Assignment3

November 30, 2017

1 CMM - Numerical Methods - Assignment 3

The included `data_files.tgz` contains a tarball of data files that will be used with this assignment.

1. [10 marks]

   The Morse potential can be defined by

   $$V(r) = D_e(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}).$$

   It can be used to fit the energy vs bond length of a diatomic molecule.

   Write a code called `Morse.py` that takes a filename as a single argument. Your code should be executable as e.g. `./Morse.py EvR.dat`.

   Your code should do the following:

   - Read the data from the filename given. You can assume it is a list of separation (Bohr) and energy (Hartree) values.
   - Fit a Morse potential to the data.
     - Note1: as the supplied data does not go zero as r increases, you will need to add an additional parameter to the fit expression to shift the large r value of the potential.
     - Note2: you may need to generate some sensible initial guesses for (some of) the fit parameters based on the input data or you could encounter convergence issues.
   - When the code is executed:
     - The fit parameters and errors associated with their values should be output to the terminal.
     - A plot of the input data along with the fit should be saved as a png file.

   The file "N2_EvR_LDA.dat" contains a Density Functional Theory calculation of the energy (Hartree) vs separation (Bohr) of a nitrogen molecule. You can use this to test your code.

2. [10 marks]

   The files suffixed `_dm` contain Density Functional Perturbation Theory calculations of the dynamical matrix of an N2 molecule at 6 different bond lengths from 2.0 to 2.5 Bohr, with the value associated with each file given in the file name. Write a Python code called `FvR.py` that when executed will:

- Parse the dynamical matrix from each file. These are in Hartree atomic units, and do not include the masses. (The electron mass is 1 in Hartree atomic units).
- Calculate the vibrational energy of the system at T=0 using only the highest vibrational frequency ($E_{\mathrm{v}ib} = \frac{1}{2}\hbar\omega$ where $\hbar = 1$ in Hartree atomic units) in Hartree for each bond length.
  - Note - while you'll get 6 frequencies, only the highest frequency is physical. The other 5 correspond to translational and rotational modes which should be comparitively small.
- Fit a straight line through the vibrational energy vs bond length.
- Your code should output the slope of this line in Ha/Bohr when executed.