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, $1.660599{\cdot}10^{-27}$ 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", $f.u.$, in the SI:

$$\begin{aligned} f.u. &= \sqrt{\frac{1\,\mathrm{eV/\AA^2}}{1\,\mathrm{a.m.u.}}} = \sqrt{\frac{\frac{1.602176487{\cdot}10^{-19}\,\mathrm{J}}{10^{-20}\,\mathrm{m^2}}}{1.660599{\cdot}10^{-27}\,\mathrm{kg}}} = \sqrt{\frac{16.021764887\,\mathrm{J/m^2}}{0.1660599{\cdot}10^{-26}\,\mathrm{kg}}} \\ &= 9.822517{\cdot}10^{13}\,\mathrm{s^{-1}}\,. \end{aligned}$$

Typical units for phonon frequencies are meV, THz, and cm^{-1}. Let's find their relations with our $f.u.$.

- meV is the measure of energy of a phonon with 1 $f.u.$:

$$\begin{aligned} f.u.{\times}\hbar &= 9.822517{\cdot}10^{13}\,\mathrm{s^{-1}}{\times}1.054572{\cdot}10^{-34}\,\mathrm{J\cdot s} = 1.035855{\cdot}10^{-20}\,\mathrm{J} \\ &= 64.652976\,\mathrm{meV}\,. \end{aligned}$$

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

$$\frac{f.u.}{2\pi} = 15.6330214\,\mathrm{THz}\,.$$

- Inverse wavelength is found from $h\nu = \frac{hc}{\lambda}$; $\quad \frac{1}{\lambda} = \frac{\omega}{2\pi{\cdot}c}$.

$$\frac{f.u.}{2\pi{\cdot}c} = \frac{9.822517{\cdot}10^{13}\,\mathrm{s^{-1}}}{2\pi{\cdot}29979245800\,\mathrm{cm/s}} = 521.461464\,\mathrm{cm^{-1}}\,.$$

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.