Chemistry 542
Fall, 2002
Problem Set 5
Due Monday, October 14

Read chapter 4, sections 1-3.

1. What is the probability of finding a harmonic oscillator in state v=1 at a distance greater than the classical turning point? First determine the turning point in reduced units and then evaluate the probability of y being greater than this value.

2. Use the recursion relation to determine the expectation value of x^4 for a harmonic oscillator in sate v. If you pay close attention to the lecture, you can save yourself a lot of work.

3. Analyze the vibrational properties of the HCl molecule, using the table from Herzberg. The date are given in wave numbers.
A. Calculate the force constant for the ground electronic state.
B. Calculate the vibrational energies the v=0 and 1 states, treating the molecule as anharmonic.
C. Calculate the wavelength of the 0-1 transituion.
D. Calculate the zero point displacement (i.e., the maximum stretch allowed classically) for v=0, assuming a harmonic wave function.
E. Repeat parts A-D for the V state of HCl.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (Å)
$^1H^{35}Cl$ (continued)							
X $^1\Sigma^+$	0	$2990.946_3{}^x$	52.8186^y	$10.59341_6{}^{xz}$	$0.30718_1{}^{a'}$	$5.3194^{zb'}$	$1.27455_2{}^{c'}$
V $^1\Sigma^+$	q 77293.$_0$	877.16 z	16.04^r	2.727	-0.026	1.02^r	2.512
	Continuous emission spectrum with maximum at 38900 cm^{-1}.						

4. Fill in the following details of the harmonic oscillator problem:
A Show that the classical kinetic energy of a harmonic oscillator is given by

$$T = \frac{1}{2}M\dot{R}^2 + \frac{1}{2}\mu\dot{r}^2$$

B Demonstrate that $\psi(y) \approx e^{-y^2/2}$ is an approximate solution derivation of the Schrodinger equation at large y.

C Using the transformation $\psi(y) = \varphi(y)e^{-\frac{1}{2}y^2}$, show that the Schrodinger equation becomes

$$\phi'' - 2y\phi' + \left(\alpha^2\beta - 1\right)\phi = 0 .$$

Levine, problems 11, 16, 25, 26, 27.