One-center close-coupling approach to two-center rearrangement collisions

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Calculations of ionization and electron-capture cross sections in ion-atom collisions usually require solving the Schrödinger equation governing the collision system by expanding the total scattering wave function in a basis of target- and projectile-centered pseudostates. This approach leads to the two-center close-coupling equations which in some cases may become ill-conditioned due to the non-orthogonality of the underlying combined basis. Here we develop a technique which allows to accurately extract the necessary collision information, including that for the rearrangement channels, from the computationally more convenient one-center close-coupling equations which are built from only target-centered pseudostates. The robustness of the method is demonstrated by considering the proton-hydrogen scattering problem across a wide incident energy range. The developed method is then applied to study proton scattering on multielectron target of lithium. The obtained results for the 2s→2p excitation and the total electron-capture cross sections are in good agreement with corresponding experimental data. It is concluded that the presented technique could be a simpler alternative when integrated cross sections are required.

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