Coulomb breakup problem and asymptotic behaviour of the three-body scattered wave

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With the progress in high-performance computing, the direct numerical integration of the Schroedinger equation has emerged as a powerful method to study scattering processes with three charged particles. Such a method, in principle, requires the knowledge of the asymptotic behavior of the scattered wave function in all asymptotic regions of the configuration space. The most studied system is that of electron-hydrogen scattering. Lack of knowledge of the complete asymptotic behavior of the scattered wave function has lead to different approaches, aimed at "avoiding" the true three-body asymptotic state, including exterior complex scaling [1] and other approaches. These approaches provide an accurate three-body scattered wave function in an "internal" region in coordinate space and the ionization amplitude is extracted by matching to ionization boundary conditions in the asymptotic region. However, the extraction process relies on approximate ionization boundary conditions. This yields an ionization amplitude with divergent phase as a function of matching radius although its magnitude converges. Despite the success of these approaches in providing accurate cross sections, formal theory of breakup with charged particles remains incomplete. Within the conventional theory there is no algorithm toward solution of the Schroedinger equation with correct boundary conditions above the breakup threshold. An asymptotic form of the scattered wave for electron-impact ionization of hydrogen obtained by Peterkop [2] is invalid when the two electrons are close to each other. For full-scale numerical calculations a representation of the wave function describing ionization in this region as well is necessary. We propose a new representation for the breakup amplitude

$$f(\vec{k}_\alpha, \vec{q}_\alpha) = \langle \Psi^{(-)}_{\vec{k}_\alpha,\vec{q}_\alpha} | \overleftarrow{H}_0 - \overrightarrow{H}_0 | \Phi^{(sc)(+)}_{\vec{k}_\alpha,\vec{q}_\alpha} \rangle,$$

Here $\Psi^{(-)}_{\vec{k}_\alpha,\vec{q}_\alpha}$ is the exact final-state 3-body scattering wave function, $\Phi^{(sc)(+)}_{\vec{k}_\alpha,\vec{q}_\alpha}$ is the three-body scattered wave function, $\vec{k}_\alpha,\vec{q}_\alpha$ are the Jacobian momenta describing the relative momentum of two particles and the relative momentum of the their c.m. and the third particle . This new representation can easily be transformed into an integral over an infinitely large surface, so that the result depends solely on the asymptotic behavior of the wave functions $\Psi^{(-)}_{\vec{k}_\alpha,\vec{q}_\alpha}$ and $\Phi^{(sc)(+)}_{\vec{k}_\alpha,\vec{q}_\alpha}$. The asymptotic form for $\Psi^{(-)}_{\vec{k}_\alpha,\vec{q}_\alpha}$ in all domains relevant for breakup has been obtained in [3]. Recently we derived an analytical expression for the asymptotic form of $\Phi^{(sc)(+)}_{\vec{k}_\alpha,\vec{q}_\alpha}$ valid in all the asymptotic domains. We demonstrate that new representation for the breakup/ionization amplitude is exact, free of divergence and suitable for numerical calculations.

References

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