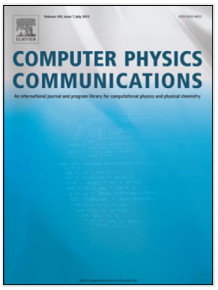
Accepted Manuscript



Reducing the dimensionality of grid based methods for electron-atom scattering calculations below ionization threshold

Jakub Benda, Karel Houfek

PII: S0010-4655(16)30365-4
DOI: http://dx.doi.org/10.1016/j.cpc.2016.12.001
Reference: COMPHY 6099

To appear in: *Computer Physics Communications*

Received date: 17 September 2016
Revised date: 29 November 2016
Accepted date: 3 December 2016

Please cite this article as: J. Benda, K. Houfek, Reducing the dimensionality of grid based methods for electron-atom scattering calculations below ionization threshold, *Computer Physics Communications* (2016), http://dx.doi.org/10.1016/j.cpc.2016.12.001

Reducing the dimensionality of grid based methods for electron-atom scattering calculations below ionization threshold

Jakub Benda, Karel Houfek

Institute of Theoretical Physics, Charles University in Prague, V Holešovičkách 2, Prague, Czech Republic

Abstract

For total energies below the ionization threshold it is possible to dramatically reduce the computational burden of the solution of the electron-atom scattering problem based on grid methods combined with the exterior complex scaling. As in the R-matrix method, the problem can be split into the inner and outer problem, where the outer problem considers only the energetically accessible asymptotic channels. The (N + 1)-electron inner problem is coupled to the one-electron outer problems for every channel, resulting in a matrix that scales only linearly with size of the outer grid.

Keywords: electron-hydrogen scattering, exterior complex scaling, B-splines

1. Introduction

The quantum collisions of electrons with atoms belong today among classical disciplines of the quantum physics. Throughout the decades several successful calculation methods emerged, which are able to simulate the collisions to a good accuracy. A few notable examples are the R-matrix method [1], the convergent close coupling [2, 3] and various formulations of direct discretization of the Schrödinger equation, like the finite element discrete variable representation with exterior complex scaling [4] and other grid based methods.

The exterior complex scaling (ECS) method has been popularized in quantum electron-atom scattering calculations by McCurdy and Rescigno [5] as a simple tool to replace outgoing-wave boundary conditions by Dirichlet boundary conditions when numerically solving the scattering Schrödinger equation discretized using the finite difference or finite element approach or using a B-spline basis. Bartlett [6] developed a modification for electron-hydrogen scattering (and other two-dimensional systems) – the "Propagating ECS" –, where the sparse two-dimensional problem is reformulated as a sequence of dense one-dimensional problems. Volkov et al [7] suggested further extension of ECS for scattering on charged ions employing the potential splitting approach. There is also a freely available implementation of the ECS method for electron-hydrogen scattering in the B-spline radial basis [8] based on the work of McCurdy and Martín [9].

While ECS has been particularly useful above the ionization threshold, where the proper boundary condition is complicated, the usage of ECS below the ionization threshold is possible, too, without any modification. However, close above the excitation thresholds it is necessary to account for the long-range dipole (and higher multipole) coupling, see [10], by extending the simulated domain to large radii: to thousands of atomic units, or even more. This can be to some degree circumvented by radial extrapolation of the calculated cross sections as suggested by Bartlett [11]. In dense environment the inter-particle Coulomb potentials are effectively damped and need not be considered to so large distances, see [12]. Generally, in an N-electron atom the scattering wave-function for a fixed angular state is $(N+1)$-dimensional, hence its size – and likewise the rank of the matrix of the system that is to be solved in a particular basis – rises with the domain size to the $(N+1)$-th power.

In further text a one-electron atom is assumed, as the main purpose of this extension is to speed up the implementation [8]. Is is, nevertheless, very straightforward to generalize the theory to many-electron atoms and other multidimensional scattering systems.

The discussion deals only with total energies below the ionization threshold. The reason for this is that the proposed method expands parts of the solution as a linear combination of energetically allowed bound states. This is not advantageous close to and above the ionization threshold, because the number of allowed channels considerably increases. But sufficiently below the ionization threshold there are only a handful of bound states and the new approach then allows more efficient application of the chosen grid based method. It is then possible to accurately simulate the scattering at low impact energies even on excited targets, where the above mentioned long-range effects are more pronounced.

In practical calculations the grid can always support only a finite number of bound states and just a discrete subset of the continuum states, so the *a priory* restriction on below-ionization energies due to an unbounded amount of states is more or less artificial. Instead of the eigenstates given by analytic expressions one could employ bound states and a discretization of the continuum obtained by some numerical approach, for example, using the Sturmian basis. This is a straightforward generalization of the present method, which allows its extension to above-ionization energies. For clarity, though, we restrict the further presentation only to the exact bound states and low energies.