CHM 6480 – Problem Set 2
Due date: Friday, September 11th (by noon)
Do all of the following problems. Show your work.

1) In solving the TISE for a particle in a box using the series solution method, the following expression was obtained:

$$\Sigma_{n=0}^{\infty} a_{n+2}\, x^n = - (2mE/\hbar^2)\, \Sigma_{n=0}^{\infty} \frac{a_n\, x^n}{(n+1)(n+2)} \qquad (1.1)$$

As discussed in class, the only way this equation can be true in general is if the coefficients on the left and right side for each term x^n are equal.

a) Using eq 1.1, find an expression for a_3 in terms of a_1.

b) Using eq 1.1, find an expression for a_5 in terms of a_3.

c) Using your result in a and b, find an expression for a_5 in terms of a_1.

d) Based on the above answers, find a general expression for a_{2n+1} in terms of a_1. (You can check your answer by comparison with the result given in Handout 2).

2) Using the boundary conditions for the particle in a box we found the following relationship for the even symmetry (cosine) solutions to the TISE

$$kb = (s + ½)\,\pi \qquad s = 1, 2, 3, \ldots \qquad k = (2mE/\hbar^2)^{1/2} \qquad (2.1)$$

a) Starting with eq 2.1, find an expression for E_s, the energy for an even symmetry solution to the particule in a box, in terms of s.

b) Define a new quantum number n as

$$n = 2\,(s + ½) \qquad (2.2)$$

Show that eq 2.2 leads to the following expression for the values of energy for the even symmetry solutions to a particle in a box

$$E_n = \frac{n^2 h^2}{32mb^2} \qquad n = 1, 3, 5, \ldots \qquad (2.3)$$

Note that by using this same procedure for the odd symmetry (sine) solutions to the particle in a box we can write all of the allowed values for energy in term of a single expression.

3) We showed in class that the expectation values for position and momentum for any state of the particle in a box (as defined in lecture) are $\langle x\rangle = 0$, $\langle p\rangle = 0$.

a) Find the values for $\langle x^2\rangle$ and $\langle p^2\rangle$ for a particle in a box in the n = 1 state.

b) The uncertainty in position and momentum can be defined as:

$$\Delta x = [\, \langle x^2\rangle - \langle x\rangle^2 \,]^{1/2} \qquad (3.1)$$

$$\Delta p = [\, \langle p^2\rangle - \langle p\rangle^2 \,]^{1/2} \qquad (3.2)$$

Find the values for Δx and Δp for a particle in a box in the n = 1 state.

c) Based on your answer in b, find the value for the product of the uncertainties in position and momentum for a particle in a box in the n = 1 state.

d) The Heisenberg uncertainty relationship predicts that your answer in c should satisfy the relationship

$$(\Delta x)\,(\Delta p) \geq \hbar/2 \qquad (3.3)$$

Is this prediction correct? Explain.

4) The following question explores the concept of the Bohr Correspondence Principle, the idea that quantum systems generally behave more and more classically in the limit of large quantum numbers.

a) For a classical particle in box, find the values for $<x>$, $<x^2>$, and Δx (Δx is defined in the previous problem). Note that your values here apply to the average values that would be observed over a long period of time, and assuming no knowledge of x_0 and p_0, the values for position and momentum at t = 0.

b) Find the values for $<x>$, $<x^2>$, and Δx for a quantum mechanical particle in a box in the limit $n \rightarrow \infty$ (where n is the quantum number for the particle).

c) Does your answer in b agree with the expectations of the Correspondence Principle? Explain.

5) In class, we claimed that the solutions to a TISE are orthogonal to one another, that is

$\int \psi_j^* \psi_i \, dx = 0$ when $i \neq j$ (note the integral is over all possible values of x) (5.1)

In this problem we will prove this statement for the case where the solutions to the TISE are singly degenerate (only one solution for each allowed value for energy). This will also give us some practice in using Dirac notation. Note that in Dirac notation the requirement that operators are Hermitian

$\int \psi_i^* \hat{O} \psi_j \, dx = (\int \psi_j^* \hat{O} \psi_i \, dx)^*$ (5.2)

can be written as

$< i | \hat{O} | j > = < j | \hat{O} | i >^*$ (5.3)

Consider two different solutions to a particular TISE

$\hat{H} | i > = E_i | i >$ (5.4)

$\hat{H} | j > = E_j | j >$ (5.5)

If we left-multiply both sides of eq 5.4 by $< j |$, and left-multiply both sides of eq 5.5 by $< i |$, the result is

$< j | \hat{H} | i > = < j | E_i | i > = E_i < j | i >$ (5.6)

$< i | \hat{H} | j > = < i | E_j | j > = E_j < i | j >$ (5.7)

. a) Take the complex conjugate of both sides of the equation 5.6. Show that the left hand side of the equation you obtain is equal to the left side of eq 5.7.

b) Based on your answer in a, show that $< i | j > = 0$.

Note that for the more general case, where there can be several states with the same value for energy, you can always find a complete set of solutions to the TISE that are orthogonal to one another, but this is more difficult to prove.

6) Let **A**, **B**, and **C** be quantum mechanical operators. Show that

$[\mathbf{A}, \mathbf{BC}] = [\mathbf{A},\mathbf{B}]\mathbf{C} + \mathbf{B}[\mathbf{A},\mathbf{C}]$ (6.1)

7) Consider the following function (sketched below)

$$f(x) = A \qquad -b/2 \le x \le b/2 \qquad (7.1)$$

$$= 0 \qquad x < -b/2 \text{ or } x > b/2$$

a) What value for A makes f(x) a normalized function?

b) The solutions to a TISE form a complete orthonormal set of functions (a basis set). Any function with the same domain and boundary conditions as the TISE can be expressed in terms of a linear combination the solutions to the TISE. In the aboce case, that means

$$f(x) = a_1 \mid 1 > + \, a_2 \mid 2 > + \, a_3 \mid 3 > + \ldots \qquad (7.2)$$

$$= \Sigma_{n=1}^{\infty} a_n \mid n >$$

Find a general expression for the coefficients a_n for the function given by eq 7.1.

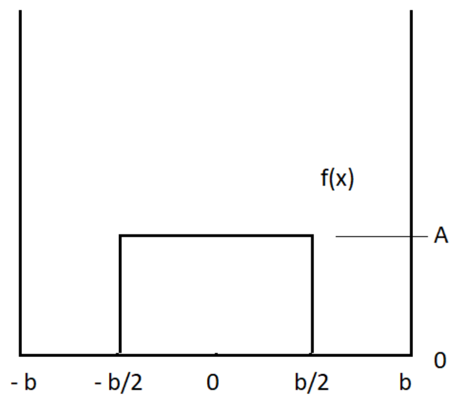

Figure 7.1 f(x), as described by eq 7.1