DUE BEFORE WORKSHOP 2 - May 12th

Write a report addressing the following problems. All computational exercises must be completed in Fortran. Submit a **PDF** of your report via Blackboard, along with any Fortran files, input and output files, gnuplot scripts, and anything else required to run your programs and replicate your results in a separate zipped directory.

Marking: There are ten marks in total. One mark is for presentation (readability, figure formatting etc), and the remaining nine marks will be split unevenly amongst the problems. For computational problems half the available marks are for the implementation, and the other half are for the discussion of theory and explanation of results wherever appropriate. A marking rubric is available on Blackboard.

Problem 1 - Laguerre basis (3 marks)

Using the recurrence relation

$$\tilde{\varphi}_{k\ell}(r) = \frac{2(k-1+\ell-\alpha r)\tilde{\varphi}_{k-1,\ell}(r) - (k+2\ell-1)\tilde{\varphi}_{k-2,\ell}(r)}{k-1} \tag{1}$$

with

$$\tilde{\varphi}_{1\ell}(r) = (2\alpha r)^{\ell+1} e^{-\alpha r} \tag{2}$$

$$\tilde{\varphi}_{2\ell}(r) = 2(\ell+1-\alpha r)(2\alpha r)^{\ell+1} e^{-\alpha r} \tag{3}$$

write a subroutine to generate the non-orthogonal radial Laguerre basis

$$\varphi_{k\ell}(r) = \sqrt{\frac{\alpha(k-1)!}{(k+\ell)(k+2\ell)!}}\tilde{\varphi}_{k\ell}(r) \tag{4}$$

The subroutine should have as input the parameters α and ℓ, the number of basis functions N to generate, and the radial grid array. The output should be a matrix containing the basis functions arranged in columns. To make your life easier you may like to read parameters from an input file rather than from standard input. You may run into problems calculating $(k+2\ell)!$:

- The maximum value of a 32-bit integer (Fortran default) is 2,147,483,647, placing an upper limit of 12 on $k+2\ell$
- The maximum value of a 64-bit integer (`integer*8`) is 9,223,372,036,854,775,807, placing an upper limit of 20 on $k+2\ell$
- The maximum integer value which can be exactly represented with a 64-bit floating-point number is 2^{53}, placing a limit of 43 on $k+2\ell$

so you will need to find an intelligent way to evaluate the normalisation constants without causing overflow.

Include the following in your report:

- Details of the relevant theory and your code, including the method used to calculate the factorial components of the normalisation constant and an indication of what bounds there are on k and ℓ in your method.
- Four figures, each with a different combination of α and ℓ, showing the first 4 basis functions. Discuss the effect changing α and ℓ has on the basis. Choose an appropriate $r_{\max}$ so you can see the exponential decay of the basis functions at large r.

Problem 2 - Analytical matrix elements (2 marks)

Making use of the following properties of the Laguerre polynomials:

$$\int_0^\infty x^t e^{-x} L_n^t(x) L_m^t(x)\,\mathrm{d}x = \frac{(n+t)!}{n!}\delta_{nm} \tag{5}$$

$$x\frac{\mathrm{d}^2}{\mathrm{d}x^2}L_n^t(x) + (t+1-x)\frac{\mathrm{d}}{\mathrm{d}x}L_n^t(x) = -nL_n^t(x) \tag{6}$$

and the operator equation for the spherical harmonics (and the fact they are orthonormal):

$$L^2 Y_\ell^m(\hat{\boldsymbol{r}}) = \ell(\ell+1)Y_\ell^m(\hat{\boldsymbol{r}}) \tag{7}$$

derive the analytical expression for the kinetic energy matrix

$$K_{ij} = \langle\phi_i| -\frac{1}{2r}\frac{\partial^2}{\partial r^2}(r\,\cdot\,) + \frac{L^2}{2r^2}|\phi_j\rangle = \alpha_{\ell_i}^2\delta_{ij} - \frac{\alpha_{\ell_i}^2}{2}\langle\varphi_{k_i\ell_i}|\varphi_{k_j\ell_j}\rangle\delta_{\ell_i\ell_j}\delta_{m_i m_j}. \tag{8}$$

Extension (optional): Derive the analytical expression for the overlap matrix elements

$$B_{ij} = \langle\phi_i|\phi_j\rangle. \tag{9}$$

This is somewhat more involved than deriving K_{ij}, and requires the following identity:

$$L_n^t(x) = L_n^{t+1}(x) - L_{n-1}^{t+1}(x). \tag{10}$$

Problem 3 - Atomic hydrogen states (4 marks)

Write a program to solve the atomic hydrogen electronic structure problem, using analytical forms for the K, B, and V matrices. Use the provided `rsg` subroutine to obtain the eigenenergies and eigenvectors, and use your subroutine from Problem 1 to generate the Laguerre basis functions and recover the coordinate-space eigenstates.

Include the following in your report:

- For $\alpha = 1.0$ a figure demonstrating convergence in the $\ell = 0$ bound spectrum and increasingly dense discretisation of the continuum as N is increased. Either replicate Fig. 15 from Igor's lecture notes, or find your own way to illustrate the same point. Note your results for small N may look different to Igor's due to the basis we're using.
- A figure similar to the one you produced for the previous point but comparing the energy levels for different values of α and fixed N. Comment on how changing α affects the distribution of energy levels and the consequences this can have on subsequent scattering calculations.
- For an N you are satisfied yields reasonably converged bound states, a figure each for $\ell = 0$ and $\ell = 1$ comparing the first three bound state radial wave functions you have calculated to the analytical solutions.

Analytical expressions for the Hydrogen radial wave functions are available online and in textbooks, and a general expression for all H-like atoms can be found here.

Extension (optional):

- Investigate the structure of the He^+ ion. Can you reproduce its analytical energies and wave functions?
- Make a surface plot showing the value of the 3D wave function in the xz plane (take $m = 0$ for simplicity).
- See if you can evaluate the V-matrix elements numerically. What can you do to avoid the singularity in $V(r)$ at the origin?