CHM 3411 – Problem Set 3
Due date: Wednesday, January 30th
Do all of the following problems. Show your work.

1) Two of the normalized solutions to the particle in a box problem discussed in class are

$$\psi_2(x) = (2/L)^{1/2} \sin(2\pi x/L) \quad (1.1)$$

$$\psi_3(x) = (2/L)^{1/2} \sin(3\pi x/L) \quad (1.2)$$

inside the box, and zero outside the box ($x < 0$ or $x > L$).

a) Show that $\psi_2(x)$ is normalized.

b) Show that $\psi_3(x)$ is orthogonal to $\psi_2(x)$.

c) Find the value for the probability of being between 040 L and 0.60 L for a particle in the n = 2 state of a particle in a box.

d) Find the value for $\langle p \rangle$ and $\langle p^2 \rangle$ for a particle in the n = 2 state of a particle in a box.

e) Using the expression for uncertainty

$$\Delta p = [\ \langle p^2 \rangle - \langle p \rangle^2\ ]^{1/2} \quad (1.3)$$

and your answers in d find the value for Δp for a particle in the n = 2 state of the particle in a box.

2) Consider the function

$$f(x) = \exp(ikx) \quad 0 < x < L \quad (2.1)$$

$$f(x) = 0 \quad x < 0 \text{ or } x > L \quad (2.2)$$

as a possible solution to the particle in a box system discussed in class.

a) Is f(x) an eigenfunction of the Hamiltonian operator for the particle in a box? If your answer is yes, what is the corresponding eigenvalue?

b) Is f(x) an acceptable wavefunction for the particle in a box? Why or why not?

3) Let ψ_1 and ψ_2 be solutions to a particular TISE

$$\hat{H}\,\psi_1 = E_1\,\psi_1 \quad (3.1)$$

$$\hat{H}\,\psi_2 = E\,\psi_2 \quad (3.2)$$

a) Show that the function

$$\phi = a\,\psi_1 + b\,\psi_2 \quad (3.3)$$

where a and b are constants is also a solution to the same TISE <u>if and only if</u> $E_1 = E_2$.

b) Assume that ψ_1 and ψ_2 are normalized functions. What is the requirement for the constants a and b that will make ϕ a normalized function?

4) The fundamental vibrational frequency for the cyanide radical CN is $\omega = 2068.7\ cm^{-1}$. Based on this, find the value for k, the force constant for the bond in the CN radical (note that a large value for k implies a strong chemical bond). The masses for the atoms involved are $m(^{12}C) = 12.000$ amu and $m(^{14}N) = 14.0031$ amu.