alpha^{\text{red}}]
\]

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

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

So

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