3rd Year B.Sc. Honours Examination 2011B4

Programming and Scientific Computation - PH306

10.00 am- 1.00 pm. May 13, 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. A continued fraction representation for the upper incomplete gamma function $\Gamma(n,x) = \int_x^\infty t^{n-1}\exp(-t)\mathrm{d}t$ (where the upper limit is fixed) is given by (as a sequence of fractions):

$$c_0 = x^n e^{-x}, \quad c_1 = \frac{x^n e^{-x}}{x+1-n+1(n-1)}, c_2 = \frac{x^n e^{-x}}{x+1-n+\cfrac{1(n-1)}{x+3-n+2(n-1)}}, \ldots$$

$$\Gamma(n,x) = \cfrac{x^n e^{-x}}{x+1-n+\cfrac{1(n-1)}{x+3-n+\cfrac{2(n-1)}{x+5-n+\cfrac{3(n-3)}{x+7-n+\cfrac{4(n-4)}{x+9-n+\cdots}}}}}$$

   (a) Write a C or C++ function `double uigamma(int n, double x,int s)`, that evaluates the s-th order iterated value of $\Gamma(n,x)$ using the above algorithm. [4]

   (b) Call the function `double uigamma(int n, double x, int s)` in a complete C or C++ program and evaluate $\Gamma(n,x)$ with $s \in [0,20]$ and write the values in a data file. Using `gnuplot`, plot `uigamma(n,x,s)` with respect to s for $s \in [0,20]$ at $n=2$ and $x=1$. Save the plot in a postscript file. [Hint: $\Gamma(2,1) \approx 0.7357588824$] [2+2]

   (c) Using `gnuplot`, plot the values of uigamm(x,n,s) versus x in the range $[0,5]$ with $s=10$ and for $n = 0.5, 1, 2, 3$ in the same plot. Save your plot as a postscript file. [2]

2. A square potential well and the transmission coefficient for it are given by

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & 0 < x < a \\ 0 & x > 0 \end{cases}$$

$$T = \left[1 + \frac{1}{4\mathcal{E}(\mathcal{E}+1)}\sin^2\left(\alpha\sqrt{1+\mathcal{E}}\right)\right]^{-1}$$

   where $\alpha = (2mV_0a^2/\hbar^2)^{1/2}$, $\mathcal{E} = E/V_0$.

   (a) Using `gnuplot`, plot the transmission coefficient T and the reflection coefficient $R = 1-T$, as functions of the reduced energy $\mathcal{E} = E/V_0$ for $\mathcal{E} \in [0,2]$ in the same plot. Save the plot as a postscript file. [2]

   (b) Write a C or C++ program that finds the resonant energies E which will give perfect transmission i.e. $T = 1$, with $\alpha = 25.598$ and $V_0 = 25$ eV, using any suitable root finding algorithm. Find the first four energy values. [Hint: Resonant values are $\mathcal{E} \approx 0.22, 0.51, \ldots$] [5+1]

3. The Fourier transform of a function $f(x)$ is defined as

$$\alpha(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} u(x)e^{-ikx}\mathrm{d}x$$

   (a) Define a `Maple` function $u(x) = \frac{1}{\sqrt{2\pi}a}\exp\left(-x^2/(2a^2)\right)$. Plot `u(x)` for $x \in [-5,5]$ for $\alpha = 1$. [1+1]

   (b) Using `Maple`, find the Fourier transforms $\alpha(k)$ of the above function $u(x)$. [2]

   (c) Using `Maple`, evaluate the following integrals:

$$\int_{-\infty}^{\infty} |u(x)|^2\,\mathrm{d}x, \quad \text{and} \quad \int_{-\infty}^{\infty} |\alpha(k)|^2\,\mathrm{d}k$$

   What conclusion can you draw from the above evaluations? [2+1]
   [Hint: The symbol for $i = \sqrt{-1}$ in `Maple` is `I`. **You may want to simplify your expressions by using `simplify` command in `Maple`.**]

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

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

(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]