Chem237: Lecture 5

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Integrals Continued

Complex Calculus

Complex Calculus is a large field (typically a 1-year course) we will highlight some useful integration techniques using the complex plane.

Analytic Function

Consider the 2D complex plane. Analytic function in domain (D) if it has derivative for any Z in D.

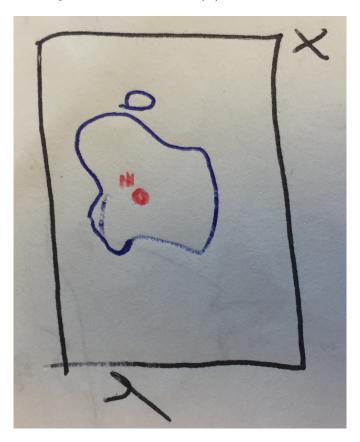


Figure 1: Under-Damped HO. The real part of the solution (blue), for the un-driven, under-damped harmonic oscillator. The dotted line (green) shows that the amplitude of the function (and the function itself) slowly decays to zero over time.

$$f'(z) = \lim_{h \to 0} \frac{f(z+h) - f(z)}{h}$$
 (1)

f(z) is regular in D if it is analytic and single valued in D. Examples of non singled valued functions are square roots $f(z) = \sqrt{z}$ and logarithm functions $f(z) = \ln{(1+z)}$

Cauchy Riemann equations

The Cauchy-Riemann equations are used to check if a complex function is analytic (sometimes referred to as holomorphic), in other words if it is differentiable. It is often useful to define complex functions into their real and complex parts as follows:

$$f(z) = u(x,y) + iv(x,y) \tag{2}$$

The Cauchy-Riemann equations are derived from taking a differential with respect to x and y and then relating the Real part and imaginary part. Note: that for the imaginary piece we multiply by i thus getting a negative:

$$\frac{\partial f}{\partial x} = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} = \frac{1}{i} \frac{\partial f}{\partial y} = \frac{1}{i} \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}
\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}
\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}$$
(3)

Example of an analytic function:

$$f(z) = z^{2} = x^{2} - y^{2} + i(2xy)$$

$$u = x^{2} + y^{2}$$

$$v = 2xy$$

$$\frac{\partial u}{\partial x} = 2x \frac{\partial v}{\partial y}$$

$$\frac{\partial v}{\partial x} = 2y - \frac{\partial u}{\partial y}$$

$$(4)$$

Example of a non-analytic:

$$f = z* = x - iy$$

$$\frac{\partial u}{\partial x} = 1 \neq \frac{\partial v}{\partial y} = -1$$
(5)

Cauchy-Theorem

The Cauchy theorem states an integral is path independent if f(z) is regular in D ϵ L. Where L denotes a path integral.

$$\int_{L}^{z_2} f(z)dz \tag{6}$$

More commonly it is written as a contour:

$$\oint_{C\epsilon D} f(z)dz = 0 \tag{7}$$

The definition of an analytic function is only the first derivative of f(z) exists. If f(z) is ? in D:

$$\frac{d^n}{dz^n}f(z) \tag{8}$$

exists for any n. $f^{(n)}(z)$ is a result function in D.

Cauchy Integral Formula

The general formula for the Cauchy integral formula is as follows:

$$f^{n}(z) = \frac{d^{n}f}{dz^{n}} \frac{n!}{2\pi i} \oint \frac{f(w)dw}{(w-z)^{n+1}}$$

$$\tag{9}$$

Where n is the order of your function.