Different representations of continuum in the positron-hydrogen scattering problem

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Synopsis

A two-centre convergent close coupling method is applied to positron-impact ionisation of hydrogen. Different ways of distributing the pseudostates representing the continuum are investigated. It is found that calculations of the grand total and total ionisation cross sections are independent of the distribution of continuum pseudostates.

Positron-hydrogen scattering is a two-centre problem. This work investigates the effect of pseudostate distribution across both centres employing the two-centre convergent close coupling method. The convergent close coupling (CCC) method, developed by Bray and Stelbovics [1], involves diagonalising the target Hamiltonian in an orthogonal Laguerre basis to produce pseudostates, which approximate the bound states and discretise the continuum. These pseudostates are used to expand the total scattering wave function of the system. Using this representation of the total wave function one obtains the Lippmann-Schwinger equation for the transition amplitudes. This was later extended by Kadyrov and Bray [2] to explicitly include positronium (Ps) formation channels by expanding the total wave function as a sum over pseudostates for both hydrogen and Ps. However, the two expansions are not mutually orthogonal and a possibility of double counting of the continuum is introduced.

The bases used in this work are denoted as $\text{CCC}(N_0^H, N_0^\text{Ps}, l_{\text{max}})$, where $l_{\text{max}}$ is the maximum orbital quantum number of the pseudostates. For each orbital quantum number $l$, the number of included pseudostates is $N_0 - l$. We consider four types of bases $\text{CCC}(30, 0, 9)$, $\text{CCC}(20, 20, 2)$, $\text{CCC}(20, 4, 3)$ and $\text{CCC}(8, 25, 2)$, where each basis uniquely represents the three-body continuum and is chosen to give a convergent result. A bar indicates the use of pseudostates and no bar means only exact bound states are included. The obtained results are given in figures 1 and 2. They show that close coupling calculations of positron-hydrogen scattering produce the same grand total cross section and also the same total break-up plus total Ps-formation cross section independent of pseudostate distribution. Interestingly, a double counting of the continuum thought to be associated with the two-centre pseudostate expansions does not appear to manifest in this scattering problem.

References


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