Phys 562 Computational Physics, Spring 2014, Midterm I

Z. Papp

1. The radial part of the wave function of the three-dimensional harmonic oscillator for angular momentum l and radial quantum number n_ρ is given by

$$u_{n_\rho,l}(\rho) = (-)^{n_\rho} \sqrt{2 \frac{n_\rho!}{(n_\rho + l + 1/2)!}} \exp(-\rho^2/2) \rho^{l+1} L_{n_\rho}^{l+1/2}(\rho^2).$$

Note that $(1/2)! = \sqrt{\pi}/2$. You should not use the gfortran Gamma function!

- Write an efficient subroutine for evaluating u.
- Plot the first 4, $l = 0$, oscillator functions in the $\rho = [0, 5]$ interval.
- Plot $u_{20,0}(\rho)$ and $u_{21,0}(\rho)$ in an interval which shows the characteristic of the functions.
- Write a small report which contains all the relevant achievements.

2. One of the incomplete gamma functions is defined by

$$\Gamma(a, z) = \int_z^\infty dt\, t^{a-1} e^{-t},$$

and it has a nice continued fraction representation

$$\Gamma(a, z) = e^{-z} z^a \cfrac{1}{z + \cfrac{1-a}{1 + \cfrac{1}{z + \cfrac{2-a}{1 + \cfrac{2}{z + \cdots}}}}}.$$

- Write a function subprogram for calculating $\Gamma(a, z)$ by evaluating the continued fraction.
- Define $f(x) = \Gamma(1/2, x^2)/\sqrt{\pi}$ if $x \geq 0$, and $f(x) = 2 - \Gamma(1/2, x^2)/\sqrt{\pi}$ if $x < 0$.
- Plot $f(x)$ in the $x = [-3, 3]$ interval. (Use just 50 points.)
- Do you have any guess what $f(x)$ might be? Test your idea numerically.