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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

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

and where

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

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

The exchange matrix elements are of the form

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

where the one-electron inner products are of the form

$$\langle f | g \rangle = \int_0^\infty f(r) g(r) \, \mathrm{d}r$$

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

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

1.1.3 Evaluation of Integrals

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

$$\int_0^\infty f(r) \, \mathrm{d}r = \lim_{n_r \to \infty} \sum_{k=1}^{n_r} w_k f(r_k) = \lim_{n_r \to \infty} \sum_{k=1}^{n_r} w_k f_k \approx \sum_{k=1}^{n_r} w_k f_k.$$

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

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

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

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

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

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

and

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

1.2 Direct Matrix Elements

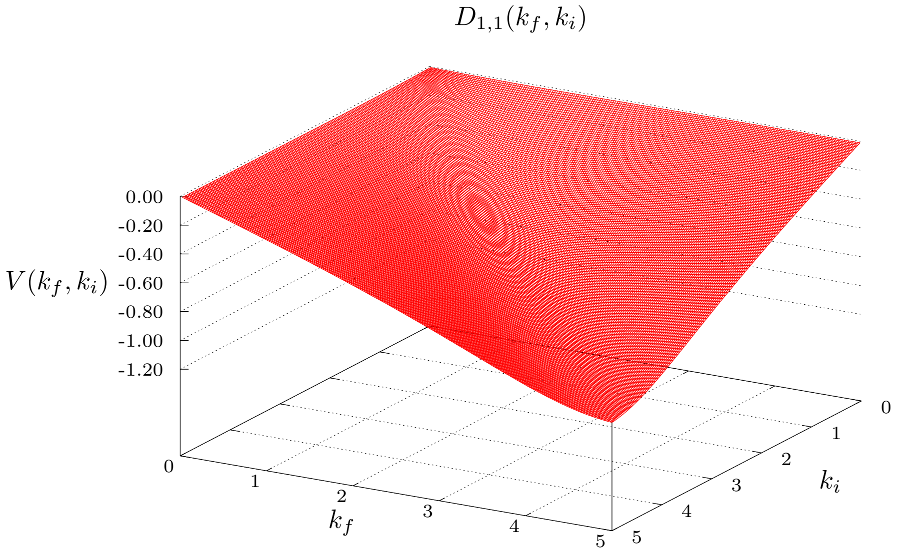

Figure 1: ...

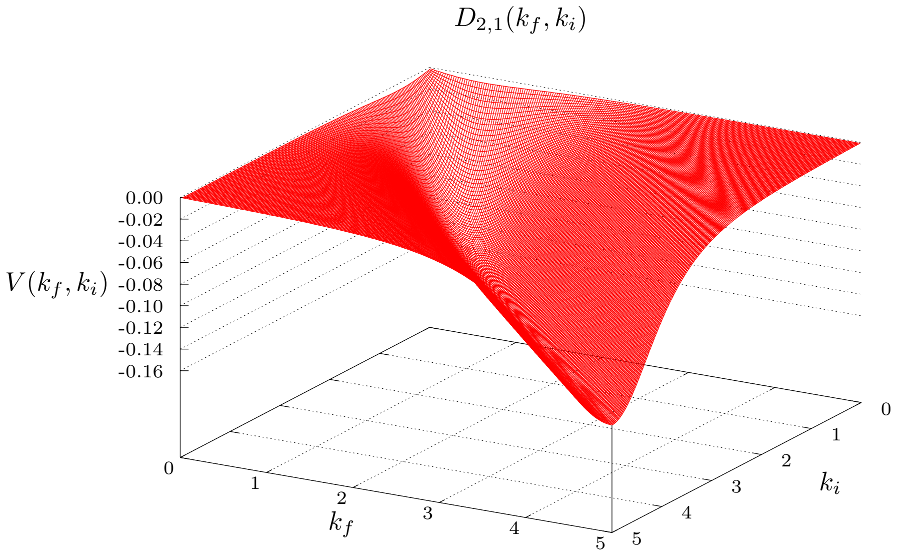

Figure 2: ...

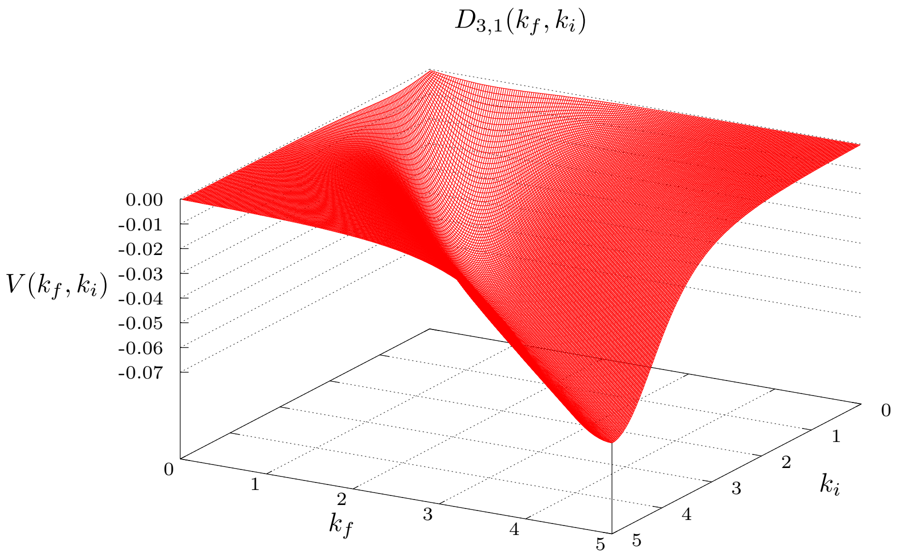
$D_{3,1}(k_f, k_i)$
$V(k_f, k_i)$
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
-0.06
-0.07
0
1
2
3
4
5
k_f
0
1
2
3
4
5
k_i

Figure 3: ...

1.3 Exchange Matrix Elements

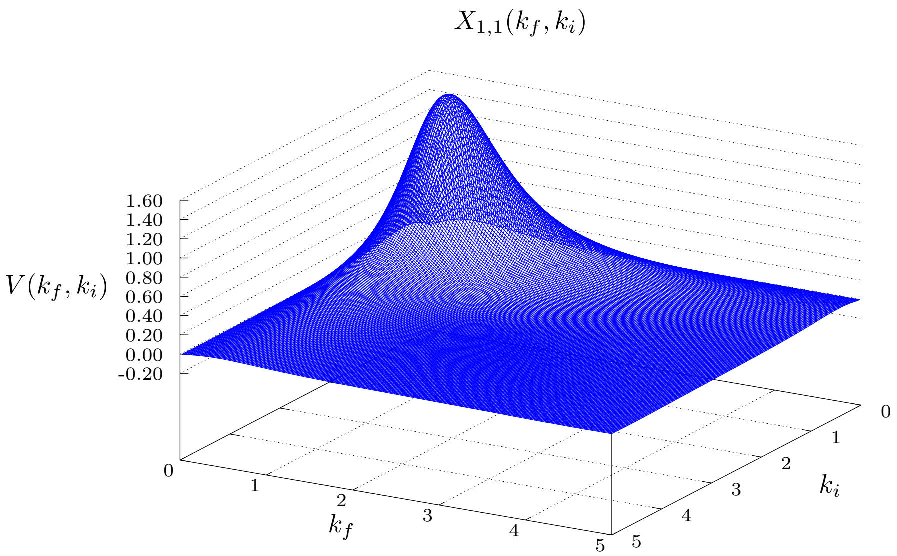

Figure 4: ...

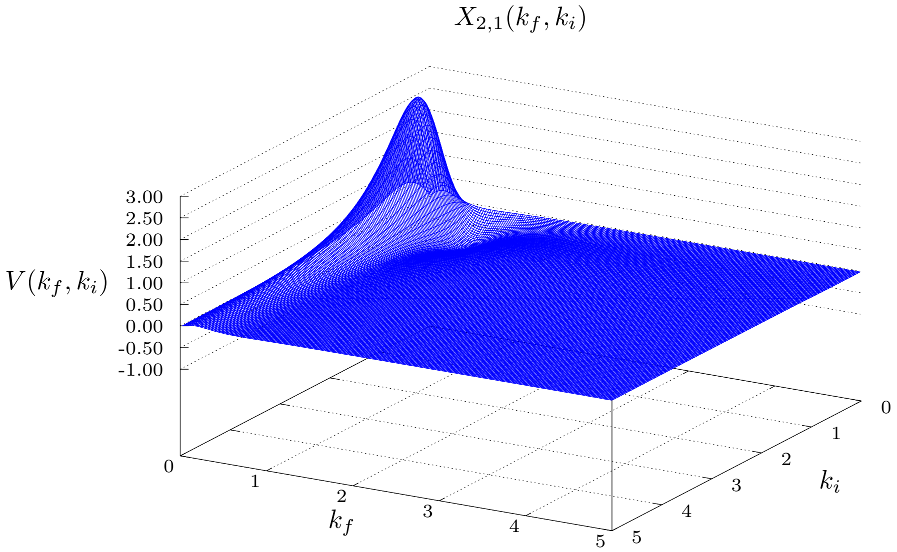

Figure 5: ...

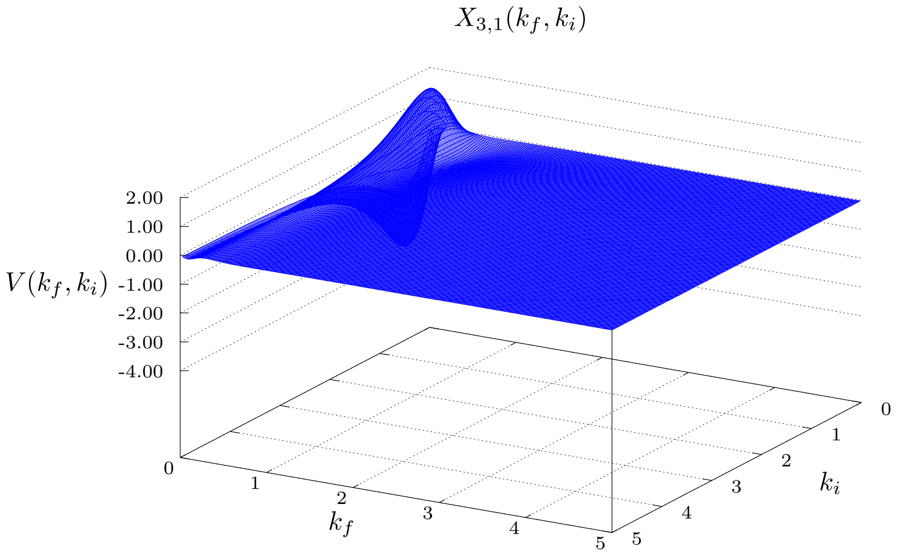

Figure 6: ...

1.4 On-Shell Matrix Elements

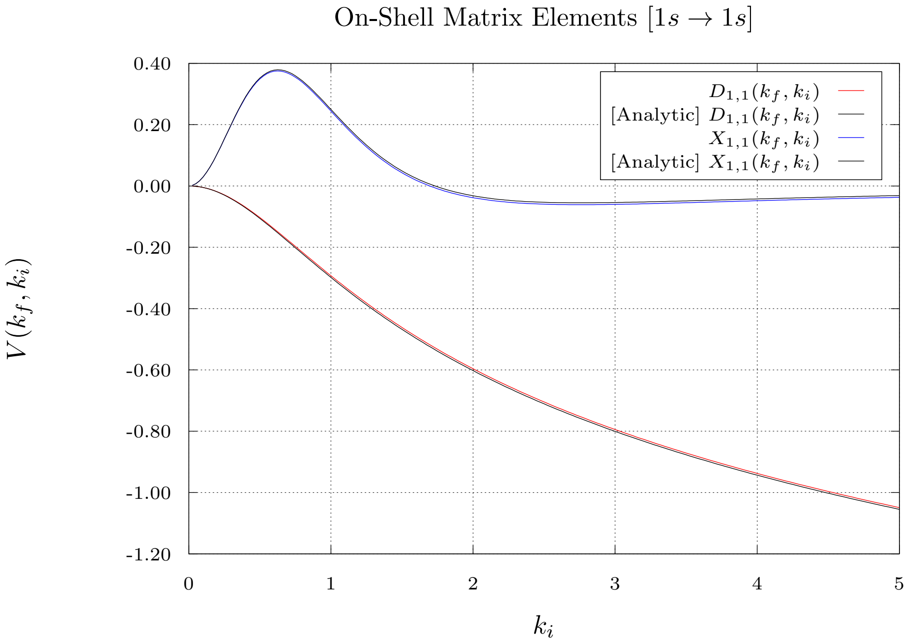

Figure 7: ...

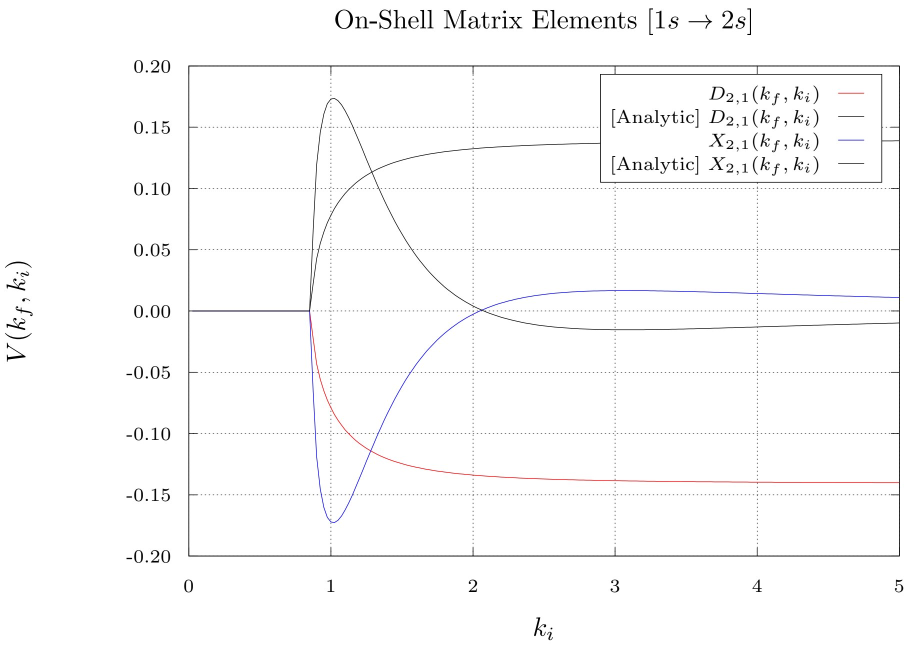

Figure 8: ...

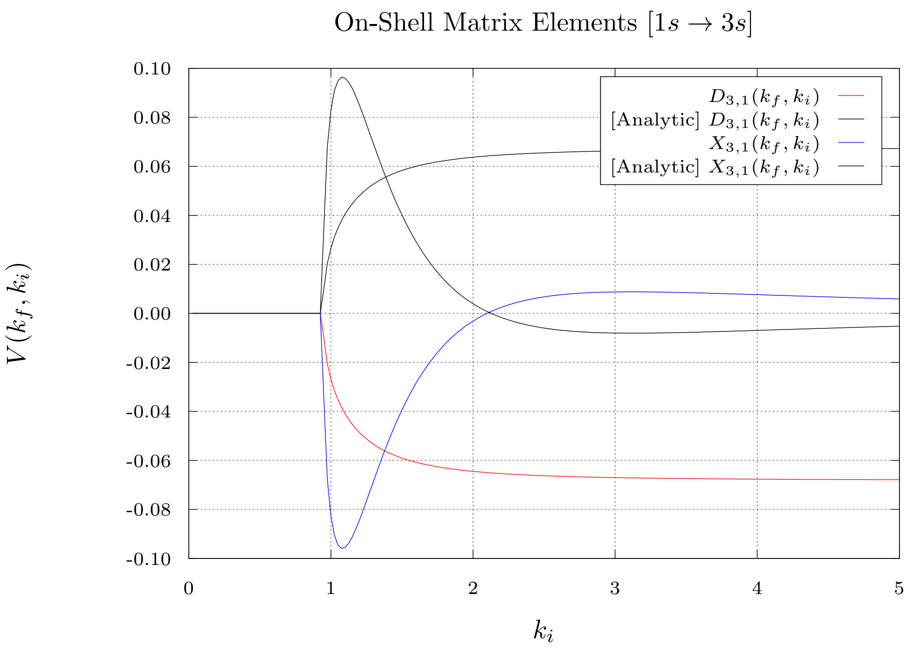

Figure 9: ...

2 V_{12} Potential in S-Wave Model

3 Reduced CCC Code