PHYSICAL REVIEW A **67**, 060704(R) (2003)

Box-based convergent close-coupling method for solving Coulomb few-body problems

I. Bray,* K. Bartschat,† and A. T. Stelbovics
Centre for Atomic, Molecular, and Surface Physics, School of Mathematical and Physical Sciences, Murdoch University, Perth 6150, Australia

(Received 3 April 2003; published 30 June 2003)

We present an implementation of the convergent close-coupling (CCC) method, in which the Laguerre-based target states are replaced with box-based eigenstates. Discrete energies are obtained by taking the states that vanish at the box radius R_0, with convergence being established by simply varying R_0. Excellent agreement between box- and Laguerre-based CCC, exterior complex scaling, and renormalized experiment is obtained for one of the most difficult three-body Coulomb breakup problems, near-threshold electron-impact ionization of atomic hydrogen. The simplicity of the box-based CCC method is expected to lead to a greater understanding of the close-coupling formalism generally.

DOI: 10.1103/PhysRevA.67.060704 PACS number(s): 34.80.Dp

Electron-impact ionization of atomic hydrogen is one of the most fundamental three-body Coulomb breakup problems. It is therefore not surprising that substantial resources have been invested in its investigation, both experimentally [1,2] (and references therein) and theoretically. At the present time, the two most successful theoretical methods for predicting the (fully) triple-differential cross section (TDCS) in $(e,2e)$ experiments are the ''exterior complex scaling'' (ECS) [3,4] and the ''convergent close-coupling'' (CCC) [5] methods. This success was illustrated in a recent joint experimental and theoretical study at the incident electron energy of 17.6 eV, where the excellent agreement between experiment and the ECS and CCC theories was demonstrated [6]. In fact, confidence among theorists has lead to statements such as ''the simplest $(e,2e)$ problem has now been reduced to practical computation'' [7].

Indeed, the aspect of practical computation is an important one, particularly in light of the need for atomic collision data for many applications in the physics of stars, plasmas, lasers, and planetary atmospheres. Hence, once theorists may be confident in their ability to simulate the real world with sufficient accuracy for a given application, the issues of generality, simplicity, and efficiency start to play an increasingly important role.

The present paper deals with the latter aspects of the close-coupling (CC) formulation, arguably the most widely applied technique in collision physics. The CCC method, in which a large coupled-channel calculation is being setup by diagonalizing the target Hamiltonian in a Laguerre basis with a fixed scaling parameter λ, has been extremely successful for Coulomb few-body breakup problems [8]. As shown in several other calculations, related but very differently implemented CC methods, such as ''R matrix with pseudostates'' [9,10], ''intermediate-energy R matrix'' (IERM) [11,12], or time-dependent close coupling [13], should also be able to solve such problems. However, so far the latter methods have not yet demonstrated their ability to reproduce $(e,2e)$ experiments as fully as the ECS and CCC theories.

Until the formulation of the CCC method using the orthogonal Laguerre basis [14], progress of the standard CC formulation had stalled due to its apparent inability to include both an infinite number of physical discrete target states and, even more critically, a continuous spectrum of true continuum states in the coupled-channel expansion. Already before the formulation of the CCC approach, attempts to approximate the effect of the omitted part of the discrete target spectrum and to simulate some coupling to the continuum part had been made by using square-integrable pseudostates in the CC expansion, but only CCC with the Laguerre basis functions outlined a mathematically sound method for treating the continuum. There are, however, several properties of the Laguerre basis that make its use potentially cumbersome are listed below.

(1) The range of a given basis function depends on both the order N of the polynomial and the exponential scaling factor λ, and hence is not immediately obvious even if these parameters are given.

(2) The energy-level distribution of the pseudostates is compressed near the ionization threshold, thereby making it comparatively difficult to put a large number of pseudostates into the high-energy regime of open or adjacent closed channels. This may lead to technical difficulties when an interpolation procedure is used to obtain T-matrix elements at any given continuum energy.

In this paper, we propose a very simple alternative basis for dealing with the discrete and the continuum spectrum in the CC expansion. We obtain the expansion states by solving the Coulomb problem

$$\left[-\frac{1}{2}\frac{d}{dr^2}-\frac{l(l+1)}{2r^2}-\frac{Z}{r}\right]u_{nl}(r)=\epsilon_{nl}\,u_{nl}(r) \qquad (1)$$

in the box $0\leqslant r\leqslant R_0$, with the boundary conditions of

$$u_{nl}(0)=u_{nl}(R_0)=0. \qquad (2)$$

Unless specified otherwise, we use atomic units throughout. If the true discrete orbital $u_{nl}(r)$ fits well into the box (i.e., it

*Electronic address: I.Bray@murdoch.edu.au
†Permanent address: Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA.

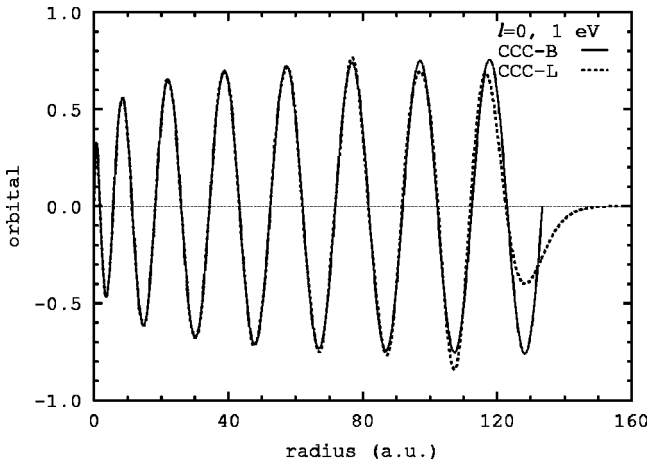

FIG. 1. The 1 eV $l=0$ orbitals that arise in the CCC-B method with $R_0=133.5$ a.u. and in the CCC-L method with $N=70$ and $\lambda=2.07$.

approaches zero in a practical sense for numerical calculations), then this orbital will become a very good approximation to the physical orbital. If it does not fit, however, the boundary condition $u_{nl}(R_0)=0$ will lead to a discretization of allowed energy levels ϵ_{nl}, some of which are still negative (i.e., simulate bound orbitals) while others become positive. The latter states are true Coulomb eigenstates, with the eigenvalues selected by the boundary condition. Increasing R_0 leads to a denser discretization of the continuum. In particular, the momenta $k_{nl}=\sqrt{2\epsilon_{nl}}$ increase approximately by π/R_0 for large energies.

This choice of basis is similar to that used by Greene and co-workers [15,16] in formulating the eigenchannel R matrix method with a large number of such ''closed'' orbitals in the R matrix expansion. However, these orbitals then had to be supplemented by a small number of ''open''orbitals (nonvanishing at $r=R_0$) to allow for a sufficiently flexible R matrix basis. A similar idea is used in the IERM method, but here some (in practice many) of the open continuum basis orbitals are also used to describe the target. To distinguish between the two implementations of the CCC method we refer to the box-based one as CCC-B and the original Laguerre-based one as CCC-L.

In Fig. 1, we present the 1 eV $l=0$ orbitals obtained by solving Eq. (1) with $R_0=133.5$, and diagonalizing the target Hamiltonian in the Laguerre basis [14] with $N=70$ and $\lambda=2.07$. Both orbitals have been normalized to range between $\pm\sqrt{2/\pi}$. We see considerable similarity of the two orbitals for $r<120$ a.u. The CCC-B orbital is a pure Coulomb orbital until the box radius R_0 is reached and is set to zero for $r>R_0$. The CCC-L orbital, on the other hand, falls off to zero gradually due to the exponential fall-off parameter λ of the Laguerre basis.

To rigorously test the new CCC-B formalism, we choose the computationally most difficult energy where detailed fully differential ionization cross-section measurements exist. This is the case for 15.6 eV e-H ionization with two 1 eV outgoing electrons. The experimental data were already well reproduced in CCC-L [17] and ECS calculations [4], provided the data were uniformly divided by two. The latter reduction is not of great concern because the experimental uncertainty is estimated as $\pm 35\%$ [1]. Also, the theoretical agreement with the absolute total ionization cross section (TICS) measurements, a flat singly differential cross section (SDCS), and agreement with the measured relative TDCS puts an upper limit on the overall TDCS normalization. This suggests that the experiment is too high by a factor of at least 2.

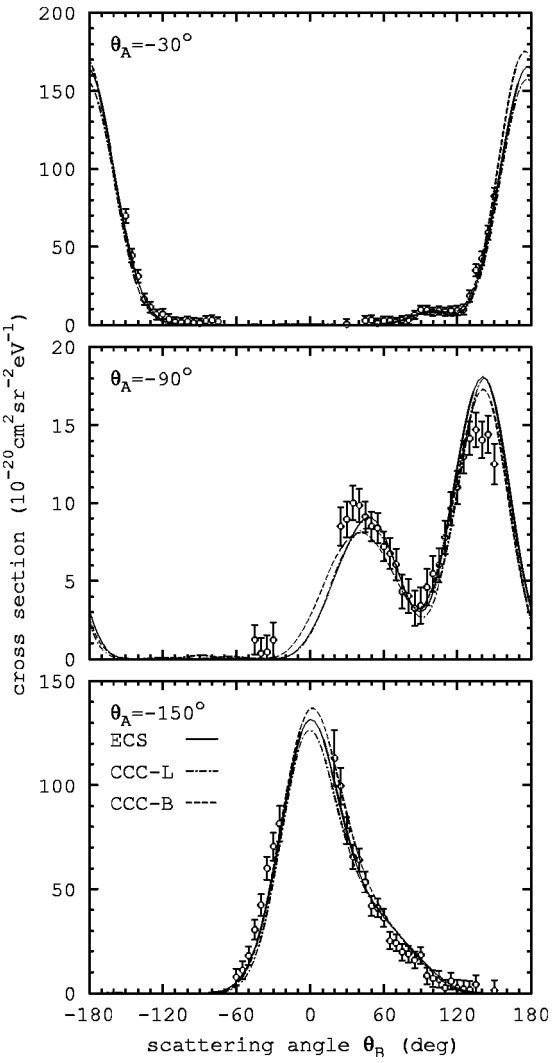

FIG. 2. The 15.6 eV e-H coplanar triply differential cross sections for two 1 eV outgoing electrons in the ''fixed-θ_A'' geometry. The present CCC-B and CCC-L predictions are compared with ECS results [4] and experimental data [1,2] divided by two (see text).

To perform CC calculations with both the box based and Laguerre bases, we took the maximum total and target orbital angular momenta to be $L_{\max}=7$ and $l_{\max}=5$, respectively. The number of states for each l were taken to be all of the open ones and the first two closed states. Setting $R_0=130$ in the CCC-B model, the total number of states and maximum number of channels were 114 and 386, respectively. Taking the Laguerre basis with $N_l=70-l$ and $\lambda=2$ in CCC-L, we obtained 119 states and a maximum of 403 channels. These choices ensured that no state had an energy numerically too

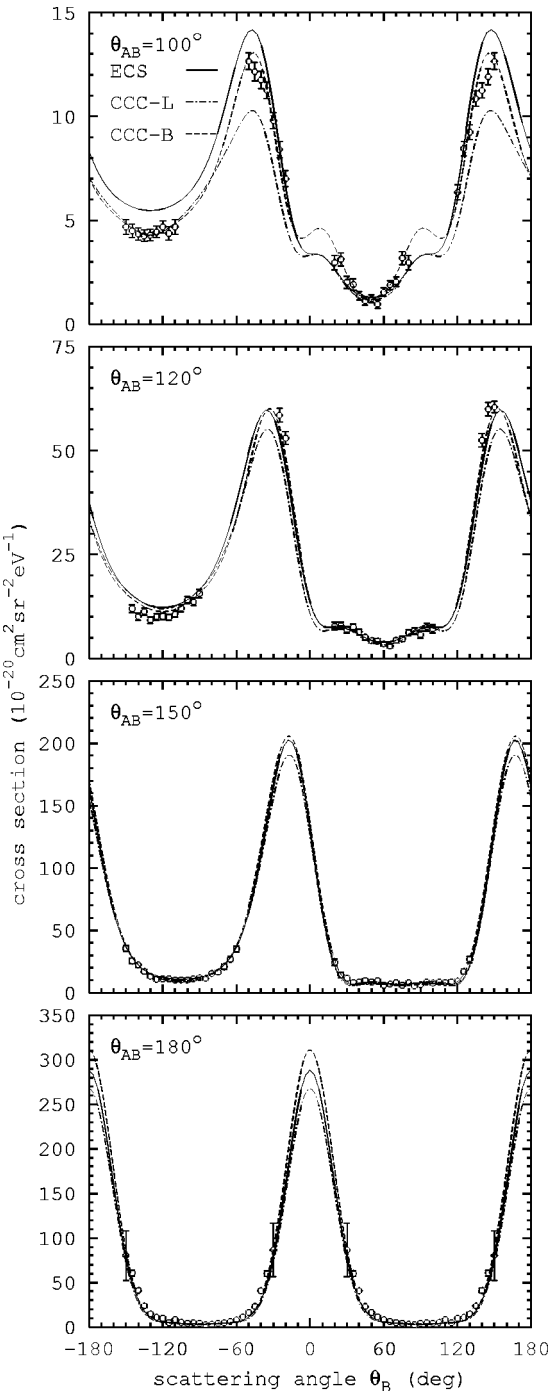

FIG. 3. As for Fig. 2, except for the ''fixed-θ_{AB}'' geometry.

close to the 2 eV total energy, with the orbitals being similar to those presented in Fig. 1.

The usual momentum-space techniques [14] were used to solve the CC equations, and the ionization amplitudes were defined directly from the *T*-matrix elements for excitation of the positive-energy states from the ground state [18]. These calculations required 8 Gb of random access memory. Our results for the TICS and the SDCS at 1 eV equal-energy sharing were 1.08×10^{-17} cm^2 and 1.09×10^{-17} cm^2 eV^{-1} in CCC-B, compared to 1.11×10^{-17} cm^2 and 1.00×10^{-17} cm^2 eV^{-1} in CCC-L. The TICS are in good agreement with the experimental result of $1.08\pm0.03\times10^{-17}$ cm^2 obtained by Shah, Elliot, and Gilbody [19], and the SDCS at 1 eV suggests a flat SDCS over the secondary energy range.

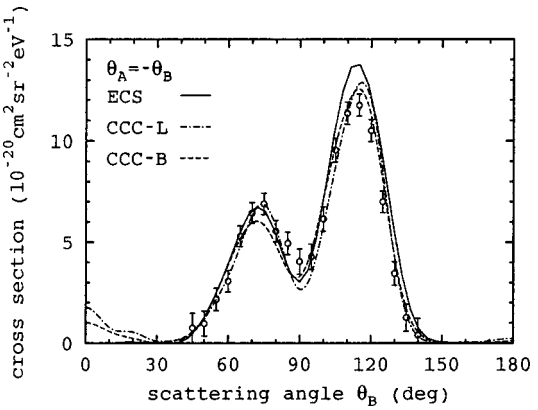

FIG. 4. As for Fig. 2, except for the ''doubly symmetric'' or ''$\theta_A=-\theta_B$'' geometry.

The 15.6-eV TDCS data [1,2] for the coplanar geometry can be thought of as a surface TDCS(θ_A,θ_B) with $-180°\leqslant\theta_{A,B}\leqslant180°$. For convenience, we use positive and negative angles to distinguish between detector positions on either side of the primary beam. The measurements take the form of slices in the TDCS(θ_A,θ_B) surface.

We begin the discussion with Fig. 2 where the TDCS for the so-called ''fixed-θ_A'' geometries are presented. The CCC-B, CCC-L, and ECS results are compared with the experimental data of Röder *et al.* [1,2], divided by two as discussed above. Excellent agreement is found between the three theories and the renormalized experimental data. This is also the case for the ''fixed-θ_{AB}'' and ''symmetric'' geometries exhibited in Figs. 3 and 4, respectively. In the fixed-θ_{AB} geometries the separation between the two detectors, $\theta_A-\theta_B$, is kept constant. These geometries show how rapidly the TDCS rise as the separation of the electrons increases. For the smallest TDCS in the $\theta_{AB}=100°$ geometry, the three calculations show the greatest variation, as might be expected. Agreement with experiment appears to be best for the CCC-B calculation, but given the experimental uncertainties and the smallness of the TDCS we do not consider this to be significant. The agreement between CCC-L and CCC-B indicates that the variation in the orbital tails has negligible effect on the collision data, i.e., the continuum orbitals extend sufficiently far in both methods for convergence.

The symmetric geometry, $\theta_A=-\theta_B$, shows some limitations of the CCC-B and CCC-L calculations. While the experimental data are well described by all three theories, only ECS correctly predicts a negligible cross section at the forward angles. The problem with both CCC-B and CCC-L is likely due to a combination of the following issues.

(1) The value of $l_{\max}=5$ may need to be increased, which would lead to a greater ability to handle long-range electron-electron correlations, but at the cost of a substantial increase in the computational resources required.

(2) To interpolate the complex ionization amplitudes,

which are available at discrete energies, to the experimental energy of 1 eV makes it difficult to obtain the required accuracy when the independent amplitudes have to combine coherently to yield near-zero cross sections.

To conclude, we have implemented a close-coupling technique that replaces the Laguerre-based pseudostates in the original CCC method with those obtained by solving the eigenstate problem in a box. Discretization of the continuum arises naturally by taking only those states that are exactly zero on the box boundary R_0. Apart from the usual angular-momentum considerations, the question of convergence has been reduced to just increasing R_0. The requirements of taking $N_l = N_0 - l$ and $\lambda_l = \lambda$ in CCC-L [5] are ''naturally'' implemented in the CCC-B method. As such, CCC-B is conceptually much simpler than CCC-L, and also explains why the original CCC method works so well. Recall from Fig. 1 that the presently used CCC-L and CCC-B orbitals are similar out to relatively large distances. We suspect that by taking a large Laguerre basis in the CCC-L calculations, we essentially ensured that a sufficiently good continuum representation was achieved, something that is much more straightforward in the CCC-B method.

We acknowledge the Merit Allocation Scheme on the National Facility of the Australian Partnership for Advanced Computing. This work was supported, in part, by the Australian Research Council and the United States National Science Foundation. K.B. would like to thank Murdoch University for the hospitality received during his visit sponsored by an international research exchange program.

[1] J. Röder, H. Ehrhardt, C. Pan, A.F. Starace, I. Bray, and D.V. Fursa, Phys. Rev. Lett. **79**, 1666 (1997).
[2] J. Röder, J. Rasch, K. Jung, C.T. Whelan, H. Ehrhardt, R.J. Allan, and H.R.J. Walters, Phys. Rev. A **53**, 225 (1996).
[3] T.N. Rescigno, M. Baertschy, W.A. Isaacs, and C.W. McCurdy, Science **286**, 2474 (1999).
[4] M. Baertschy, T.N. Rescigno, and C.W. McCurdy, Phys. Rev. A **64**, 022709 (2001).
[5] I. Bray, Phys. Rev. Lett. **89**, 273201 (2002).
[6] J. Röder, M. Baertschy, and I. Bray, Phys. Rev. A **67**, 010702 (2003).
[7] C.W. McCurdy, M. Baertschy, W.A. Isaacs, and T.N. Rescigno, in *Photonic, Electronic and Atomic Collisions*, edited by J. Burgdörfer, J.S. Cohen, S. Datz, and C.R. Vane (Rinton Press, Princeton, 2002), Vol. 500, pp. 38–49.
[8] I. Bray, D.V. Fursa, A.S. Kheifets, and A.T. Stelbovics, J. Phys. B **35**, R117 (2002).
[9] K. Bartschat, E.T. Hudson, M.P. Scott, P.G. Burke, and V.M. Burke, J. Phys. B **29**, 115 (1996).
[10] K. Bartschat and I. Bray, J. Phys. B **29**, L577 (1996).
[11] P.G. Burke, C.J. Noble, and M.P. Scott, Proc. R. Soc. London, Ser. A **410**, 289 (1987).
[12] M.P. Scott, T. Stitt, N.S. Scott, and P.G. Burke, J. Phys. B **35**, L323 (2002).
[13] M.S. Pindzola and D.R. Schultz, Phys. Rev. A **53**, 1525 (1996).
[14] I. Bray and A.T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[15] C.H. Greene and L. Kim, Phys. Rev. A **36**, 2706 (1987).
[16] M. Aymar, C.H. Greene, and E. Luc-Koenig, Rev. Mod. Phys. **68**, 1015 (1996).
[17] I. Bray, J. Phys. B **32**, L119 (1999).
[18] I. Bray and D.V. Fursa, Phys. Rev. A **54**, 2991 (1996).
[19] M.B. Shah, D.S. Elliot, and H.B. Gilbody, J. Phys. B **20**, 3501 (1987).