Chemistry 60649 Fall 2008
Professor J. Daniel Gezelter Due Wed. 9/3/2008

Problem Set 1

1. We will make extensive use of complex numbers in this class. Complex numbers include all of the real numbers, and are also extended by the addition of the imaginary number i, with

$$i = \sqrt{-1}$$

For any real numbers a and b, we have the complex number c

$$c = a + bi$$

Examples include: 7 ($a = 7, b = 0$); $2.37i$ ($a = 0, b = 2.37$); $22.3 + 0.61477\overline{7}i$, etc.

We can also define the *complex conjugate* of c, written as c^*:

$$c^* = a - bi$$

The main purpose of this is to provide a definition for the *square modulus* of a complex number, $|c|^2$:

$$|c|^2 \equiv cc^*$$

Prove:

a) The complex conjugate is *distributive* — i.e., for two complex numbers c_1 and c_2,

$$(c_1 c_2)^* = c_1^* c_2^*$$

b) For any complex number c, the square modulus $|c|^2$ is always a positive real number.

2. A Taylor series can be used to represent many functions. The definition of a Taylor series of the function f around an arbitrary point a is:

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d^n f}{dx^n} \right)_{x=a} (x-a)^n$$

Show explicitly that the first three terms of each of the functions e^x, $\cos x$, and $\sin x$ are given by:

$$\begin{aligned} e^x &= 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots \\ \cos x &= 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \\ \sin x &= x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \end{aligned}$$

3. When we first learn about exponential and trigonometric functions, we usually work with an argument (x) that is real. Now consider an *imaginary* exponent, $x = i\theta$ (θ real):

   a) Use the power series in problem 2 to derive **Euler's relation**:

   $$e^{i\theta} = \cos\theta + i\sin\theta$$

   [Note that this provides the interesting identity, $e^{i\pi} + 1 = 0$]

   b) Show that

   $$\left(e^{i\theta}\right)^* = e^{-i\theta}$$

   and thus

   $$\left|e^{i\theta}\right|^2 = 1$$

   for any value of θ.

   c) Show that *any* complex number c can be expressed as

   $$c = a + bi = re^{i\theta}$$

   where a, b, r, and θ are all real. Express a and b in terms of r and θ.

4. If we have two complex variables ψ and χ where

$$\begin{aligned} \psi &= |\psi|e^{i\alpha_1} \\ \chi &= |\chi|e^{i\alpha_2} \end{aligned}$$

(where α_1 and α_2 are real variables) show that

$$|\psi + \chi|^2 = |\psi|^2 + |\chi|^2 + 2|\psi\chi|\cos(\alpha_1 - \alpha_2)$$

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

   (Hint: you should have a non-zero result here)

6. Determine whether or not the following pairs of operators commute:

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

7. 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?

8. A particle constrained to move in one dimension (x) is in the potential field

$$V(x) = \frac{V_0(x-a)(x-b)}{(x-c)^2} \qquad (0 < a < b < c < \infty)$$

a) Make a sketch of V.

b) Discuss the possible classical motions, forbidden domains, and turning points. Specifically, if the particle is known to be at $x = -\infty$ with

$$E = \frac{3V_0}{c-b}(b - 4a + 3c)$$

at which value of x does it reflect?