Explicit Demonstration of the Convergence of the Close-Coupling Method for a Coulomb Three-Body Problem

Igor Bray[a]
Electronic Structure of Materials Centre, School of Physical Sciences, The Flinders University of South Australia, G.P.O. Box 2100, Adelaide 5001, Australia

Andris T. Stelbovics[b]
Centre for Atomic, Molecular and Surface Physics, School of Mathematical and Physical Sciences, Murdoch University, Perth 6150, Australia

(Received 24 February 1992)

Convergence as a function of the number of states is studied and demonstrated for the Poet-Temkin model of electron-hydrogen scattering. In this Coulomb three-body problem only the $l = 0$ partial waves are treated. By taking as many as thirty target states, obtained by diagonalizing the target Hamiltonian in a Laguerre basis, complete agreement with the smooth results of Poet is obtained at all energies. We show that the often-encountered pseudoresonance features in the cross sections are simply an indication of an inadequate target state representation.

PACS numbers: 34.80.Bm, 34.80.Dp, 34.80.Nz

The close-coupling equations [1] have formed the framework for detailed modeling of electron-atom collisions since the late 1950s. An approach based on the Faddeev formalism has also been applied to such systems of few interacting particles with Coulomb potentials [2], but this has not proved as successful as the former approach. The close-coupling equations are derived by making an expansion over the complete set of target states including the continuum. Typically, neglecting the contribution of the continuum states leads to an overestimation of the cross sections above the ionization threshold. Burke and Webb [3] used a basis of L^2 Slater functions to diagonalize the hydrogen-atom target. The positive energy states (pseudostates), when included in the close-coupling formalism, gave improved cross sections. A further study of the approximation of the continuum by L^2 states was reported by Burke and Mitchell [4] for a model electron-hydrogen problem, first analyzed in detail by Temkin [5] and Kyle and Temkin [6], in which only $l = 0$ target states were used and the $L = 0$ partial wave amplitude was studied as a function of energy. While this is a simplification of the full Coulomb three-body problem, it still contains the essential difficulties associated with it, namely, the Coulomb continuum. For singlet scattering the pseudostate expansions were accompanied by resonance features above the ionization threshold which persisted for the largest basis used. Away from the resonance features the amplitudes for the different bases appeared to converge. The pseudoresonances varied in number and energy with different bases.

A J-matrix calculation was carried out for the same model problem by Heller and Yamani [7]. In the J-matrix method one similarly makes use of L^2 expansions of the target and they also observed unphysical resonance features. Their expansions included up to ten basis states for the hydrogen-atom target. An interesting aspect of the J-matrix method is that it leads to a physical interpretation of the nature of the L^2 discretization of the continuum. Yamani and Reinhardt [8] showed for the hydrogen atom that an expansion of the target in a basis of Laguerre functions could be given in a form where the coefficients were obtainable analytically. The coefficients are essentially Pollazeck polynomials. The energy of the pseudostates can be readily identified with the zeros of the polynomials of order N for a set of N Laguerre functions. The pseudostates apart from an overall normalization factor can be shown to converge conditionally to the continuum Coulomb functions [9].

Further investigations of the convergence of the pseudostate method were carried out by Oza and Callaway [10] and Oza [11]. Their largest calculations ($N \leq 9$) still contained pseudoresonance features although it was noted [11] that their effect was diminishing with increase in basis. An important advance to the theory of electron-hydrogen scattering for this model was made by Poet [12]. He noted that the Schrödinger equation was of a separable form enabling the general solutions of the differential equation to be found analytically. The matching to obtain the physical solutions required numerical solution of an integral equation, which was done to a high accuracy. The cross sections he obtained in the region where close coupling suffered from pseudoresonances were very smooth. Where the close-coupling results were convergent, i.e., away from the resonance regions, they were in good agreement with Poet. Callaway and Oza [13] extended Poet's methods to calculate the total and ionization cross sections and compared the results with their pseudostate calculations which were averaged over the pseudoresonances. Bransden, Hewitt, and Plummer [14] applied the Schwinger variational method to this

model with the wave function expanded in a basis of pseudostates. This approach also suffered from pseudoresonance behavior which was difficult to remove.

The above pseudostate investigations still leave open the question of whether the pseudoresonances can be completely eliminated directly, without having to resort to averaging techniques such as in [10] or [14]. In this Letter we employ a Laguerre basis to generate target expansions of up to thirty states and solve the close-coupling equations using the momentum space approach of McCarthy and Stelbovics [15]. The results we present show that convergence to the model results is obtained over the whole energy range treated by Poet [12]. We extend the scale of his calculation and give results for higher level inelastic and ionization scattering from 0 to 400 eV incident electron energy. In such an application a Laguerre basis is ideal because with an appropriate choice the functions are orthogonal and hence large basis diagonalizations pose no numerical difficulties (N up to 100 has been achieved). Moreover, the convergence can be studied systematically by simply increasing the basis size N. A very important feature of the Laguerre basis is that the lower-energy states rapidly converge to the exact hydrogen eigenstates as N is increased. The Laguerre basis $\xi_{kl}(r)$ we choose has the form

$$\xi_{kl}(r) = \left(\frac{\lambda(k-1)!}{(2l+1+k)!}\right)^{1/2} (\lambda r)^{l+1} \times \exp(-\lambda r/2) L_{k-1}^{2l+2}(\lambda r), \quad (1)$$

where the $L_{k-1}^{2l+2}(\lambda r)$ are the associated Laguerre polynomials, l is set to zero for this model, and k ranges from 1 to the basis size N. The constant λ is arbitrary and is chosen so that the lowest-energy states are essentially the exact hydrogen eigenstates. By taking $\lambda = 2$ or $\lambda = 1$ the exact $1s$ or $2s$ state, respectively, is obtained from the diagonalization for $N \geq 1$. The rate of convergence to the higher exact hydrogen bound states for $\lambda = 2$ as a function of N has been given by Bray, Konovalov, and McCarthy [16]. A preliminary study of the close-coupling expansion and its convergence properties for $N \leq 10$ were given by Winata and Stelbovics [17].

We solve the close-coupling equations using the Lippmann-Schwinger equation for the T matrix elements

$$\langle k_n n|T^S|n_0 k_0\rangle = \langle k_n n|V^S|n_0 k_0\rangle + \sum_{n'}^{N} \int_0^\infty dk' k'^2 \frac{\langle k_n n|V^S|n' k'\rangle \langle k' n'|T^S|n_0 k_0\rangle}{E - \epsilon_{n'} - k'^2/2 + i0}, \quad (2)$$

where S denotes total spin, and $E = \epsilon_0 + k_0^2/2 = \epsilon_n + k_n^2/2$ is the on-shell energy. Note that all orbital angular momenta are set to zero, and have been omitted from the notation. Denoting the total Hamiltonian by H, and the space-exchange operator by P_r, the potential matrix elements in (2) are [15]

$$\langle k_n n|V^S|n' k'\rangle = \langle k_n n|v_1 + v_{12} + (-1)^S (H - E) P_r|n' k'\rangle, \quad (3)$$

where v_1 and v_{12} are the electron-proton and electron-electron potentials, respectively. The space-exchange operator arises by demanding that the singlet-triplet coordinate-space wave functions have the symmetry required on application of the Pauli principle. The target states $|n'\rangle$ are obtained by diagonalizing the atomic hydrogen Hamiltonian in the Laguerre basis. The basis size N must be sufficiently large that the states $|n\rangle$ and $|n_0\rangle$ in (2) come out from the diagonalization to be essentially the exact hydrogen eigenstates for the transition of interest. The incident projectile is denoted by $|k_0\rangle$ and the initial target state is $|n_0\rangle$, which we take to be the ground state of hydrogen. The method of solution of (2) is given by McCarthy and Stelbovics [15]. The corresponding cross section σ_n^S in units of πa_0^2 is given by

$$\sigma_n^S = \pi^2 (k_n/k_0) |\langle k_n n|T^S|n_0 k_0\rangle|^2. \quad (4)$$

In Fig. 1 we present the singlet cross sections σ_n^0 for a number of transitions and compare them with the exact results of Poet [12,18]. The projectile energy ranges from 1 to 400 eV, with approximately 100 energy steps chosen to represent the essential structures. The calculations were done over a large range of N from 5 to 30. The results are shown for three sets of target states $N = 5$ and $N = 10$ calculated with $\lambda = 1$, and $N = 30$ calculated with $\lambda = 2$. Quantitative results may be obtained upon request.

We chose $\lambda = 1$ for the smaller sets as then on diagonalization the $2s$ state is exact while the $1s$ and $3s$ are quite good, whereas if we had $\lambda = 2$ then the $1s$ state would be exact, but the $3s$ state would be quite bad. For the $N = 30$ runs we can take either value of λ. We took $\lambda = 2$ to show that the convergent answers are independent of λ.

We see that the characteristic pseudoresonance behavior is evident for the smaller sets. However, the thirty-state runs do not exhibit this phenomenon and are in complete agreement with Poet, indicating that pseudoresonances can be simply thought of as a lack of convergence with N. A very narrow genuine resonance in the $2s$ cross section around 10 eV is well reproduced by the thirty-state runs. The ionization cross section is calculated by adding the cross sections of the positive energy target states. It is the most difficult to get convergent. Even with thirty states some minor oscillations are visible at the intermediate energies.

In Fig. 2 the corresponding triplet results σ_n^1 are given.

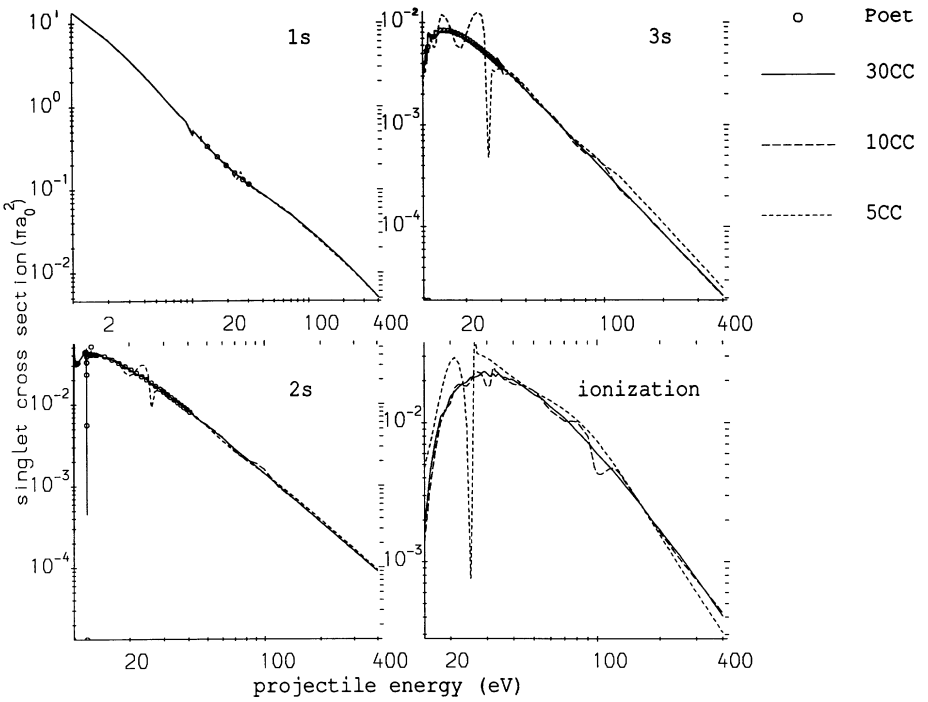

FIG. 1. Singlet cross sections of the simplified model of electron-hydrogen scattering that treats only states with zero orbital angular momentum. The exact results, denoted by open circles, are due to Poet [12, 18]. The curves denote close-coupling calculations with thirty (solid line), ten (long-dashed line), and five (short-dashed line) L^2 states generated using the Laguerre basis.

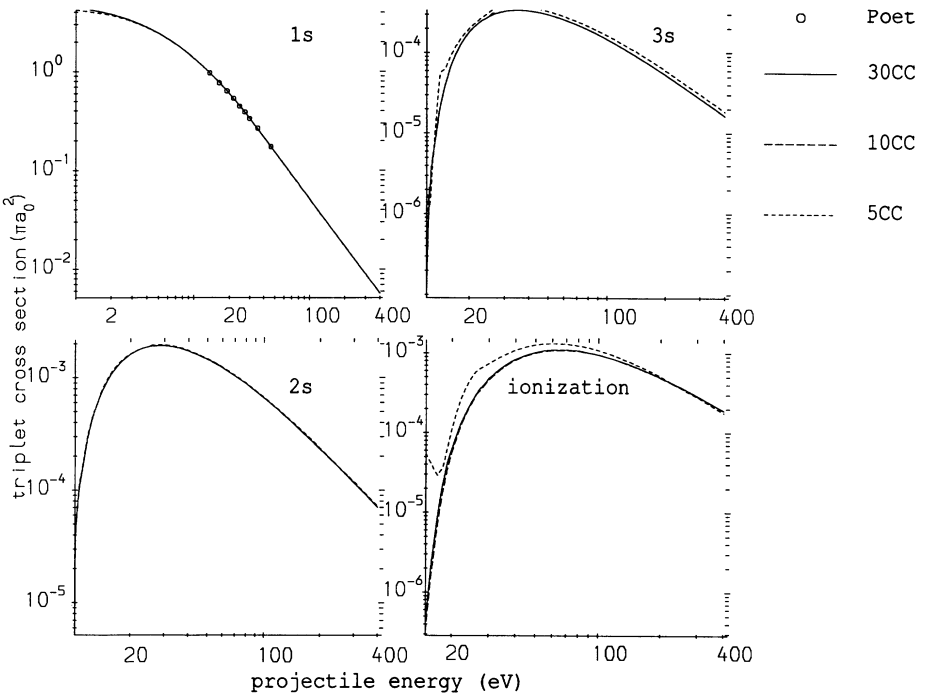

FIG. 2. Triplet cross sections of the simplified model of electron-hydrogen scattering that treats only states with zero orbital angular momentum. The exact results, denoted by open circles, are due to Poet [12]. The curves denote close-coupling calculations with thirty (solid line), ten (long-dashed line), and five (short-dashed line) L^2 states generated using the Laguerre basis.

We see that there is no pseudoresonance structure here, and for most of the transitions $N = 5$ is sufficient. The reason that the $3s$ transition is a little higher for the $N = 5$ set is that with only five states in the Laguerre basis it is not possible to get simultaneously the exact $1s$, $2s$, and $3s$ hydrogen wave functions to a high precision, for any λ.

The major conclusion that we draw from this work is that close-coupling equations can be made to yield convergent results at all energies for a Coulomb three-body problem. The basis size required is at least a factor of 2 larger than employed in previous applications. Convergence is independent of the value of λ, though the convergence rate probably does depend on λ. The rate of convergence depends on the transition, e.g., convergence for the elastic channel is much faster than for the ionization channel, and it is more difficult to get convergent singlet channels than triplet channels, at least in this model. Last, the convergence rates critically depend on the energy of the incident projectile. While at energies a little above the ionization threshold as many as thirty states may be necessary, at the higher energies as few as five states are often sufficient. Further studies of the full electron-hydrogen scattering system, by allowing arbitrary partial waves for both the target and projectile, indicate that the conclusions regarding convergence are carried over to the general case.

We would like to thank Professor Ian McCarthy for some useful discussions, and to acknowledge support from the Australian Research Council.

[a] Electronic address: igor@esm.cc.flinders.edu.au.
[b] Electronic address: stelbovi@atsibm.csu.murdoch.edu.au.

[1] I. C. Percival and M. J. Seaton, Proc. Camb. Philos. Soc. **53**, 654 (1957).
[2] H. Bürger, W. Sandhas, and E. O. Alt, Phys. Rev. A **30**, 2965 (1984).
[3] P. G. Burke and T. G. Webb, J. Phys. B **3**, L131 (1970).
[4] P. G. Burke and J. F. Mitchell, J. Phys. B **6**, 320 (1973).
[5] A. Temkin, Phys. Rev. **126**, 130 (1962).
[6] H. L. Kyle and A. Temkin, Phys. Rev. **134**, A600 (1964).
[7] E. J. Heller and H. A. Yamani, Phys. Rev. A **9**, 1209 (1974).
[8] H. A. Yamani and W. P. Reinhardt, Phys. Rev. A **11**, 1144 (1975).
[9] A. T. Stelbovics and T. Winata, Aust. J. Phys. **43**, 485 (1990).
[10] D. H. Oza and J. Callaway, Phys. Rev. A **27**, 2840 (1983).
[11] D. H. Oza, Phys. Rev. A **30**, 1101 (1984).
[12] R. Poet, J. Phys. B **11**, 3081 (1978).
[13] J. Callaway and D. H. Oza, Phys. Rev. A **29**, 2416 (1984).
[14] B. H. Bransden, R. Hewitt, and M. Plummer, J. Phys. B **21**, 2645 (1988).
[15] I. E. McCarthy and A. T. Stelbovics, Phys. Rev. A **28**, 2693 (1983).
[16] I. Bray, D. A. Konovalov, and I. E. McCarthy, Phys. Rev. A **43**, 1301 (1991).
[17] T. Winata and A. T. Stelbovics, in *Proceedings of the Sixth International Symposium on Correlations and Polarization in Electronic and Atomic Collisions and (e,2e) Reactions*, edited by P. Teubner and E. Weigold (Flinders University, S. Australia, 1991).
[18] R. Poet, J. Phys. B **13**, 2995 (1980).