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 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.1.1, for each l, that the Laguerre radial basis functions, $\{\xi_{k,l}(r)\}_{k=1}^{\infty}$, forms a complete basis for the Hilbert space $L^2_{\mathbb{C}}([0,\infty))$. Similarly, it is also shown in subsubsection A.2.1, 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.

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 Appendix A.

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. 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, the total state of the projectile-target system can be constructed as a tensor product of the individual projectile and target states. That is, the total state, $|\Phi\rangle$, may be written as $|\Phi\rangle = |\phi, \boldsymbol{k}\rangle$, where $|\phi\rangle$ is the target state, and $|\boldsymbol{k}\rangle$ is the projectile state. It now remains to construct the projectile states, and the target states.

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 Structure The target states, $|\phi\rangle$ are constructed by expanding the target Hamiltonian,

$$\hat{H}_2 |\phi\rangle = [\hat{K}_2 + \hat{V}_2] |\phi\rangle \tag{6}$$

in a Laguerre basis, and diagonalising to yield the target pseudostates $\{|\phi_i\rangle\}_{i=1}^{N}$

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