

CHEMISTRY 373 – TUTORIAL 5
PRACTICE FOR THE HARMONIC OSCILLATOR AND THE UNCERTAINTY
PRINCIPLE

February 9, 2000

A. Questions regarding the harmonic oscillator.

1. The wave functions for the harmonic oscillator can be written

$$\psi_n(x) = \sqrt{\frac{1}{n!}} (a^\dagger)^n \psi_0,$$

where n is a nonnegative integer and ψ_0 is the ground state wave function. Using the fact that a and a^\dagger are hermitian conjugates (adjoints), show that for $m \neq n$,

$$\int_{-\infty}^{+\infty} dx \psi_m^*(x) \psi_n(x) = 0,$$

that is ψ_m and ψ_n are orthogonal.

2. For the $n = 1$ state of the harmonic oscillator, find the most probable position(s) of a particle of reduced mass, μ .
3. Using the wave function from Question 1, show that

$$a\psi_n(x) = \sqrt{n} \psi_{n-1}(x), \quad a^\dagger \psi_n(x) = \sqrt{n+1} \psi_{n+1}(x).$$

4. For the ground state of a one-dimensional harmonic oscillator, find the average value of the kinetic energy, $\hat{T} = \frac{\hat{p}_x^2}{2\mu}$, and the potential energy, $\hat{V} = \frac{1}{2}k\hat{x}^2$. Verify that $\langle T \rangle = \langle V \rangle$.
5. The vibrations of a diatomic molecule can be approximated by a harmonic oscillator. Diatomic molecules undergoing vibrational transitions absorb and/or emit energy in the infrared part of the electromagnetic spectrum. The infrared spectrum of $^1\text{H}^{35}\text{Cl}$ has its strongest band at 8.65×10^{13} Hz. Calculate the force constant of the bond in this molecule. Predict the frequency of the strongest infrared band of $^1\text{H}^{37}\text{Cl}$. What assumption must you make in order to perform this calculation. Isotopic masses are: ^1H , 1.007852 amu; ^{35}Cl , 34.968854 amu; ^{37}Cl , 36.965896 amu.

B. General questions on quantum mechanics.

1. What are the similarities and differences between the particle in a box (1D) and the harmonic oscillator wave functions and energies.
2. Why are Hermitian operators important in quantum mechanics?
3. How do the differences between the classical and quantum mechanical harmonic oscillator exemplify the two major differences between the classical and quantum that we discussed earlier in the course?

C. Questions pertaining to uncertainty relations.

1. The uncertainty in a dynamical variable A is denoted by ΔA and is defined as $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$. Calculate the uncertainty in the position and momentum for a particle in a box (1D) of length, L , and show that the Heisenberg uncertainty relation for position and momentum is satisfied for each state, i.e., each value of the quantum number n .
2. Consider a one-dimensional system whose Hamiltonian, \hat{H} , is

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(x).$$

Suppose that the system is in an eigenstate, $\psi(x)$, of the Hamiltonian. Show that the uncertainty in the energy is zero. This is true in the general case, when the system is in an eigenstate of any operator, \hat{A} , the uncertainty in, A , is zero.

3. Compute Δx and Δp_x for the harmonic oscillator ground state. What value does the product of uncertainties $\Delta x \Delta p_x$ have? Does it obey Heisenberg's uncertainty relation?
4. In general, it can be shown that for two operators \hat{A} and \hat{B} , the uncertainty product is

$$(\Delta A)(\Delta B) \geq \frac{1}{2} \left| \int d^3 r \Psi^* [\hat{A}, \hat{B}] \Psi \right|.$$

Use this result to prove that $(\Delta x)(\Delta p_x) \geq \frac{\hbar}{4\pi}$ and $(\Delta y)(\Delta p_y) \geq \frac{\hbar}{4\pi}$, but $(\Delta x)(\Delta p_y) = (\Delta y)(\Delta p_x) = 0$. What do the latter two relationships imply?