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, $\{|\varphi_i\rangle\}_{i=1}^{N}$, for which the coordinate-space representation is of the form

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

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 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 $k_i \in \{1, \dots, N_l\}$, $l_i \in \{0, \dots, l_{max}\}$ and $m_i \in \{-\ell_i, \dots, \ell_i\}$, for each $i \in \{1, 2, \dots, N\}$, where N_l is the total number of radial basis functions for each l.
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, $\{Y_l^{-l}(\Omega), \dots, Y_l^{l}(\Omega)\}_{l=0}^{\infty}$, 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.
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