Fall 2011 CHEM 760: Introductory Quantum Chemistry

Homework 1

1 a) Find the real and imaginary parts of the following quantities

$(2\text{-}i)^3$, $e^{-2+i\pi/2}$, and $(\sqrt{2}+2i)e^{-i\pi/2}$

b) Express the following complex numbers in the form $re^{i\theta}$

$4-\sqrt{2}i$, and $\pi + ei$

2. If $g(x) = \hat{A}f(x)$, where $g(x)$and $f(x)$ are functions and $\hat{A}$ is an operator, find $g(x)$ for the system below. Does this system represent an eigensystem? If so, label the eigenfunction and the eigenvalue.

$\hat{A} = \frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx}$, and $f(x) = 4x^3$

3. The Laplace transform operator $\hat{L}$ is defined as $\hat{L}f(x) = \int_0^\infty e^{-px}f(x)dx$.

Is this operator linear? Justify your answer.

4. The operators $\hat{A}$ and $\hat{B}$ are defined as $\hat{A} = \frac{d^2}{dx^2}$, and $\hat{B} = x^2$.

Use these definitions to prove $\hat{A}\hat{B} - \hat{B}\hat{A} = 2 + 4x\frac{d}{dx}$.

5. Writ out $\hat{A}^2$ for $\hat{A} = \frac{d}{dx} + x$.

Hint: include f(x) before carrying out the operation.

6. Determine whether the following functions are acceptable or not as wave functions over the indicated intervals.

a) $\frac{1}{x}\,[0,\infty]$, b) $e^{-2x}cosx\ [0,\infty]$, and c) $e^x[-\infty.\infty]$.

7. Which of the following wave functions are normalized over the indicated two-dimensional intervals?

a) $e^{-\frac{x^2+y^2}{2}}, 0 \le x \le \infty, 0 \le y \le \infty$

b) $e^{-\frac{x+y}{2}}, 0 \le x \le \infty, 0 \le y \le \infty$

c) $(\frac{4}{ab})^{1/2} sin\frac{\pi x}{a} sin\frac{\pi y}{b}, 0 \le x \le a, 0 \le y \le b$

Normalize those that aren't.

8. Why does $\Psi^*\Psi$ have to be everywhere real, nonnegative, finite and definite value?

9. Consider the linear differential equation

$$a(x)y''(x) + b(x)y'(x) + c(x)y(x) = 0$$

where $y''(x)$ and $y'(x)$ are standard notation for d^2y/dx^2 and dy/dx, respectively. Show that if $y_1(x)$and $y_2(x)$ are each solutions to the above differential equation, then so is $y(x) = c_1y_1(x) + c_2y_2(x)$ where c_1 and c_2 are constants.

10. Calculate the values of $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$ for a particle in a box in the state described by

$$\Psi(x) = \left(\frac{630}{a^9}\right)^{\frac{1}{2}} x^2 (a-x)^2 \text{ }, 0 \leq x \leq a$$

11. Show that if $\hat{A}$ is Hermitian, then $\hat{A} - \langle a \rangle$ is Hermitian.
12. Given that $f_0(x) = a_0$ and $f_1(x) = a_1 + b_1 x$, find the constants such that $f_0(x)$ and $f_1(x)$ are orthonormal over the interval $0 \leq x \leq 1$.