Chemical Physics Cumulative Examination
February 20, 2008

This exam covers the Schrödinger equation and its applications. To receive full credit you will need to show all work, equations and units used to reach the final answer. Indicate clearly your final answers to each question. A total of 100 points are available.

1) The time-independent Schrödinger equation is a linear, homogeneous, second order differential equation. Find the roots of the following differential equation for the given trial solution and express the general solution for y(x) in terms of sin and cos functions. (15 points)

$$\text{Equation: } y'' + 2y' + 10y = 0$$

$$\text{Trial Solution: } y(x) = e^{\alpha x}$$

2) a) Define the requirements for an acceptable wavefunction. (5 points)

b) Determine which of the following functions are acceptable or not as wavefunctions over the indicated intervals. If the function is unacceptable state why. (10 points)

$$(1-x^2)^{-1}, \quad -1 \le x \le 1$$

$$e^{-x}\cos x, \quad 0 \le x \le \infty$$

$$\tan^{-1} x, \quad 0 \le x \le \infty$$

3) Consider a particle trapped in a potential well defined by: (30 points)

$$V = \infty \quad \text{for} \quad x < 0$$

$$V = 0 \quad \text{for} \quad 0 \le x \le a$$

$$V = \infty \quad \text{for} \quad x > a$$

a. Draw the potential well.
b. Write a general expression for the wavefunction in each region and solve for the energy.
c. Calculate the probability that the particle is between 0 and a/2.
d. Assuming an electron in a carbon chain can be treated as a particle in a box, calculate the energy difference between the n=1 and n=2 states for an electron trapped in a 1,3-pentadiene chain which has a length of 5.60Å. (m_e=9.10x10^{-31} kg, h=6.63x10^{-34} J*s)
e. How does this value compare with the actual absorption spectrum that has a maximum of 224nm? (c=2.998x10^{8} m/s)

4) Consider an electron trapped in a well defined by: (30 points)

$$V = \infty \quad \text{for} \quad x < 0$$

$$V = 0 \quad \text{for} \quad 0 \le x \le a$$

$$V = +V_0 \quad \text{for} \quad x > a$$

a) Draw the potential well.
b) Write a general expression for the wavefunction in each region and solve for the energy.
c) How many bound levels will the potential well support assuming V_0=10eV and a=5nm? (m_e=9.10x10^{-31} kg, h=6.63x10^{-34} J*s, 1eV=1.602x10^{-19}J)
d) For what range of a are there *no* bound levels?