

Homework 4

Due Mon Oct 22 at the start of lecture (in class)

CIRCLE YOUR ANSWERS AND KEY INTERMEDIATE RESULTS

USE MAPLE WHENEVER POSSIBLE

STAPLE YOUR PAPERS TOGETHER

INCLUDE ALL COMPUTER PRINTOUTS (with commentary)

Levine Problems (5th Ed. in parenthesis) 6th Ed.

(4.16) 4.14 most likely particle position

(4.18) 4.19 3D SHO (note: you don't need to resolve you've already solved)

(4.27) 4.25 vibrations in LiH and ICl

(4.29) 4.28 Morse Potential – also: **c)** Given that $D_e = 7.31\text{E-}19$ J/molecule, and $a = 1.82\text{E}10$ m⁻¹ for HCl, calculate the force constant k for the HCl bond. Plot the Morse Potential for HCl and the corresponding Harmonic oscillator potential on the same graph.

d) for what displacements from equilibrium is the harmonic oscillator (HO) potential a good approximation of the Morse potential (*this requires only a qualitative answer*)?

e) For what physical situations would the HO potential yield a poor approximation to the actual potential? (*again, requires a qualitative answer*)

Additional Problems:

1) In lecture we derived the density of states for particle in a 3D box as:

$$D(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2},$$

starting with an approximation for the number of states with $n_x^2 + n_y^2 + n_z^2 \leq n^2$ as a function of n . Test this starting approximation by writing a program or routine in Maple (or C or Fortran or Basic or Labview or whatever) to calculate the ACTUAL number of states below the energy corresponding to a given n and compare it to the formula (and calculate % error of the formula) for values of n from $n=1$ to $n=200$ (i.e. $n^2=1$ to 40000).

2) In lecture we introduced the lowering operator as $a^- = \frac{1}{\sqrt{2\hbar\mu\omega}} (+ip + \mu\omega x)$

By arguing that energy can't be negative, we reasoned that there must be some state $|\psi_0\rangle$ for which $a^-|\psi_0\rangle = 0$. Use this relationship to generate a first-order differential equation for ψ_0 and solve the resulting differential equation (it should be a "simple" first-order equation) to find ψ_0 . The answer is the same as obtained with the power series solution in Levine.

3) Find ψ_1 , the first excited state of the SHO, by explicitly applying the raising operator, a^+ to ψ_0

4) The frequencies of the three normal modes of H₂O are $\omega_1=3833$ cm⁻¹ $\omega_2=1649$ cm⁻¹ and $\omega_3=3943$ cm⁻¹. If we describe a vibrationally excited state by the notation $(n_1 n_2 n_3)$ where n_i is the quantum number associated with the i^{th} normal mode, what is the energy of the (121) state? What is the energy difference between the (112) and (010) state? Side note not needed for the problem: anharmonicity in real bonds tends to mix the normal modes over time so energy will spread out between the modes.