Normal Mode Analysis - Spectroscopy

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What is Normal Mode Analysis?

Normal mode analysis provides information on the equilibrium modes accessible to a system, assuming that the system is stabilized by harmonic potentials.

Water

The given .xyz file is of the water molecule.

We have to perform normal mode analysis on that water molecule.

First we write a potential energy function for two atoms. After generalising this function to all atoms, we then calculate it's Hessian.

What is the Hessian?

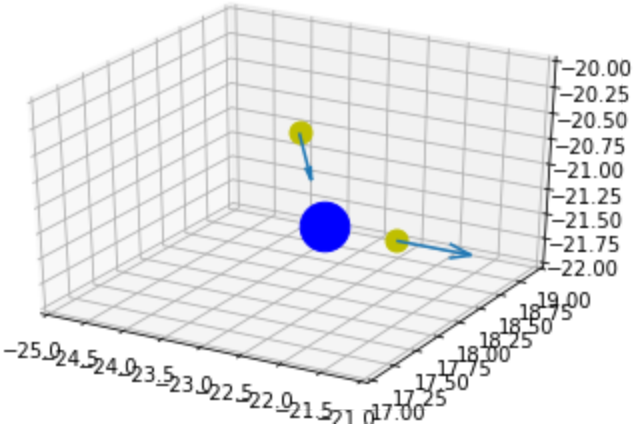
The Hessian matrix is a square matrix of second-order partial derivatives of a scalar-valued function. In our case, the scalar function is the Potential.

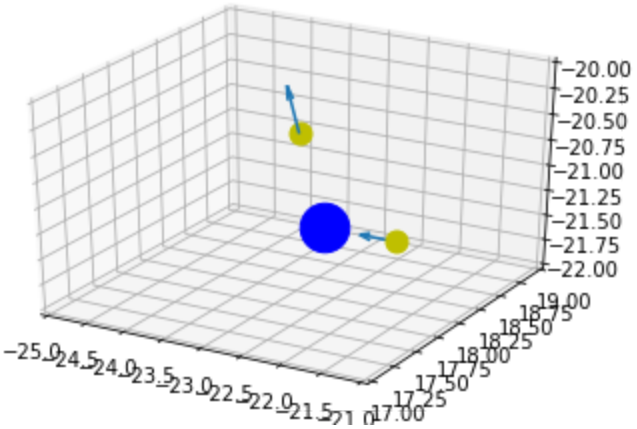
After calculating the Hessian, we can find the frequencies and hence the normal modes of the water molecules.

Normal Modes

For a single water molecule, the normal modes are outputted in this manner:

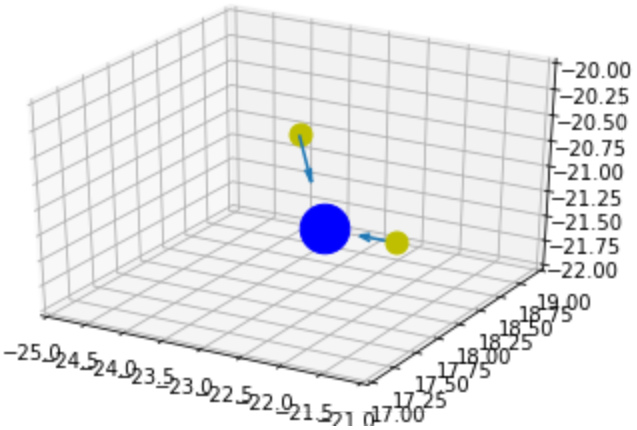
- Hydrogen-Oxygen Bonds - Alternate Stretching

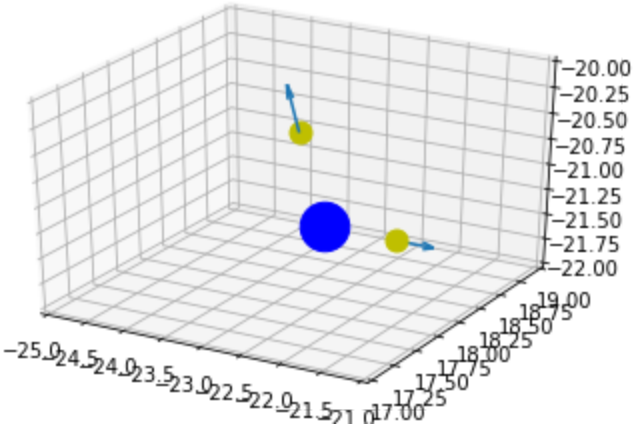




When one hydrogen bond shrinks, the other bond stretches

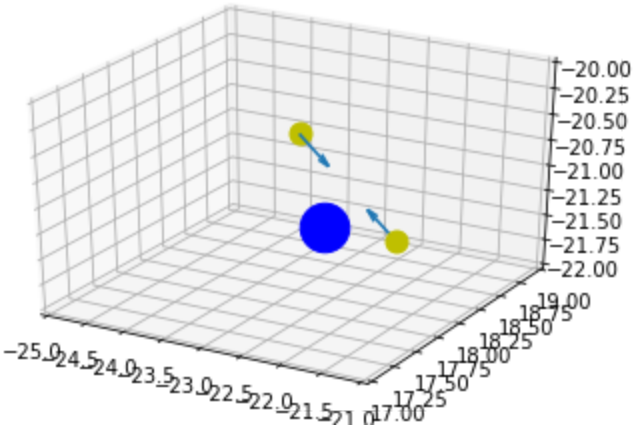
- Hydrogen-Oxygen Bonds - Stretching Together

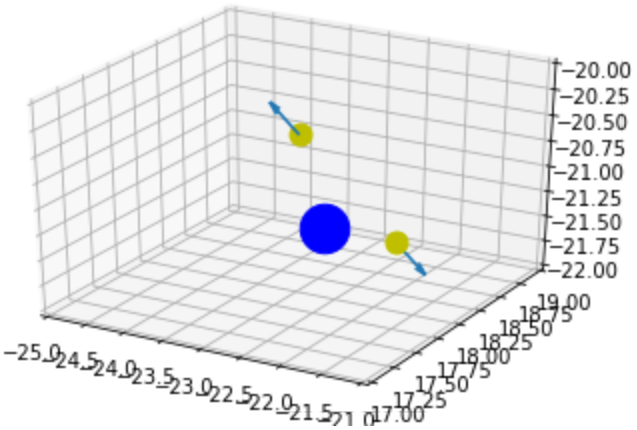




When both hydrogen bonds stretch and shrink together.

- HOH bond - Changing Angles





The bond angle between H-O-H increases and decreases with a given frequency.