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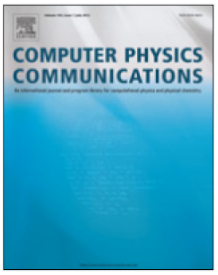

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Solving close-coupling equations in momentum space without singularities for charged targets

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Abstract

The analytical treatment of the Green's function in the convergent close-coupling method [Bray *et al.* Comp. Phys. Comm. **203** 147 (2016)] has been extended to charged targets. Furthermore, we show that this approach allows for calculation of cross sections at zero channel energy. For neutral targets this means the electron scattering length may be obtained from a single calculation with zero incident energy. For charged targets the non-zero excitation cross sections at thresholds can also be calculated by simply setting the incident energy to the exact threshold value. These features are demonstrated by considering electron scattering on H and He^+.

1. Introduction

There has been immense progress in the field of atomic and molecular scattering theory during the last two decades. Computational methods such as R-matrix with pseudostates [1–3], exterior complex scaling [4, 5], time-dependent close-coupling [6], and convergent close-coupling (CCC) [7, 8] all set out to fully solve the underlying Schrödinger equation without approximation. Collisions involving electron, positron, or photon scattering on few-electron atoms and ions can now be routinely calculated accurately at any energy of interest. The CCC approach has also been recently extended to molecular targets [9] and heavy projectiles like antiprotons and protons[10–14]. A review of the CCC approach to positron scattering has recently been given by Kadyrov and Bray [15].

Generally, further progress in the field comes from extending the capability to more complex collision systems. However, recently we found that a novel approach to the solution of the CCC equations yields greater utility when applied to ill-conditioned systems such as two-centre positron-atom scattering [16–18]. Starting with the electron-hydrogen S-wave model, it was shown that the Green's function in the CCC coupled Lippmann-Schwinger equations may be treated analytically, and thereby removing a somewhat problematic principal-value integral [19]. The full implementation [16] is applicable to electron or positron scattering on neutral targets. However, in the case of ionic targets there is considerable extra complexity due to the requirement for the inclusion of projectile bound states. Extension to ionic targets is useful in its own right, and is also a requirement for the application of the CCC method to photon scattering [20–24].

Another interesting consequence of the analytical approach is that the elimination of the singularity allows the application of the method at exact threshold energies. In the case of neutral targets this is useful when calculating the scattering length. For charged targets the excitation cross sections are non zero at threshold, and as we shall show, may also be directly calculated.

When considering electron scattering on charged targets the e-He^+ S-wave model, where only wavefunctions of zero orbital angular momentum are retained, is the ideal starting point [25, 26]. Having demonstrated the utility of the analytic treatment of the Green's function in the Lippmann-Schwinger equation of the S-wave model for the e-H system [19], we consider the full e-He^+ system here from the outset. Atomic units are used throughout unless specified otherwise.

2. Theory

The general ideas behind the analytic treatment of the Green's function in the Lippmann-Schinger equations have already been discussed earlier [16, 19]. Here we concentrate on the extra complexity associated with charged targets. In such cases the projectile asymptotic Hamiltonian contains the potential due to the asymptotic nuclear charge Z_a, leading to the projectile wave satisfying

$$\left(K + \frac{z_p Z_a}{r} - \varepsilon_k\right)|\boldsymbol{k}_p\rangle = 0, \tag{1}$$

where K is the projectile kinetic energy operator and $\boldsymbol{k}_p$ is projectile momentum. In the case of electron scattering we have $z_p = -1$, and for the He^+ target $Z_a = +1$. Consequently, the complete set in projectile space includes the countably infinite number of discrete states as well as the continuum. The resulting coupled Lippmann-Schwinger equations [27] take almost an identical form to the case of neutral targets except for the requirement to also include the bound states of the projectile of

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