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

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[ABSTRACT]

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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.

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

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

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, for each l, that the Laguerre radial basis functions, $\{\xi_{k,l}(r)\}_{k=1}^{\infty}$, forms a complete basis for the Hilbert space $L_{\mathbb{C}}^2([0,\infty))$. 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 $L_{\mathbb{C}}^2(S^2)$. Hence, the Laguerre basis functions $\{\varphi_i(r,\Omega)\}_{i=1}^{\infty}$, forms a complete basis for the Hilbert space $L_{\mathbb{C}}^2(\mathbb{R}^3)$ 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 construct the two into a total state.

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

$$\hat{H}_1 |\boldsymbol{k}\rangle = \hat{K}_1 |\boldsymbol{k}\rangle = \tfrac{k^2}{2} |\boldsymbol{k}\rangle . \tag{4}$$

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 states, $|\phi\rangle$ are constructed by expanding the target Hamiltonian, $\hat{H}_2 = \hat{K}_2 + \hat{V}_2$, 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

$$\langle \phi_i^{(N)}|\, \hat{H}_2\, |\phi_j^{(N)}\rangle = \epsilon_i^{(N)} \delta_{i,j}. \tag{6}$$

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.

Total State As a result of the asymptotic initial conditions, in which the projectile and the target are assumed to be sufficiently far apart as to be non-interacting, we might naively suppose the total state of the projectile-target system can be constructed as a tensor products of the individual projectile and target states. That is, we might suppose that the total asymptotic state, $|\Psi^{(+)}\rangle$, may be written as $|\Psi^{(+)}\rangle = |\phi, \boldsymbol{k}\rangle$, where $|\phi\rangle$ is the target state, and $|\boldsymbol{k}\rangle$ is the projectile state. However, this neglects to account for the effects of spin and Pauli's exclusion principle, or more generally symmetrisation / anti-symmetrisation.

For the case where the projectile is a fermion, and the target contains one such fermion, then the fermions are necessarily indistinguishable. Additionally, Pauli's exclusion principle states that two fermions cannot occupy the same state (including spin) within a system. To account for this principle, we may write the total state, $|\Psi^{(S+)}\rangle$, for a given total spin S, in the form

$$|\Psi^{(S+)}\rangle = [1 + (-1)^S \hat{P}_r] \, |\psi^{(S+)}\rangle \tag{7}$$

where $\hat{P}_r$ is the spatial exchange operator, and where $|\psi^{(S+)}\rangle$ is the two-fermion state. It follows that the total state, in this form, is guaranteed to adhere to Pauli's exclusion principle.

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