Due: Next Workshop-3d

Physical Chemistry II

Exercises and Homework Set 1

1. Concepts in Complex Dynamics

Briefly answer the following questions:

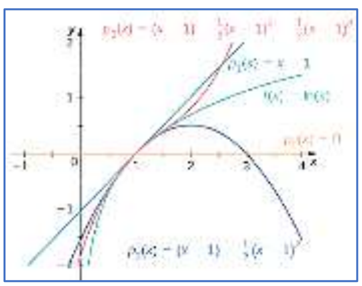
a) What properties of Edward Lorenz' mathematical weather model make it non-linear, and in what components (variables, parameters,..)

b) How can one discover from a variation of starting values in positions and momenta of a particle system whether or not it would likely obey deterministic dynamics?

c) What is a positive or negative feed-back effect? Are there some feed-back effects that could influence Earth' climate?

d) What are reaction constants and equilibrium constants, how are they similar or different?

2. Differentiation and Taylor Expansion



A differentiable function $f(x)$ of variable x can be approximated by a Taylor expansion series about a specific value $x = x_0$ of the variable. The expansion has the form

$$f(x) = f(x_0) + \sum_{n=1}^{N} \frac{1}{n!} \cdot \left(\frac{df}{dx}\right)^n \Bigg|_{x=x_0} \cdot (x - x_0)^n$$

Here, $\left(\frac{df}{dx}\right)^n \Big|_{x=x_0}$ denotes the n^{th} derivative of $f(x)$, evaluated at $x = x_0$. The summation limit $N \le \infty$ determines the accuracy of the representation of $f(x)$ in the vicinity of $x \approx a$ by the above polynomial series. Use this method to approximate the function $\sin(\alpha)$ of phase α, with $-\pi \le \alpha \le +\pi$.

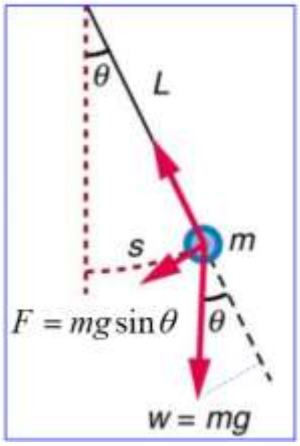
a) Derive the first $N = 5$ terms of the Taylor expansion for $\sin(\alpha)$.

b) Use the MS-Excel utility to compare numerically the exact function $\sin(\alpha)$ to its second-order Taylor expansion around $\alpha = \pi/2$. For this comparison, use at least 21 data α_i points.

c) For which range in values of α is the expansion better than 1%?

d) Plot the function and its expansion versus α

3. Mechanical Harmonic Oscillator (XLS Computational Practice)



Spatial vibrations represent the time evolution of an ubiquitous degree of freedom of mode of systems in vastly different length scales. For small amplitudes of vibrations, this mode can be modeled with a "harmonic oscillation" about an equilibrium configuration. Consider the pictured pendulum, a mass ***m*** subtended by a rigid rod of length ***L*** from an anchor point, as a representation of a larger class of vibrational systems. Its time evolution is determined by the differential equation for the angle $\theta(t)$ relative to the vertical

$$\frac{d^2\theta(t)}{dt^2} = -(g/L)\cdot\sin\theta(t) = -\varpi_0^2\cdot\sin\theta(t)$$

And the conditions for initial amplitude $\theta_0 = \theta(t=0)$ and velocity $\dot{\theta}_0 = d\theta/dt(t=0)$. In the DEq. above, the characteristic angular vibrational frequency ϖ_0 (in 1/sec) is given in terms of period T (in seconds) as $\varpi_0 = 2\pi/T = \sqrt{(g/L)}$; $g = 9.81\,m/s^2$.

a) Write down expressions for a discretized time evolution trajectory as a sequence $\{\theta_i = \theta(t_i), \dot{\theta}_i = \dot{\theta}(t_i), \ddot{\theta}_i = \theta(t_i)\}$ of amplitudes, velocities, and accelerations for the time steps t_i. Successive time steps follow at small intervals $\Delta t = t_{i+1} - t_i \ll T$.

b) Write down similar expressions for the trajectory $\{\theta_i = \theta(t_i), \dot{\theta}_i = \dot{\theta}(t_i), \ddot{\theta}_i = \theta(t_i)\}$ but for a linearized force law. Apply a first-order Taylor expansion for $\theta_{i+1} = \theta_i + \Delta\theta(t_i)$ etc.

c) Produce a Microsoft Excel Worksheet for the numerical simulation of motion under the linear driving force $F(t) = -m\cdot g\cdot\theta(t)$. Assume $\varpi_0 = 2\pi/T = 2\pi/100\,s$ and about $N \approx 200$ time steps $\Delta t = const. \leq 1\,s$.

d) Perform and describe results of simulation runs for at least 2 sets $\{\theta_0, \dot{\theta}_0\}$ of initial conditions, for example $\{\theta_0, \dot{\theta}_0\} = \{-1, +0.01 s^{-1}\}$ etc. Show plots of amplitude vs. time and phase curves $\{\theta_i, \dot{\theta}_i\}$.

e) Produce a copy of the above Worksheet c), but for the non-linear driving force $F(t) = -m\cdot g\cdot\sin\theta(t)$.

f) Perform and discuss simulation runs, like in d, but for at least 2 sets $\{\theta_0, \dot{\theta}_0\}$ of initial conditions, for the non-linear driving force.