

## Contents

<b>1</b>	<b>e-H V-Matrix</b>	<b>2</b>
1.1	Implementation . . . . .	2
1.1.1	Calculation of Direct Matrix Elements $D_{f,i}(k', k)$ . . . . .	2
1.1.2	Calculation of Exchange Matrix Elements $X_{f,i}(k', k)$ . . . . .	3
1.1.3	Evaluation of Integrals . . . . .	3
1.2	Direct Matrix Elements . . . . .	4
1.3	Exchange Matrix Elements . . . . .	6
1.3.1	$X_{f,i}(k', k)$ for $E = 10 \text{ eV}$ . . . . .	6
1.3.2	$X_{f,i}(k', k)$ for $E = 1 \text{ eV}$ . . . . .	8
1.4	On-Shell Matrix Elements . . . . .	10
<b>2</b>	<b><math>V_{12}</math> Potential in S-Wave Model</b>	<b>12</b>
<b>3</b>	<b>Reduced CCC Code</b>	<b>14</b>

## List of Figures

1	Direct Matrix Elements 1s-1s . . . . .	4
2	Direct Matrix Elements 1s-2s . . . . .	5
3	Direct Matrix Elements 1s-3s . . . . .	5
4	Exchange Matrix Elements 1s-1s . . . . .	6
5	Exchange Matrix Elements 1s-2s . . . . .	7
6	Exchange Matrix Elements 1s-3s . . . . .	7
7	Exchange Matrix Elements 1s-1s . . . . .	8
8	Exchange Matrix Elements 1s-2s . . . . .	9
9	Exchange Matrix Elements 1s-3s . . . . .	9
10	On-Shell Matrix Elements 1s-1s . . . . .	10
11	On-Shell Matrix Elements 1s-2s . . . . .	11
12	On-Shell Matrix Elements 1s-3s . . . . .	11

## List of Tables

The entire code repository used to calculate the data for this report can be found at <https://github.com/dgsaf/acqm-workshop-5>. Note that section 3 has not yet been attempted - it may be at a later date if time permits.

## 1 e-H V-Matrix

### 1.1 Implementation

We denote the hydrogen target states by  $|\phi_i\rangle$ , and we denote the electron projectile states by  $|\mathbf{k}\rangle$  corresponding to continuum waves with energy  $\frac{1}{2}k^2$ , where  $k = \|\mathbf{k}\|$ . We shall work in the s-wave model; that is, we only consider target states with  $\ell_i = 0$  and  $m_i = 0$ , and continuum states with

$$\langle \mathbf{r} | \mathbf{k} \rangle = N_k \sin(rk).$$

Note that we shall neglect the normalisation constants  $N_k$  henceforth. We calculate potential matrix elements of the form

$$\begin{aligned} V_{f,i}^{(S)}(k', k) &= \langle k', \phi_f | \hat{V}^S | \phi_i, k \rangle \\ &= \langle k', \phi_f | \hat{V} - (-1)^S (E - \hat{H}) \hat{P}_r | \phi_i, k \rangle \\ &= \langle k', \phi_f | \hat{V}_1 + \hat{V}_{1,2} | \phi_i, k \rangle - (-1)^S \langle k', \phi_f | E - \hat{H} | k, \phi_i \rangle \\ &= D_{f,i}(k', k) - (-1)^S X_{f,i}(k', k) \end{aligned}$$

where  $D_{f,i}(k', k)$  is the direct matrix element,  $X_{f,i}(k', k)$  is the exchange matrix element, and where  $\hat{V}_1$  is the electron-nuclear potential of the form

$$\hat{V}_1 = -\frac{1}{r_1},$$

and where  $\hat{V}_{1,2}$  is the electron-electron potential of the form

$$\hat{V}_{1,2} = \frac{1}{\|\mathbf{r}_1 - \mathbf{r}_2\|} = \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}} \sum_{\mu=-\lambda}^{\lambda} Y_{\lambda}^{\mu}(\Omega_1) Y_{\lambda}^{\mu*}(\Omega_2)$$

where  $r_{<} = \min(r_1, r_2)$ ,  $r_{>} = \max(r_1, r_2)$ , and where  $Y_{\lambda}^{\mu}$  are the spherical harmonics. However, within the s-wave model this potential reduces to the form

$$\hat{V}_{1,2} = \frac{1}{r_{>}} = \frac{1}{\max(r_1, r_2)}.$$

#### 1.1.1 Calculation of Direct Matrix Elements $D_{f,i}(k', k)$

The direct matrix elements are of the form

$$D_{f,i}(k', k) = \langle k', \phi_f | \hat{V}_1 + \hat{V}_{1,2} | \phi_i, k \rangle$$

where

$$\begin{aligned} \langle k', \phi_f | \hat{V}_1 | \phi_i, k \rangle &= \langle k' | \hat{V}_1 | k \rangle \langle \phi_f | \phi_i \rangle \\ &= - \int_0^{\infty} \frac{1}{r_1} \sin(k'r_1) \sin(kr_1) dr_1 \int_0^{\infty} \phi_f(r_2) \phi_i(r_2) dr_2 \\ &= - \int_0^{\infty} \frac{1}{r_1} \sin(k'r_1) \sin(kr_1) dr_1 \delta_{f,i} \end{aligned}$$

and where

$$\begin{aligned} \langle k', \phi_f | \hat{V}_{1,2} | \phi_i, k \rangle &= \int_0^{\infty} \int_0^{\infty} \sin(k'r_1) \phi_f(r_2) \frac{1}{\max(r_1, r_2)} \sin(kr_1) \phi_i(r_2) dr_1 dr_2 \\ &= \int_0^{\infty} \sin(k'r_1) \sin(kr_1) \left( \int_0^{\infty} \frac{1}{\max(r_1, r_2)} \phi_f(r_2) \phi_i(r_2) dr_2 \right) dr_1 \\ &= \int_0^{\infty} \sin(k'r_1) \sin(kr_1) \left( \frac{1}{r_1} \int_0^{r_1} \phi_f(r_2) \phi_i(r_2) dr_2 + \int_{r_1}^{\infty} \frac{1}{r_2} \phi_f(r_2) \phi_i(r_2) dr_2 \right) dr_1. \end{aligned}$$

### 1.1.2 Calculation of Exchange Matrix Elements $X_{f,i}(k', k)$

The exchange matrix elements are of the form

$$\begin{aligned} X_{f,i}(k', k) &= \langle k', \phi_f | E - \hat{H} | k, \phi_i \rangle \\ &= (E - \frac{1}{2}k'^2 - \frac{1}{2}k^2) \langle k' | \phi_i \rangle \langle \phi_f | k \rangle \\ &\quad - \langle k' | \hat{V}_1 | \phi_i \rangle \langle \phi_f | k \rangle - \langle k' | \phi_i \rangle \langle \phi_f | \hat{V}_2 | k \rangle \\ &\quad - \langle k', \phi_f | \hat{V}_{1,2} | k \phi_i \rangle \end{aligned}$$

where the one-electron inner products are of the form

$$\langle f | g \rangle = \int_0^\infty f(r)g(r) dr$$

and where the two-electron inner product is of the form

$$\begin{aligned} \langle k', \phi_f | \hat{V}_{1,2} | k \phi_i \rangle &= \int_0^\infty \int_0^\infty \sin(k'r_1) \phi_f(r_2) \frac{1}{\max(r_1, r_2)} \phi_i(r_1) \sin(kr_2) dr_1 dr_2 \\ &= \int_0^\infty \sin(k'r_1) \phi_i(r_1) \left( \int_0^\infty \frac{1}{\max(r_1, r_2)} \phi_f(r_2) \sin(kr_2) dr_2 \right) dr_1 \\ &= \int_0^\infty \sin(k'r_1) \phi_i(r_1) \left( \frac{1}{r_1} \int_0^{r_1} \phi_f(r_2) \sin(kr_2) dr_2 + \int_{r_1}^\infty \frac{1}{r_2} \phi_f(r_2) \sin(kr_2) dr_2 \right) dr_1 \end{aligned}$$

### 1.1.3 Evaluation of Integrals

We suppose that the radial functions are to be plotted on a radial grid of the form  $\mathcal{R} = \{k\delta_r\}_{k=1}^{n_r}$  for  $n_r > 0$  and small  $\delta_r > 0$ , and with a corresponding set of weights  $\mathcal{W} = \{w_k\}_{k=1}^{n_r}$  such that

$$\int_0^\infty f(r) dr = \lim_{n_r \rightarrow \infty} \sum_{k=1}^{n_r} w_k f(r_k) = \lim_{n_r \rightarrow \infty} \sum_{k=1}^{n_r} w_k f_k \approx \sum_{k=1}^{n_r} w_k f_k.$$

The one-electron integrals, of the form  $\langle f | g \rangle$ , are then evaluated in the following manner

$$\langle f | g \rangle = \int_0^\infty f(r)g(r) dr \approx \sum_{k=1}^{n_r} w_k f_k g_k.$$

The two electron integrals  $\langle F | | G \rangle$  where

$$\langle F | | G \rangle = \int_0^\infty F(r_1) \left( \frac{1}{r_1} \int_0^{r_1} G(r_2) dr_2 + \int_{r_1}^\infty \frac{1}{r_2} G(r_2) dr_2 \right) dr_1,$$

are evaluated in the following manner

$$\langle F | | G \rangle \approx \sum_{k=1}^{n_r} w_k F_k \left( \frac{1}{r_k} A_k + B_k \right)$$

where

$$A_k = \sum_{m=1}^k w_m G_m = \begin{cases} A_{k-1} + w_k G_k & \text{for } k = 2, \dots, n_r \\ w_k G_k & \text{for } k = 1 \end{cases}$$

and

$$B_k = \sum_{m=k}^{n_r} \frac{1}{r_m} w_m G_m = \begin{cases} B_{k+1} + \frac{1}{r_k} w_k G_k & \text{for } k = 1, \dots, n_r - 1 \\ \frac{1}{r_k} w_k G_k & \text{for } k = n_r \end{cases}.$$

For these calculations, we have used: a radial grid of the form  $\mathcal{R} = \{i\delta_r\}_{i=1}^{n_r}$ , with  $\delta_r = 0.01$  and  $\max(\mathcal{R}) = 100$ , and a momentum grid of the form  $\mathcal{K} = \{i\delta_k\}_{i=1}^{n_k}$ , with  $\delta_k = 0.025$  and  $\max(\mathcal{K}) = 5$ .

## 1.2 Direct Matrix Elements

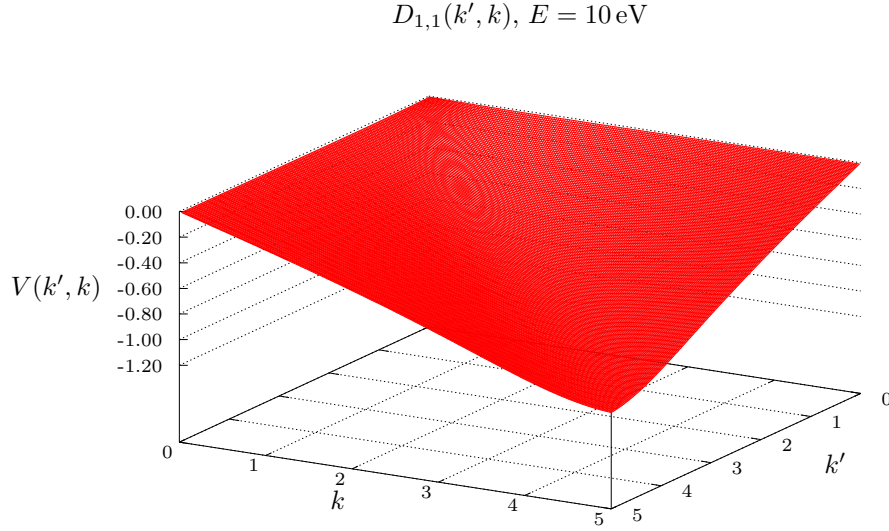


Figure 1: The  $D_{f,i}(k', k)$  direct matrix elements (shown in red) are presented for the  $1s \rightarrow 1s$  transition, with  $E = 10 \text{ eV}$ .

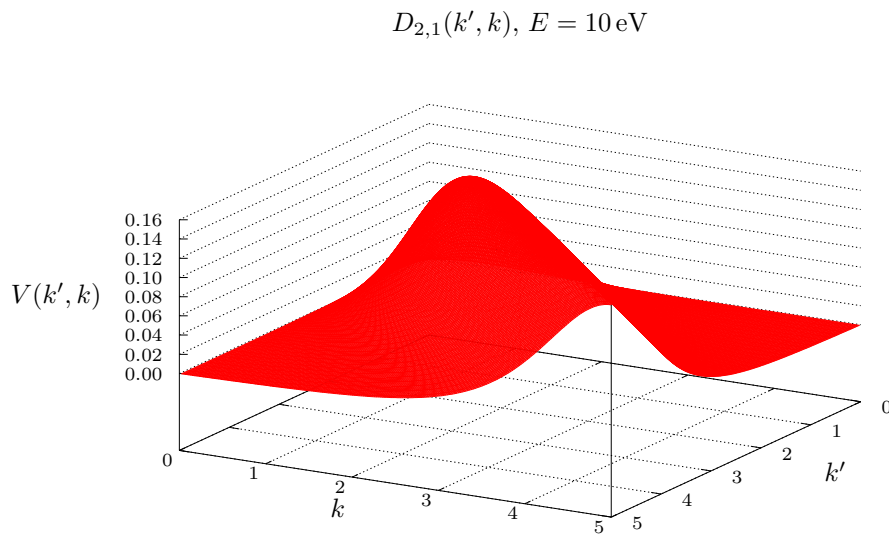


Figure 2: The  $D_{f,i}(k', k)$  direct matrix elements (shown in red) are presented for the  $1s \rightarrow 2s$  transition, with  $E = 10 \text{ eV}$ .

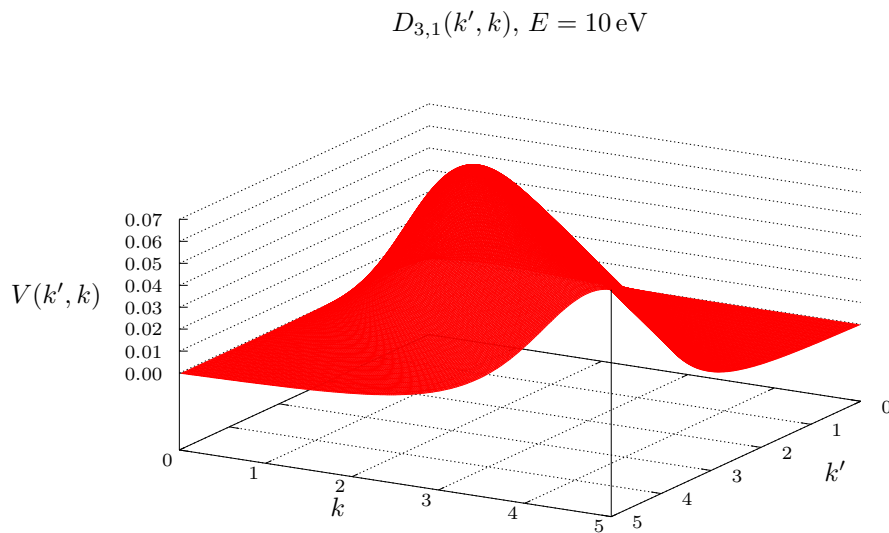


Figure 3: The  $D_{f,i}(k', k)$  direct matrix elements (shown in red) are presented for the  $1s \rightarrow 3s$  transition, with  $E = 10 \text{ eV}$ .

### 1.3 Exchange Matrix Elements

#### 1.3.1 $X_{f,i}(k', k)$ for $E = 10 \text{ eV}$

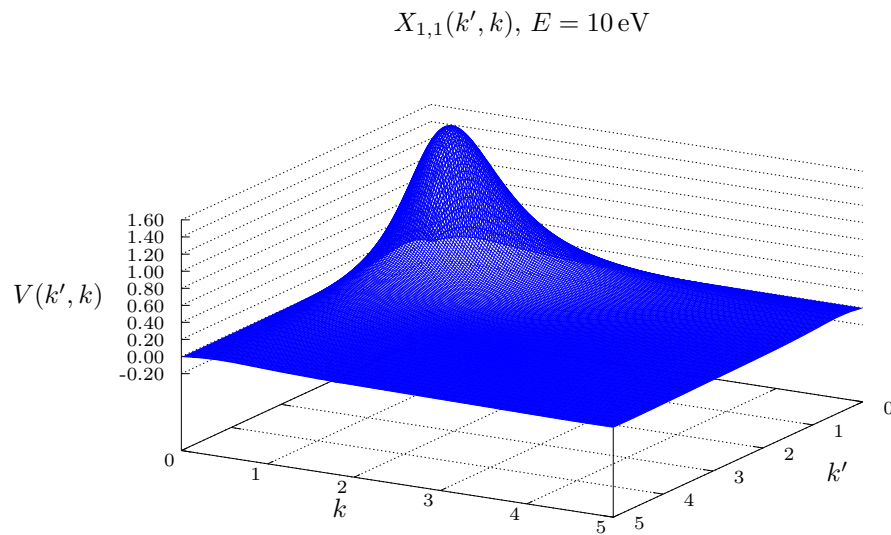


Figure 4: The  $X_{f,i}(k', k)$  exchange matrix elements (shown in blue) are presented for the  $1s \rightarrow 1s$  transition, with  $E = 10 \text{ eV}$ .

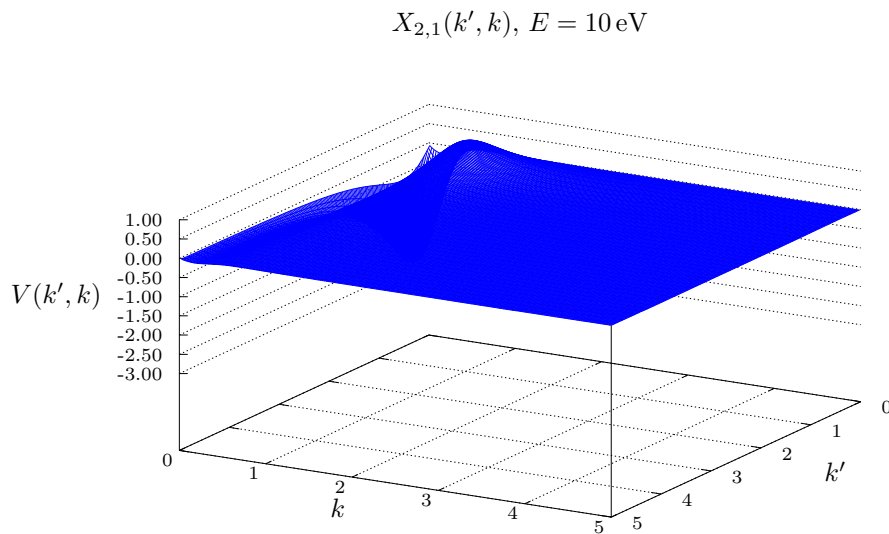


Figure 5: The  $X_{f,i}(k', k)$  exchange matrix elements (shown in blue) are presented for the  $1s \rightarrow 2s$  transition, with  $E = 10 \text{ eV}$ .

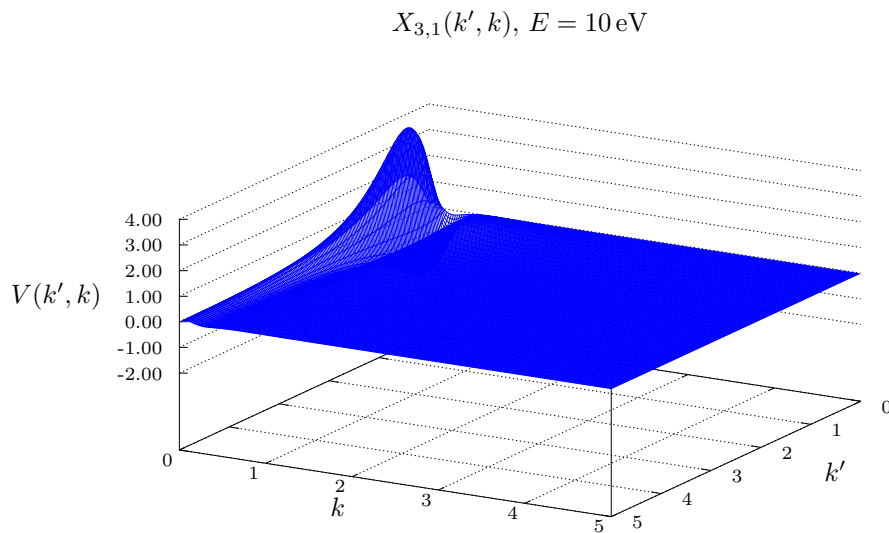


Figure 6: The  $X_{f,i}(k', k)$  exchange matrix elements (shown in blue) are presented for the  $1s \rightarrow 3s$  transition, with  $E = 10 \text{ eV}$ .

### 1.3.2 $X_{f,i}(k',k)$ for $E = 1 \text{ eV}$

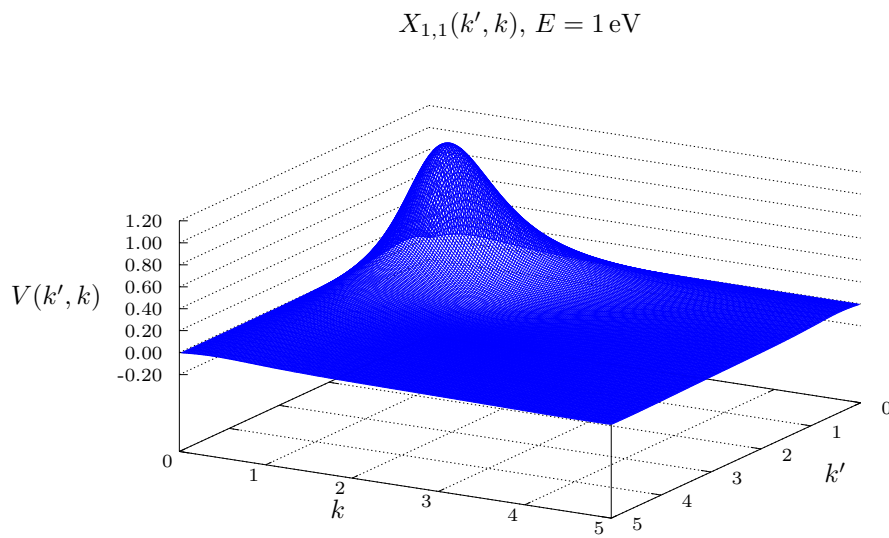


Figure 7: The  $X_{f,i}(k',k)$  exchange matrix elements (shown in blue) are presented for the  $1s \rightarrow 1s$  transition, with  $E = 1 \text{ eV}$ .



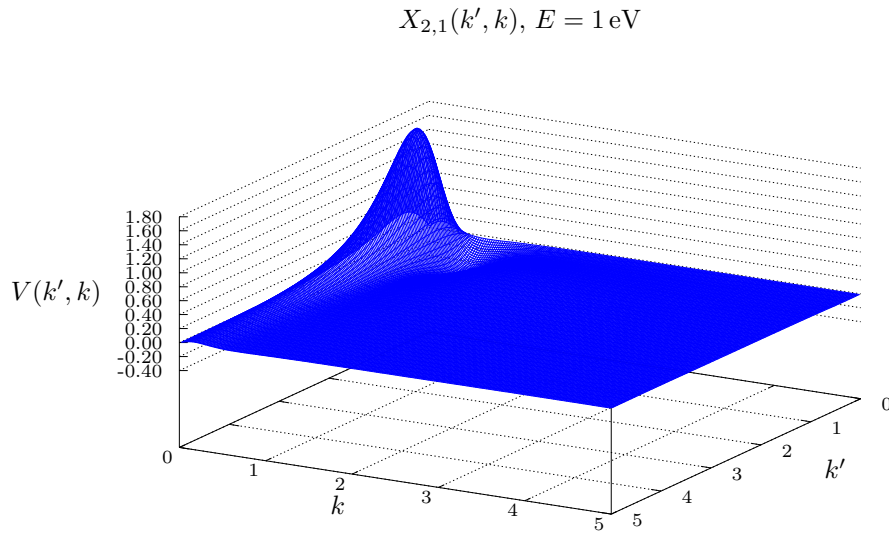


Figure 8: The  $X_{f,i}(k', k)$  exchange matrix elements (shown in blue) are presented for the  $1s \rightarrow 2s$  transition, with  $E = 1 \text{ eV}$ .

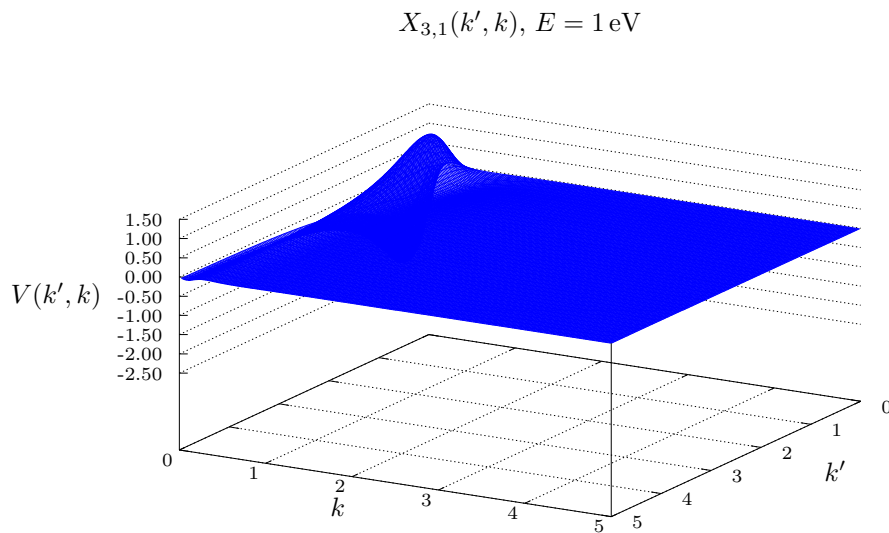


Figure 9: The  $X_{f,i}(k', k)$  exchange matrix elements (shown in blue) are presented for the  $1s \rightarrow 3s$  transition, with  $E = 1 \text{ eV}$ .

## 1.4 On-Shell Matrix Elements

For the transition  $[i \rightarrow f]$ , the on-shell energy is of the form

$$\epsilon_i + \frac{1}{2}k^2 = E = \epsilon_f + \frac{1}{2}k'^2$$

whence the on-shell value for  $k'$  is defined by

$$\frac{1}{2}k'^2 = E - \epsilon_f = \frac{1}{2}k^2 + \epsilon_i - \epsilon_f$$

where for the case of a hydrogen target, with  $\epsilon_n = -\frac{1}{2n^2}$ , and  $i = 1$ , we have have that

$$k' = \sqrt{k^2 - \frac{f^2 - 1}{f^2}}.$$

Note that transitions are forbidden for

$$k^2 < \frac{f^2 - 1}{f^2} = 1 - \frac{1}{f^2}.$$

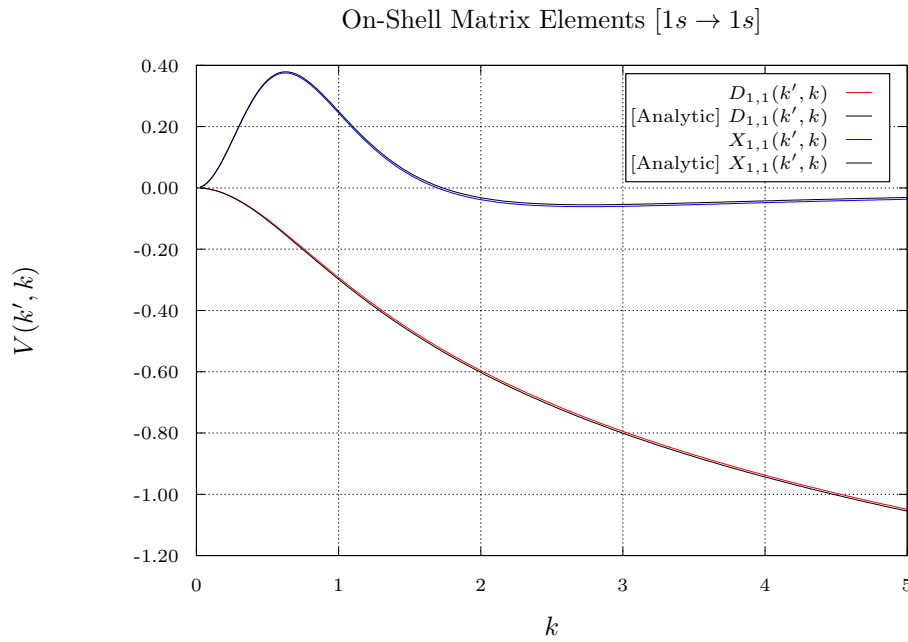


Figure 10: The  $D_{f,i}(k', k)$  direct and  $X_{f,i}(k', k)$  exchange on-shell matrix elements (shown in red and blue respectively) are presented for the  $1s \rightarrow 1s$  transition, and are compared with their respective analytic expressions (shown in black).

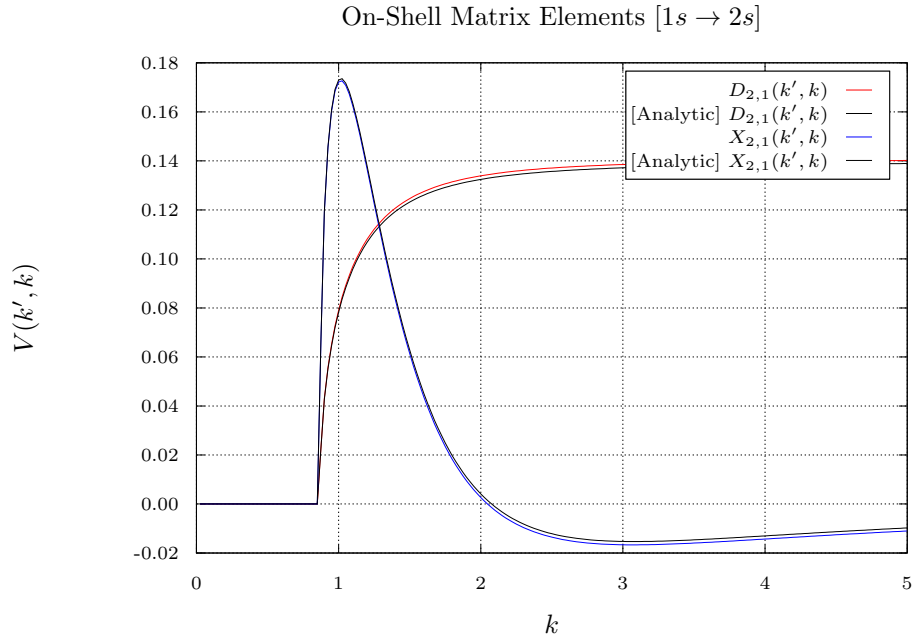


Figure 11: The  $D_{f,i}(k', k)$  direct and  $X_{f,i}(k', k)$  exchange on-shell matrix elements (shown in red and blue respectively) are presented for the  $1s \rightarrow 2s$  transition, and are compared with their respective analytic expressions (shown in black).

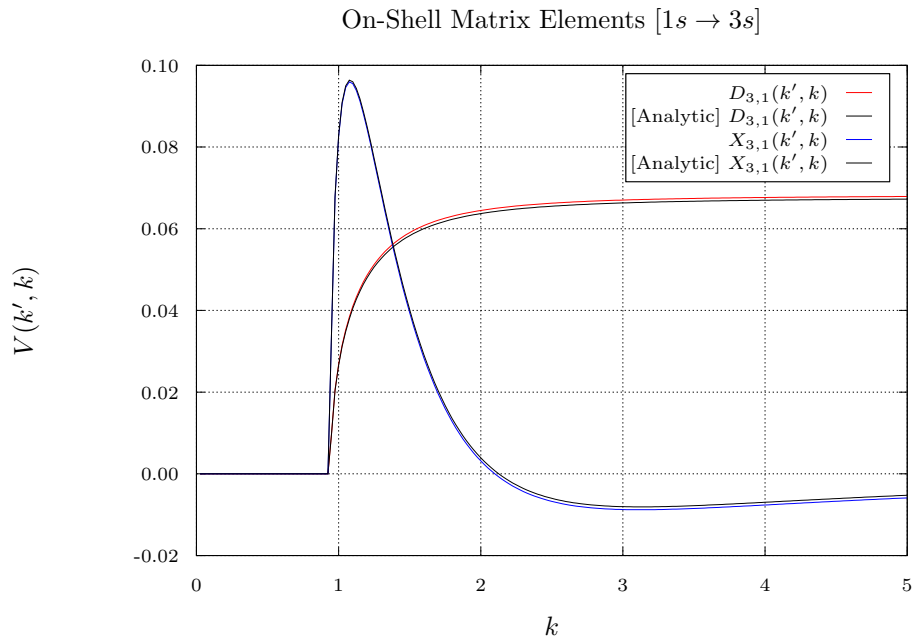


Figure 12: The  $D_{f,i}(k', k)$  direct and  $X_{f,i}(k', k)$  exchange on-shell matrix elements (shown in red and blue respectively) are presented for the  $1s \rightarrow 3s$  transition, and are compared with their respective analytic expressions (shown in black).

## 2 $V_{12}$ Potential in S-Wave Model

We note that the general form for a continuum wave  $|\mathbf{k}\rangle = |k, \ell, m\rangle$  is

$$\langle \mathbf{r} | \mathbf{k} \rangle = \frac{1}{r} u_\ell(r; k) Y_\ell^m(\Omega),$$

and that the general form for the hydrogen target states  $|\phi_i\rangle = |\phi_{n_i, \ell_i, m_i}\rangle$  is

$$\langle \mathbf{r} | \phi_i \rangle = \frac{1}{r} \phi_i(r) Y_{\ell_i}^{m_i}(\Omega).$$

Recall that the electron-electron potential is of the form

$$\hat{V}_{1,2} = \frac{1}{\|\mathbf{r}_1 - \mathbf{r}_2\|} = \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} \sum_{\mu=-\lambda}^{\lambda} Y_\lambda^\mu(\Omega_1) Y_\lambda^{\mu*}(\Omega_2)$$

where  $r_{<} = \min(r_1, r_2)$ ,  $r_{>} = \max(r_1, r_2)$ , and where  $Y_\lambda^\mu$  are the spherical harmonics. We now consider the form of the two-electron term in  $D_{f,i}(\mathbf{k}', \mathbf{k})$ ,

$$\langle \mathbf{k}', \phi_f | \hat{V}_{1,2} | \phi_i, \mathbf{k} \rangle = \int \int \langle \mathbf{r}_1 | \mathbf{k}' \rangle^* \langle \mathbf{r}_2 | \phi_f \rangle^* \frac{1}{\|\mathbf{r}_1 - \mathbf{r}_2\|} \langle \mathbf{r}_1 | \mathbf{k} \rangle \langle \mathbf{r}_2 | \phi_i \rangle d\mathbf{r}_1 d\mathbf{r}_2$$

for which the partial wave expansion is of the form

$$\begin{aligned} \langle \mathbf{k}', \phi_f | \hat{V}_{1,2} | \phi_i, \mathbf{k} \rangle &= \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \sum_{\mu=-\lambda}^{\lambda} \int_0^\infty \int_0^\infty \frac{u_{\ell'}(r_1; k')}{r_1} \frac{\phi_f(r_2)}{r_2} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} \frac{\phi_i(r_2)}{r_2} \frac{u_\ell(r_1; k)}{r_1} r_1^2 r_2^2 dr_1 dr_2 \\ &\quad \times \int_{S^2} Y_{\ell'}^{m'*}(\Omega_1) Y_\lambda^\mu(\Omega_1) Y_\ell^m(\Omega_1) d\Omega_1 \\ &\quad \times \int_{S^2} Y_{\ell_f}^{m_f*}(\Omega_2) Y_\lambda^{\mu*}(\Omega_2) Y_{\ell_i}^{m_i}(\Omega_2) d\Omega_2 \\ &= \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} \sum_{\mu=-\lambda}^{\lambda} \int_0^\infty \int_0^\infty u_{\ell'}(r_1; k') \phi_f(r_2) \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} \phi_i(r_2) u_\ell(r_1; k) dr_1 dr_2 \\ &\quad \times \int_{S^2} Y_{\ell'}^{m'*}(\Omega_1) Y_\lambda^\mu(\Omega_1) Y_\ell^m(\Omega_1) d\Omega_1 \\ &\quad \times \int_{S^2} Y_{\ell_f}^{m_f*}(\Omega_2) Y_\lambda^{\mu*}(\Omega_2) Y_{\ell_i}^{m_i}(\Omega_2) d\Omega_2. \end{aligned}$$

However, in the s-wave model, we have that that all  $\ell, m$  terms (for the continuum wave) are zero, where therefore all  $Y_\ell^m(\Omega) = Y_0^0(\Omega) = \frac{1}{\sqrt{4\pi}}$ . It then follows that

$$\int_{S^2} Y_{\ell'}^{m'*}(\Omega_1) Y_\lambda^\mu(\Omega_1) Y_\ell^m(\Omega_1) d\Omega_1 = \frac{1}{\sqrt{4\pi}} \int_{S^2} Y_{\ell'}^{m'*}(\Omega_1) Y_\lambda^\mu(\Omega_1) d\Omega_1 = \frac{1}{\sqrt{4\pi}} \delta_{\ell', \lambda} \delta_{m', \mu}$$

and as  $\ell', m' = 0$ , the only non-zero term in the sum is where  $\lambda = \mu = 0$ . Whence, we have that

$$\begin{aligned} \langle \mathbf{k}', \phi_f | \hat{V}_{1,2} | \phi_i, \mathbf{k} \rangle &= \sqrt{4\pi} \int_0^\infty \int_0^\infty u_{\ell'}(r_1; k') \phi_f(r_2) \frac{r_{<}^0}{r_{>}^1} \phi_i(r_2) u_\ell(r_1; k) dr_1 dr_2 \\ &\quad \times \int_{S^2} Y_{\ell_f}^{m_f*}(\Omega_2) Y_0^{0*}(\Omega_2) Y_{\ell_i}^{m_i}(\Omega_2) d\Omega_2 \\ &= \int_0^\infty \int_0^\infty u_{\ell'}(r_1; k') \phi_f(r_2) \frac{1}{r_{>}} \phi_i(r_2) u_\ell(r_1; k) dr_1 dr_2 \\ &\quad \times \int_{S^2} Y_{\ell_f}^{m_f*}(\Omega_2) Y_{\ell_i}^{m_i}(\Omega_2) d\Omega_2 \\ &= \int_0^\infty \int_0^\infty u_{\ell'}(r_1; k') \phi_f(r_2) \frac{1}{r_{>}} \phi_i(r_2) u_\ell(r_1; k) dr_1 dr_2 \\ &\quad \times \delta_{\ell_f, \ell_i} \delta_{m_f, m_i} \end{aligned}$$

and so we may restrict our attention to the case where  $\ell_f = \ell_i$  and  $m_f = m_i$ ; that is, where the angular momentum of the target is left unchanged. Finally, we have that

$$\langle \mathbf{k}', \phi_f | \hat{V}_{1,2} | \phi_i, \mathbf{k} \rangle = \langle k', \phi_f | \hat{V}_{1,2} | \phi_i, k \rangle = \int_0^\infty \int_0^\infty u_{\ell'}(r_1; k') \phi_f(r_2) \frac{1}{r_{>}} \phi_i(r_2) u_\ell(r_1; k) dr_1 dr_2$$

yielding the result as required.

### 3 Reduced CCC Code