Homework 4

Due Mon Oct 22 at 9:30 am in Prof. Ginger's mailbox

CIRCLE YOUR ANSWERS AND KEY INTERMEDIATE RESULTS

USE MAPLE WHENEVER POSSIBLE

STAPLE YOUR PAPERS TOGETHER

INCLUDE ALL COMPUTER PRINTOUTS (with commentary)

Levine Problems

4.16 most likely particle position

4.18 3D SHO

4.27 vibrations in LiH and ICl

Additional Problems

0) Additional Problem #6 From Homework #3

1) 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 $|\psi_0>$ for which $a^-|\psi_0>=0$ Use this relationship to generate a first-order differential equation for ψ_0 and solve the differential equation (it should be a "simple" first-order equation) to verify that ψ_0 is the same as obtained with the power series solution in Levine.

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

3) The frequencies of the three normal modes of H_2O are ω_1=3833 cm^{-1} ω_2=1649 cm^{-1} and ω_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: the anharmonicity in real bonds tends to mix the normal modes over time.

4) The spatial Parity operator P satisfies the eigenvalue equation: $P\ \psi = p\psi$ where the eigenvalues of P are $p=+1$ (if ψ is even) and $p=-1$ (if ψ is odd) . Only even and odd functions are eigenfunctions of P. We claimed in lecture that he symmetry of the Hamiltonian has important consequences for the symmetry of the allowed wave functions that we examine below.

4a) Show that if the Hamiltonian is a symmetric (even) function, then [P,H]=0 (hint: what is the parity of an even function times an even function, or an odd function times an odd function, i.e. $P(f_1f_2)$=?)

4b) *Two operators will commute if and only if they have a simultaneous set of eigenfunctions*. Use this fact, and your result from a) to justify that statement that "for a symmetric Hamiltonian, the only allowed energy eigenfunctions will be even and odd functions." The analysis of the spatial symmetry of a wavefunction is a very powerful tool that allows you to predict properties (i.e. IR and Raman activity of vibrational modes).