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

Tom Ross supervised by Professor Igor Bray

[ABSTRACT]

Contents

List of Figures

List of Tables

1 Introduction

Applications of Electron-Impact Hydrogen Scattering

Specific Applications of Electron-Impact Hydrogen Ionisation

Development of Quantum Scattering Theory

2 Theory

We shall describe the development of the Convergent Close-Coupling (CCC) method for generalised projectile-target scattering, before describing its application to the cases of: electron-impact hydrogen (e-H) scattering, and electron-impact helium (e-He) scattering. In particular, we shall explore the treatment of target ionisation within the CCC method. Note that in the general treatment, we restrict our attention to electron projectiles and atomic/ionic targets.

2.1 Convergent Close-Coupling Method

In brief, the CCC method utilises the method of basis expansion, discussed in further detail in subsection B.1, to numerically solve the Lippmann-Schwinger equation, for a projectile-target system, to yield the transition amplitudes, which are convergent as the size of the basis is increased. The rate of convergence depends on many factors, such as the complexity and geometry of the projectile-target system for example, as well as the choice of basis used in the expansion. Furthermore, by selecting a complete basis, ionisation transition amplitudes can be treated in a similar manner to discrete excitation transition amplitudes.

2.1.1 Laguerre Basis

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

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

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 α_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 $i \in \{1,2,\ldots\}$.

It is shown in subsubsection A.2.1, that the Laguerre radial basis functions, $\{\xi_{k,l}(r)\}_{k=1}^{\infty}$, for each l, forms a complete basis for the Hilbert space $L^2_{\mathbb{C}}([0,\infty))$. Similarly, it is also shown in subsubsection A.1.1, that the set of spherical harmonics, $\{Y_l^{-l}(\Omega),\ldots,Y_l^{l}(\Omega)\}_{l=0}^{\infty}$, forms a orthonormal, complete basis for the Hilbert space $L^2_{\mathbb{C}}(S^2)$. Hence, the Laguerre basis functions $\{\varphi_i(r,\Omega)\}_{i=1}^{\infty}$, forms a complete basis for the Hilbert space $L^2_{\mathbb{C}}(\mathbb{R}^3)$ space.

This Laguerre basis is utilised due to being a complete basis, the short-range and long-range behaviour of the radial basis functions, and because it allows the matrix elements of certain operators to be calculated analytically.

Practically, we cannot utilise a 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.

Further properties of the Laguerre basis are provided in subsection A.3.

2.1.2 Projectile-Target System

Possessing now a suitable basis to work with, we proceed to represent the projectile-target system in this basis by the method of basis expansion. We first construct the projectile states, and the target states, before considering how to combine the two into a set of total states. Recall that we restrict our attention to the case of an electron projectile, and an atomic/ionic target consisting of n_e electrons. We shall adopt the convention that the projectile electron space is acted on by operators indexed by 0, and the m-th target electron space is acted on by operators indexed by m.

Projectile States The projectile states, $|\boldsymbol{k}\rangle$, are defined to be eigenstates of the free Hamiltonian; that is,

$$\hat{K}_0 \, |\boldsymbol{k}\rangle = \tfrac{k^2}{2} \, |\boldsymbol{k}\rangle \, . \tag{4}$$

It follows that the projectile states are plane waves, for which the coordinate-space representation is of the form

$$\langle \boldsymbol{r} | \boldsymbol{k} \rangle = (2\pi)^{-\frac{3}{2}} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}). \tag{5}$$

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

$$\hat{H}_T = \sum_{m=1}^{n_\mathrm{e}} \hat{K}_m + \sum_{m=1}^{n_\mathrm{e}} \hat{V}_m + \tfrac{1}{2} \sum_{m=1}^{n_\mathrm{e}} \sum_{n=1}^{n_\mathrm{e}} \hat{V}_{m,n} \tag{6}$$

where $\hat{K}_m$ and $\hat{V}_m$ are the target electron kinetic and electron-nuclei potential operators, for $m = 1, \ldots, n_\mathrm{e}$, and where $\hat{V}_{m,n}$ are the electron-electron potential operators, for $m, n = 1, \ldots, n_\mathrm{e}$. The target states, $|\phi\rangle$, are constructed by expanding the target Hamiltonian, $\hat{H}_T$, in a Laguerre basis, $\{|\varphi_i\rangle\}_{i=1}^{N}$, and diagonalising to yield the target pseudostates $\{\, |\phi_i^{(N)}\rangle\}_{i=1}^{N}$, which are orthonormal and satisfy

$$\langle \phi_i^{(N)} | \, \hat{H}_T \, | \phi_j^{(N)} \rangle = \epsilon_i^{(N)} \delta_{i,j}. \tag{7}$$

Furthermore, the target pseudostates are anti-symmetric under pairwise electron exchange. Note 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 Laguerrre basis, and that these

pseudostates and their pseudoenergies are dependent on the size of the Laguerre basis utilised. The procedure of diagonalising the target Hamiltonian is discussed in further detail in subsection B.2.

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. In general, bounded states have negative energy and unbounded states have positive energy, however this is not necessarily the case - a note which will be relevant in the treatment of the meta-stable positive-energy discrete states of helium. To do (??) For clarity, we shall adjourn the treatment of these meta-stable states until required, and proceed with the assumption that bounded states have negative energy. To do (??) We order the target pseudostates by increasing pseudoenergy, $\epsilon_1^{(N)} < \ldots < \epsilon_N^{(N)}$, which allows us to express the separability of the spectrum in the form

$$\{\,|\phi_i^{(N)}\rangle\}_{i=1}^{N} = \{\,|\phi_i^{(N)}\rangle\}_{i=1}^{N_B} \cup \{\,|\phi_i^{(N)}\rangle\}_{i=N_B+1}^{N} \tag{8}$$

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

We note that the identity operator for the space of target states can be represented in the form

$$\hat{I}_2 = \sum_{i=1}^{\infty} |\phi_i\rangle\ \langle\phi_i| + \int_{\boldsymbol{q}:q^2\geq 0} \mathrm{d}\boldsymbol{q}\ |\boldsymbol{q}\rangle\ \langle\boldsymbol{q}| \tag{9}$$

where $\{\,|\phi_i\rangle\}_{i=1}^{\infty}$ is the true target discrete spectrum and where $\{\,|\boldsymbol{q}\rangle : q^2 \geq 0\}$ is the true continuum spectrum. Furthermore, we note that the projection operator for the target pseudostates, $\hat{I}_2^{(N)}$, is To do (??) of the form

$$\hat{I}_2^{(N)} = \sum_{i=1}^{N} |\phi_i^{(N)}\rangle\ \langle\phi_i^{(N)}| = \sum_{i=1}^{N_B} |\phi_i^{(N)}\rangle\ \langle\phi_i^{(N)}| + \sum_{i=N_B+1}^{N} |\phi_i^{(N)}\rangle\ \langle\phi_i^{(N)}| \tag{10}$$

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

$$\lim_{N\to\infty} \sum_{i=1}^{N_B} |\phi_i^{(N)}\rangle\ \langle\phi_i^{(N)}| = \sum_{i=1}^{\infty} |\phi_i\rangle\ \langle\phi_i| \tag{11}$$

and the sum over the unbounded pseudostates will converge to a discretisation of the integral over the true continuum spectrum

$$\lim_{N\to\infty} \sum_{i=N_B+1}^{N} |\phi_i^{(N)}\rangle\ \langle\phi_i^{(N)}| = \int_{\boldsymbol{q}:q^2\geq 0} \mathrm{d}\boldsymbol{q}\ |\boldsymbol{q}\rangle\ \langle\boldsymbol{q}|\,. \tag{12}$$

Whence, it follows that projection operator for the target pseudostates converges to the identity operator, for the space of target states, in the limit as $N \to \infty$; that is,

$$\lim_{N\to\infty} I_2^{(N)} = I_2. \tag{13}$$

Total State The total Hamiltonian of the projectile-target system, $\hat{H}$, is of the form

$$\hat{H} = \hat{H}_T + \hat{K}_0 + \hat{V}_0 + \sum_{m=1}^{n_e} \hat{V}_{0,m} \tag{14}$$

where $\hat{H}_T$ is the target Hamiltonian, defined in Equation 6, $\hat{K}_0$ 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 total state of the projectile-target system, $|\Psi^{(+)}\rangle$, specified to have outgoing spherical-wave boundary conditions, is an eigenstate of the total Hamiltonian, $\hat{H}$,

$$\hat{H}\,|\Psi^{(+)}\rangle = E\,|\Psi^{(+)}\rangle \tag{15}$$

with total energy E. Since the construction of the total state will depend upon the target pseudostates, $\{\,|\psi_i^{(N)}\rangle\}_{i=1}^{N}$, obtained by the diagonalisation of the target hamiltonian, Equation 7, we shall make explicit it's dependence on the size of the basis by writing, $|\Psi^{(N,+)}\rangle$, and note that

$$|\Psi^{(+)}\rangle = \lim_{N\to\infty} |\Psi^{(N,+)}\rangle\,. \tag{16}$$

To ensure that the total state is anti-symmetric (that is, that it respects the indistinguishableness of individual electrons, as well as Pauli's exclusion principle), we construct it using a multichannel expansion of the form

$$|\Psi^{(N,+)}\rangle = \left[1 - \sum_{m=1}^{n_e} \hat{P}_{0,m}\right] |\psi^{(N,+)}\rangle \tag{17}$$

where $\hat{P}_{0,m}$ are the electron exchange operators, for $m = 1, \ldots, n_e$, exchanging the projectile electron state and m-th target electron state. We neglect to anti-symmetrise the target electrons with each other, since the target pseudostates, $\{\,|\phi_i^{(N)}\rangle\}_{i=1}^{\infty}$ are already anti-symmetric by construction. However, we observe that the multichannel expansion is not uniquely defined, since for any state in the kernel of the multichannel operator, $|\omega^{(N,+)}\rangle \in \ker(1 - \sum_{m=1}^{n_e} \hat{P}_{0,m})$, and constant θ, the multichannel expansion of $|\psi^{(N,+)}\rangle + \theta\,|\omega^{(N,+)}\rangle$ will be identical to that of $|\psi^{(N,+)}\rangle$. This dilemma can be resolved in the following To resolve this dilemma, we impose the constraint that for any of the one-electron states, $|\eta\rangle$, used to construct the target state, $|\phi_i^{(N)}\rangle$, that

$$\langle \eta, \phi_i^{(N)}|\,\hat{P}_{0,m}\,|\gamma^{(N,+)}\rangle = -\,\langle \eta, \phi_i^{(N)}|\gamma^{(N,+)}\rangle \quad \text{for all} \quad |\gamma^{(N,+)}\rangle\,. \tag{18}$$

Whence it follows that the multichannel expansion of $|\psi^{(N,+)}\rangle + \theta\,|\omega^{(N,+)}\rangle$ will be identical to that of $|\psi^{(N,+)}\rangle$, only in the case where $\theta = 0$, or $|\omega\rangle = |0\rangle$; that is, $|\psi^{(N,+)}\rangle$ will now uniquely determine $|\Psi^{(N,+)}\rangle$.

2.1.3 Close-Coupling Equations

2.1.4 Transition Amplitudes

2.1.5 Cross Sections

Total Cross Sections

Differential Cross Sections

References

A Properties of Utilised Bases

A.1 Spherical Harmonics

A.1.1 Completeness

A.2 Laguerre Radial Basis

A.2.1 Completeness

A.3 Laguerre Basis

A.4 Plane Waves

B Numerical Techniques

B.1 Basis Expansion

B.2 Diagonalisation