Chemistry 3730 Fall 2002 Test 1

Write all your answers in the booklets provided. You are entitled to *one* $8\frac{1}{2} \times 11$-inch piece of paper containing any information you want. (Some data is also given at the end of this test paper.) Hand-held calculators are allowed. You may use Maple and its help system. No other aids, printed or electronic, are allowed.

If you use Maple to solve a problem, it is *your responsibility* to make it clear what you are doing. I expect to see the mathematical expressions evaluated using Maple, but *not* the Maple commands used to evaluate them.

Time: 2 h

Total marks: 50

1. Calculate the probability that a particle in a two-dimensional square box of side L occupies the rectangle defined by $L/5 \leq x \leq L/3$, $0 \leq y \leq L/8$ if the quantum numbers are $n_x = 2$, $n_y = 1$. Report your answer to four digits. [8 marks]

   Maple hints: Don't forget that π is `Pi` in Maple and that square roots are obtained with the `sqrt()` function. To get a numerical value from an exact result, use the `evalf()` function.

2. (a) Explain what it means for a wavefunction to be normalized and why this is an important property. [4 marks]

   (b) We will see later that we can use approximate methods to solve quantum mechanical problems. Suppose that $\phi(x) = x(L-x)$ is an approximate particle-in-a-box wavefunction and normalize it. [6 marks]
   See the syntactic hints for question 1.

   (c) To which of the true particle-in-a-box wavefunctions is the approximate wavefunction $\phi(x)$ orthogonal? [8 marks]

   Maple hints: See the syntactic hints for question 1. Maple may need to know that the quantum number n in the exact wavefunctions is an integer.

3. For the particle in a one-dimensional box, calculate a general expression for the expectation value of x^2. How does this quantity behave in the limit of large quantum number n? [8 marks]

   Maple hints: See the hints for question 2c. It may be necessary to use the `simplify()` command to get the simplest form of the general expression.

4. Is L_x compatible (a) with x? (b) with y? [10 marks]

5. True or false: If $\hat{A}$ commutes with $\hat{B}$ and $\hat{B}$ commutes with $\hat{C}$, then $\hat{A}$ commutes with $\hat{C}$. If the statement is true, provide a proof. If false, provide a counterexample. [6 marks]

Useful information

Particle-in-a-one-dimensional-box wavefunctions:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right).$$

Particle-in-a-two-dimensional-box wavefunctions:

$$\psi_{n_x,n_y}(x) = \frac{2}{\sqrt{L_x L_y}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right).$$