3rd Year B.Sc. Honours Examination 2011B8

Programming and Scientific Computation - PH306

2.00 pm- 5.00 pm. May 12, 2012

Instructions: Answer the following questions. The mark for each part of a question is indicated on the right. Once done writing and executing codes, **please copy them in the exam book**. Any plot that you make, **must be saved for later viewing**.

Time: 3 hours. **Total Marks**: 25

1. The $\mathrm{Ber}_n(x)$ and $\mathrm{Bei}_n(x)$ (or Kelvin functions) functions are the real and the imaginary parts of the spherical Bessel's function $J_n(x\exp(3\pi i/4))$ and are defined by the infinite series representations (for $n=0$) as:

$$\mathrm{Ber}(x) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n (x/2)^{4n}}{[(2n)!]^2}, \qquad \mathrm{Bei}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{4n+2}}{[(2n+1)!]^2}$$

   Here $(2n)!$ represents the factorial of $2n$, etc.

   (a) Write two C or C++ functions `double ber(double x, int n)` and `double ber(double x, int n)` that evaluate the Ber and Bei functions using the above definitions and using the first n-th term in the infinite series. You may want to define your own factorial function in evaluating the series. Start with $i_0 = 0$ in the iterations. [3+3]

   (b) Plot, using `gnuplot` the functions $\mathrm{Ber}(x)$ and $\mathrm{Bei}(x)$ in the range $x \in [-10, 10]$ using the above C/C++ functions for $n = 2, 4, 8, 10$ in the same plot for each function. Save the two plots as postscript files. [2+2]

2. In circuit with a diode and a resistor of resistance 10Ω connected in series with a dc voltage source of 5 V, the current in the diode is modelled as $i = i_s(\exp(-V/(\eta V_T)) - 1)$, where V is the potential difference across the diode, i_s is the reverse saturation current equal to 8.3×10^{-6} A, η is a parameter, taken as $\eta = 2$ and V_T is the knee voltage equal to 0.7 V for silicon semiconductor-diode.

   To solve for the current in the circuit, we need to apply Kirchhoff's voltage law around the circuit which gives

$$-5 + 1.4\ln\left(i/i_s + 1.0\right) + 10.0i = 0$$

   (a) Write a C or C++ program that solves for the current in the circuit in the forward bias case (i.e. the above equation) using any suitable root finding method. [4]

   (b) Modify the program such that the value of the current is written in a file for successive iterations in the root finding algorithm. Write the number of iteration in the first column, the value of the current in the previous step in the second column and the value of the current in the current iteration/step in the third column of a file. [3]

   (c) Plot the values of $|i_n - i_{n-1}|$ vs n, using `gnuplot`, where n is the iteration number. Save the plot as a postscript file. [2]

3. The Bohr model of the atom is based on three basic equations:

$$\begin{aligned} mvr &= nh/(2\pi) && \text{angular momentum quantization rule} \\ \frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2} &= m\frac{v^2}{r} && \text{for balance equation} \\ E &= \frac{1}{2}mv^2 - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} && \text{Energy equation} \end{aligned}$$

   (a) Using `Maple` define three equations `Eq1`, `Eq2` and `Eq3` corresponding to the three equations given above. [1]

   (b) Using `Maple` command `solve` get the solutions for r, v and E which correspond to the radius, speed of the electron and the energy of the Bohr atom. Define a `Maple` expression `soln1` which correspond to the solution set. [Hint: `soln1[1]` is equal to r, `soln1[2]` is equal to v, etc.] [3]

   (c) Use `Maple` command `assign` and define three quantities r_n, v_n and E_n which correspond to r, v and E. [1]

   (d) Using `Maple` command `subs` evaluate the Bohr radius $a_0 = r_1$ and Rydberg energy $E_R = -E_1$ by using the values $c = 2.99792458e8, h = 6.626069e{-34}, m = 9.109382e{-31}, e = 1.602176e{-19}, \epsilon_0 = 8.854187e-12, n = 1$. [2]

   Save the worksheet that contains the `Maple` commands that you wrote and the plot .

p is the momentum and c is the speed of light. The element of momentum space is $\mathrm{d}p = 4\pi(\epsilon^2/c^3)\mathrm{d}\epsilon$.
For bosons and fermions, the distribution laws are:

$$f_{\mathrm{BE}}(\epsilon) = \frac{1}{\exp(\epsilon/kT) - 1} \qquad , \qquad f_{\mathrm{FD}}(\epsilon) = \frac{1}{\exp(\epsilon/kT) + 1}$$

(a) Define $\eta = \epsilon/(kT)$. Using `Maple`, plot f_{BE} and f_{BE} as functions of η for $\eta \in [-2, 3]$ and $y \in [0, 2]$. [2]

(b) Using `Maple`, evaluate the total number of particles N in a volume V at temperature T for both bosons and fermions using the formula: $N = (gV/h^3)\int_0^\infty f(\epsilon)\mathrm{d}p$. Here, g is the degeneracy and h is Planck's constant. [1+1]

(c) Using `Maple`, evaluate the total internal energy U of particles in a volume V at temperature T for both bosons and fermions using the formula: $U = (gV/h^3)\int_0^\infty \epsilon f(\epsilon)\mathrm{d}p$. [1+1]

(d) For photons, degeneracy $g = 2$. Using `Maple`, plot the energy density $\rho = U/V$ as a function of energy ϵ in the range $[0, 20]$. Take $c = h = 1$. This is the famous Planck's distribution law. [1]

Save the worksheet that contains the `Maple` commands that you wrote and the plot(s).

$$P_n(x) = \frac{1}{\pi}\int_0^\pi \left[x + \sqrt{x^2-1}\cos\phi\right]^n \mathrm{d}\phi$$

(a) Write a `Maple` procedure or function, `legendre(n,x)`, that evaluates the Legendre Polynomial of order n, using the above relations, at some point x. [3]

(b) Using `Maple`, evaluate

$$\int_{-1}^{1} P_m(x)P_n(x)\mathrm{d}x$$

for $m \neq n$ and $m = n$. Take $m, n = 1, 2, 3, \ldots$ etc. [2]

(c) Using `Maple`, plot $P_3(x)$ and $P_5(x)$. [2]

(d) Using `Maple`, find the zeros of $P_3(x)$. [1]

2. The generating function for the Legendre polynomials $P_n(x)$ is $g(x,t) = 1/\sqrt{1-2xt+t^2}$, with $0 < t < 1$ such that

$$\sum_{n=0}^{\infty} P_n(x)t^n = g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}}$$

(a) Use the `taylor` command to generate the first five Legendre polynomials from the above definition of the generating function. [2]

(b) Use the `coeftayl` command to write a `Maple` function, `legendre(n,x)`, that evaluates the Legendre polynomials of order n, using the above relation, at some point x. [2]

(c) Using `Maple`, plot $P_3(x)$ and $P_5(x)$. [1]

(d) Using `Maple`, find the zeros of $P_3(x)$. [2]

Save the worksheet that contains the `Maple` commands that you wrote and the plot .

1. Random numbers may be used to calculate integrals. This method is known as Monte Carlo Integration. Consider the following integral

$$I = \int_{-1}^{1} \frac{2}{1+x^2}\mathrm{d}x$$

(a) Generate a sequence of pair of random numbers (x, y) with $x \in [-1, 1]$ and $y \in [0, 1]$. Write a `C` or `C++` function `double integral2(int N)` to calculate the value of the integral by comparing the area under the curve $y = \frac{2}{1+x^2}$ and that of the rectangular region with sides 2 and 1 using N pairs of random numbers, i.e. N points. [4]

(b) Increase the number of points used to evaluate the area and find the errors in each case. Take $N \in [10, 10^7]$. The exact value of the integral is π. [2]

(c) Write the number of points and the errors in two columns of a file. Plot the error vs the number of points used and the save the plot as a postscript file. [2+1]

2. The Euler's method for solving the second order ordinary differential equation $\mathrm{d}^2x/\mathrm{d}t^2 + \omega^2 x = 0$, written as a set of coupled first order difference equations is

$$\begin{aligned} x_{n+1} &= x_n + f(x_n, t_n)(t_{n+1} - t_n) = x_n + z_n h \\ z_{n+1} &= z_n + g(z_n, x_n, t_n)h = z_n - \omega^2 x_n h \end{aligned}$$

Consider the initial conditions $x_0 = 0$, $z_0 = 1$.

(a) Write a C/C++ code that solves the above initial value problem. Your code should write the values of t, x and z in different columns of a file. [6]

(b) Plot the values of $z = \frac{\mathrm{d}x}{\mathrm{d}t}$ vs. x for $\omega = 1, 4, 9, 16$. [3]

$$\rho_e(r) = -\frac{q}{\pi}e^{-2r}, \qquad \rho_p(r) = q\delta(\vec{r})$$

where we have adopted the system of units in which the Bohr radius $a_0 = 1$ and $k_e = 1/(4\pi\epsilon_0) = 1$. The system is spherically symmetric and hence volume integration of a radial function $f(r)$ can be expressed as $\int f(r)\mathrm{d}^3r = 4\pi \int_{r=0}^{\infty} f(r)\, r^2\mathrm{d}r$. Also, recall that $\int \delta(\vec{r})\mathrm{d}^3r = 1$
Hint: The `Maple` function for the Dirac delta function $\delta(r)$, is `Dirac(r)`. Use `Pi` for π in `Maple` instead of `pi`.

(a) Using `Maple` find the total positive and negative charges of the atom. Do your answers make sense? [2]

(b) Using `Maple` evaluate

$$\int_{-\infty}^{\infty} j_m(x) j_n(x)\mathrm{d}x, \qquad m,\, n \geq 0$$

for (a) $m \neq n$ and (b) $m = n$ taking $m, n = 0, 1, 2, \ldots$ etc. Can you interpret the result? Can you guess the value of the integral for general m, n? [2+0.5+0.5]

4. (a) Using `Maple`, evaluate the magnetic field at a distance D for in infinitely long wire procedure `laguerre:=proc(n,x)`, that recursively calculates the Laguerre Polynomial of order n, using the above relations, at some point x. [5]

(b) Use the above procedure `laguerre(n,x)` to calculate the values of $n!L_n(x)$ for $n = 1, 2, \ldots 4$ and plot them. [2]