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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_{λ}^{μ} 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

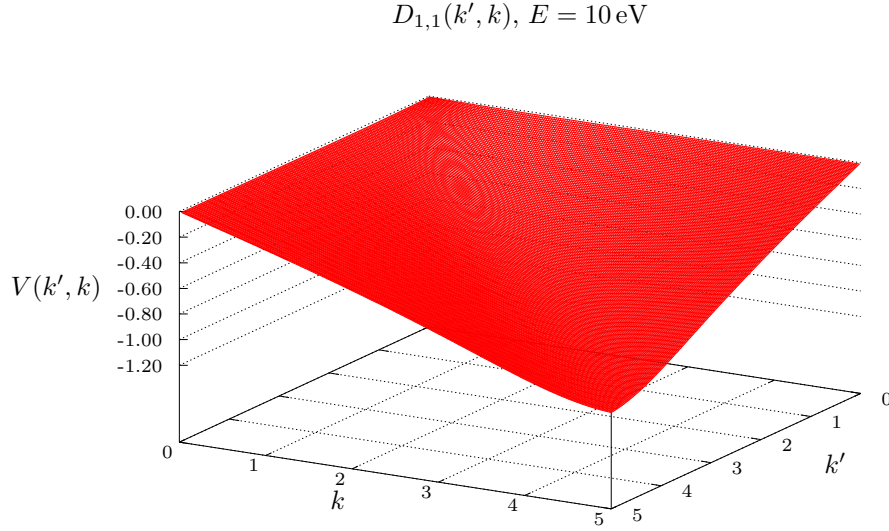


Figure 1: The $D_{f,i}(k', k)$ direct matrix elements (shown in red) are presented for the $1s \rightarrow 1s$ transition, with $E = 10 \text{ eV}$.

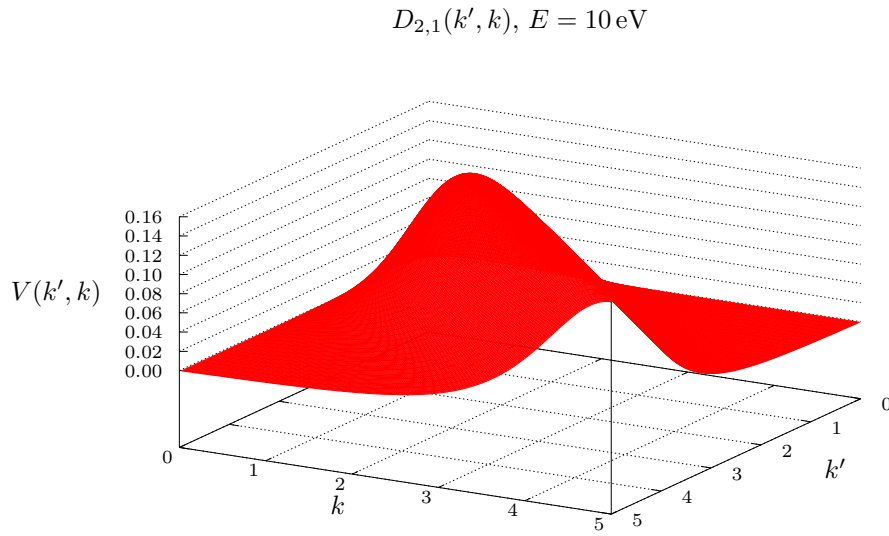


Figure 2: The $D_{f,i}(k', k)$ direct matrix elements (shown in red) are presented for the $1s \rightarrow 2s$ transition, with $E = 10 \text{ eV}$.

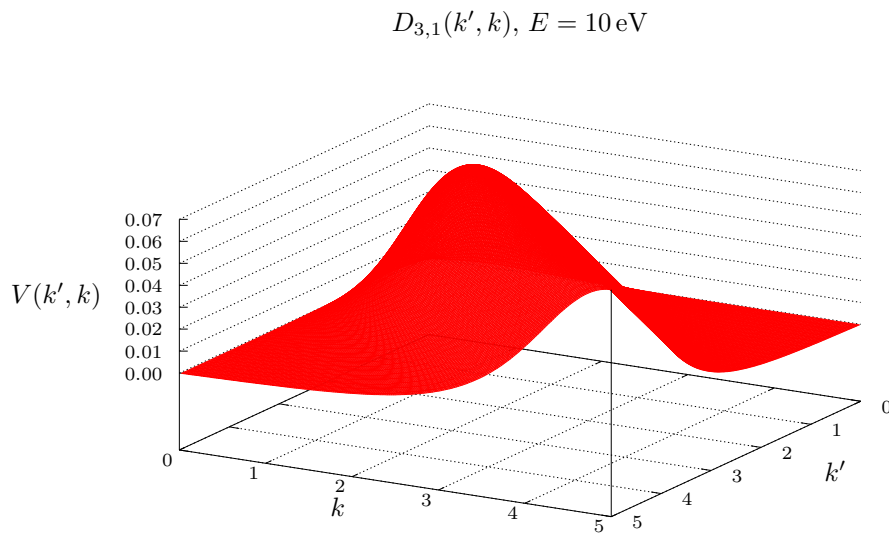


Figure 3: The $D_{f,i}(k', k)$ direct matrix elements (shown in red) are presented for the $1s \rightarrow 3s$ transition, with $E = 10 \text{ eV}$.

1.3 Exchange Matrix Elements

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

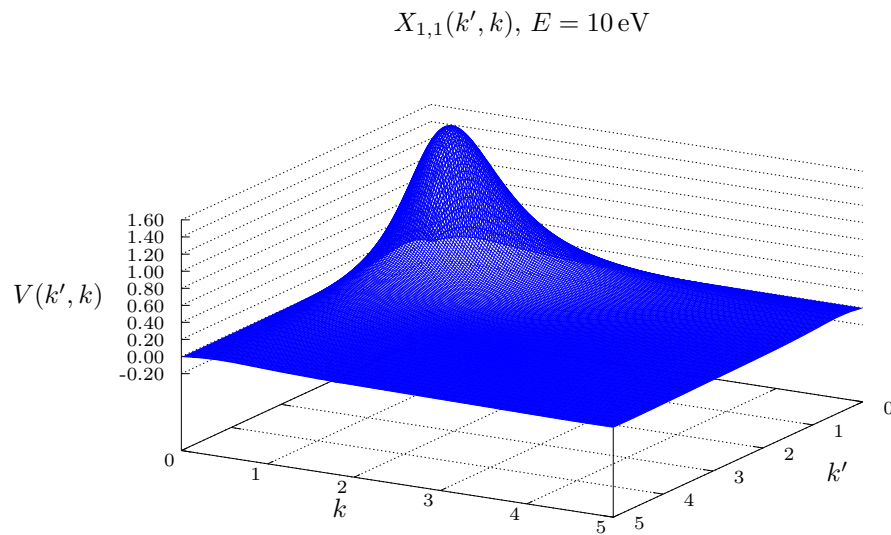


Figure 4: The $X_{f,i}(k', k)$ exchange matrix elements (shown in blue) are presented for the $1s \rightarrow 1s$ transition, with $E = 10 \text{ eV}$.

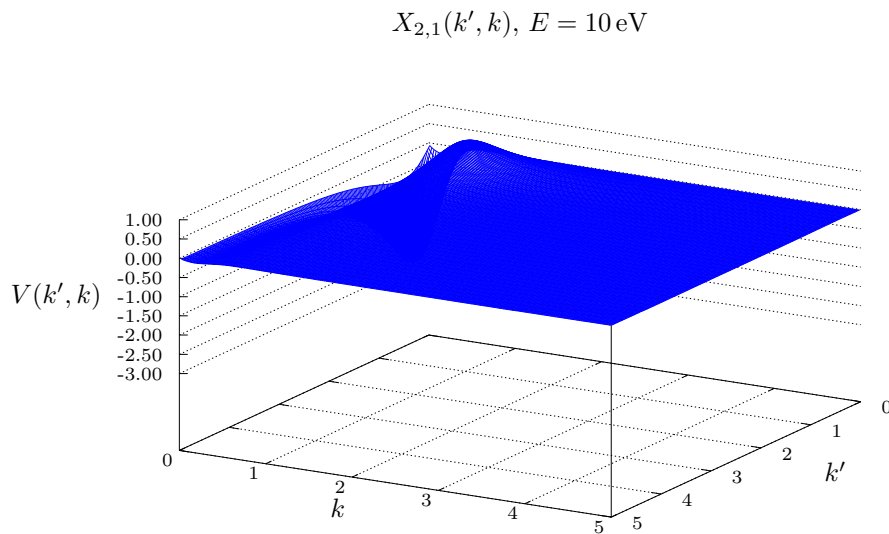


Figure 5: The $X_{f,i}(k', k)$ exchange matrix elements (shown in blue) are presented for the $1s \rightarrow 2s$ transition, with $E = 10 \text{ eV}$.

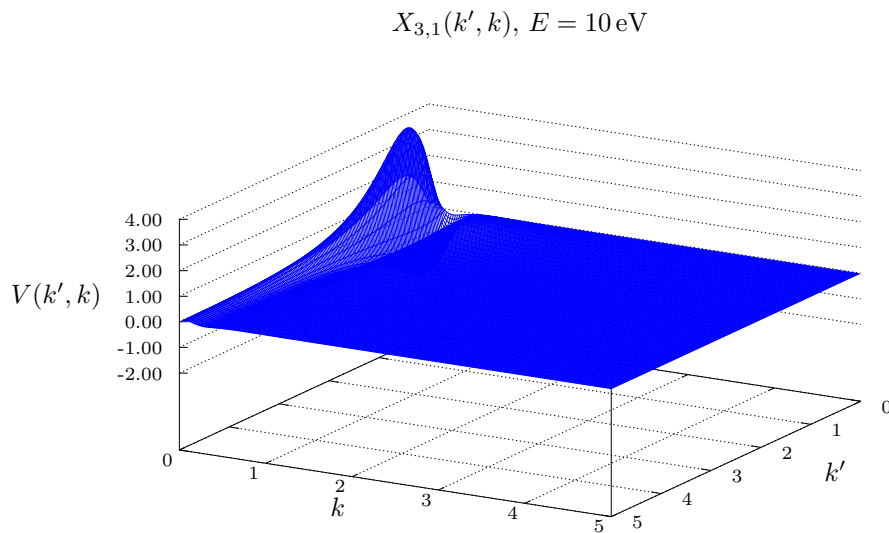


Figure 6: The $X_{f,i}(k', k)$ exchange matrix elements (shown in blue) are presented for the $1s \rightarrow 3s$ transition, with $E = 10 \text{ eV}$.

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

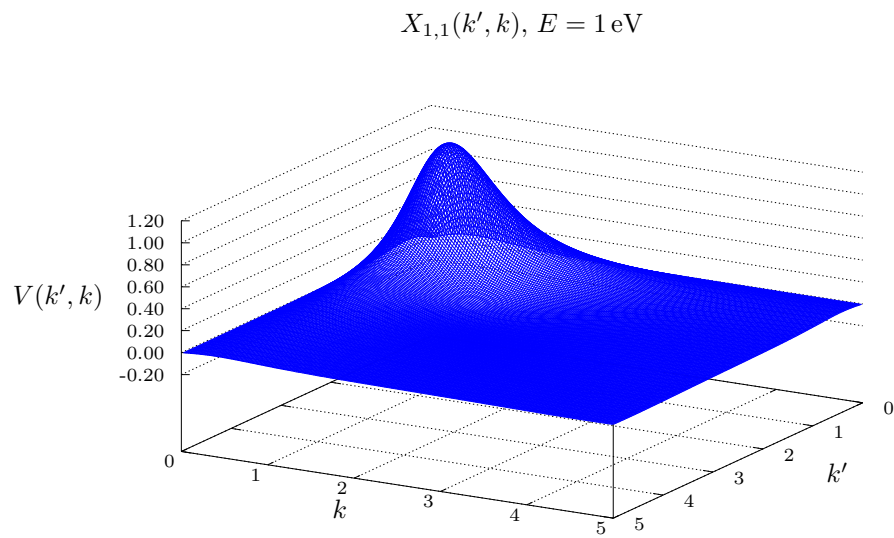


Figure 7: The $X_{f,i}(k', k)$ exchange matrix elements (shown in blue) are presented for the $1s \rightarrow 1s$ transition, with $E = 1 \text{ eV}$.

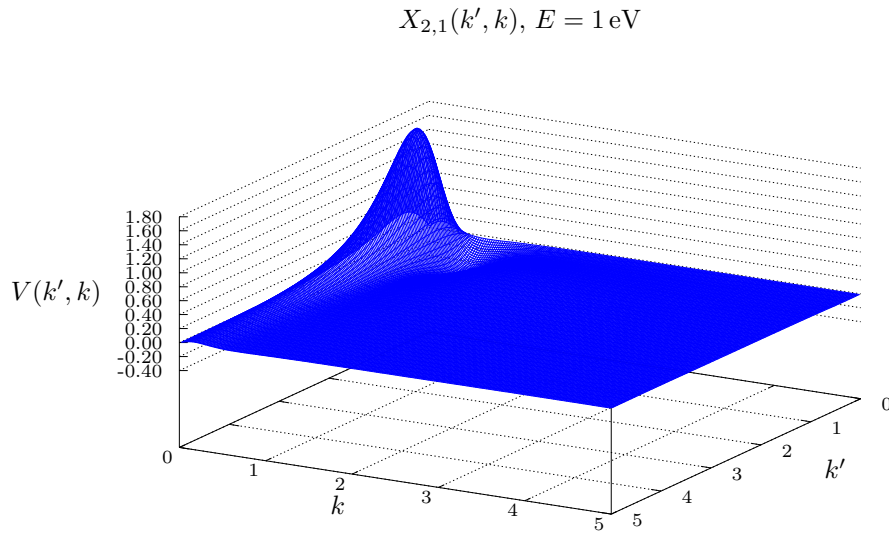


Figure 8: The $X_{f,i}(k', k)$ exchange matrix elements (shown in blue) are presented for the $1s \rightarrow 2s$ transition, with $E = 1 \text{ eV}$.

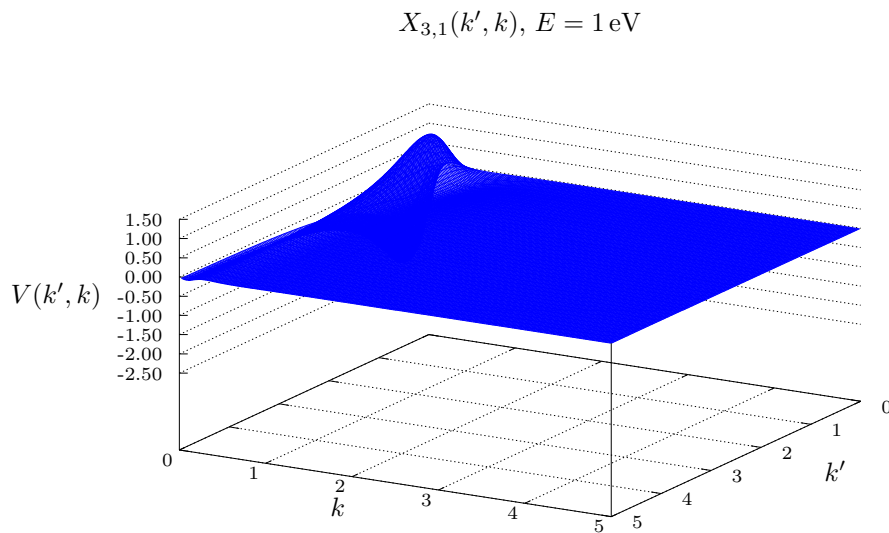


Figure 9: The $X_{f,i}(k', k)$ exchange matrix elements (shown in blue) are presented for the $1s \rightarrow 3s$ transition, with $E = 1 \text{ eV}$.

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

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

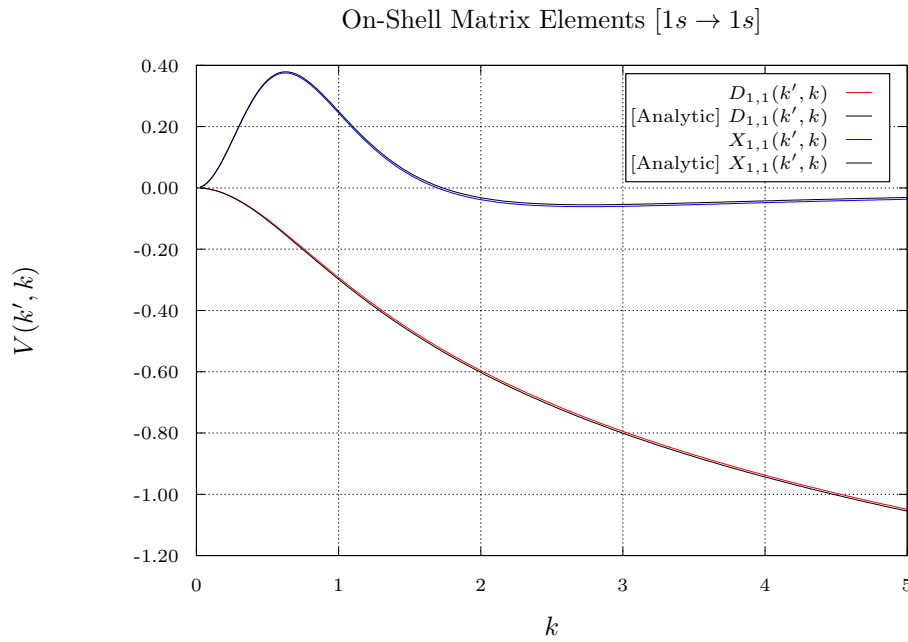


Figure 10: The $D_{f,i}(k', k)$ direct and $X_{f,i}(k', k)$ exchange on-shell matrix elements (shown in red and blue respectively) are presented for the $1s \rightarrow 1s$ transition, and are compared with their respective analytic expressions (shown in black).

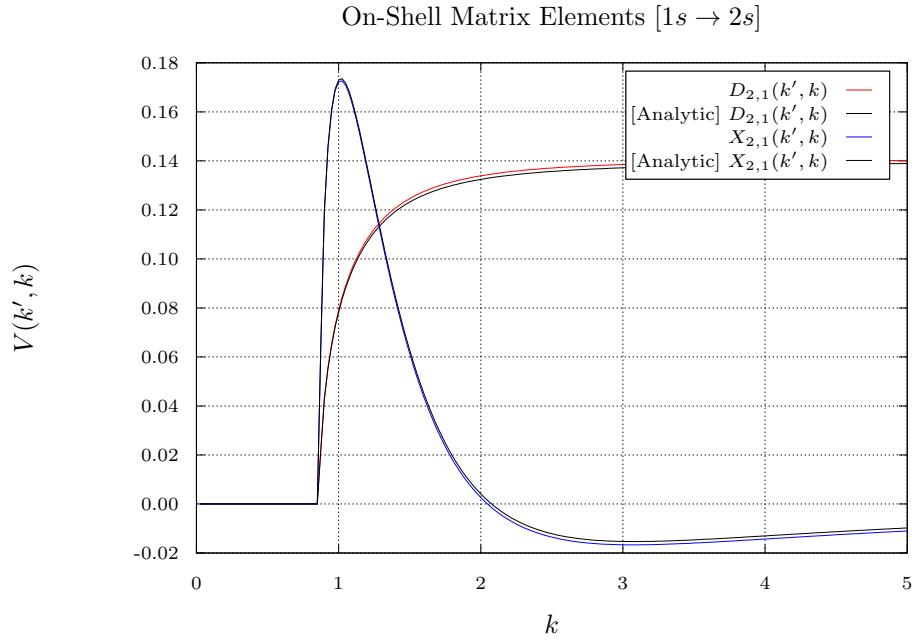


Figure 11: The $D_{f,i}(k', k)$ direct and $X_{f,i}(k', k)$ exchange on-shell matrix elements (shown in red and blue respectively) are presented for the $1s \rightarrow 2s$ transition, and are compared with their respective analytic expressions (shown in black).

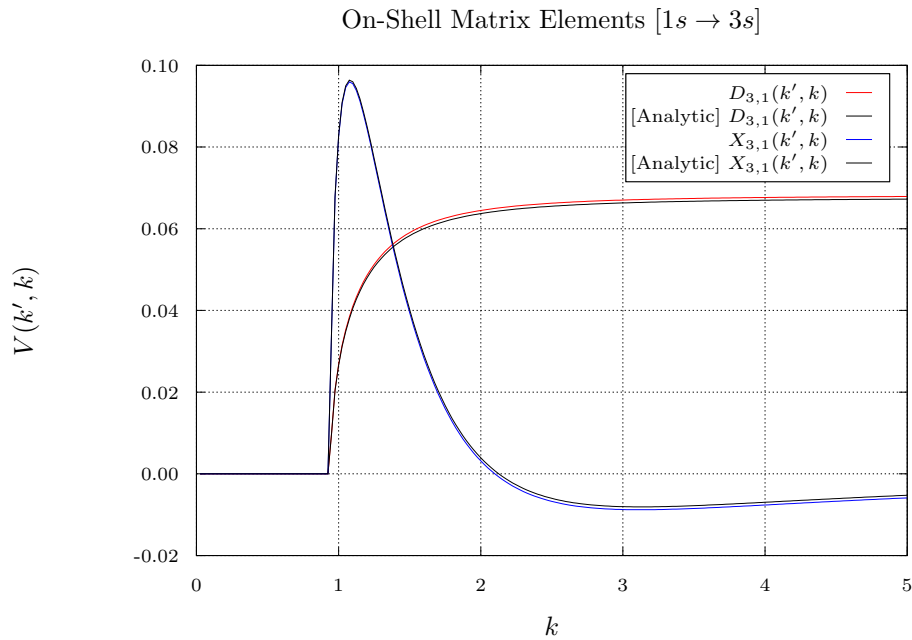


Figure 12: The $D_{f,i}(k', k)$ direct and $X_{f,i}(k', k)$ exchange on-shell matrix elements (shown in red and blue respectively) are presented for the $1s \rightarrow 3s$ transition, and are compared with their respective analytic expressions (shown in black).

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_λ^μ 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 ℓ, 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

3.1 Triplet Half-on-Shell Matrix Elements

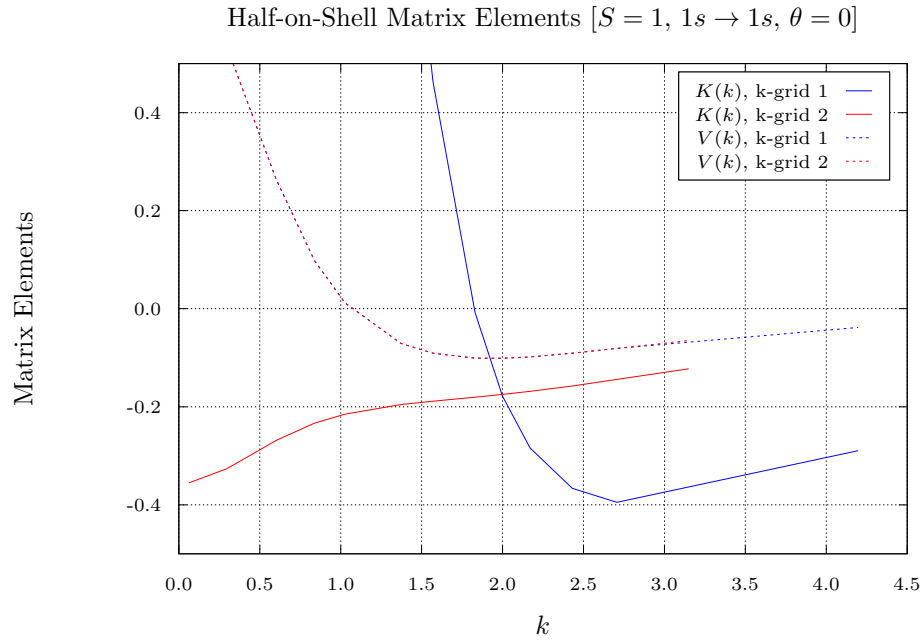


Figure 13: The triplet half-on-shell direct matrix elements, $K(k)$ (shown in solid lines) and $V(k)$ (shown in dashed lines), are presented for the $1s \rightarrow 1s$ transition, with $\theta = 0$, for both k -grids (shown in blue and red). Note that the $V(k)$ matrix elements overlap for both grids, on their common domain.

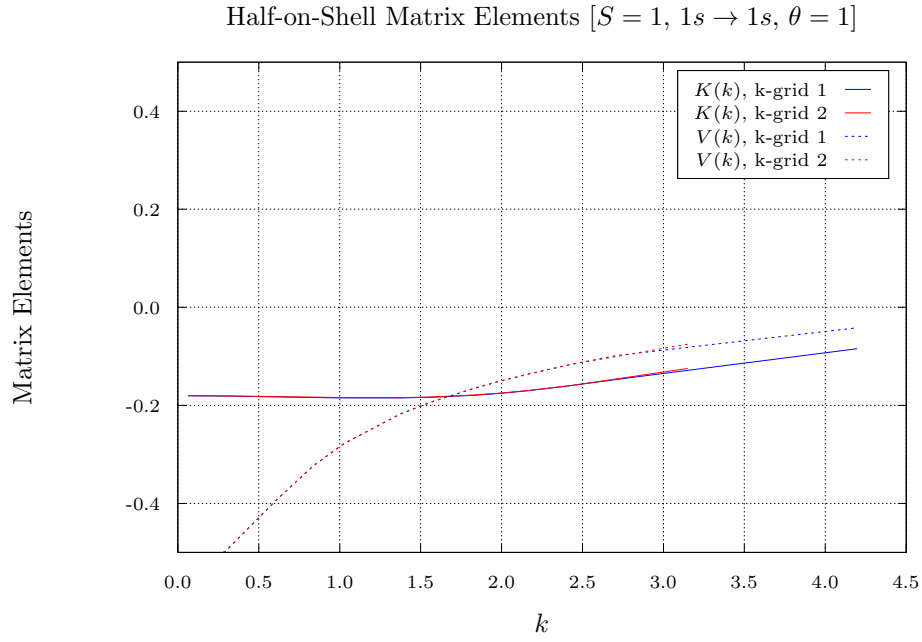


Figure 14: The triplet half-on-shell direct matrix elements, $K(k)$ (shown in solid lines) and $V(k)$ (shown in dashed lines), are presented for the $1s \rightarrow 1s$ transition, with $\theta = 1$, for both k -grids (shown in blue and red). Note that the $K(k)$ and $V(k)$ matrix elements overlap for both grids, on their common domain.

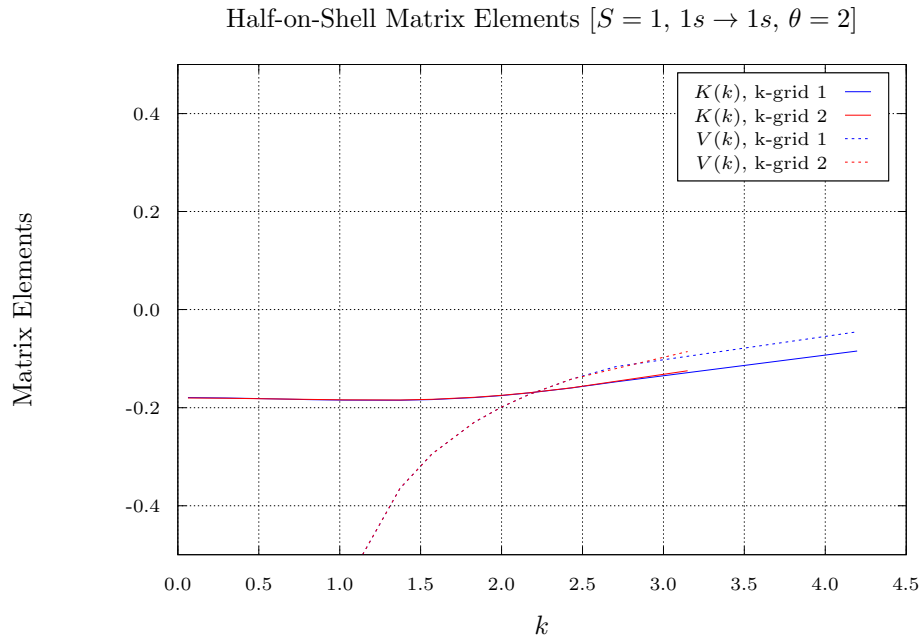


Figure 15: The triplet half-on-shell direct matrix elements, $K(k)$ (shown in solid lines) and $V(k)$ (shown in dashed lines), are presented for the $1s \rightarrow 1s$ transition, with $\theta = 2$, for both k -grids (shown in blue and red). Note that the $K(k)$ and $V(k)$ matrix elements overlap for both grids, on their common domain. Note also that the $K(k)$ matrix elements are essentially equivalent to those for $\theta = 1$, presented in Figure 14, even though the $V(k)$ matrix elements are different.

3.2 Total Cross Sections

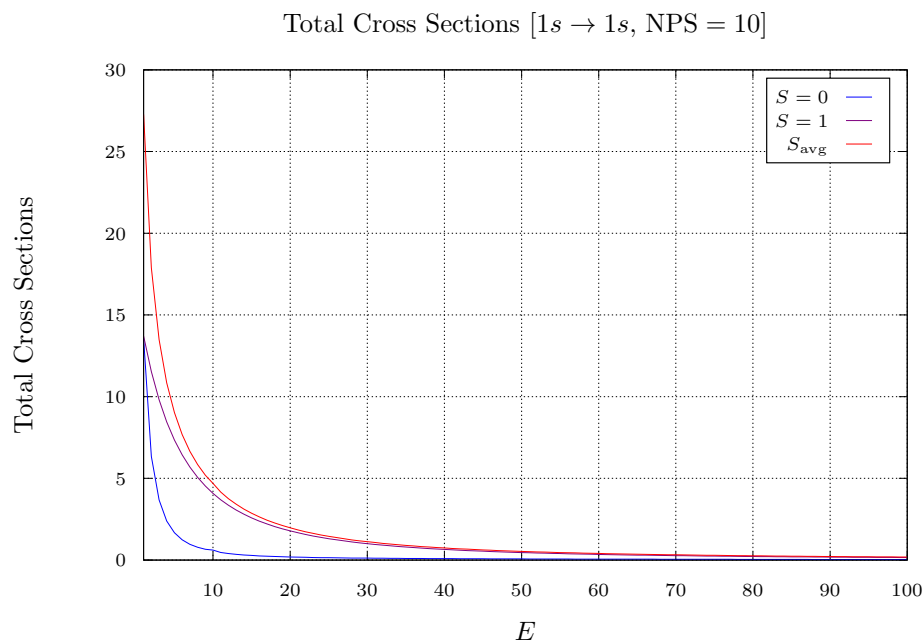


Figure 16: The total cross sections, for $S = 0$ (shown in blue), $S = 1$ (shown in purple), and S averaged (shown in red), are presented for the $[1s \rightarrow 1s]$ transition, from 1 eV to 100 eV. Note that this calculation was performed with NPS = 10.

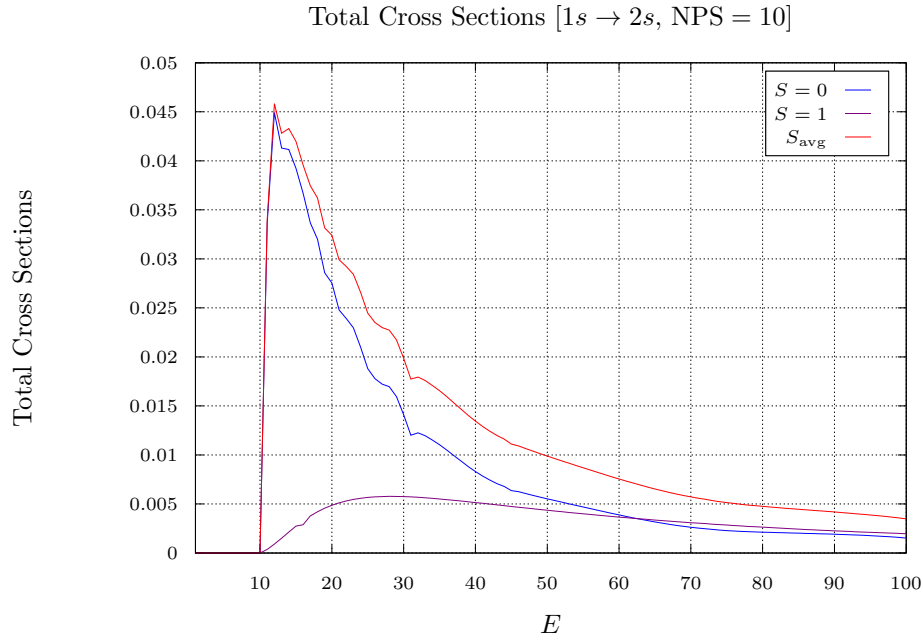


Figure 17: The total cross sections, for $S = 0$ (shown in blue), $S = 1$ (shown in purple), and S averaged (shown in red), are presented for the $[1s \rightarrow 2s]$ transition, from 1 eV to 100 eV. Note that this calculation was performed with NPS = 10.

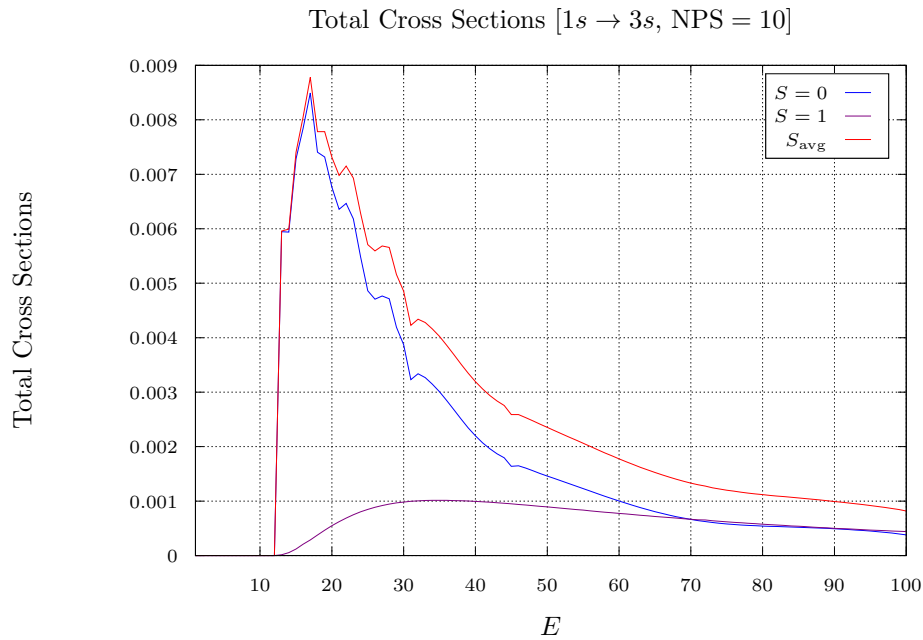


Figure 18: The total cross sections, for $S = 0$ (shown in blue), $S = 1$ (shown in purple), and S averaged (shown in red), are presented for the $[1s \rightarrow 3s]$ transition, from 1 eV to 100 eV. Note that this calculation was performed with NPS = 10.

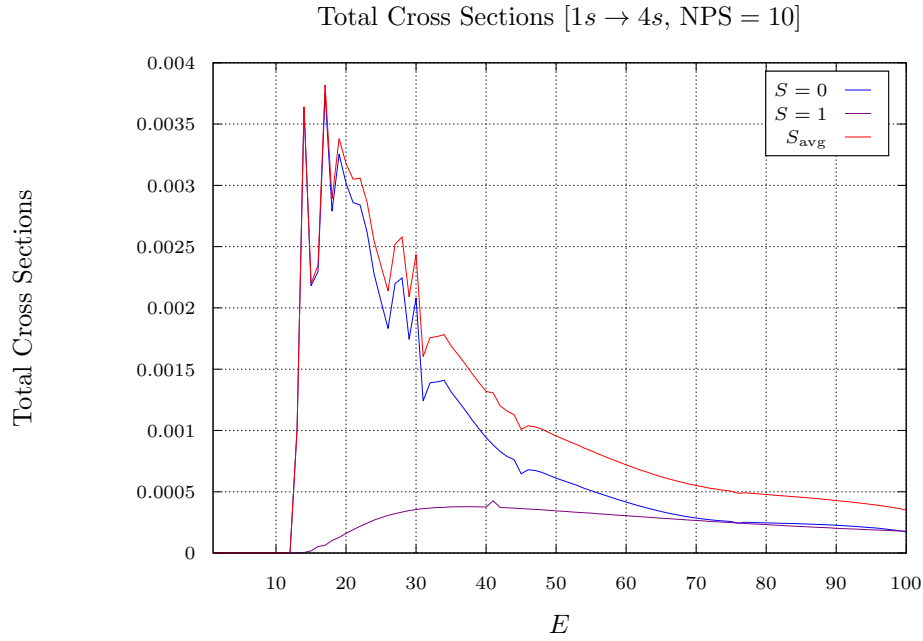


Figure 19: The total cross sections, for $S = 0$ (shown in blue), $S = 1$ (shown in purple), and S averaged (shown in red), are presented for the $[1s \rightarrow 4s]$ transition, from 1 eV to 100 eV. Note that this calculation was performed with NPS = 10.

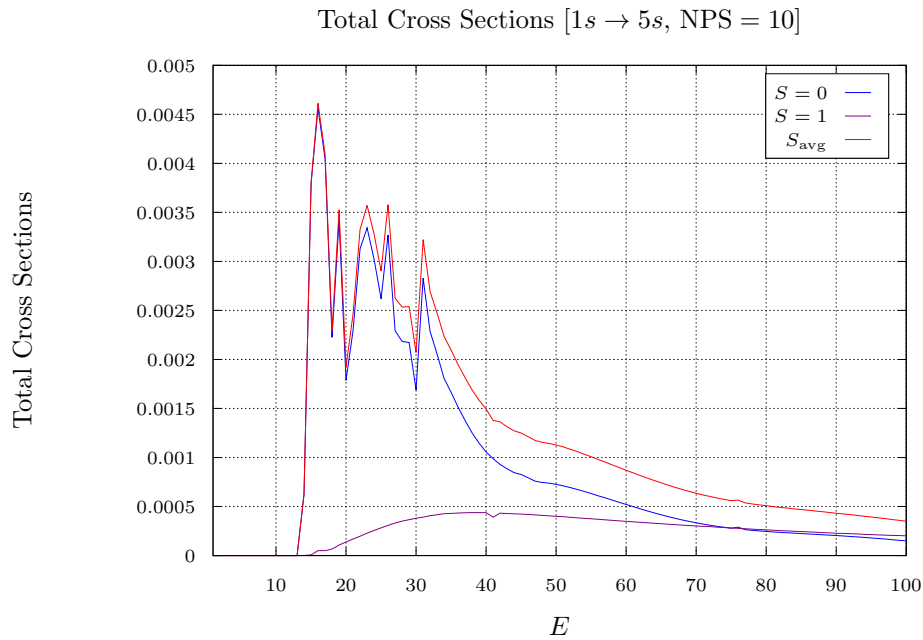


Figure 20: The total cross sections, for $S = 0$ (shown in blue), $S = 1$ (shown in purple), and S averaged (shown in red), are presented for the $[1s \rightarrow 5s]$ transition, from 1 eV to 100 eV. Note that this calculation was performed with NPS = 10.