Ionisation Amplitudes in Electron-Impact Helium Collisions within the S-Wave Model

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[ABSTRACT]

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We shall describe a brief derivation of the Convergent Close-Coupling (CCC) method for generalised electron-projectile atomic/ionic-target scattering, similar in form to the derivations presented in [1, 5]. The specific considerations for the application of the CCC method to the cases of electron-impact hydrogen (e-H) scattering, and electron-impact helium (e-He) scattering, are discussed in subsubsection 3.1.1 and subsubsection 3.2.1 respectively. We shall focus on the treatment of target ionisation, both with and without excitation, by consideration of the ionisation amplitudes within the CCC method.

2.1   Convergent Close-Coupling Method

In brief, the CCC method utilises the method of basis expansion to numerically solve the Lippmann-Schwinger equation in a momentum-space representation, for a projectile-target system, to yield the transition amplitudes, which are checked for convergence as the size of the basis is increased. The scattering statistics can then be extracted from the transistion amplitudes.

The rate of convergence, depends on many factors, such as the complexity of the target structure, the coupling between transition channels, and the choice of basis used in the expansion. With the selection of an appropriate basis, unbounded continuum waves can be accurately represented by a finite amount of basis states, which allows ionisation amplitudes to be treated in a similar manner to discrete excitation amplitudes within the CCC method. A Laguerre basis is well-suited to this task; the benefits of this basis are discussed in further detail in [5, 5-9].

2.1.1   Laguerre Basis

To describe the target structure, the CCC method utilises a Laguerre basis $\{|\varphi_i\rangle\}_{i=1}^{\infty}$ for the Hilbert space $L^2(\mathbb{R}^3)$, for which the coordinate-space representation is of the form

$$\langle\mathbf{r}|\varphi_i\rangle = \varphi_i(r,\Omega) = \tfrac{1}{r}\xi_{k_i,li}(r)Y_{l_i}^{m_i}(\Omega), \tag{1}$$

where $Y_{l_i}^{m_i}(\Omega)$ are the spherical harmonics, and where $\xi_{k_i,l_i}(r)$ are the Laguerre radial basis functions, which are of the form

$$\xi_{k,l}(r) = \sqrt{\frac{\lambda_l(k-1)!}{(2l+1+k)!}}(\lambda_l r)^{l+1}\exp\left(-\tfrac{1}{2}\lambda_l r\right)L_{k-1}^{2l+2}(\lambda_l r), \tag{2}$$

where λ_l is the exponential fall-off, for each l, and where $L_{k-1}^{2l+2}(\lambda_l r)$ are the associated Laguerre polynomials. Note that we must have that $k_i \in \{1,2,\ldots\}$, $l_i \in \{0,1,\ldots\}$ and $m_i \in \{-\ell_i,\ldots,\ell_i\}$, for each $i \in \{1,2,\ldots\}$.

This Laguerre basis is utilised due to: the Laguerre basis functions $\{\varphi_i(r, \Omega)\}_{i=1}^{\infty}$ forming a complete basis for the Hilbert space $L^2(\mathbb{R}^3)$, the short-range and long-range behaviour of the radial basis functions being well suited to describing bound target states and providing a basis for expanding continuum states in, and because it allows the matrix representation of numerous operators to be calculated analytically.

Practically, we cannot utilise a basis of infinite size. Hence, we truncate the Laguerre radial basis $\{\xi_{k,l}(r)\}_{k=1}^{N_l}$ to a certain number of radial basis functions N_l, for each l, and we also truncate $l \in \{0, \ldots, l_{max}\}$, limiting the maximum angular momentum we consider in our basis. Hence, for a given value of m, we have a basis size of

$$N = \sum_{l=0}^{l_{max}} N_l. \tag{3}$$

In the limit as $N \to \infty$, the truncated basis will tend towards completeness, and it is in this limit that we discuss the convergence of the Convergent Close-Coupling method. We have presented the Laguerre basis with full generality, however we note that in the S-wave model we have $l_{max} = 0$, which allows for the simplification of numerous expressions and computations.

2.1.2   Target States

Possessing now a suitable basis to work with, we proceed to represent the target in this basis by the method of basis expansion. Firstly, we note that electrons are indistinguishable fermionic particles; that is, no two electrons can be distinguished from each other, and they must satisfy Pauli's exclusion principle - that an electron state cannot be occupied by more than one electron. Since electrons are indistinguishable, we might naively suppose that the space of states consisting of n electrons is simply the n-th tensor power of the one-electron space, $T^n(\mathcal{H})$, defined by

$$T^n(\mathcal{H}) = \{|\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle : |\psi_1\rangle, \ldots, |\psi_n\rangle \in \mathcal{H}\}, \tag{4}$$

where $\mathcal{H}$ is the space of one-electron states. However this fails to account for Pauli's exclusion principle, since any one-electron state may be occupied up to n times. Hence, the space of states consisting of n electrons is instead defined to be the quotient space $\Lambda^n(\mathcal{H})$ of $T^n(\mathcal{H})$ by $\mathcal{D}^n$,

$$\Lambda^n(\mathcal{H}) = T^n(\mathcal{H})/\mathcal{D}^n, \tag{5}$$

where $\mathcal{D}^n \subset T^n(\mathcal{H})$ is the subspace of tensor products which contain any one-electron state more than once. The space $\Lambda^n(\mathcal{H})$ is known as the n-th exterior power of $\mathcal{H}$, and is identifiable as the subspace of $T^n(\mathcal{H})$ consisting of anti-symmetric tensors. Note that we shall adopt the following notation for tensor products

$$|\psi_1, \ldots, \psi_n\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle \tag{6}$$

and the following notation for anti-symmetric tensor products

$$|[\psi_1, \ldots, \psi_n]\rangle = |\psi_{[1,\ldots,n]}\rangle = \sqrt{n!}\hat{A} |\psi_1, \ldots, \psi_n\rangle \tag{7}$$

where $\hat{A} : T^n(\mathcal{H}) \to \Lambda^n(\mathcal{H})$ is the anti-symmetriser operator which we define to be of the form

$$\hat{A} |\psi_1, \ldots, \psi_n\rangle = \frac{1}{n!} \sum_{\sigma \in S_n} \text{sgn}(\sigma) |\psi_{\sigma(1)}, \ldots, \psi_{\sigma(n)}\rangle, \tag{8}$$

where S_n is the symmetric group on n elements, the sum is taken over all permutations $\sigma \in S_n$, and where $\text{sgn}(\sigma)$ is the signature of the permutation σ. It follows from this construction that

$$\left|\psi_{[a_1,\ldots,a_n]}\right\rangle = 0 \quad \text{if any} \quad a_i = a_j, \tag{9}$$

hence satisfying Pauli's exclusion principle. Furthermore, we have that

$$\hat{P}_{i,j}\left|\psi_{[1,\ldots,n]}\right\rangle = -\left|\psi_{[1,\ldots,n]}\right\rangle, \tag{10}$$

where $\hat{P}_{i,j}$ is the pairwise exchange operator, permuting the states $|\psi_i\rangle$ and $|\psi_j\rangle$. We note that in this context, the states $|\psi_i\rangle$ include both coordinate and spin states.

It follows that for an atomic/ionic target, consisting of n_e electrons, the space of target states is of the form $\mathcal{H}_T = \Lambda^{n_\text{e}}(\mathcal{H})$. We shall adopt the convention that operators which act on the m-th electron space (including the projectile electron), will be indexed by m, for $m = 0, 1, \ldots, n_\text{e}$.

Target Hamiltonian   The target Hamiltonian, for an atomic/ionic target with n_e electrons, is of the form

$$\hat{H}_T = \sum_{m=1}^{n_\text{e}} \hat{K}_m + \sum_{m=1}^{n_\text{e}} \hat{V}_m + \sum_{m=1}^{n_\text{e}} \sum_{n=m+1}^{n_\text{e}} \hat{V}_{m,n}, \tag{11}$$

where $\hat{K}_m$ and $\hat{V}_m$ are the target electron kinetic and electron-nuclei potential operators, for $m = 1, \ldots, n_\text{e}$, and where $\hat{V}_{m,n}$ are the electron-electron potential operators, for $m, n = 1, \ldots, n_\text{e}$.

Target Diagonalisation   The target Hamiltonian, restricted to just one target electron,

$$\hat{H}_{T,\text{e}} = \hat{K}_1 + \hat{V}_1, \tag{12}$$

is expanded in a Laguerre basis $\{|\varphi_i\rangle\}_{i=1}^N$ and diagonalised to yield a set of one-electron atomic orbitals $\{|\phi_i^{(N)}\rangle\}_{i=1}^N$ which are orthonormal and satisfy

$$\langle\phi_i^{(N)}|\,\hat{H}_{T,\text{e}}\,|\phi_j^{(N)}\rangle = \varepsilon_i^{(N)}\delta_{i,j}. \tag{13}$$

From these one-electron atomic orbitals, we generate a set of one-electron spin orbitals $\{|\chi_i^{(N)}\rangle\}_{i=1}^{2N}$ for which $|\chi_{2i-1}^{(N)}\rangle$ and $|\chi_{2i}^{(N)}\rangle$ both correspond to $|\phi_i^{(N)}\rangle$ but have spin projection $\frac{1}{2}$ and $-\frac{1}{2}$ respectively. These one-electron spin orbitals are then combined to construct Slater determinants; for any selection of n_e one-electron spin orbitals $|\chi_{a_1}^{(N)}\rangle, \ldots, |\chi_{a_{n_\text{e}}}^{(N)}\rangle \in \{|\chi_i^{(N)}\rangle\}_{i=1}^{2N}$, the Slater determinant of these spin orbitals is of the form

$$|\chi_{[a_1,\ldots,a_{n_\text{e}}]}^{(N)}\rangle = \sqrt{n_\text{e}!}\hat{A}\,|\chi_{a_1}^{(N)},\ldots,\chi_{a_{n_\text{e}}}^{(N)}\rangle = \frac{1}{\sqrt{n_\text{e}!}}\sum_{\sigma \in S_{n_\text{e}}}\text{sgn}(\sigma)\,|\chi_{a_{\sigma(1)}}^{(N)},\ldots,\chi_{a_{\sigma(n_\text{e})}}^{(N)}\rangle, \tag{14}$$

as per Equation 7 and Equation 8. We note that Slater determinants are anti-symmetric under pairwise exchange of any two orbitals, and are zero if constructed with two spin orbitals in the same state. Hence adhere to Pauli's exclusion principle and are indeed elements of $\mathcal{H}_T = \Lambda^{n_\text{e}}(\mathcal{H})$.

The true target states $\{|\Phi_\alpha\rangle\} \in \mathcal{H}_T$ are then approximated by expanding the full target Hamiltonian $\hat{H}_T$ in a basis of Slater determinants,

$$\left\{|\chi_{[a_1,\ldots,a_{n_\text{e}}]}^{(N)}\rangle : a_1, \ldots, a_{n_\text{e}} \in \{1, \ldots, 2N\}\right\}, \tag{15}$$

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and diagonalising to yield a set of target pseudostates $\{|\Phi_n^{(N)}\rangle\}_{n=1}^{N_T}$ which are orthonormal and satisfy

$$\langle\Phi_i^{(N)}|\,\hat{H}_T\,|\Phi_j^{(N)}\rangle = \epsilon_i^{(N)}\delta_{i,j}, \tag{16}$$

where $\epsilon_n^{(N)}$ is the pseudoenergy corresponding to the pseudostate $|\Phi_n^{(N)}\rangle$. Note that the number of target pseudostates N_T depends on the number of Slater determinants utilised in the expansion of $\hat{H}_T$. Note also that the (N) superscript has been introduced to indicate that these are not true eigenstates of the target Hamiltonian, only of its representation in the truncated Laguerre basis, and that these pseudostates and their pseudoenergies are dependent on the size of the Laguerre basis utilised.

The process of selecting which Slater determinants to use in the expansion is not trivial, as the number of Slater determinants scales as $\binom{2N}{n_e}$. A common method of mitigating this computationaly complexity, is to partition the target orbitals into a core set and valence set of orbitals, with the core orbitals being limited to a much smaller set of states, while the valence orbitals are not so constrained. This provides an effective model for targets with a mostly fixed set of core electron states, while allowing the valence electrons to interact fully with the projectile.

Completeness of Target Pseudostates   As a result of the completeness of the Laguerre basis, the set of target pseudostates will be separable into a set of bounded pseudostates which will form an approximation of the true target discrete spectrum, and a set of unbounded pseudostates which will provide a discretisation of the true continuum of unbounded states. Without loss of generality, we order the target pseudostates by increasing pseudoenergy, $\epsilon_1^{(N)} < \ldots < \epsilon_{N_T}^{(N)}$, which allows us to express the separability of the spectrum in the form

$$\{|\Phi_n^{(N)}\rangle\}_{n=1}^{N_T} = \{|\Phi_n^{(N)}\rangle\}_{n=1}^{N_B} \cup \{|\Phi_n^{(N)}\rangle\}_{n=N_B+1}^{N_T}, \tag{17}$$

where $\epsilon_n^{(N)} < 0$ for $n = 1, \ldots, N_B$, and where $\epsilon_n^{(N)} \geq 0$ for $n = N_B + 1, \ldots, N_T$. Note that N_B is the number of bounded pseudostates, and we write $N_U = N_T - N_B$ to represent the number of unbounded pseudostates, both of which are dependent on N by consequence of the construction of the target pseudostates.

The projection operator for the target pseudostates, $\hat{I}_T^{(N)}$, is of the form

$$\hat{I}_T^{(N)} = \sum_{n=1}^{N_T} |\Phi_n^{(N)}\rangle\langle\Phi_n^{(N)}| = \sum_{n=1}^{N_B} |\Phi_n^{(N)}\rangle\langle\Phi_n^{(N)}| + \sum_{n=N_B+1}^{N_T} |\Phi_n^{(N)}\rangle\langle\Phi_n^{(N)}|, \tag{18}$$

and so in the limit as $N \to \infty$, the sum over the bounded pseudostates will converge to the sum over the true target discrete states and the sum over the unbounded pseudostates will converge to a discretisation of the integral over the true continuum spectrum. Whence, it follows that projection operator for the target pseudostates converges to the identity operator, for $\mathcal{H}_T$, in the limit as $N \to \infty$; that is,

$$\lim_{N\to\infty} \hat{I}_T^{(N)} = \hat{I}_T. \tag{19}$$

A more rigorous discussion on the suitabiliy of representing unbounded states in the Laguerre basis is provided in [5, 5-9].

2.1.3   Total Wavefunction

The total wavefunction $|\Psi^{(+)}\rangle \in \Lambda^{1+n_e}(\mathcal{H})$ is defined to be an eigenstate of the total Hamiltonian $\hat{H}$ with total energy E and specified to have outgoing spherical-wave boundary conditions,

$$\hat{H}|\Psi^{(+)}\rangle = E|\Psi^{(+)}\rangle, \tag{20}$$

where $\hat{H}$ is of the form

$$\hat{H} = \hat{H}_T + \hat{K}_0 + \hat{V}_0 + \sum_{m=1}^{n_e} \hat{V}_{0,m}, \tag{21}$$

where $\hat{H}_T$ is the target Hamiltonian, defined in Equation 11, $\hat{K}_0$ is the projectile electron kinetic operator, $\hat{V}_0$ is the projectile electron-nuclei potential operator, and $\hat{V}_{0,m}$ are the projectile electron-target electron potential operators. The following treatment of the total wavefunction is of a similar form to [1, 202-204].

   To ensure that the total wavefunction is anti-symmetric we utilise the anti-symmetriser, defined in Equation 8, to construct it explicitly

$$|\Psi^{(+)}\rangle = \hat{A}|\psi^{(+)}\rangle = \left[1 - \sum_{m=1}^{n_e} \hat{P}_{0,m}\right]|\psi^{(+)}\rangle, \tag{22}$$

where $\hat{P}_{0,m}$ are the pairwise electron exchange operators defined in Equation 10, and where $|\psi^{(+)}\rangle \in \mathcal{H}_T \otimes \mathcal{H}$ is the un-symmetrised total wavefunction. As the target states are already anti-symmetric by construction, the anti-symmetriser has assumed a simpler form - requiring only permutations of the un-symmetrised projectile state with the spin-orbital states of the target electrons. Note that we have omitted the $(1 + n_e)!$ term in $\hat{A}$, since it is a scalar term which can be normalised away when required.

   To construct the un-symmetrised total wavefunction $|\psi^{(+)}\rangle$ we perform a multichannel expansion, projecting it onto the target psuedostates,

$$|\psi^{(N,+)}\rangle = \hat{I}_T^{(N)}|\psi^{(+)}\rangle = \sum_{n=1}^{N_T} |\Phi_n^{(N)}\rangle \langle\Phi_n^{(N)}|\psi^{(+)}\rangle = \sum_{n=1}^{N_T} |\Phi_n^{(N)}F_n^{(N)}\rangle, \tag{23}$$

where $|F_n^{(N)}\rangle = \langle\Phi_n^{(N)}|\psi^{(+)}\rangle$ are the multichannel weight functions, and note that as a result of Equation 19, that

$$|\psi^{(+)}\rangle = \lim_{N\to\infty} \hat{I}_T^{(N)}|\psi^{(+)}\rangle = \lim_{N\to\infty} |\psi^{(N,+)}\rangle. \tag{24}$$

Similarly, the total wavefunction constructed from the projection of the un-symmetrised total wavefunction onto the target pseudostates is written in the form

$$|\Psi^{(N,+)}\rangle = \hat{A}|\psi^{(N,+)}\rangle = \left[1 - \sum_{m=1}^{n_e} \hat{P}_{0,m}\right]|\psi^{(N,+)}\rangle, \tag{25}$$

and we note that as a result of Equation 19, that

$$|\Psi^{(+)}\rangle = \lim_{N\to\infty} |\Psi^{(N,+)}\rangle. \tag{26}$$

However, after projecting the un-symmetrised total wavefunction with the projection operator for the target pseudostates, the multichannel expansion is not uniquely defined, since for any state $|\omega^{(N)}\rangle \in \ker(\hat{A}\hat{I}_T^{(N)})$ and scalar $\alpha \in \mathbb{C}$, the multichannel expansion of $|\psi^{(N,+)}\rangle + \alpha|\omega^{(N)}\rangle$ will be identical to that of $|\psi^{(N,+)}\rangle$. To resolve this dilemma, we first note that the multichannel weight functions $|F_n^{(N)}\rangle$ are within the span of the one-electron spin orbitals $\{|\chi_i^{(N)}\rangle\}_{i=1}^{2N}$, used to construct the Slater determinants, Equation 14, with which the target states are expanded. Hence, we impose the constraint that for any of the one-electron spin orbitals $|\chi_i^{(N)}\rangle$, that

$$\hat{P}_{0,m} |\Phi_n^{(N)}\chi_i^{(N)}\rangle = - |\Phi_n^{(N)}\chi_i^{(N)}\rangle. \tag{27}$$

which can be seen as an explicit imposition of Equation 10. With this constraint in place, it can then be shown that $\dim \ker(\hat{A}\hat{I}_T^{(N)}) = 0$, whence it follows that the multichannel expansion of $|\psi^{(N,+)}\rangle$ is now unique in determining $|\Psi^{(N,+)}\rangle$.

2.1.4 Convergent Close-Coupling Equations

We present a derivation for the Convergent Close-Coupling (CCC) equations, beginning with the Schrödinger equation for the total wavefunction $|\Psi^{(+)}\rangle$ presented in Equation 20. This shall be re-arranged to yield the Lippmann-Schwinger equation, which will then be solved using the CCC formalism to obtain the matrix elements of the $\hat{T}$ operator - with which scattering statistics can be calculated.

Lippmann-Schwinger Equation We consider an eigenstate $|\Psi\rangle$ of a Hamiltonian $\hat{H}$, with eigenenergy E, for which the Schrödinger equation is of the form

$$\hat{H}|\Psi\rangle = \hat{H}_A|\Psi\rangle + \hat{V}|\Psi\rangle = E|\Psi\rangle, \tag{28}$$

where $\hat{H}_A$ is the unbounded asymptotic Hamiltonian and $\hat{V}$ is a potential. This expression can be rearranged to the form

$$[E - \hat{H}_A]|\Psi\rangle = \hat{V}|\Psi\rangle. \tag{29}$$

Suppose that $\{|\Omega_\alpha\rangle\}$ are the (countably and uncountably infinite) eigenstates of the asymptotic Hamiltonian, with corresponding eigenvalues ε_α,

$$\hat{H}_A|\Omega_\alpha\rangle = \varepsilon_\alpha|\Omega_\alpha\rangle. \tag{30}$$

We note that where $\varepsilon_\alpha = E$, it follows that $|\Omega_\alpha\rangle \in \ker(E - \hat{H}_A)$; for a given energy E, we denote these particular asymptotic states by $|\Omega_\alpha^{(E)}\rangle$ and say that they are on-shell states, and that the energies of these states are on-shell. We now define the Green's operator $\hat{G}_{(E)}$, to be such that

$$\hat{G}_{(E)}[E - \hat{H}_A] = \hat{I} = [E - \hat{H}_A]\hat{G}_{(E)}, \tag{31}$$

whence we obtain a general form of the Lippmann-Schwinger equation,

$$|\Psi\rangle = \sum_{\alpha:\varepsilon_\alpha=E} \int C_\alpha |\Omega_\alpha^{(E)}\rangle + \hat{G}_{(E)}\hat{V}|\Psi\rangle, \tag{32}$$

where C_α are arbitrary scalar coefficients. We note that in this context, the sum taken over the indexes of the asymptotic eigenstates represents a sum over the countably infinite states, and an

integration over the uncountably infinite states, for which the eigenenergy ε_α is equal to E. The inclusion of the selected asymptotic eigenstates is required as they are in the kernel of $[E - \hat{H}_A]$, thus forming the homogenous solutions to the Lippmann-Schwinger equation. This can be demonstrated by applying the operator $[E - \hat{H}_A]$ on the left of Equation 32,

$$
\begin{aligned}
[E - \hat{H}_A] \, |\Psi\rangle &= \sum_{\alpha : \varepsilon_\alpha = E} \int C_\alpha [E - \hat{H}_A] \, |\Omega_\alpha^{(E)}\rangle + [E - \hat{H}_A] \hat{G}_{(E)} \hat{V} \, |\Psi\rangle \\
&= \sum_{\alpha : \varepsilon_\alpha = E} \int C_\alpha \, |0\rangle + \hat{I} \hat{V} \, |\Psi\rangle \\
&= \hat{V} \, |\Psi\rangle \, .
\end{aligned}
$$

At this point, we note that selecting the values of the coefficients C_α amounts to specifying a boundary condition for the eigenstate $|\Psi\rangle$. By consequence of the linearity of Equation 32, we may therefore simplify the generalised sum/integral, without loss of generality, by considering eigenstates of the form

$$
|\Psi_\alpha\rangle = |\Omega_\alpha^{(E)}\rangle + \hat{G}_{(E)} \hat{V} \, |\Psi_\alpha\rangle , \tag{33}
$$

for a particular $|\Omega_\alpha^{(E)}\rangle \in \ker(E - \hat{H}_A)$, and we say that $|\Psi_\alpha\rangle$ is the eigenstate of $\hat{H}$ corresponding to the boundary condition specified by the asymptotic eigenstate $|\Omega_\alpha^{(E)}\rangle$. We now define the $\hat{T}$ operator to be such that

$$
|\Psi_\alpha\rangle = [\hat{I} + \hat{G}_{(E)} \hat{T}] \, |\Omega_\alpha^{(E)}\rangle , \tag{34}
$$

which is equivalently defined by writing

$$
\hat{T} \, |\Omega_\alpha^{(E)}\rangle = \hat{V} \, |\Psi_\alpha\rangle . \tag{35}
$$

Furthermore, we have that

$$
\begin{aligned}
|\Psi_\alpha\rangle &= |\Omega_\alpha^{(E)}\rangle + \hat{G}_{(E)} \hat{V} \, |\Psi_\alpha\rangle \\
&= |\Omega_\alpha^{(E)}\rangle + \hat{G}_{(E)} \hat{V} \big[\hat{I} + \hat{G}_{(E)} \hat{T} \big] \, |\Omega_\alpha^{(E)}\rangle \\
&= \big[\hat{I} + \hat{G}_{(E)} \hat{V} + \hat{G}_{(E)} \hat{V} \hat{G}_{(E)} \hat{T} \big] \, |\Omega_\alpha^{(E)}\rangle \\
&= \big[\hat{I} + \hat{G}_{(E)} (\hat{V} + \hat{V} \hat{G}_{(E)} \hat{T}) \big] \, |\Omega_\alpha^{(E)}\rangle ,
\end{aligned}
$$

whence it follows that $\hat{T}$ can be written in the form

$$
\hat{T} \, |\Omega_\alpha^{(E)}\rangle = [\hat{V} + \hat{V} \hat{G}_{(E)} \hat{T}] \, |\Omega_\alpha^{(E)}\rangle , \tag{36}
$$

yielding the formulation of the Lippmann-Schwinger equation in terms of the $\hat{T}$ operator. At this point we consider the explicit form of the Green's operator $\hat{G}_{(E)}$. First, we note that the asymptotic eigenstates are complete in the sense that they provide a resolution of the identity

$$
\hat{I} = \sum_\gamma \int |\Omega_\gamma\rangle\langle\Omega_\gamma| , \tag{37}
$$

and a spectral decomposition of the asymptotic Hamiltonian

$$
\hat{H}_A = \sum_\gamma \int \varepsilon_\gamma \, |\Omega_\gamma\rangle\langle\Omega_\gamma| .
$$

It therefore follows from the definition of the Green's operator, Equation 31, that we must have

$$\hat{G}_{(E)}[E - \hat{H}_A] = \hat{I}$$

$$\sum_\gamma \int (E - \varepsilon_\gamma)\hat{G}_{(E)} |\Omega_\gamma\rangle\langle\Omega_\gamma| = \sum_\gamma \int |\Omega_\gamma\rangle\langle\Omega_\gamma|,$$

whence it follows that the spectral decomposition of the Green's operator is of the form

$$\hat{G}_{(E)} = \sum_\gamma \int \frac{|\Omega_\gamma\rangle\langle\Omega_\gamma|}{E - \varepsilon_\gamma}. \tag{38}$$

However, this expression is not well-defined, as it is singular for the asymptotic states $|\Omega_\gamma^{(E)}\rangle$ for which $\varepsilon_\gamma = E$. This problem can be overcome by regularising the Green's operator to either the incoming $\hat{G}_{(E,-)}$ or outgoing $\hat{G}_{(E,+)}$ forms,

$$\hat{G}_{(E,\pm)} = \lim_{\eta \to 0} \sum_\gamma \int \frac{|\Omega_\gamma\rangle\langle\Omega_\gamma|}{E - \varepsilon_\gamma \pm i\eta} = \sum_\gamma \int \frac{|\Omega_\gamma\rangle\langle\Omega_\gamma|}{E - \varepsilon_\gamma \pm i0}, \tag{39}$$

where the presence of the imaginary limit ensures that the integral is well-defined for all ε_γ. We elect to use the outgoing Green's operator $\hat{G}_{(E,+)}$ as we are concerned with the outgoing behaviour of the eigenstate $|\Psi_\alpha^{(+)}\rangle$. We can now re-write the Lippmann-Schwinger equation in the following form

$$\langle\Omega_\alpha|\hat{T}|\Omega_\beta^{(E)}\rangle = \langle\Omega_\alpha|\hat{V}|\Omega_\beta^{(E)}\rangle + \sum_\gamma \int \frac{\langle\Omega_\alpha|\hat{V}|\Omega_\gamma\rangle \, \langle\Omega_\gamma|\hat{T}|\Omega_\beta^{(E)}\rangle}{E - \varepsilon_\gamma + i0}, \tag{40}$$

which expresses the representation of the operator $\hat{T}$, for a given energy E, in terms of the asymptotic eigenstates $\{|\Omega_\alpha\rangle\}$ and the on-shell asymptotic eigenstates $\{|\Omega_\beta^{(E)}\rangle\}$.

Convergent Close-Coupling Formalism   In the Convergent Close-Coupling formalism, the Lippmann-Schwinger equation in terms of the $\hat{T}$ operator, Equation 40, is solved in momentum space. We preface this discussion with a minor note, that the notation for the asymptotic Hamiltonian $\hat{H}_A$ is to be distinguished from the notation for the anti-symmetriser $\hat{A}$.

We split the Hamiltonian, from Equation 21, into an asymptotic Hamiltonian and a potential in the form

$$\hat{H} = \hat{H}_T + \hat{K}_0 + \hat{V}_0 + \sum_{m=1}^{n_e} \hat{V}_{0,m} = \hat{H}_A + \hat{W}, \tag{41}$$

where the asymptotic Hamiltonian is of the form

$$\hat{H}_A = \hat{H}_T + \hat{K}_0 + \hat{U}_0, \tag{42}$$

and where the potential, modelling the interaction between the projectile and target states, is of the form

$$\hat{W} = \hat{V}_0 + \sum_{m=1}^{n_e} \hat{V}_{0,m} - \hat{U}_0, \tag{43}$$

where $\hat{U}_0$ is an asymptotic potential acting on the projectile, which can be chosen arbitrarily. A suitable choice for this potential is that of a Coulomb potential with a charge corresponding to the asymptotic charge of the target system, whence $\langle \mathbf{r} | \hat{W} \rangle = W(r, \Omega) \to 0$ as $r \to \infty$. Such a selection for $\hat{U}_0$ adapts the projectile states to the target system, without loss of generality, and can lead to improvement in computational performance, as discussed in [1, 204].

The asymptotic eigenstates are therefore taken to be of the form

$$|\Omega_\alpha\rangle = |\Phi_\alpha \mathbf{k}_\alpha\rangle \approx |\Phi_{n_\alpha}^{(N)} \mathbf{k}_\alpha\rangle, \tag{44}$$

where $\{|\Phi_n^{(N)}\rangle\}_{i=1}^{N_T}$ are the target pseudostates, defined in Equation 16, which satisfy

$$\langle \Phi_i^{(N)} | \hat{H}_T | \Phi_j^{(N)} \rangle = \epsilon_i^{(N)} \delta_{i,j}, \tag{45}$$

and where $|\mathbf{k}_\alpha\rangle$ are the continuum waves (which could be plane, distorted, or Coulomb waves depending on the choice of $\hat{U}_0$), defined to be eigenstates of the projectile component of the asymptotic Hamiltonian,

$$[\hat{K}_0 + \hat{U}_0] |\mathbf{k}_\alpha\rangle = \tfrac{1}{2} k_\alpha^2 |\mathbf{k}_\alpha\rangle, \tag{46}$$

whence it can be seen that the asymptotic eigenenergies are of the form

$$\varepsilon_\alpha = \epsilon_{n_\alpha} + \tfrac{1}{2} k_\alpha^2 \approx \epsilon_{n_\alpha}^{(N)} + \tfrac{1}{2} k_\alpha^2. \tag{47}$$

Furthermore, the total wavefunction is taken to be of the form

$$|\Psi_\alpha^{(+)}\rangle = \hat{A} |\psi_\alpha^{(+)}\rangle \approx \hat{A} \hat{I}_T^{(N)} |\psi_\alpha^{(+)}\rangle = \hat{A} |\psi_\alpha^{(N,+)}\rangle = |\Psi_\alpha^{(N,+)}\rangle, \tag{48}$$

as in Equation 22, where $\hat{A}$ is the anti-symmetriser operator, defined in Equation 8, and is subject to the constraints imposed in Equation 27 to ensure uniqueness. We note that with these expressions for the asymptotic eigenstates and the total wavefunction, that the $\hat{T}$ operator is related to the potential $\hat{W}$ by the expression

$$\hat{T} |\Phi_{n_\alpha}^{(N)} \mathbf{k}_\alpha\rangle = \hat{W} |\Psi_\alpha^{(N,+)}\rangle = \hat{W} \hat{A} \hat{I}_T^{(N)} |\psi_\alpha^{(+)}\rangle = \hat{W} \hat{A} |\psi_\alpha^{(N,+)}\rangle. \tag{49}$$

However, it is possible to recast the potential $\hat{W}$ in a form $\hat{V}$ which accounts for the explicit anti-symmetrisation of the total wavefunction; that is, which allows us to write the CCC equations without direct reference to the anti-symmetriser $\hat{A}$. To do this, we first note that

$$0 = [E - \hat{H}] |\Psi_\alpha^{(+)}\rangle = [E - \hat{H}] \hat{A} |\psi_\alpha^{(+)}\rangle,$$

with the operator on the right hand side expanding to the form

$$[E - \hat{H}]\hat{A} = \left[E - \hat{H} - [E - \hat{H}] \sum_{m=1}^{n_e} \hat{P}_{0,m} \right] = \left[E - \hat{H}_A - \hat{W} - [E - \hat{H}] \sum_{m=1}^{n_e} \hat{P}_{0,m} \right],$$

where again we make sure to distinguish the notation for the asymptotic Hamiltonian $\hat{H}_A$ and the anti-symmetriser $\hat{A}$. We therefore define the explicitly anti-symmetrised potential $\hat{V}$ to be of the form

$$\hat{V} = \hat{W} + [E - \hat{H}] \sum_{m=1}^{n_e} \hat{P}_{0,m} = \hat{V}_0 + \sum_{m=1}^{n_e} \hat{V}_{0,m} - \hat{U}_0 + [E - \hat{H}] \sum_{m=1}^{n_e} \hat{P}_{0,m}, \tag{50}$$

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for which we can see that

$$0 = [E - \hat{H}]\hat{A}\,|\psi_\alpha^{(+)}\rangle = [E - [\hat{H}_A + \hat{V}]]\,|\psi_\alpha^{(+)}\rangle,$$

which is to say that the Lippmann-Schwinger equation Equation 40 can be written in terms of the un-symmetrised total wavefunction $|\psi_\alpha^{(+)}\rangle$, rather than the anti-symmetric total wavefunction $|\Psi_\alpha^{(+)}\rangle$. Specifically, this allows us to write the $\hat{T}$ operator in the form

$$\hat{T}\,|\Phi_{n_\alpha}^{(N)}\mathbf{k}_\alpha\rangle = \hat{V}\hat{I}_T^{(N)}\,|\psi_\alpha^{(+)}\rangle = \hat{V}\,|\psi_\alpha^{(N,+)}\rangle. \tag{51}$$

We then have the Convergent Close-Coupling equations in terms of the $\hat{T}$ operator

$$\langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{T}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle = \langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{V}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle \tag{52}$$
$$+ \sum_{n=1}^{N_T}\int \mathrm{d}\mathbf{k}\,\frac{\langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{V}|\Phi_n^{(N)}\mathbf{k}\rangle\,\langle \mathbf{k}\Phi_n^{(N)}|\hat{T}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle}{E - \epsilon_n^{(N)} - \frac{1}{2}k^2 \pm \mathrm{i}0},$$

forming a set of $\mathbb{C}$-valued matrix equations which are numerically solved to yield the T matrix, from which information about the total wavefunction $|\Psi_i^{(N,+)}\rangle$ can be derived. However, it is possible to re-write the Convergent Close-Coupling equations in terms of an operator $\hat{K}$,

$$\langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{K}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle = \langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{V}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle \tag{53}$$
$$+ \sum_{n=1}^{N_T}\mathcal{P}\int \mathrm{d}\mathbf{k}\,\frac{\langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{V}|\Phi_n^{(N)}\mathbf{k}\rangle\,\langle \mathbf{k}\Phi_n^{(N)}|\hat{K}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle}{E - \epsilon_n^{(N)} - \frac{1}{2}k^2},$$

where $\mathcal{P}$ indicates that the principal value of the integral is taken, which forms a set of $\mathbb{R}$-valued matrix equations which can be solved more efficiently, to yield the K matrix. The T matrix can then be reconstructed from the K matrix by the identity [5, 9]

$$\langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{K}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle = \sum_{n=1}^{N_T}\langle \mathbf{k}_f \Phi_{n_f}^{(N)}|\hat{T}|\Phi_n^{(N)}\mathbf{k}_n\rangle\left(\delta_{n,i} + \mathrm{i}\pi k_n\,\langle \mathbf{k}_n \Phi_n^{(N)}|\hat{K}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle\right), \tag{54}$$

where k_n are the on-shell projectile momenta which satisfy

$$E = \epsilon_n^{(N)} + \tfrac{1}{2}k_n^2 \quad \text{for} \quad n = 1, \ldots, N_T. \tag{55}$$

We note that the matrix equations Equation 52, as well as Equation 53 and Equation 54, are computationally parameterised by the set of target pseudostates $\{\,|\Phi_n^{(N)}\rangle\}_{n=1}^{N_T}$ and the discretisation of the projectile spectrum. In turn, the target pseudostates are parameterised by the number of Slater determinants N_T used in their construction, and the number of basis functions N used to construct the one-electron orbitals from which the Slater determinants are built. Furthermore, we note that matrix equations in this form do not explicitly include the constraints, detailed in Equation 27, which guarantee the uniqueness of the explicitly anti-symmetrised multichannel expansion. The manifestation of these constraints for the case of a hydrogen target is discussed in section 3.1.1.

2.2   Scattering Statistics

At this point, we shall utilise the S-wave model, wherein we restrict our attention to the asymptotic eigenstates for which the target pseudostate $\{|\Phi_n^{(N)}\rangle\}_{n=1}^{N_T}$ and projectile both have $l = 0$. This allows for a simpler presentation of theoretical results, and calculations performed in the S-wave model are often sufficient to explore the behaviour of scattering phenomena with the benefit of a significant reduction in computational complexity. Much of the following treatment is generalisable to a full treatment of angular momentum.

2.2.1   Scattering Amplitudes

Once calculated, the matrix elements of the $\hat{T}$ operator yield the transition amplitudes between asymptotic states, which can then be used to calculate the scattering amplitudes. In general terms, the scattering amplitudes can be written in the form

$$F_{\alpha,\beta} = F_{\alpha,\beta}(\mathbf{k}_\alpha, \mathbf{k}_\beta) = \langle \mathbf{k}_\alpha \Phi_\alpha | \hat{V} | \Psi_\beta \rangle = \langle \mathbf{k}_\alpha \Phi_\alpha | \hat{T} | \Phi_\beta \mathbf{k}_\beta \rangle, \tag{56}$$

where the target state $|\Phi_\alpha\rangle$ can be a bounded discrete state or an unbounded continuum state, corresponding to either an elastic scattering / a discrete excition transition, or an ionisation transition. Note that despite the duplicated notation, we are referring to the scattering amplitudes $F_{\alpha,\beta}$, not the multichannel weight functions $|F_n^{(N)}\rangle$ defined in [Equation 23](#).

For discrete excitations, the numerically calculated scattering amplitude is simply of the form

$$F_{f,i}^{(N)} = F_{n_f,n_i}^{(N)}(\mathbf{k}_f, \mathbf{k}_i) = \langle \mathbf{k}_f \Phi_{n_f}^{(N)} | \hat{T} | \Phi_{n_i}^{(N)} \mathbf{k}_i \rangle, \tag{57}$$

for on-shell transitions,

$$\epsilon_{n_f}^{(N)} + \tfrac{1}{2}k_f^2 = E = \epsilon_{n_i}^{(N)} + \tfrac{1}{2}k_i^2, \tag{58}$$

with elastic scattering occuring in the case where $n_f = n_i$,

$$F_i^{(N)}(\mathbf{k}_f, \mathbf{k}_i) = F_{n_i,n_i}^{(N)}(\mathbf{k}_f, \mathbf{k}_i) = \langle \mathbf{k}_f \Phi_{n_i}^{(N)} | \hat{T} | \Phi_{n_i}^{(N)} \mathbf{k}_i \rangle. \tag{59}$$

However, the numerically calculated scattering amplitudes for ionisations require a more carefully considered treatment - which we present in a form similar to that described in [2, 4]. We shall restrict our attention to the case of single ionisation, but leave open the consideration of ionisation with excitation. The ionised asymptotic state $|\Phi_\alpha \mathbf{k}_\alpha\rangle$ corresponds to the breakup of the target state $|\Phi_\alpha\rangle$ into a singly-ionised target state $|\Phi_{n_\alpha}^+\rangle$ (which may be excited) and an ionised electron in the form of a Coulomb wave $|\mathbf{q}_\alpha\rangle$; that is,

$$|\Phi_\alpha \mathbf{k}_\alpha\rangle = |\Phi_{n_\alpha}^+ \mathbf{q}_\alpha \mathbf{k}_\alpha\rangle, \tag{60}$$

where the energy of the ionised asymptotic state is of the form

$$E = \epsilon_\alpha + \tfrac{1}{2}k_\alpha^2 = \epsilon_{n_\alpha}^+ + \tfrac{1}{2}q_\alpha^2 + \tfrac{1}{2}k_\alpha^2 \tag{61}$$

where $\epsilon_{n_\alpha}^+$ is the energy of the singly-ionised target state, and where $\tfrac{1}{2}q_\alpha^2$ is the energy of the Coulomb wave. It is important to note that in this formulation, the asymptotic state $|\Phi_\alpha \mathbf{k}_\alpha\rangle$ separates into the asymptotic projectile state $|\mathbf{k}_\alpha\rangle$ and the asymptotic target state $|\Phi_\alpha\rangle = |\Phi_{n_\alpha}^+ \mathbf{q}_\alpha\rangle$, within which the Coulomb wave $|\mathbf{q}_\alpha\rangle$ is modelled - thus excluding from consideration a three-body boundary condition. This presents an issue however as Coulomb waves are not bounded

states, and thus their coordinate-space representations are not elements of $L^2(\mathbb{R}^3)$. This is the space wherein the coordinate-space representations of the one-electron states, comprising the target pseudostates, are spanned in terms of the Laguerre basis, Equation 1. However it can be shown, as discussed in [5], that the projection of a continuum wave onto a N-dimensional Laguerre basis is conditionally convergent as N increases, but is numerically stable. Hence, for ionisations, the numerically calculated scattering amplitude can be written in the form

$$
\begin{aligned}
F_{\alpha,i}^{(N)} = F_{n_\alpha,n_i}^{(N)}(\mathbf{q}_\alpha;\mathbf{k}_\alpha,\mathbf{k}_i) &= \langle \mathbf{k}_\alpha\mathbf{q}_\alpha\Phi_{n_\alpha}^+|\hat{I}_T^{(N)}\hat{T}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle \\
&= \sum_{n=1}^{N_T} \langle \mathbf{k}_\alpha\mathbf{q}_\alpha\Phi_{n_\alpha}^+|\Phi_n^{(N)}\rangle \, \langle\Phi_n^{(N)}|\hat{T}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle \\
&= \sum_{n=1}^{N_T} \langle \mathbf{q}_\alpha\Phi_{n_\alpha}^+|\Phi_n^{(N)}\rangle \, \langle\mathbf{k}_\alpha\Phi_n^{(N)}|\hat{T}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle .
\end{aligned}
\tag{62}
$$

However, this expression is problematic as it involves a summation over not necessarily on-shell terms $\langle \mathbf{k}_\alpha\Phi_n^{(N)}|$. If we restrict our attention to only evaluating the ionisation scattering amplitudes $F_{\alpha,i}^{(N)}$ for ionised asymptotic states $|\Phi_{n_\alpha}^+\mathbf{q}_\alpha\mathbf{k}_\alpha\rangle$ for which the ionised target energy satisfies

$$
\epsilon_\alpha = \epsilon_{n_\alpha}^+ + \tfrac{1}{2}q_\alpha^2 = \epsilon_{n_\alpha}^{(N)},
\tag{63}
$$

for one of the target pseudoenergies $\epsilon_{n_\alpha}^{(N)}$, corresponding to the target pseudostate $|\Phi_{n_\alpha}^{(N)}\rangle$, then we must have that

$$
\langle \mathbf{q}_\alpha\Phi_{n_\alpha}^+|\Phi_n^{(N)}\rangle = \delta_{n_\alpha,n} \langle \mathbf{q}_\alpha\Phi_{n_\alpha}^+|\Phi_n^{(N)}\rangle ,
\tag{64}
$$

whence the ionisation scattering amplitudes can be evaluated as

$$
F_{n_\alpha,n_i}^{(N)}(\mathbf{q}_\alpha;\mathbf{k}_\alpha,\mathbf{k}_i) = \langle \mathbf{q}_\alpha\Phi_{n_\alpha}^+|\Phi_{n_\alpha}^{(N)}\rangle \, \langle\mathbf{k}_\alpha\Phi_{n_\alpha}^{(N)}|\hat{T}|\Phi_{n_i}^{(N)}\mathbf{k}_i\rangle ,
\tag{65}
$$

at these q_α which satisfy Equation 63. This is the approach taken in the CCC method to calculate the ionisation scattering amplitudes, and we note that it is constrained to evaluating these amplitudes only at certain energies permitted by the target pseudoenergies. Evaluating the ionisation scattering amplitudes at any other energy requires an interpolation between these energies.

2.2.2 Cross Sections

We present expressions for the partial and total cross sections, in a manner similar to [5, 10]. In general terms, the partial cross sections are of the form

$$
\sigma_{\alpha,\beta} = \sigma_{\alpha,\beta}(\mathbf{k}_\alpha,\mathbf{k}_\beta) = \frac{k_\alpha}{k_\beta}|F_{\alpha,\beta}|^2 = \frac{k_\alpha}{k_\beta}|\langle \mathbf{k}_\alpha\Phi_\alpha|\hat{T}|\Phi_\beta\mathbf{k}_\beta\rangle|^2,
\tag{66}
$$

with the specific notation for elastic, discrete excitation, and ionisation cross sections paralleling the notation used in Equation 57, Equation 59, and Equation 62 respectively.

The total cross section (TCS), for a given initial asymptotic state, is obtained as a sum of all partial cross sections for which the outgoing asymptotic projectile energy is positive,

$$
\sigma_{\mathrm{T};i}^{(N)} = \sum_{f:k_f>0} \sigma_{f,i}^{(N)},
\tag{67}
$$

while the total ionisation cross section (TICS), for a given initial asymptotic state, is obtained as a sum of all partial cross sections for which the outgoing asymptotic target state is positive (and thus unbounded),

$$\sigma_{\mathrm{I};i}^{(N)} = \sum_{f:k_f>0,\epsilon_\alpha^{(N)}>0} \sigma_{\alpha,i}^{(N)}. \tag{68}$$

We also consider the various differential cross sections in the context of ionisation transitions, following in the form of [3]. Evaluating the partial cross sections, for an ionisation transition, yields the triple-differential cross section (TDCS). Integrating the TDCS over the spherical coordinates of either the outgoing asymptotic projectile electron, or the outgoing ionised target electron, yields the double-differential cross section (DDCS). Furthermore, integrating the DDCS over the spherical coordinates of the remaining electron, whichever one that may be, yields the single-differential cross section (SDCS). Integration of the SDCS over the projectile (or target) electron energy yields the total ionisation cross section.

3 Survey of Literature

3.1 Electron-Impact Hydrogen Ionisation

3.1.1 Considerations for a Hydrogen Target

Spin

Uniqueness

3.1.2 Convergent Close-Coupling Calculations

Triplet Case

Singlet Case

Step Function Behaviour of TICS

3.1.3 Exterior-Complex-Scaling Calculations

3.1.4 Ansatz of Zatsarinny and Bartschat

3.2 Electron-Impact Helium Ionisation

3.2.1 Additional Considerations for a Helium Target

Frozen-Core Model

Autoionising States

3.2.2   Convergent Close-Coupling Calculations

3.2.3   Exterior-Complex-Scaling Calculations

4   Conclusion

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