Homework 12: Boundary Value Problems

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1 Question 1: Legendre Polynomial

In this question I calculated the values of Legendre polynomials of first kind of order three, four, and five. I chose the range of x-values from -0.9999 to 0.9999 and relative precision 1e-6. We can see in the data files that all three polynomials converges to 1.0000 when x=1. I also compared some of the values from my data and the Abramovich-Stegun Table (page 342) for n=3. We can also check other values in Wolfram Alpha, which are pretty much accurate.

x	0.250	0.500	0.750	1.000
table	-0.33 59 375	-0.43 75 000	-0.07 03 125	1.000
mv value	-0.33 59 367	-0.43 74 972	-0.07 03 093	1.000

The table shows values are accurate upto third decimal points. For the order four and five I used Wolfram Alpha to find the values. command: legendre p(n, x).

X	my p(4,x)	wolfram p(4,x)	my p(5,x)	wolfram $p(5,x)$
0.701001	-0.374935221	-0.41130010	-0.366720672	-0.366725162
0.801001	-0.229389047	-0.2300239	-0.398291064	-0.3982963965
0.901001	0.159050061	0.213968570	-0.034653366	-0.0346544594

The solution directory is:

location : hw12/qn1/
source code : hw12qn1.f90
plots : hw12qn1.eps

datafiles : n3.dat, n4.dat, n5.dat

datafiles : n3compare.dat, n4compare.dat, n5compare.dat (for comparison)

provided subroutines : rk4.f90

The figures are shown below:

Plot of legendre polynomials

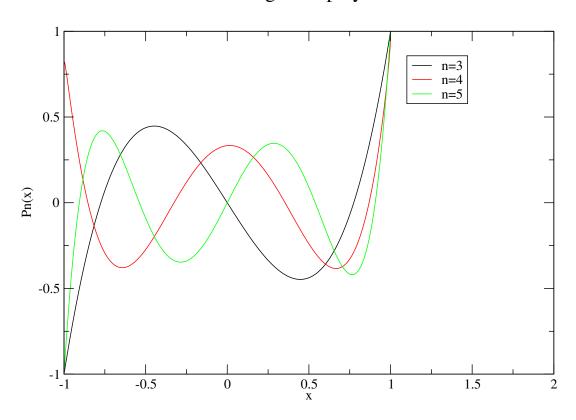


Figure 1: Legendre Polynomials

2 Question 2: 3D Isotropic Harmonic Oscillator

The potential of 3D harmonic oscillator is given by:

$$V(r) = \frac{1}{2}m\omega^2 r^2 \tag{1}$$

Where, m is mass of oscillator, ω is angular frequency and r is radial distance. The energy of three dimensional oscillator is:

$$E_n = (n + \frac{3}{2})\hbar\omega \tag{2}$$

The energy state n is given by:

$$n = 2k + l \tag{3}$$

Here, k = no. of nodes.

l= angular momentum quantum number.

 $hbar = \frac{h}{2\pi}$ = reduced planck's constant.

The radial schrodinger equation is:

$$-\frac{\hbar^2}{2m}u'' + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{4}$$

Rearranging yields:

$$u'' = \left[\frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}(E-V)\right]u\tag{5}$$

2.1 part 2.1: Solving radial equation

In this part I solved the radial differential equation using a subroutine from the internet mentioned below. I calculated the ground state energy and its value is:

The solution directory is:

location : hw12/qn2/ source code : hw12qn2.f90

plots : hw12qn2.eps, hw12qn2d.eps

datafiles : hw12qn2.dat, hw12qn2d.dat downloded subroutine : nsolve.f90 and ho.f90

reference : http://infty.net/nsolve/nsolve.html

The figures are shown below:

3d Harmonic Oscillator wavections

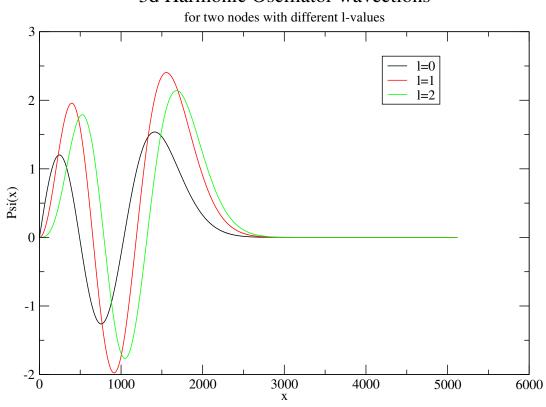


Figure 2: 3d harmonic oscillator

2.2 part 2.4: Perturbed 3d harmonic oscillator

In this part I added a quartic perturbation term $\lambda \rho^4$ to the potential of the oscillator and calculated the ground state energy and wavefunction for l=0. I chose $\lambda=0.1$.

The value of perturbed ground state energy is :

 $E_{0(perturbed)} = 7.899$

The plot of wavefunction is shown below:

3d Harmonic Oscillator with perturbation

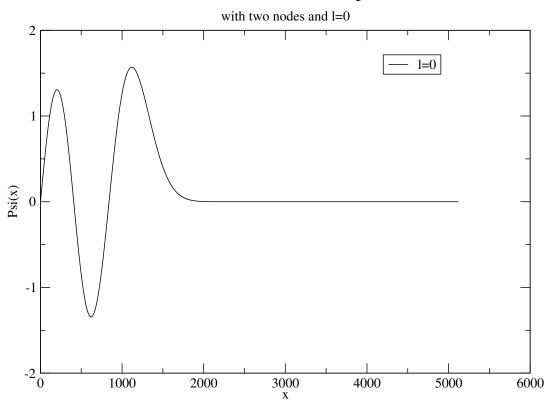


Figure 3: Perturbed 3d harmonic oscillator