Chemistry 30321 Professor J. Daniel Gezelter

Fall 2012 Due Fri. 8/31/2012

Problem Set 1 (Complex Numbers, Taylor Series, Euler's Relation) This one is longer, but should still be largely a review of previous material.

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 z

$$z = a + bi \tag{1}$$

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

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

$$z^* = a - bi \tag{2}$$

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

$$|z|^2 \equiv zz^*$$

a) Prove that the complex conjugate is *distributive* — i.e., for two complex numbers z_1 and z_2 ,

$$(z_1 z_2)^* = z_1^* z_2^*$$

- b) Prove that for any complex number z, the square modulus $|z|^2$ 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:

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d^n f}{dx^n}\right)_{x=a} (x-a)^n \tag{3}$$

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

$$e^{x} = 1 + x + \frac{x^{2}}{2} + \frac{x^{3}}{3!} + \frac{x^{4}}{4!} + \cdots$$

$$\cos x = 1 - \frac{x^{2}}{2} + \frac{x^{4}}{4!} - \frac{x^{6}}{6!} + \cdots$$

$$\sin x = x - \frac{x^{3}}{3!} + \frac{x^{5}}{5!} - \frac{x^{7}}{7!} + \cdots$$

(You can stop after you get the first three terms).

- 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 series expressions 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. Do problem A-6 in McQuarrie and Simon.
- 5. Do problem C-3 in McQuarrie and Simon.
- 6. Do problem C-8 in McQuarrie and Simon.
- 7. Extra Credit: Do problem A-9 in McQuarrie and Simon.