

In the name of God

Department of Physics Shahid Beheshti University

ADVANCED COURSE ON COMPUTATIONAL PHYSICS

Exercise Set 11: Mathematica by Adeela Afzal

(Due Date: 1403/10/05)

1. In tracing the circle $x = \cos(t)$, $y = \sin(t)$, both the x motion and the y motion repeat every 2π . This means that we trace the same circle over and over and over again. If we change the frequency of one of the two motions, then we get a more complicated curve called a **Lissajous figure**. Mathematically,

$$x = \cos(at + \delta); \quad y = \sin(bt).$$

- (i) First set $\delta = 0$, $b = 1$ and a equal to a small integer, like 1, 2, or 3. These are the simplest kinds of Lissajous figures, plot them in Mathematica.
(ii) Now set $b = 1$, $\delta = 0$, a equal to a simple fraction, like $3/2$ or $5/2$ or $2/3$ or $3/4$. What happens? When $a = p/q$, how many times does the curve go up and down before it repeats? How many times does it go side to side?
(iii) Now set $a = 9$, $b = 8$, $\delta = \pi/2$ and plot the result in Mathematica.

2. Wave functions for the hydrogen atom take the form,

$$\psi_{\ell m n}(r, \theta, \phi) \propto e^{-\kappa r} (\kappa r)^\ell L_{n-\ell-1}^{2\ell+1}(2\kappa r) Y_\ell^m(\theta, \phi)$$

where n is the principal (radial) quantum number, ℓ is the orbital angular momentum in units of \hbar , m is the magnetic (azimuthal) quantum number, and $\hbar\kappa = \sqrt{2\mu E_b}$ is the wave number for positive binding energy E_b . The radial dependence involves generalized Laguerre functions and the angular dependence spherical harmonics. Note that we are not interested in normalizing these functions at this time. The probability density is given by the absolute square of the wave function, namely $|\psi|^2$. Write a function that plots the probability density in the xy plane ($\theta = \pi/2$) given values of the quantum numbers $n\ell m$ using **Plot3D**. You will need to express the Cartesian coordinates in terms of spherical coordinates. Write a similar function that uses **DensityPlot**. Show several cases of each. Do the proper labeling of the plot.

3. The damped harmonic oscillator is given by

$$\frac{d^2x}{dt^2} + 2\beta \frac{dx}{dt} + \omega_0^2 x = 0,$$

where $b = 2m\beta$ and $\omega_0^2 = k/\omega$. Find the solution for x and plot

- 1) Under damped ($\omega_0^2 > \beta^2$)
- 2) Over damped ($\omega_0^2 < \beta^2$)
- 3) Critical damped ($\omega_0^2 = \beta^2$)

4. A diffusion system is given by,

$$\frac{\partial u}{\partial t} = D_u \frac{\partial^2 u}{\partial x^2} + u(1-u) - v, \quad \frac{\partial v}{\partial t} = D_v \frac{\partial^2 v}{\partial x^2} + \epsilon u,$$

Solve this system in Mathematica numerically under the valid range of x for $D_u = 0.1$, $D_v = 0.05$, $\epsilon = 0.01$, and $u(x, 0) = e^{-x^2}$, $v(x, 0) = 0.1e^{-x^2}$.

5. Numerically compute:

$$I = \int_{-1}^1 \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \int_{-\sqrt{1-x^2-y^2}}^{\sqrt{1-x^2-y^2}} e^{-(x^2+y^2+z^2)} dz dy dx.$$

This integral calculates the weighted volume of a unit sphere with a Gaussian weight $e^{-x^2+y^2+z^2}$. Also,

- 1) Generate the data points for I as a function of x and y .
- 2) Export as *.csv* file in your system.
- 3) Import data and plot it as an interpolating function of x and y .

Good luck, Movahed
