Notes on units of phonon frequencies
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The vibration equations we want to solve have a form like

\[ M \omega^2 u = \left( \frac{\partial^2 E}{\partial u \partial u} \right) u \]

(omitting indices and possible “symmetrization” of force constant matrix). Therefore, in what regards units, the frequency comes out as

\[ [\omega] = \sqrt{\frac{1}{M} \left( \frac{\partial^2 E}{\partial u \partial u} \right)} . \]

We’d like to have \( M \) in atomic mass units, \( 1.660599 \times 10^{-27} \) kg, and energy derivatives – in “conventional” units of a DFT calculation, i.e., \( E \) in eV or Ry, and displacements – in Å or Bohr. Assume for the following that the force constants are in eV/Å\(^2\), and note that alternatively 1 Ry = 13.605692 eV; 1 Bohr = 0.529177 Å. Let’s find the corresponding “frequency unit”, \( \text{f.u.} \), in the SI:

\[
\text{f.u.} = \sqrt{\frac{1 \text{eV/Å}^2}{1 \text{ a.m.u.}}} = \sqrt{\frac{1.602176487 \times 10^{-19} \text{J}}{1.660599 \times 10^{-27} \text{kg}}} = \sqrt{\frac{16.021764887 \text{J/m}^2}{0.1660599 \times 10^{-26} \text{kg}}} = 9.822517 \times 10^{13} \text{s}^{-1} .
\]

Typical units for phonon frequencies are meV, THz, and cm\(^{-1}\). Let’s find their relations with our \( \text{f.u.} \):

- meV is the measure of energy of a phonon with 1 \( \text{f.u.} \):

\[
\text{f.u.} \times \hbar = 9.822517 \times 10^{13} \text{s}^{-1} \times 1.054572 \times 10^{-34} \text{J} \cdot \text{s} = 1.035855 \times 10^{-20} \text{J}
\]

\[ = 64.652976 \text{ meV} . \]

- \( \nu \), expressed in THz, is \( \omega/(2\pi) \):

\[
\frac{\text{f.u.}}{2\pi} = 15.6330214 \text{ THz} .
\]

- Inverse wavelength is found from \( h\nu = \hbar c / \lambda \); \( \frac{1}{\lambda} = \frac{\omega}{2\pi c} \).

\[
\frac{\text{f.u.}}{2\pi c} = 9.822517 \times 10^{13} \text{s}^{-1} = 521.461464 \text{ cm}^{-1} .
\]

Units conversion:
1 THz = 4.136 meV = 33.356 cm\(^{-1}\);
1 meV = 0.242 THz = 8.066 cm\(^{-1}\);
1 cm\(^{-1}\) = 0.030 THz = 0.124 meV.