Chemistry 542
Fall, 2002
Problem Set 10
Due Monday, December 2

Read Chapter 8. This problem set covers parts of chapter 7 and 8.3, 8.4, 8.6. The remaining parts of chapter 8, and hopefully parts of chapter 9 will be covered next week, as time allows.

1. This problem fills in the details of the derivation of the Uncertainty Principle.

A. Show that $\left\langle \left[\hat{A}-\langle\hat{A}\rangle\right]^2 \right\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$ (This is a one line proof.)

B. Show that for any pair of linear operators, $\hat{A}$ and $\hat{B}$, the following identity holds:

$$\left(\hat{A}-\langle\hat{A}\rangle\right)\left(\hat{B}-\langle\hat{B}\rangle\right)=\frac{1}{2}\hat{F}+\frac{1}{2}\left[\hat{A},\hat{B}\right],$$

where

$$\hat{F}=\left\{\left(\hat{A}-\langle A\rangle\right)\left(\hat{B}-\langle B\rangle\right)+\left(\hat{B}-\langle B\rangle\right)\left(\hat{A}-\langle A\rangle\right)\right\}.$$

In class we proved that if $\hat{A}$ and $\hat{B}$ are Hermitian, their commutator equals $i\hat{C}$, where $\hat{C}$ is also Hermitian. Note that in class the first ½ was missing.

C. Show that if $\hat{A}$ and $\hat{B}$ are Hermitian, then $\hat{A}\hat{B}+\hat{B}\hat{A}$ is also Hermitian.

D. The Schwarz inequality was given in class for real functions. Levine gives the following more general result, which applies to complex functions as well. You can think of this inequality as a statement about overlap integrals,

$$4\langle f\,|\,f\rangle\langle g\,|\,g\rangle \ge \left[\langle f\,|\,g\rangle+\langle g\,|\,f\rangle\right]^2$$

Demonstrate this inequality for the real functions,

$$f = x$$
$$g = x-1,$$

over the interval $0 \le x \le L$.

At this point, you should be able to piece together the entire derivation of the Uncertainty Principle..

2. Using the matrix representations of $\hat{L}_{x,}\hat{L}_{y,}\hat{L}_z$ derived in class for $l=1$, demonstrate that

$$\left[\hat{L}_{x,}\hat{L}_y\right]=i\hbar\hat{L}_z$$

Also show that the identity $\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = \hat{L}^2$ is satisfied.

3. Derive the matrix representation of the operators $\hat{L}^2, \hat{L}_{+}, \hat{L}_{-}, \hat{L}_{x}, \hat{L}_{y}, \hat{L}_z$ for the case of $l = 2$.

4. Repeat problem 3 for l = ½. The matrices for $\hat{L}_{x}, \hat{L}_{y}, \hat{L}_z$ are called the Pauli spin matrices.

Levine 7.55, 7.56, 8.37, 8.42.