Chem 532: Problem Set #1

Due by 5pm: Friday, Sept. 9th

(1) Demonstrate whether $x^2 \frac{d}{dx}$ and $x \frac{d^2}{dx^2}$ commute. What about $x \frac{d}{dx}$ and $x^2 \frac{d^2}{dx^2}$?

(2) If A and B are hermitian operators, prove

(a) that their product AB is hermitian only if A and B commute

(b) that $\frac{1}{2}(AB+BA)$ is hermitian

(c) that A + *i*B and A – *i*B are not hermitian

(3) Consider the following normalized hydrogen atom wave functions that are degenerate eigenfunctions of the (hermitian) total angular momentum operator L^2.

$$2p_1 = \frac{-1}{8\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{5/2} re^{-r/(2a_0)}\sin\theta\, e^{i\phi}$$

$$2p_{-1} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{5/2} re^{-r/(2a_0)}\sin\theta\, e^{-i\phi}$$

$$2p_x = \frac{1}{\sqrt{2}}\left(2p_{-1}+2p_1\right) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{5/2} re^{-r/(2a_0)}\sin\theta\cos\phi$$

where a_0 is a constant.

(a) Show that $2p_x$ and $2p_1$ are not orthogonal. (Note: $2p_1$ and $2p_{-1}$ are orthonormal)

(b) Use Schmidt orthogonalization to construct linear combinations of the functions of part (a) that will be orthogonal and then normalize these functions.
(Note: you can do both parts without actually doing any integrals)

(4) The (hermitian) operators for energy and angular momentum for an electron constrained to move in a ring of constant potential are, respectively, $-\left(\frac{1}{2}\right)\frac{d^2}{d\phi^2}$ and $\left(\frac{1}{i}\right)\frac{d}{d\phi}$.

(a) Discuss/show whether or not there should be a set of functions that are simultaneously eigenfunctions for both operators.

(b) Discuss whether or not there is a set of functions that are eigenfunctions for one of these operators but not the other.