Homework #3

Computational Physics: Fall 2023
Professor Coan & Olness

Due Wednesday 06 September 11:59pm in Canvas upload

0) PROGRAM SUBMISSION:
For problems where you submit code please use the following format so I can EASILY run your code.

1. Make a new sub-directory with your name and homework # (e.g., olness3)
2. Copy the source code ONLY (not the big executable) into this directory
3. Make a 'doit' file that will compile the code; be sure to use debugging flag '-g'
4. Move up to the upper level directory (where 'olness2' directory is located)
5. Zip this into a zip file: **`zip olness2.zip ./olness2/*`**
6. Upload the zip file to canvas.

1) [10 points] Particle in a 1-dimensional infinite square well: Consider a particle in an infinite square well of width "a" and potential V(x)=0 for x=[0,a] and V=∞ otherwise.
BY HAND: Compute the energy E_n and normalized wave functions $\psi_n(x)$.
You can copy this from your Modern Physics course notes, but I want you to show the steps.

2) [10 points] Plot the wave functions you found in problem #1.
BY COMPUTER: Using GnuPlot plot the first 4 wave functions and ensure they satisfy the correct boundary conditions. Submit the plots in a PDF document. Also include the GnuPlot scripts.
Suggestion: you can put the GnuPlot commands in a file and then: gnuplot> load "file"

***) WARMUP #1**: [Don't hand in] Go to the example for Gnu Scientific Library and run the example for the function: **int gsl_sf_bessel_J0_e (x, &result);**

LINK: https://www.gnu.org/software/gsl/doc/html/specfunc.html#examples

***) WARMUP #2**: [Don't hand in] Modify the above example to use the Bessel function without the error checking and with order "nu": **double gsl_sf_bessel_Jnu(double nu, double x):**

3) [10 points] With GnuPlot, plot J[L+1/2, r] for L={0,1,2}. Be sure to show at least 4 zeros for each function. [We do NOT want to use any zeros at r=0 for physical reasons, so ignore these.]
Submit the plots in a PDF document.

4) [10 points] Create a program to find the first 4 roots (k_n) EACH of the Bessel function J[L+1/2, r] for L={0,1,2}. Use the bisection method to find the root and specify the accuracy to be 0.001.
[We do NOT want to use any zeros at r=0 for physical reasons, so ignore these.]
Suggestion: You don't have to use any fancy method to automate this as we only need 3x4=12 roots. I suggest you write a program where you input L={0,1,2} and x_{min} and x_{max}, and have the program search for a root in the interval. When you are done, I want the following table:

L	k1	k2	k3	k4
0				
1				
2				

Submit the table in a PDF document. **Submit the code in a zip file.**
Include a 'doit' file, and be sure to prompt the user for the format of the input, *i.e.*, "enter: L, xmin, xmax"

5) [10 points] 3-D Schrodinger Equation. Particle in an Infinite, Spherical Well. Consider a three-dimensional well with infinite depth and radius a defined by V[r] = 0 if r<a; V[r]=∞ if a<r.
We find the wave function separates and is of the form:

$$R(r) = \frac{\sqrt{2L+1}}{\sqrt{r}}\; J\left[L + \frac{1}{2}, k\, r\right] \qquad \text{with} \quad E_n = \frac{\hbar^2 k^2}{2m}$$

With GnuPlot, plot R(r) for each L={0,1,2} showing the first 4 eigenvalues (i.e., kn from the previous problem). If things work correctly, this should satisfy the boundary conditions R(1)=0.
Plot each L={0,1,2} separately, so I have 3 plots, each with 4 curves, and all 4 curves vanish at r=1.
Submit the plots in PDF.
Submit the GnuPlot data file and script files in a zip file.