The phonon eigenvectors indicate how each atom moves for a given vibrational mode. It is important to note that there are several different conventions as to the form of the eigenvectors that are output from codes, such as for use in visualisation programs. By default, the eigenvectors in GULP prior to version 6.1 were those that diagonalise the dynamical matrix as given above (i.e. the Cartesian second derivative matrix divided by the product of the square roots of the masses of the atoms for the matrix element). From version 6.1 onwards an alternative form is used in which the phase due to the position of the atom is removed by multiplying the components of the eigenvectors, e, by:

$$e'_{i\alpha} = e_{i\alpha} exp\left(-ik.r_i\right)$$

Here k represents the reciprocal lattice vector for the phase of the phonon k point, while r_i is the position vector of atom i. As a further option, it is also possible to output the eigenvectors in a form where the effect of the mass-weighting is removed. In this case a further transformation of the eigenvectors is performed according to:

$$e''_{i\alpha} = \frac{e_{i\alpha}}{m_i^{\frac{1}{2}}} \left(\frac{1}{\sum_{i,\alpha}^{N} \frac{e^*_{i\alpha} e_{i\alpha}}{m_i^2}} \right)^{\frac{1}{2}}$$

The option `eigenvector_type` can be used to change between the different possible conventions.