Assignment 5

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1 Problem 1: Electron-Hydrogen V-matrix elements

Electron-hydrogen scattering involves interaction of an incoming electron with a hydrogen atom. We solve the the Schrödinger equation for the system, accounting for the electron-electron interactions by calculating the partial-wave V-matrix elements. This can later be used to calculate scattering amplitudes and cross sections to gain better understanding of the scattering procerss. The calculations involve both direct and exchange matrix elements, and we employ numerical techniques to evaluate these integrals efficiently.

1.1 Partial-Wave V-Matrix Elements

The partial-wave V-matrix elements for electron-hydrogen scattering are given by:

$$V^S_{f,i}(k',k) = \langle k'\Phi_f|V^S|\Phi_i k\rangle \tag{1}$$

This can be decomposed into direct and exchange terms as:

$$V^S_{f,i}(k',k) = \langle k'\Phi_f|V_1+V_{12}|\Phi_i k\rangle - (-1)^S\langle k'\Phi_f|E-H|k\Phi_i\rangle \tag{2}$$

where V_1 and V_{12} are the incident electron-nuclear potential and electron-electron potential, respectively.

1.1.1 Direct Term

The direct V-matrix elements represent the interaction where the incident electron directly interacts with the target electron in the hydrogen atom without any exchange of identities between the incident and target electrons and is given by:

$$\langle k'\Phi_f|V_1+V_{12}|\Phi_i k\rangle = \frac{2}{\pi}\int_0^\infty\int_0^\infty \sin(k'r_1)\Phi_f(r_2)\left(\frac{1}{r_>}-\frac{1}{r_1}\right)\Phi_i(r_2)\sin(kr_1)\,dr_1\,dr_2 \tag{3}$$

where we use the s-wave model and use partial wave expansion (only for $\ell = 0$ in this case) for the incident electron. This can be simplified and computed efficiently by evaluating the integral in the form:

$$\langle k'\Phi_f|V_1+V_{12}|\Phi_i k\rangle = \frac{2}{\pi}\int_0^\infty \sin(k'r_1)\sin(kr_1)\left[\frac{1}{r_1}\int_0^{r_1}\Phi_f(r_2)\Phi_i(r_2)\,dr_2 + \int_{r_1}^\infty \frac{\Phi_f(r_2)\Phi_i(r_2)}{r_2}\,dr_2 - \frac{\delta_{fi}}{r_1}\right]dr_1 \tag{4}$$

1.1.2 Exchange Term

The exchange term in electron-electron scattering represents the interaction where the incident and target electrons exchange their identities. This term arises due to the indistinguishability of the electrons and the need for the overall wavefunction to be anti-symmetric. The exchange term is expressed below and is dependent on the total energy of the system:

$$\langle k'\Phi_f|E-H|k\Phi_i\rangle = (E-\frac{k'^2}{2}-\frac{k^2}{2})\langle k'|\Phi_i\rangle\langle\Phi_f|k\rangle-\langle k'|V_1|\Phi_i\rangle\langle\Phi_f|k\rangle-\langle k'|\Phi_i\rangle\langle\Phi_f|V_2|k\rangle-\langle k'\Phi_f|V_{12}|k\Phi_i\rangle \tag{5}$$

The non-separable term $\langle k'\Phi_f|V_{12}|k\Phi_i\rangle$ has the same form as the V_{12} term in the direct matrix element and is calculated similarly:

$$\langle k'\Phi_f|V_{12}|k\Phi_i\rangle = \frac{2}{\pi}\int_0^\infty \sin(k'r_1)\Phi_i(r_1)\left[\frac{1}{r_1}\int_0^{r_1}\Phi_f(r_2)\sin(kr_2)\,dr_2+\int_{r_1}^\infty\frac{\Phi_f(r_2)\sin(kr_2)}{r_2}\,dr_2\right]dr_1 \tag{6}$$

1.2 Implementation

The program calculates the direct and exchange V matrix elements using the $\ell = 0$ wave functions. For this program we only consider the initial target states always being $1s$ with the final states are allowed to be $1s, 2s, 3s$, ..etc. The program reads in the projectile energy, the number of radial grid points and spacing and also the final state `fstate` which is just an integer representing the final target state. It then sets up the kgrid and calculates the radial laguerre basus functions to represent the hydrogen wavefunctions. Using these wavefunctions the program calculates the direct and exchange V-matrix elements using the following subroutines described below.

1.2.1 Direct V-matrix calculation

The `calc_direct_V_mat_elements` subroutine calculates the direct V-matrix elements by numerically evaluating equation 4. In the implementation, the `krond` variable is set to 1.0 if there is no transition (when `fstate` equals 1) and 0.0 otherwise. This is crucial for correctly computing the Kronecker delta term, which ensures the proper treatment of the direct and exchange interactions. Since this involves a non-separable integral, the two inner integrals must be evaluated for all values of r_1 in our `rgrid`. The integral takes the form,

$$\int_0^\infty f(r_1)\left(\frac{1}{r_1}\int_0^{r_1}g(r_2)\,\mathrm{d}r_2+\int_{r_1}^\infty\frac{1}{r_2}g(r_2)\,\mathrm{d}r_2\right)\mathrm{d}r_1 \approx \sum_{i=1}^n w_i f(r_i)\left(\frac{1}{r_i}\sum_{j=1}^i w_j g(r_j)+\sum_{j=i}^n w_j\frac{1}{r_j}g(r_j)\right)$$

where we have discretised it for numerical evaluation using simpson's rule, where w_i are integration weights and n is the number of discrete radial grid points. The method we use to calculate this efficiently is shown below,

Step 1: Forward Iteration

Iterate forwards over the radial grid from $i = 1$ to n, and compute an array A1(i) which calculates the inner sum of $\int_0^{r_1} g(r_2)\,\mathrm{d}r_2$ where each element contains the integral for a given r_1 value. The function $g(r_2)$ is calculated before hand as the product of the final and initital target state wavefunctions:

$$\mathrm{A1}(i) = \sum_{j=1}^{i} w_j g(r_j) = \mathrm{A1}(i-1) + w_i g(r_i) \tag{7}$$

Step 2: Backward Iteration

Iterate backwards over the radial grid from $i = n$ to 1, and compute an array $\mathrm{A2}(i)$ which accumulates the inner sum of $\int_{r_1}^{\infty} \frac{1}{r_2} g(r_2)\, dr_2$:

$$\mathrm{A2}(i) = \sum_{j=i}^{n} w_j \frac{1}{r_j} g(r_j) = \mathrm{A2}(i+1) + w_i \frac{1}{r_i} g(r_i) \tag{8}$$

Step 3: Final Summation

Combine the results of the forward and backward sums to approximate the outer integral:

$$\sum_{i=1}^{n} w_i f(r_i) \left(\frac{1}{r_i} \mathrm{A1}(i) + \mathrm{A2}(i) \right) \tag{9}$$

This method is efficient because it avoids recalculating the inner sums for each value of r_1 in the outer sum by precomputing them in the forward and backward passes. Last step is achieved in the double for loop over the k' and k indices. For each pair, the function $f(r_1)$ is calculated for each k' and k value. Then the integral is evaluated using the precomputed `A1` and `A2` arrays, ensuring the kronecker delta term is included. After computing matrix elements, the subroutine calculates the on-shell elements for all the incident `kgrid` values, by considering energy conservation, where the initial sum of the target and $1s$ energy must equal to the energy of the outgoing electron and the final target state energy. We do this by calculating the final momentum of the electron k' using k and the final state energy ϵ_f and storing k' in an array called `kprime`. We then iterate over the number of k-grid points and evaluate $V(k, k')$ storing the on-shell points in an array called `Von`.

```
subroutine calc_direct_V_mat_elements(nrmax, nkmax, fstate, dr,
   kgrid, r, wf, rweights, V, Von, kprime)
                        ...

        ! Check if there is a transition
        krond = 1.0d0
        if (fstate /= 1) krond = 0.0d0

        V = 0.0d0
        Von = 0.0d0
        ! Calculate g(r2)
        g(:) = wf(:,fstate) * wf(:, 1)

        ! Calculate A1 array
        A1(1) = rweights(1) * g(1)
        do i = 2, nrmax
            A1(i) = A1(i-1) + rweights(i) * g(i)
        end do
        ! Calculate A2 array
        A2(nrmax) = rweights(nrmax) * g(nrmax) / r(nrmax)
```

```
        do i = nrmax-1, 1, -1
            A2(i) = A2(i+1) + rweights(i) * g(i) / r(i)
        end do

        ! Loop over k' and k
        do ki = 1, nkmax
            do kj = 1, nkmax
                ! Calculate f(r1)
                    f(:) = sin(kgrid(ki) * r) * sin(kgrid(kj) * r
                       )
                    ! Loop over r1
                     V(ki, kj) = 2.0d0 / pi * sum(f(:) * (A1(:) /
                         r(:) + A2(:) - krond / r(:)) * rweights
                        (:))

            end do
        end do

        !loop to calculate onshell Values
        do ki = 1, nkmax
            f(:) = sin(kgrid(ki) * r) * sin(kprime(ki) * r)
            Von(ki) = 2.0d0 / pi * sum(f(:) * (A1(:) / r(:) + A2(:)
               - krond / r(:)) * rweights(:))
        end do
end subroutine calc_direct_V_mat_elements
```

1.2.2 Exchange V-matrix calculation

In order to calculate the exchange V-matrix elements we numerically evaluate the terms in equation 5 using the `calc_exchange_V_mat_elements` subroutine. The last term (equation 6) is calculated using a similar method to calculating the direct terms, however the inner integrals now involve integrands depending on k meaning we would have to repeat the previous method for each value of k as we iterate through k and k'. For computational efficiency, we precompute the `A1` and `A2` values for each k by making them a 2-D array and storing backwards and forwards iterations in the rows for each k, before the double for loop starts to avoid recalculating the values again for the next iterations of k' values in the for loop. This is also done for the remaining terms that have k or k' dependence, to avoid recalculating sums.

```
subroutine calc_exchange_V_mat_elements(nrmax, nkmax, fstate, dr,
   kgrid, r, wf, rweights, V, Von, kprime, E)
    ...
    ! Calculate g(r2), f(r1), A1, A2 and other matrix element terms
    do i = 1, nkmax
        f(i,:) = sin(kgrid(i) * r(:)) * wf(:,1)
        Of(i) = sum(sin(kgrid(i) * r(:)) * wf(:,1) * rweights(:))
        V1(i) = sum(-sin(kgrid(i) * r(:)) *wf(:,1) * rweights(:) / r
           (:))
        Oi(i) = sum(sin(kgrid(i) * r(:)) * wf(:,fstate) * rweights
           (:))
        V2(i) = sum(-sin(kgrid(i) * r(:)) * wf(:,fstate) * rweights
           (:) / r(:))
```

```
10          g(i,:) = wf(:,fstate) * sin(kgrid(i) * r)
11          ! Calculate A1 array
12          A1(i,1) = rweights(1) * g(i,1)
13          do j = 2, nrmax
14              A1(i,j) = A1(i,j-1) + rweights(j) * g(i,j)
15          end do
16          ! Calculate A2 array
17          A2(i,nrmax) = rweights(nrmax) * g(i,nrmax) / r(nrmax)
18          do j = nrmax-1, 1, -1
19                  A2(i,j) = A2(i,j+1) + rweights(j) * g(i,j) / r(j)
20          end do
21      end do
22
23      ! Loop over k' and k
24      do ki = 1, nkmax
25          do kj = 1, nkmax
26                  ! Calculate V12 term
27                  V(ki, kj) = sum(f(ki,:) * (A1(kj,:) / r(:) + A2(kj
                        ,:)) * rweights(:))
28                  ! Calculate V(k',k)
29                  V(ki,kj) = (E - kgrid(ki)**2 / 2.0d0 - kgrid(kj)**2
                        / 2.0d0) * Oi(kj) * Of(ki) &
30                  -V1(ki) * Oi(kj) - Of(ki) * V2(kj) - V(ki,kj)
31          end do
32      end do
33      V = 2.0d0 / pi * V
34
35      !loop to calculate onshell Values
36      do i = 1, nkmax
37              !we want to recalculate the k' terms from before
38              f(i,:) = sin(kprime(i) * r(:)) * wf(:,1)
39              Of(i) = sum(sin(kprime(i) * r(:)) * wf(:,1) * rweights
                    (:))
40              V1(i) = sum(-sin(kprime(i) * r(:)) *wf(:,1) * rweights
                    (:) / r(:))
41
42              Von(i) = sum(f(i,:) * (A1(i,:) / r(:) + A2(i,:)) *
                    rweights(:))
43              Von(i) = (kgrid(i)**2 / 2.0d0 -0.5 - kprime(i)**2 / 2.0
                    d0 - kgrid(i)**2 / 2.0d0) * Oi(i) * Of(i) &
44              -V1(i) * Oi(i) - Of(i) * V2(i) - Von(i)
45      end do
46      Von = 2.0/pi * Von
47  end subroutine calc_exchange_V_mat_elements
```

1.3 Results

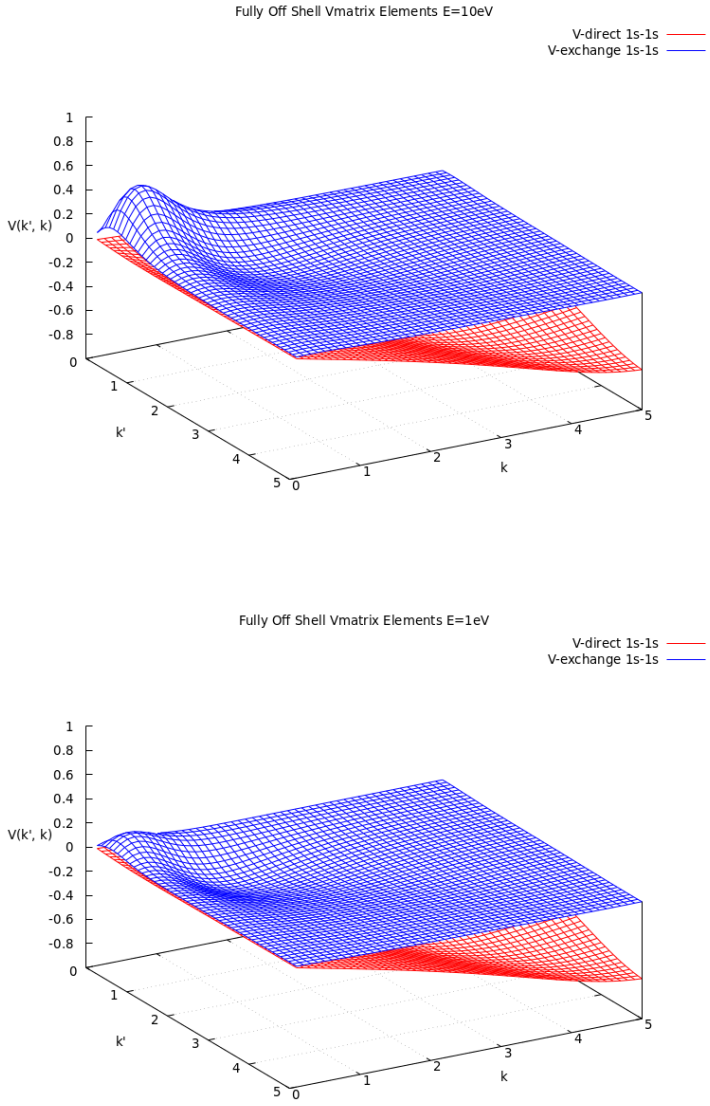

Figure 1: 1s-1s V-direct and V-exchange matrix elements for both 10eV and 1eV incident electron energies.

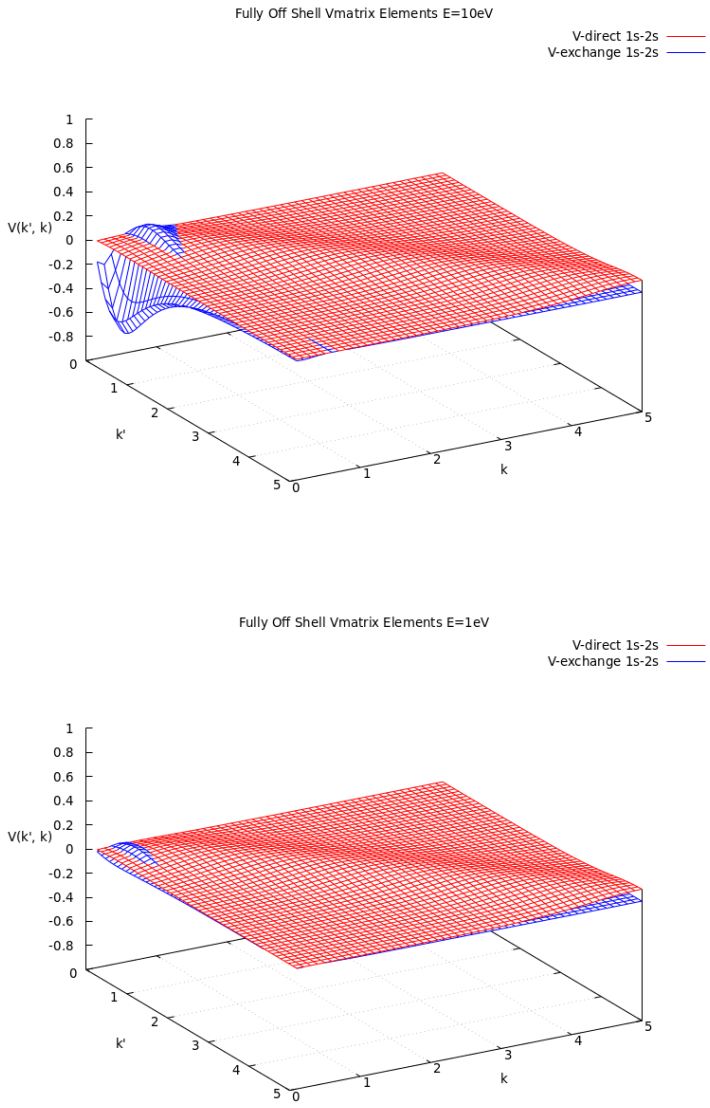

Figure 2: 1s-2s V-direct and V-exchange matrix elements for 10ev and 1ev incident electron energies.

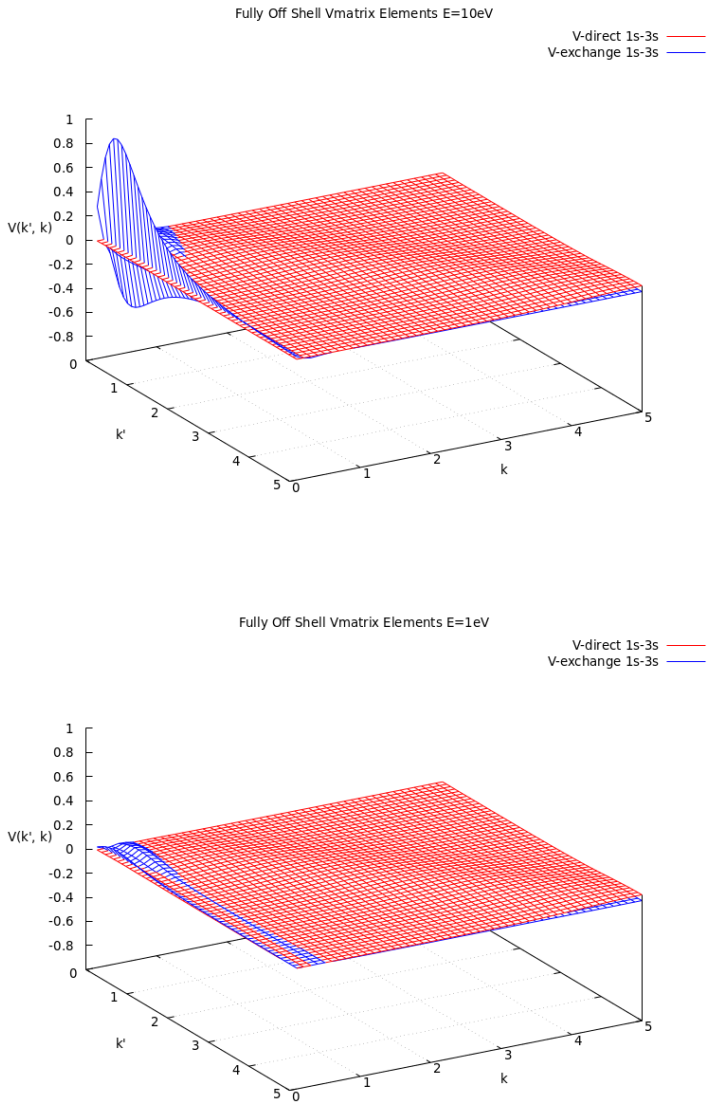

Figure 3: 1s-3s V-direct and V-exchange matrix elements for 10ev and 1ev incident electron energies.

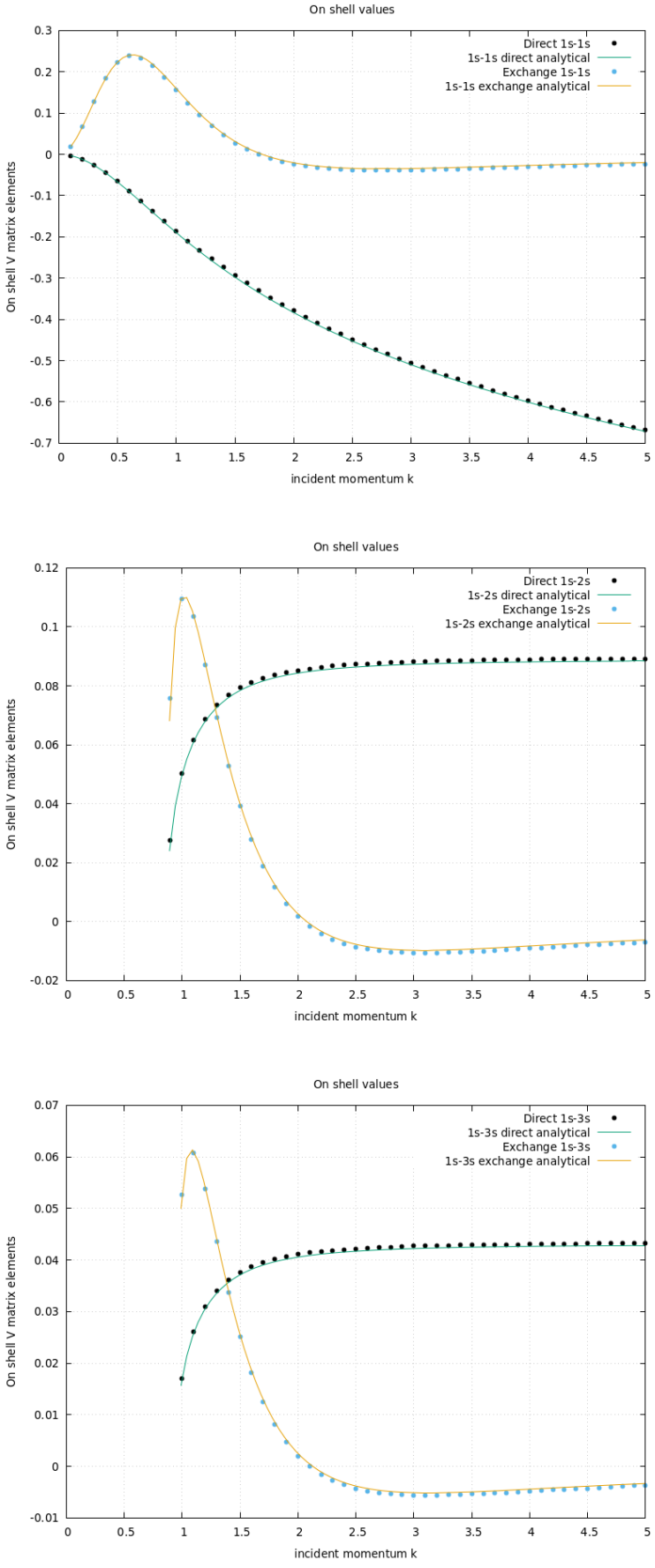

Figure 4: Analytical vs computed V-direct and V-exchange, on-shell matrix elements for an arbitrary k-grid. Top to bottom shows different transitions of the target state.

In figure 1, for elastic scattering, the direct and exchange V-matrix elements clearly exhibit symmetry with respect to the interchange of k' and k. We also see that the V-direct elements are independent of the total energy of the system and remain unchanged, while the exchange matrix elements show a decrease in magnitude when incident energy is 1eV. For higher values of $k = k'$ we see the V-direct elements become more negative while the exchange elements flatten out to zero probably due to reduced overlap between the incident and target electron wave functions? For the in-elastic scattering the V matrix elements are no longer symmetric due to having different final states and we see the same behaviour as before for when the projectile energy is decreased the magnitude of the exchange elements decrease. The direct elements are all positive values and flatten out more for higher transitional states. Looking at figure 4 the direct on-shell values, which respect energy conservation, are generally higher in magnitude over large k compared to the exchange values, reflecting the dominance of direct interactions. This might be because, at higher energies, the incoming electron spends less time in the vicinity of the target electron, reducing the likelihood of significant exchange interactions. For in-elastic cases we see no on-shell values for lower incident momenta due to these values not being sufficient to account for the energy difference between the initial and final states for the transition to occur.

2 Problem 3- Single-channel s-wave CCC

Non-uniqueness issues can arise when solving the Lippmann-Schwinger equation for the K-matrix. These issues are particularly prevalent in triplet scattering where $S = 1$. To address this, we use the "theta trick" which introduces a parameter θ to modify the total energy in the exchange matrix elements. This modification helps to resolve the non-uniqueness by effectively shifting the energy and breaking the symmetry that causes the issue and resolves ambiguities in calculation of scattering amplitudes and cross-sections.

2.1 Non-Uniqueness in the Exchange Matrix Elements

The exchange matrix element for electron-hydrogen scattering in the partial-wave expansion was given in equation 5. To resolve the non-uniqueness, we replace the total energy E with:

$$E(1 - \theta + (-1)^S\theta) \tag{10}$$

where θ is a parameter used to resolve the non-uniqueness, and S is the spin state (0 for singlet and 1 for triplet). The modified total partial-wave V-matrix element then becomes:

$$\langle k'\Phi_f|V^S(\theta)|\Phi_i k\rangle = \langle k'\Phi_f|V_1 + V_{12}|\Phi_i k\rangle - (-1)^S\langle k'\Phi_f|E(1 - \theta + (-1)^S\theta) - H|k\Phi_i\rangle$$

For singlet scattering, the V-matrix is independent of θ, thus there is no non-uniqueness issue. For triplet scattering, non-uniqueness is addressed by introducing the θ parameter, making the V-matrix element dependent on θ.

2.2 Implementation

To calculate the K matrix values we use the code from assignment 4 and use our subrotuines from problem 1 to calculate the total V-matrix by changing the `calculate_Vmatrix` subroutine. We change the total energy using equation 10 and input it to our exchange subroutine and then calculate the total V-matrix elements.

```
subroutine calculate_Vmatrix(nkmax,kgrid,nrmax,rgrid,rweights,wf,
    energy,theta,Vmat)
   ...
   !use the theta trick
   E = energy*(1.0d0 - 2.0d0*theta)
   call calc_direct_V_mat_elements(nrmax, nkmax, kgrid, rgrid, wf,
      rweights, Vdir)
   call calc_exchange_V_mat_elements(nrmax, nkmax, kgrid, rgrid, wf,
      rweights, Vex, E)
   Vmat = Vdir+Vex
end subroutine calculate_Vmatrix
```

2.3 Results

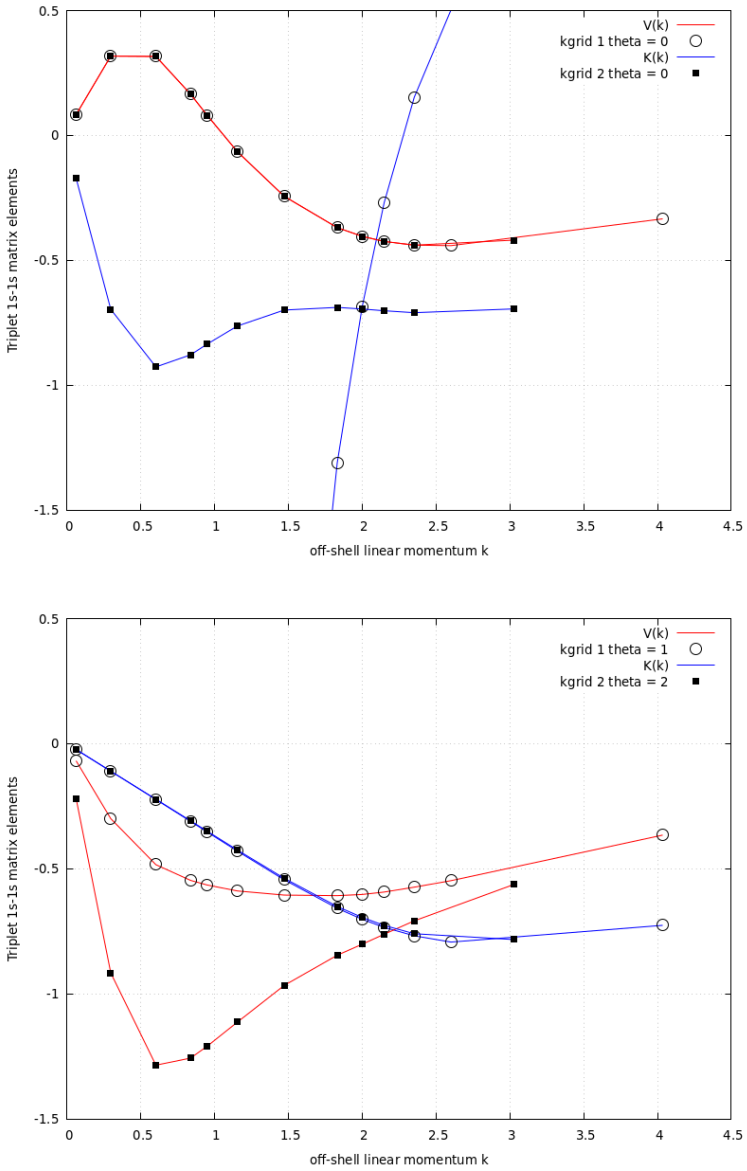

Figure 5: Triplet half off-shell 1s-1s V and K matrix elements for an incident energy of 54.4232eV for $\theta = 0, 1, 2$ using 2 different k-grids.

The results from implementing the theta trick in the calculation of the exchange matrix elements are illustrated in the provided graphs. The graphs show the behavior of the triplet half-offshell 1s-1s V and K matrix elements for different values of θ. The top graph compares the matrix elements for $\theta = 0$ using two different k-grids. The $V(k')$ values exhibit the same behavior as expected. The $K(k')$ values show differences for the two k-grids, while containing the same on-shell values. This indicates that the non-uniqueness issue is present when $\theta = 0$, as the off-shell K-matrix elements differ for the same incident energy. This non-uniqueness means that there are multiple possible values for the K-matrix elements, leading to ambiguity in the scattering calculations. The bottom graph shows the matrix elements for $\theta = 1$ and $\theta = 2$. Here, the introduction of θ resolves the non-uniqueness issue. The $K(k')$ values for $\theta = 1$ and $\theta = 2$ are the same for both k-grids, demonstrating that the theta trick successfully works. The consistency of the K-matrix elements across different k-grids and θ values indicates that the non-uniqueness problem has been resolved, ensuring that the results are physically meaningful.

Φ_f

Direct V-matrix elements are given: $\langle k'\ell'm'|V_1+V_{12}|\Phi_i k\ell m\rangle$

$= \langle k'\Phi_f|V_1+V_{12}|\Phi_i k\rangle = \langle k'\Phi_f|V_1|\Phi_i k\rangle + \langle k'\Phi_f|V_{12}|\Phi_i k\rangle$

where we wrote $|k\ell m\rangle = |k\rangle$ for simplicity.

term 1 $\Rightarrow \langle k'\Phi_f|V_1|\Phi_i k\rangle = \iiint\int \langle k'\Phi_f|\vec{r}_2\vec{r}_1'\rangle\langle\vec{r}_1'\vec{r}_2'|V_1|\vec{r}_2\vec{r}_1\rangle\langle\vec{r}_1\vec{r}_2|\Phi_i k\rangle d^3\vec{r}_1' d^3\vec{r}_2' d^3\vec{r}_1 d^3\vec{r}_2$

$\langle\vec{r}_2'\vec{r}_1'|V_1|\vec{r}_2\vec{r}_1\rangle = -\dfrac{\delta(\vec{r}_2'-\vec{r}_2)\,\delta(\vec{r}_1'-\vec{r}_1)}{r_1}$ since $V_1|\vec{r}_1\rangle = \frac{1}{r_1}|\vec{r}_1\rangle$

this simplifies integral to,

$$-\iint \frac{\langle k'\Phi_i|\vec{r}_2\vec{r}_1\rangle\langle\vec{r}_1\vec{r}_2|\Phi_i k\rangle}{r_1} d^3\vec{r}_1 d^3\vec{r}_2 = -\int \frac{\langle k'|\vec{r}_1\rangle\langle\vec{r}_1|k\rangle}{r_1} d^3\vec{r}_1 \int \langle\Phi_f|\vec{r}_2\rangle\langle\vec{r}_2|\Phi_i\rangle d^3\vec{r}_2$$

$$= \frac{2}{\pi}\int_0^\infty \frac{u_{\ell_f}(r_1;k')\,u_{\ell_i}(r_1;k)}{r_1} dr_1 \int_0^\infty \overline{\Phi}_{n_f\ell_f}(r_2)\,\overline{\Phi}_{n_i\ell_i}(r_2)\,dr_2 \int_{\Omega_1} Y_\ell^m(\hat{r}_1)\,Y_{\ell'}^{m'}(\hat{r}_1)\,d\Omega_1 \int_{\Omega_2} Y_{\ell_i}^{m_i}(\hat{r}_2)\,Y_{\ell_f}^{m_f}(\hat{r}_2)\,d\Omega_2$$

where $\int_{\Omega_1} Y_\ell^m(\hat{r}_1)\,Y_{\ell'}^{m'}(\hat{r}_1)\,d\Omega_1 = \delta_{mm'}\delta_{\ell\ell'}$

and $\int_{\Omega_2} Y_{\ell_i}^{m_i}(\hat{r}_2)\,Y_{\ell_f}^{m_f}(\hat{r}_2)\,d\Omega_2 = \delta_{m_i m_f}\delta_{\ell_i\ell_f}$

In the s-wave model ($\ell=0$, $m=0$), the spherical harmonics terms disappear (Y_0^0) and so only the radial integrals remain, due to spherical symmetry.

second term $\Rightarrow \langle k'\Phi_f|V_{12}|\Phi_i k\rangle = \iiint\int \langle k'\Phi_f|\vec{r}_2'\vec{r}_1'\rangle\langle\vec{r}_1'\vec{r}_2'|V_{12}|\vec{r}_2\vec{r}_1\rangle\langle\vec{r}_1\vec{r}_2|\Phi_i k\rangle d^3\vec{r}_1' d^3\vec{r}_2' d^3\vec{r}_1 d^3\vec{r}_2$

using similar method to before and using $V_{12}|\vec{r}_2\vec{r}_1\rangle = \frac{1}{|\vec{r}_1-\vec{r}_2|}|\vec{r}_2\vec{r}_1\rangle$

we get $\langle k'\Phi_f | V_{12} | \Phi_i k\rangle = \iint \frac{\langle k'\Phi_f | V_2 r_1\rangle \langle r_1 r_2 | \Phi_i k\rangle}{|\vec{r}_1 - \vec{r}_2|} d^3\vec{r}_1 \, d\vec{r}_2$

$$\frac{1}{|\vec{r}_1 - \vec{r}_2|} = \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \sum_{\mu=-\lambda}^{\lambda} (-1)^{\mu} \frac{r_<^{\lambda}}{r_>^{\lambda+1}} Y_{\lambda}^{-\mu}(\hat{r}_1) Y_{\lambda}^{\mu}(\hat{r}_2)$$

and so,

$$\langle k'\Phi_f | V_{12} | \Phi_i k\rangle = \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \sum_{\mu=-\lambda}^{\lambda} (-1)^{\mu} \int \langle k'|\vec{r}_1\rangle \langle \vec{r}_1|k\rangle \int \langle \Phi_f | \vec{r}_2\rangle \langle \vec{r}_2 | \Phi_i\rangle \frac{r_<^{\lambda}}{r_>^{\lambda+1}} Y_{\lambda}^{-\mu}(\hat{r}_1) Y_{\lambda}^{\mu}(\hat{r}_2) \, d^3r_1 d^3r_2$$

$$= \frac{2}{\pi} \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \sum_{\mu=-\lambda}^{\lambda} (-1)^{-\mu} \int_0^{\infty} u_{\ell}(r_1;k') u_{\ell}(r_1;k) \int_0^{\infty} \underset{n_f \ell_f}{\Phi}(r_2) \underset{n_i \ell_i}{\Phi}(r_2) \frac{r_<^{\lambda}}{r_>^{\lambda+1}} dr_1 dr_2 \int_{\Omega_1} Y_{\ell'}^{m'}(\hat{r}_1) Y_{\lambda}^{-\mu}(\hat{r}_1) Y_{\ell}^{m}(\hat{r}_1) d\Omega_1$$

$$\cdots \times \int_{\Omega_2} Y_{\ell_f}^{m_f}(\hat{r}_2) Y_{\lambda}^{\mu}(\hat{r}_2) Y_{\ell_i}^{m_i}(\hat{r}_2) d\Omega_2$$

$$= \sum_{\lambda=0}^{\infty} \frac{8}{2\lambda+1} \sum_{\mu=\lambda}^{\lambda} (-1)^{-\mu} \int_0^{\infty} u_{\ell}(r_1;k') u_{\ell}(r_1;k) \int_0^{\infty} \underset{n_f \ell_f}{\Phi}(r_2) \underset{n_i \ell_i}{\Phi}(r_2) \frac{r_<^{\lambda}}{r_>^{\lambda+1}} dr_1 dr_2 \langle Y_{\ell'}^{m'} | Y_{\lambda}^{-\mu} | Y_{\ell}^{m}\rangle \langle Y_{\ell_f}^{m_f} | Y_{\lambda}^{\mu} | Y_{\ell_i}^{m_i}\rangle$$

in the s-wave model $\ell = 0$ ∴ this indicates $\lambda = 0$ and so

$\frac{r_<^{\lambda}}{r_>^{\lambda+1}}$ reduces to $\frac{1}{r_>}$ and the spherical harmonic parts turn to constants, and we obtain a non-separable integral over radial coordinates.