Chemistry 30321 Fall 2012
Professor J. Daniel Gezelter Due Fri. 9/14/2012

Problem Set 3
(Operators, Particles in Boxes)

1. Do problem 3-3 in McQuarrie and Simon.
2. Evaluate the operator $\hat{A}^2$ for $\hat{A} =$

   a) $\frac{\partial^2}{\partial x \partial y}$

   b) $\frac{d^2}{dx^2} + x\frac{d}{dx}$

   c) $\frac{\partial}{\partial x}\hat{\mathbf{i}} + \frac{\partial}{\partial y}\hat{\mathbf{j}} + \frac{\partial}{\partial z}\hat{\mathbf{k}}$

   ($\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$, and $\hat{\mathbf{k}}$ are the unit vectors along the x, y, and z axes.)

   (Hint: Be sure to include $f(x,y,z)$ before carrying out the operations.)
3. Determine whether or not the following pairs of operators commute, and be careful with partial vs. total derivatives!

$\hat{\mathbf{A}}$	$\hat{\mathbf{B}}$
$\sqrt{}$	x
$\frac{d^2}{dx^2}$	$\frac{d^3}{dx^3} + x\frac{d}{dx}$
$\frac{\partial}{\partial x}$	$\frac{\partial^2}{\partial y \partial z}$
$\frac{d}{dx}$	$\frac{d^2}{dx^2} + y\frac{d}{dx}$

4. Calculate the value of a that makes e^{-ax^2} an eigenfunction of the operator $\hat{A} = \frac{d^2}{dx^2} - Bx^2$, where B is a constant. What is the corresponding eigenvalue?
5. Do problem 3-9 in McQuarrie and Simon
6. Do problem 3-11 in McQuarrie and Simon
7. Do problem 3-13 in McQuarrie and Simon