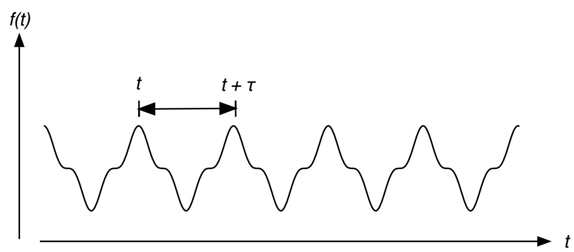
Chemistry 20262 | Spring 2018
Professor J. Daniel Gezelter | Due Fri. 3/2/2018

Problem Set 5
(Differential Equations)

1. McQuarrie, problem 6-12.

2. McQuarrie, problem 6-13. If a function $f(t)$ is periodic, it will repeat itself with *period* τ. This means that:

$$f(t+\tau) = f(t)$$



Since the frequency (ν) is inversely related to the period ($\nu = 1/\tau$), this means that a function with frequency ν will have this property,

$$f(t+\frac{1}{\nu}) = f(t)$$

The problem asks you to show that a function has a frequency, $\nu = \omega/2\pi$. What you are being asked to do is to prove the following:

$$f(t+\frac{2\pi}{\omega}) = f(t)$$

for the function in question.

3. McQuarrie, problem 6-14.

4. McQuarrie, problem 6-20.

5. The rates of chemical reaction mechanisms can be written as differential equations. For the reaction mechanism

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C},$$

we have differential equations,

$$\begin{aligned} \frac{d\mathrm{A}}{dt} &= -k_1\mathrm{A} \\ \frac{d\mathrm{B}}{dt} &= k_1\mathrm{A} - k_2\mathrm{B} \\ \frac{d\mathrm{C}}{dt} &= k_2\mathrm{B} \end{aligned}$$

Solve the first equation with the initial condition $\mathrm{A}(0) = \mathrm{A}_0$ and substitute the result into the second equation to obtain

$$\frac{d\mathrm{B}}{dt} = k_1\mathrm{A}_0 e^{-k_1 t} - k_2\mathrm{B}$$

Solve this equation with the initial condition $\mathrm{B}(0) = 0$. Plot (using Mathematica or QtGrace) the concentrations of A, B, and C for the cases: (a) when $k_1 >> k_2$ and (b) when $k_1 << k_2$.

6. Extra credit: Find the value of R so that

$$\int\int_{x^2+y^2 \le R^2} dxdy\; e^{-\sqrt{x^2+y^2}} = 0.5 \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\; e^{-\sqrt{x^2+y^2}}$$

That is, find the radius of the circle that encloses 50 % of the volume under a 2-dimensional exponential function.

(Although it may not seem so right now, solving this problem this is *directly* related to finding the distance from the nucleus that encompasses 50 % of the probability of observing an electron in a hydrogen atom.)