3rd Year B.Sc. Honours Examination 2012$_{\text{B8}}$

Programming and Scientific Computation - PH306

9.00 am- 12.00 pm. April 20, 2013

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 zeta function $\zeta(s)$ has an infinite series representation as:

$$\zeta(s) = \frac{1}{1-2^{1-s}} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^s}$$

   (a) Write a `C` or `C++` function `double zeta(int s,int M)` that evaluates the zeta function from the above definition and using the first M terms in the infinite series. Take suitable value of M for evaluating the function $\zeta(s)$. [4]

   (b) In a complete `C` or `C++` program write the values of s in the first column and the values of the function $\zeta(s)$ in second column. Plot, using `gnuplot` the functions $\zeta(s)$ in the range $s \in [2, 5]$ and in the range $s \in [0.1, 0.8]$ using the above C/C++ function. Save the two plots as postscript files. [2+2+2]

2. The energy eigenvalues E for a particle of mass m in a one-dimensional square-well potential of half-size a and depth V_0 satisfy the following transcendental equation

$$\sqrt{2m(E+V_0)}\tan\left(\sqrt{2m(E+V_0)}\right)\frac{a}{\hbar} - \sqrt{-2mE} = f(E) = 0$$

   The parameter values are chosen to be representative of the energy levels of a neutron or proton in a nucleus. Take $\hbar = 1$, $m = 938$, (MeV) $a = 197.3$ (MeV) $V_0 = 70$ (MeV) and note that E should be negative for bound system.

   (a) Using `gnuplot` plot $\sqrt{2m(E+V_0)}\tan\left(\sqrt{2m(E+V_0)}\right)a/\hbar$ and $\sqrt{-2mE}$ with respect to $E \in [-4, 0]$ in the same plot and save it as a postscript file. Can you identify the singularities of the functions? Change the $x-$range of your plot to identify the first two solutions of the above equation. [2+1+2]

   (b) Write a C or C++ program to find the lowest bound state i.e. energy eigenvalue E from the above equations using any suitable root finding algorithm. [6]

3. An integral representation for the Anger function $\mathrm{J}_n(x)$ is are given by:

$$\mathrm{J}_n(x) = \frac{1}{\pi}\int_0^{\pi} \cos\left(nt - x\sin(t)\right)\mathrm{d}t$$

   (a) Write a `Maple` functions `J(n,x)` that evaluates the Anger function $\mathrm{J}_n(x)$ using the above definition, at some point x. [Hint: The `Maple` symbol for π is `Pi`]. [1]

   (b) Using `Maple`, plot $\mathrm{J}_n(x)$ for $n = 0.0, 0.5, 1.0, 1.5, 2.0$ in the same plot for $x \in [-8, 8]$. [2]

   (c) Using `Maple` evaluate the first, second and third derivatives of the Anger function i.e. $\mathrm{J'}_n(x)$, $\mathrm{J}''_n(x)$ and $\mathrm{J}^{(3)}_n(x)$ for $n = 0, 1$. [0.5+0.5]

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

$$csch(x) = \frac{1}{x} + 2x \sum_{k=1}^{\infty} \frac{(-1)^k}{x^2 + (k\pi)^2}$$

for $x \neq 0$

(a) Define a C or C++ function `double cosech(double x, int n)` that evaluates the series expansion for the Fresnel integral using the expansion up to the n-th term in the series for a given value of the arguments x and n. [5]

(b) Plot your function `cosech(x,n)` with $n = 20$, for $x \in [0.1, 1.0]$ using `gnuplot` and save the plot as a postscript file. [2+1]

2. The Legendre Polynomials have the integral representation

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

(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]

1. 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]

2. The electron and the nuclear charge densities of the hydrogen atom are given by

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

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 $\int \delta(\vec{r})\mathrm{d}^3 r = 1$
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]

3. (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]