DUE BEFORE WORKSHOP 4 - June 2nd

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 - Potential scattering (8 marks)

Take the potential scattering template code provided and write the missing subroutines. Comments are given throughout the files to direct you. Comments beginning with "`!>>>`" show you where you need to write your own code. The potential you should implement is

$$V(r) = z\left(1 + \frac{1}{r}\right)e^{-2r}, \tag{1}$$

where $z$ is the projectile charge.

Run your code for a range of energies up to 50 eV, for both electrons and positrons, and include the following in your report:

- A figure for each projectile of the ICS as a function of energy, demonstrating convergence as $\ell_{\text{max}}$ is increased. Comment on the rate of convergence for different energies. Use a log scale on the vertical axis to clearly show the contributions from higher partial waves.
- A figure with the DCS as a function of scattering angle for a few energies of your choosing.
- A figure showing the convergence of the DCS with increasing $\ell_{\text{max}}$ for one energy. Comment on and explain the shape of the $\ell_{\text{max}} = 0$ DCS.

*Troubleshooting tips:*

- Check your continuum waves for $\ell = 0$ by comparing to $\sin(kr)$. For higher $\ell$ find analytical formulas for the spherical Bessel functions and use Eq. (134) in the slides.
- The half-onshell $V$-matrix elements on Slide 70 were calculated with an incident energy of 8.708 eV. Check that you are able to reproduce them.
- Check that you are able to reproduce both the ICS and DCS given as examples in the lecture slides.

*Extension (optional):* at very low incident energies the cross section approaches a constant value. What is it?

# Problem 2 - Derivation (0.5 marks)

Derive the partial-wave Lippmann-Schwinger equation (94) by substituting the $T$- and $V$-matrix partial-wave expansions (92–93) into the 3D Lippmann-Schwinger equation (82).

# Problem 3 - Dimensional analysis (0.5 marks)

What are the units of the partial-wave $T$-matrix elements $T_\ell(k_f, k_i)$? Figure this out by looking at the partial-wave Lippmann-Schwinger equation (Eq. (94) in the slides), and because we are working in a system of units where factors of $m_\text{e}$ and $\hbar$ can be neglected, only consider the length component of each variable's dimension. As an example, the momentum of a particle can be expressed as

$$p = \hbar k, \tag{2}$$

where $k$ is the particle's *wavenumber* and has dimensions of inverse length. For the sake of this problem you could then treat any variables with dimensions of momentum as having dimensions of inverse length because we disregard $\hbar$

Substitute the dimensions of $T_\ell(k_f, k_i)$ into Eq. (126) to show that the cross section has the correct dimension.