DUE June 9th

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 each problem half the available marks are for the implementation, and the other half are for the discussion of theory and explanation of results wherever appropriate.

Problem 1 - Electron-hydrogen V-matrix elements (6 marks)

Using your code from assignment 1 to generate the hydrogen wave functions, write a code to calculate the direct and exchange electron-hydrogen V-matrix elements. Your program should calculate the matrix elements $V(k', k)$ for k' and k in a k-grid determined by specifying δk and $k_{\max}$. To facilitate plotting of the V matrix as a surface in gnuplot, write the matrix elements to file in the following format:

```
#k'   k     V(k',k)
1.0   1.0   V(1,1)
1.0   2.0   V(1,2)
1.0   3.0   V(1,3)
 ⋮     ⋮     ⋮

2.0   1.0   V(2,1)
2.0   2.0   V(2,2)
2.0   3.0   V(2,3)
 ⋮     ⋮     ⋮

3.0   1.0   V(3,1)
3.0   2.0   V(3,2)
3.0   3.0   V(3,3)
 ⋮     ⋮     ⋮
```

Note the blank line between each `k'` block which is required for a nice looking plot. Then you can plot in gnuplot using [`splot 'file' u 1:2:3 with lines`].
Include the following in your report:

- Details of the methods for calculating the matrix elements
- Surface plots of the direct $1s$-$1s$, $1s$-$2s$, and $1s$-$3s$ matrix elements
- Surface plots of the exchange $1s$-$1s$, $1s$-$2s$, and $1s$-$3s$ matrix elements for 1 and 10 eV incident energies
- Plots of the $1s$-$1s$, $1s$-$2s$, and $1s$-$3s$ on-shell direct and exchange matrix elements as a function of incident momentum k, compared to the analytical formulas given in the slides. Recall that the *on-shell* matrix element has k' decided by conservation of energy. This will require a separate loop to evaluate the V-matrix elements $V(k', k)$ for each k in the input k grid and k' calculated specifically for each k and transition.

Extension (optional): Modify your potential scattering code to allow multi-channel scattering and use the electron-hydrogen V-matrix elements you have implemented to write your own version of the s-wave CCC code. This is best left as an exercise for the holidays.

Problem 2 - V_{12} potential in the s-wave model (1 mark)

The Legendre polynomials are orthonormal on $[-1, 1]$:

$$\int_{-1}^{1} P_{\ell'}(x) P_{\ell}(x)\, \mathrm{d}x = \frac{2}{2\ell + 1} \delta_{\ell'\ell}, \tag{1}$$

and the zeroth Legendre polynomial is

$$P_0(x) = 1. \tag{2}$$

Therefore, beginning by writing the partial-wave direct matrix element in terms of the general partial-wave function

$$\langle \boldsymbol{r} | k\ell m \rangle = \frac{1}{r} u_{\ell}(r; k) Y_{\ell}^{m}(\hat{\boldsymbol{r}}), \tag{3}$$

justify the simplification we have employed for the electron-electron potential.

Problem 3 - Reduced CCC code (2 marks)

Compile and run the reduced CCC code using the supplied input files `kgrid1.in` and `kgrid2.in` (copy each to `ccc.in` before running the code). The output files `singlet.`n`1` and `triplet.`n`1` contain the half-onshell K- and V-matrix elements for the $1 \rightarrow n$ transition as a function of the offshell k. Run the calculations for both k grids with $\theta = 0$, 1, and 2, and use the output to recreate Fig. 8.1 in the book chapter (same as the figure on slide 81). Comment on the results in the context of the issue of non-uniqueness.

Using the `book.in` input file supplied, run the reduced CCC code over a range of incident energies from 1 to 100 eV. The cross sections are printed to the file `totalcs`, and are listed per transition first for $S = 0$, then $S = 1$, then finally the spin-averaged cross sections. Plot the cross sections for a selection of transitions of your choosing as a function of energy.

Extension (optional): Implement non-zero θ in your V-matrix elements and see if you can reproduce the V-matrix elements from Fig. 8.1 of the book chapter. Note you will need to multiply your V-matrix elements by $\dfrac{1}{\pi} \dfrac{1}{k_f k_i}$ to compare with CCC.