CHM 3411, Dr. Chatfield, Spring 2018
Problem Set 3
Due Monday, Feb 5

Suggested "warmups" (not to turn in): Discussion questions 7C.1-3; Exercises [all (b)] 7C.1-7 (except the assigned ones below)

Problems 1-5 explore principles of quantum mechanics (operators, orthogonality, Heisenberg's uncertainty principle). Problems 5-8 explore the particle in a box. Note that in some cases, Atkins' Exercises are assigned.

1. Exercise 7C.1b (constructing an operator)

2. Exercises 7C.3b and 7C.4b (same topic: orthogonality)

3. Exercise 7C.5b (construct a quantum mechanical operator)

4. (This is Problem 7C.10 omitting the last part. It is a more advanced problem on operators and superposition) The wavefunction of an electron in a linear accelerator is $\psi = (\cos\chi)e^{ikx} + (\sin\chi)e^{-ikx}$, where χ (chi) is a parameter. (i) What is the probability that the electron will be found with a linear momentum (a) $+k\hbar$, (b) $-k\hbar$? (ii) What form would the wavefunction have if it were 90 per cent certain that the electron had linear momentum $+k\hbar$?

5. Consider the n=3 wavefunction for the one dimensional particle in a box of length L:

$$\psi_3(x) = \left(\tfrac{2}{L}\right)^{1/2}\sin\left(\tfrac{3\pi x}{L}\right) \qquad \text{where } 0 < x < L$$

(a) Calculate the probability that the particle is in the region between 0 and 0.2 L.
(b) Calculate Δx and Δp, and show that the Heisenberg uncertainty principle is satisfied. To do this, you will need to calculate the expectation values $<x>$, $<x^2>$, $<p>$ and $<p^2>$. The first is the average position, the second is the average of the square of the position, and likewise for the momentum expectation values. Note that the interval for the integrations is 0 to L (the wavefunction is defined as 0 outside of this range). From these expectations values, Δx and Δp can be calculated using:

$$\Delta x = [<x^2> - <x>^2]^{1/2} \qquad \text{and} \qquad \Delta p = [<p^2> - <p>^2]^{1/2}$$

6. Exercise 8A.3b (1-D particle in a box energies)

7. Exercise 8A.9b (3-D particle in a box energies)

8. (This is Problem P8A.1 slightly adjusted.) (a) Calculate the separation between the two lowest energy levels for an O_2 molecule in a one-dimensional container of length 5.0 cm. [you are to imagine a particle that is one-dimensional (to keep things simple) but has the mass of normal O_2] (b) The average energy of such a particle is ½ kT. Determine the value of the quantum number *n* that this energy corresponds to when T=300 K.