Definitions, conventions and useful facts

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1 Terminology

$\mathbf{G}$ Vector on the reciprocal lattice $\mathcal{R}^*$

$\mathbf{k}$ Vector inside the first Brillouin zone

$\mathbf{q}$ Reciprocal-space vector $\mathbf{q} = \mathbf{k} + \mathbf{G}$

$\mathbf{R}$ Vector on the lattice $\mathcal{R}$

$\mathbf{r}$ Vector inside the unit cell

$\mathbf{x}$ Real-space vector, $\mathbf{x} = \mathbf{r} + \mathbf{R}$

Ω Unit cell / unit cell volume

$e_{\mathbf{G}}$ Normalized plane wave

$$e_{\mathbf{G}} = \frac{1}{\sqrt{\Omega}} \exp(i\mathbf{G} \cdot \mathbf{r})$$

$T_{\mathbf{R}}$ Lattice translation operator

$$T_{\mathbf{R}} u(\mathbf{x}) = u(\mathbf{x} - \mathbf{R})$$

Y_l^m complex spherical harmonics

Y_{lm} real spherical harmonics

$\mathbf{x} = x\hat{\boldsymbol{x}}$ Separation of a vector into its radial and angular part

j_l Spherical Bessel functions. $j_0(x) = \frac{\sin x}{x}$

2 Conventions and useful formulas

- The Fourier transform is

$$\widehat{f}(\mathbf{q}) = \int_{\mathbb{R}^3} e^{-i\mathbf{q}\cdot\mathbf{x}} \, \mathrm{d}\mathbf{x}$$

- Plane wave expansion

$$e^{i\mathbf{q}\cdot\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(qr) Y_l^m(\hat{\boldsymbol{q}}) Y_l^{m*}(\hat{\boldsymbol{r}})$$

- Spherical harmonics orthogonality
$$\int_{\mathbb{S}^2} Y_l^{m*}(\hat{\boldsymbol{r}}) Y_{l'}^{m'}(\hat{\boldsymbol{r}})\,\mathrm{d}\hat{\boldsymbol{r}} = \delta_{l,l'}\delta_{m,m'}$$
This also holds true for real spherical harmonics.

- Fourier transforms of centered functions. If
$$f(\mathbf{x}) = R(x) Y_l^m(\hat{\boldsymbol{x}}),$$
then
$$\begin{aligned}
\hat{f}(\mathbf{q}) &= \int_{\mathbb{R}^3} R(x) Y_l^m(\hat{\boldsymbol{x}}) e^{-i\mathbf{q}\cdot\mathbf{x}}\,\mathrm{d}\mathbf{x} \\
&= \sum_{l=0}^{\infty} 4\pi i^l \sum_{m=-l}^{l} \int_{\mathbb{R}^3} R(x) j_{l'}(qx) Y_{l'}^{m'}(-\hat{\boldsymbol{q}}) Y_l^m(\hat{\boldsymbol{x}}) Y_{l'}^{m'*}(\hat{\boldsymbol{x}})\,\mathrm{d}\mathbf{x} \\
&= 4\pi Y_l^m(-\hat{\boldsymbol{q}}) i^l \int_{\mathbb{R}^+} x^2 R(x)\ j_l(qx)\ \mathrm{d}x,
\end{aligned}$$
This also holds true for real spherical harmonics.

3 Discretization and normalization

The periodic part of Bloch waves is discretized in a set of normalized plane waves $e_{\mathbf{G}}$:
$$\begin{aligned}
\psi_k(x) &= e^{i\mathbf{k}\cdot\mathbf{x}} u_{\mathbf{k}}(\mathbf{r}) \\
&= \sum_{\mathbf{G}\in\mathcal{R}^*} c_{\mathbf{G}} e^{i\mathbf{k}\cdot\mathbf{x}} e_{\mathbf{G}}(\mathbf{r})
\end{aligned}$$
The $c_{\mathbf{G}}$ are ℓ^2-normalized. The summation is truncated to a "spherical" basis set
$$S_k = \left\{ G \in \mathcal{R}^* \,\middle|\, \frac{1}{2}\left|\mathbf{k}+\mathbf{G}\right|^2 \le E_{\text{cut}} \right\}$$
Densities involve terms like $|\psi_k|^2 = |u_k|^2$ and therefore products $e_{-\mathbf{G}} e_{\mathbf{G}'}$ for $\mathbf{G}, \mathbf{G}'$ in X_k. To represent these we use a "cubic" basis set large enough to contain the set $\{\mathbf{G}-\mathbf{G}' \,|\, \mathbf{G},\mathbf{G}' \in S_k\}$. We can obtain the decomposition of densities on the $e_{\mathbf{G}}$ basis by a convolution, which can be performed efficiently with FFTs. Potentials are discretized on this same set. The normalization conventions used in the code is that quantities stored in reciprocal space are coefficients in the $e_{\mathbf{G}}$ basis, and quantities stored in real space use real physical values. This means for instance that wavefunctions in the real space grid are normalized as $\frac{|\Omega|}{N}\sum_r |f(r)|^2 = 1$ where N is the number of grid points.

4 Relative and Cartesian coordinates

Let A be a set of primitive lattice vectors for $\mathcal{R}$, and B for $\mathcal{R}^*$, with $A^*B = 2\pi I$. Then $x_c = Ax_r$ and $q_c = Bq_r$, where the subscripts c and r stand for Cartesian and relative. Other names for relative coordinates are **integer coordinates** (usually for $\mathbf{G}$-vectors) and **fractional coordinates** (usually for $\mathbf{k}$-points). We have
$$x_c \cdot q_c = 2\pi x_r \cdot q_r.$$