Electron-helium scattering in the S-wave model using exterior complex scaling

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Electron-impact excitation and ionization of helium is studied in the S-wave model. The problem is treated in full dimensionality using a time-dependent formulation of the exterior complex scaling method that does not involve the solution of large linear systems of equations. We discuss the steps that must be taken to compute stable ionization amplitudes. We present total excitation, total ionization and single differential cross sections from the ground and $n = 2$ excited states and compare our results with those obtained by others using a frozen-core model.

I. INTRODUCTION

Since the early years of quantum mechanics and the development of scattering theory, an accurate description of the correlated motion of three unbound particles interacting via Coulomb forces has been a difficult problem to treat theoretically. Indeed, this problem was only reduced to computation in the last decade [1]. The difficulty stems from the long-range nature of the Coulomb potential which introduces a number of formal and practical complications. Although the formal theory of e-H ionization was developed in the 1960's by Peterkop [2] and by Rudge and Seaton [3, 4], it has not provided a practical path to computation. The asymptotic form of the wave function they derived is valid only in specific and limited geometries of the interacting particles and has proved to be too complicated to use as a boundary condition for solving the time-independent Schrödinger equation. Consequently, much of the work on electron-impact ionization has been carried out using perturbative, distorted-wave type methods or with close-coupling approaches that apply approximate two-body boundary conditions.

A practical path to accurate computation at low collision energies was only fully realized in the past few years. The key to overcoming the difficulties posed by the formal theory has been to formulate methods that do not rely on explicitly enforcing the boundary conditions for three-body Coulomb breakup. Several theoretical methods can be mentioned in this context. One such approach is the "time-dependent close-coupling" method developed by Pindzola, Schultz, Robicheaux and coworkers [5, 6]. In that approach, a wave packet is fired at the target atom and the time-dependent Schrödinger equation describing its dynamics is solved in a close-coupling formulation. Asymptotic boundary conditions are avoided since the time-dependent Schrödinger equation is solved as an initial value problem. Another successful method, which has been applied to the atomic double photoionization problem, is the hyperspherical R-matrix method with semi-classical outgoing waves [7]. In that approach, the time-independent Schrödinger equation is solved without detailed specification of three-body Coulomb boundary conditions by merging two different approaches: an R-matrix treatment of the entire system in the vicinity of the nucleus along with a semiclassical description of the evolution of the system in the asymptotic region. Exterior complex scaling (ECS) [8] avoids the explicit enforcement of boundary conditions entirely and has been successful in solving all aspects of the prototypical three-body Coulomb problem, electron-impact ionization of atomic hydrogen, to arbitrary accuracy [9, 10].

Most of the currently successful methods have been applied to study electron-impact ionization of multi-electron atoms by treating all but one active target electron in a frozen-core approximation, which reduces the problem to an effective three-body Coulomb system. The question we want to address here is whether the ECS method offers a practical approach to studying ionization of atoms with two *active* electrons. The method, as originally applied, involves solving large, sparse systems of linear equations. Extending this implementation, directly, to three electrons leads to linear systems that are extremely large and prohibitively expensive to solve. We have addressed that issue previously [11] by showing how the ECS method could be cast in a time-dependent formulation that scales more favorably with the number of electrons than the original time-independent formulation. The time-dependent ECS (TD-ECS) method was successfully applied to a problem involving four particles interacting via short range potentials.

Here we take the first steps toward applying ECS to the full electron-helium system. In this paper we extend the time-dependent ECS method to a system of four charged particles and consider the S-wave model of e^--He ionization. The S-wave model provides a distillation of the full, 9-dimensional, problem into a system involving just three radial coordinates. While the problem we consider here is a model, it has the complexity of a true four-body Coulomb problem - involving long-range forces and

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