University of the Witwatersrand

Computational Physics : 2004

Project 1 : Semi-Classical Quantisation of Molecular Vibrations in a Lennard - Jones Potential

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1. String together modules from Numerical Recipes in a "driver program" to perform the elementary mathematical operations discussed in Lecture 1. You can the calculate E_n, the energies of the quantised vibration states.

   (a) You will have to think quite carefully about the structure of your calculation in order to achieve the correct relationships between the various numerical components.

   (b) Usually, if this is your first excursion into Computational Physics, your calculation will initially be unstable and subject to run time errors and crashing, because of numerical issues related to external errors, internal errors and stability. At this stage, try to visualise the program flow and the values of variables with debugging software.

   (c) Once you have the program running, devise methods to explore the reliability of the results from a purely numerical point of view. Document these.

2. Now you can study the reliability of the results using your physics insight. Here, you would consider analgous problems, which may be simpler, or analytically solvable, or problems where your intuition about the behaviour is better informed. For example, if you have designed your code to be modular, then switch the Lennard-Jones potential for the Harmonic Oscillator potential. Note that it is sensible to tune the parameters of the Harmonic Oscillator potential by matching it to the Taylor expansion of the Lennard-Jones potential up to second order. Do you get evenly spaced energy levels ? Does the Lennard-Jones potential correspond to the Harmonic Oscillator potential at least near the minimum ? Now you can try the Square Well potential. This is also analytic.

3. Derive the result

$$\frac{\hbar\omega}{V_0} \sim \frac{10.7}{\gamma}$$

   Now run your program for different values of γ. To be realistic, consider that for H_2, $\gamma = 25$ and for O_2, $\gamma = 150$. Interpret the result. Does it conform to your intuition ?

4. Finally, visualise the energy levels within the potential and sketch the corresponding phase space trajectories. The simplest way is to generate output files of your results and read these into a scientific plotting program.