Interatomic force constants
and
phonon dispersion

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Real-space interatomic force constants (IFCs)

\[ C_{st}^{ab}(R) = \frac{\partial^2 E}{\partial u_s^a(0) \partial u_t^b(R)} = \frac{1}{N_c} \sum_q e^{i q \cdot R} \tilde{C}_{st}^{ab}(q) \]

- Calculation of \( C_{st}^{ab}(q) \) on a suitable grid of \( q \)-vectors
- Fourier transform to real space
Real space interatomic force constants

The shorter the range of real-space IFCs, the coarser will be the reciprocal-space grid needed for the Fourier transform. The size of the grid is assessed \textit{a posteriori} by verifying that it yields vanishing real-space constants beyond a certain cutoff radius.

For \textbf{non polar systems}, the IFCs are relatively short range, thus requiring a moderate number of calculations at different $q$.

For \textbf{polar systems}, the IFCs are long ranged. But Fourier interpolation is efficiently applicable to the \textit{analytic} contribution to IFC, while the \textit{nonanalytic} behavior is restored by adding the IFC of a suitable point charge model.
Phonon dispersion

Once real-space IFCs have been computed, dynamical matrices in reciprocal space (and, hence, vibrational frequencies) can be obtained at any wave vector (*not necessarily contained in the original grid*) by Fourier transform.

\[
\tilde{C}^{ab}_{st}(q) = \sum_{R} e^{-i\mathbf{q} \cdot \mathbf{R}} C^{ab}_{st}(\mathbf{R})
\]

The comparison of the results of this procedure with the full calculation on some points *not* included in the original grid (used to compute the IFCs) is a check of the accuracy of the Fourier interpolation.
Phonon dispersion of MgO
Phonon dispersion of MgO

- Calculation of $C_{s,t}^{a,b}(q)$ on a 4 x 4 x 4 grid ---> ph.x
- Calculation of the real-space IFCs ---> q2r.x
- Calculation of the phonon dispersion ---> matdyn.x
- Calculation of the vibrational density of states ---> matdyn.x