S-wave model for electron-hydrogen scattering

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The R matrix with pseudostates and convergent close-coupling methods are applied to the calculation of elastic, excitation, and total as well as single-differential ionization cross sections for the simplified S-wave model of electron-hydrogen scattering. Excellent agreement is obtained for the total-cross-section results obtained at electron energies between 0 and 100 eV. The two calculations also agree on the single-differential ionization cross section at 54.4 eV for the triplet spin channel, while discrepancies are evident in the singlet channel, which shows remarkable structure. [S1050-2947(96)50208-8]

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The simplified S-wave model of electron scattering from hydrogen atoms, introduced by Temkin [1], has received much attention during recent years. For elastic scattering and excitation, accurate solutions have been given by Poet [2–4]. Furthermore, results for the total ionization cross section in the singlet spin channel were derived by Callaway and Oza [5].

Although the ionization results are not exact, they have been used as a standard for comparison with predictions from other methods. Such methods include the intermediate energy R-matrix method [6], a two-dimensional R-matrix propagator [7], the convergent close-coupling (CCC) approach [8], hyperspherical close coupling [9], the J-matrix method [10], and the eigenchannel R-matrix method [11]. Since the applicability of these methods is not restricted to the solution of the Temkin-Poet (TP) model for electron-hydrogen scattering, a successful reproduction of the known results for this model should provide confidence in applying the techniques to more complex and realistic problems. This is particularly true for the description of the two-electron continuum—a long-standing problem in electron-atom collision theory.

We have used the recently developed R matrix with pseudostates (RMPS) method [12] to investigate its applicability to the TP model. This is particularly important, since the RMPS method has been implemented in the general R-matrix codes of the Belfast group that are designed to handle complex many-electron targets. If this method is able to describe ionization accurately, such calculations become immediately possible for a large variety of targets.

Since details of the method have been described elsewhere [12], we only summarize the most important details for the present study. We are interested in transitions involving discrete levels up to $n=3$, and thus the analytically known $1s$, $2s$, and $3s$ orbitals were included in the R-matrix expansion. In addition, pseudo-orbitals $n\ell$ were constructed to represent the target continuum by taking the minimum linear combination of Sturmian-type orbitals $r^i e^{-\alpha r}$ orthogonal to the above-mentioned orbitals. The pseudostates were then obtained through diagonalization of the target Hamiltonian.

An important aspect in the present work concerns the range parameter α. Although it is, in principle, arbitrary, the convergence of the results for specific transitions depends on its choice. We performed several RMPS calculations and varied α while keeping a fixed basis size. In the CCC calculations a fixed α is taken, but the basis size is increased until convergence is obtained. Both approaches correspond to a varying effective size of the box into which all states have to be squeezed. Consequently, they result in a variation of the pseudothresholds for consecutive calculations.

As shown by Meyer, Greene, and Bray [11], R-matrix calculations with box sizes determined by the range of the physical target states of interest can be expected to exhibit pseudoresonance structure. It is essentially impossible to eliminate these resonances by simply increasing the number of pseudo-orbitals with the same value of α (as is done in the CCC method), since such an increase would enlarge the R-matrix box significantly. To preserve the strengths of R-matrix approaches, other methods, like box averaging, frame transformations, or energy convolution have to be designed. (For a detailed discussion, see Ref. [11].) Although an energy convolution over pseudoresonances could be used for the TP model without losing potentially important information about true resonances in the two-electron continuum, the results presented here were obtained entirely through box averaging via a range of α values. In order to keep some correlation between the two electrons when both have positive energies, we chose an R-matrix radius of $60a_0$ and α values between 0.52 and 0.78. This range of α ensured that in all cases the first eight states fit into the box, with one pseudostate being bound and four lying in the continuum. For this rather large box size, 72 continuum orbitals had to be included in the R-matrix expansion to obtain converged results for collision energies up to 100 eV. Note that these continuum orbitals must be Schmidt orthogonalized to all pseudo-orbitals in the calculation. This causes numerical problems that have been addressed in Ref. [12]; without the revised algorithm, the present calculation would have been numerically intractable.

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The convergent close-coupling approach solves the coupled momentum-space Lippmann-Schwinger equations derived from the full three-body Schrödinger equation. A Laguerre basis set is chosen to diagonalize the target Hamiltonian. This choice of basis functions eliminates numerical problems associated with convergence and linear dependence. The basis set size is systematically increased until the observable of interest converges. Most importantly for the present study, accurate CCC cross sections for elastic scattering, excitation of the $2s$ and $3s$ states, and ionization in both the singlet and triplet total spin channels have been tabulated for the TP model in the energy range from 1 to 400 eV incident energy [13]. Further details of the CCC method, including its application to realistic quasi-one- and -two-electron targets can be found in Refs. [14] and [15].

In Figs. 1 and 2, we present total-cross-section results for elastic scattering, excitation of the $2s$ and $3s$ levels, and ionization as a function of the incident electron energy. The RMPS curves were obtained from 27 calculations with $\alpha=0.52,0.53,\ldots,0.78$, which were averaged by ordering the results according to size and assigning a weighting factor to the individual terms. Tests with several weighting schemes (where the center is given at least as much weight as the edges) showed that the results are essentially independent of the details of the averaging procedure. The CCC results [13] are from a 30-state calculation. In both methods the ionization cross sections are obtained by simply summing the cross sections for the positive-energy pseudostates. In the RMPS method, due to the small number of states, a contribution to the ionization from the bound $4\bar{s}$ pseudostate is estimated to be $\sigma_{4\bar{s}}\simeq 1.08\sigma_{3s}$, when positive [5]. Tests without this correction term showed that it is essentially responsible for the difference between the present results and those of the eigenchannel approach [11], which used a frame transformation of the scattering matrix.

The agreement between the RMPS and the CCC results is excellent over the whole energy range of interest, both for the singlet discrete transitions (see Fig. 1) and for ionization in both spin channels (see Fig. 2). The results for the triplet discrete channels (not shown) converge very fast with the number of states included in the close-coupling expansion and are also in excellent agreement. The problem with pseudoresonances is almost entirely confined to the singlet spin channel and becomes most pronounced in the results for the $1s$-$3s$ excitation. This is illustrated by the curves labeled ''0.65'' which represent the RMPS results obtained with $\alpha=0.65$. Clearly, performing a series of calculations with variable α is an effective, though somewhat expensive, way of dealing with pseudoresonances. It should be pointed out, however, that neither 27 eight-state RMPS calculations nor a CCC calculation with 30 S states is expected to be necessary to obtain accurate results for a realistic scattering problem where several partial waves interfere with each other.

Having checked the results of the RMPS and CCC methods against each other, we now extend our treatment of the TP model to the calculation of single-differential ionization cross sections $d\sigma/dq$. Ways to extract this parameter in a close-coupling formalism have been discussed by Konovalov, Bray, and McCarthy [16], and by Bray and Fursa [17].

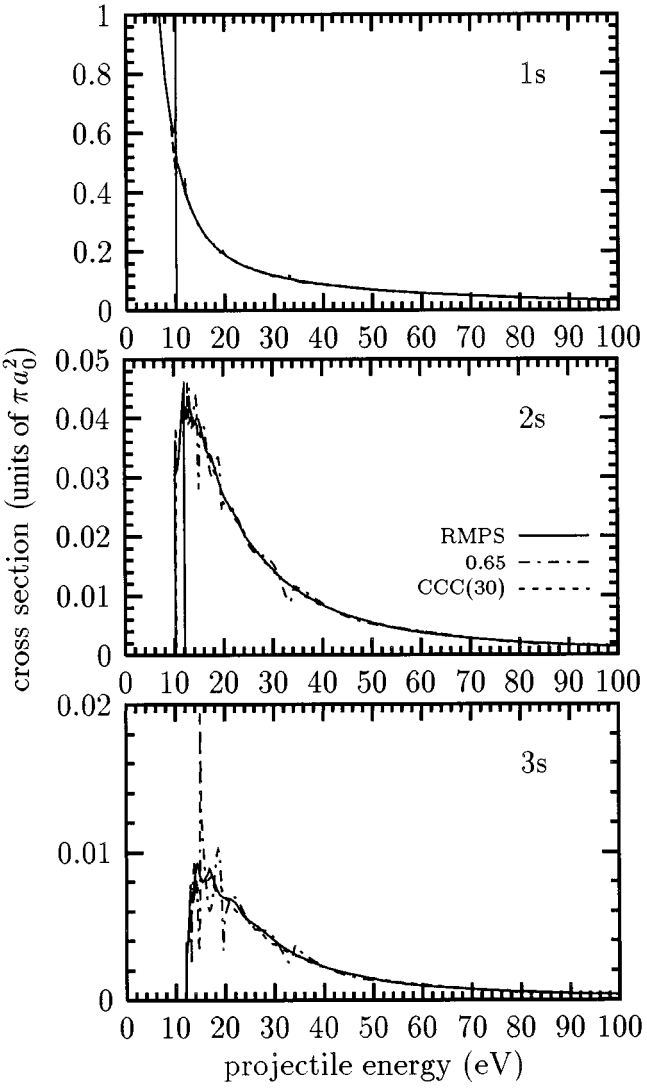

FIG. 1. Singlet total cross section for elastic scattering and excitation of the $2s$ and $3s$ levels for the Temkin-Poet model of e-H scattering as a function of the incident electron energy. The curve labeled ''0.65'' corresponds to the RMPS calculation with $\alpha=0.65$. The CCC(30) results are from Ref. [13].

Both techniques should be equivalent, with the former one being simpler to implement and used here by the RMPS method, while the latter was used by the CCC method. The general idea is based on the fact that we obtain the total ionization cross section as the sum of the excitation cross sections for the pseudostates with positive energy. Hence it is possible to obtain an estimate for the single-differential cross section for energies ($\epsilon_{n\bar{s}}>0$) of the ''ejected'' electron (described by square-integrable functions) that correspond to the excitation thresholds for the pseudostates. One can expect that these estimates will improve with the number of pseudothresholds that lie, for a fixed total energy E, in the region $0<\epsilon_{n\bar{s}}<E$. The total ionization cross section must be equal to the integral (dq, $0<q<\sqrt{2E}$) over $d\sigma/dq$.

In Fig. 3, we show results for the differential ionization cross section $d\sigma/dq$ for the TP model at an incident electron energy of 54.4 eV, corresponding to a total (projectile plus

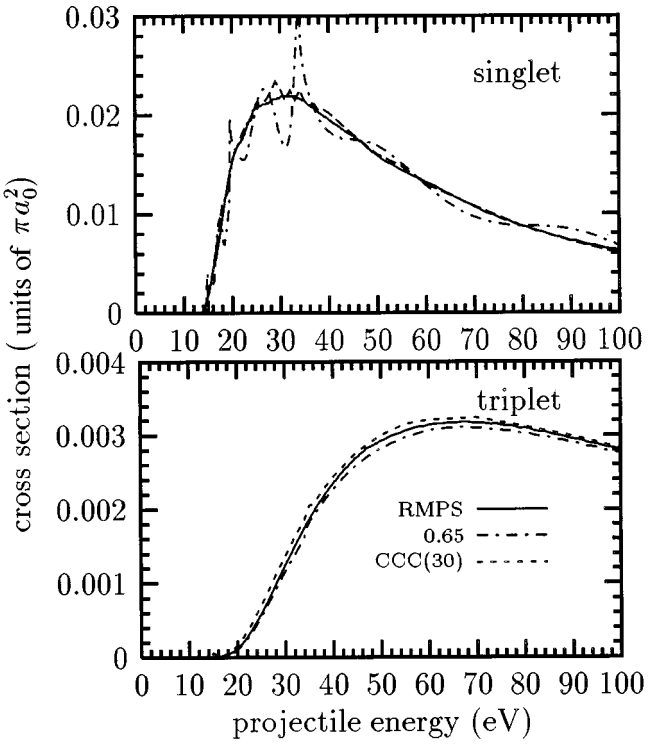

FIG. 2. Same as Fig. 1 for the ionization cross sections in the singlet and triplet spin channels.

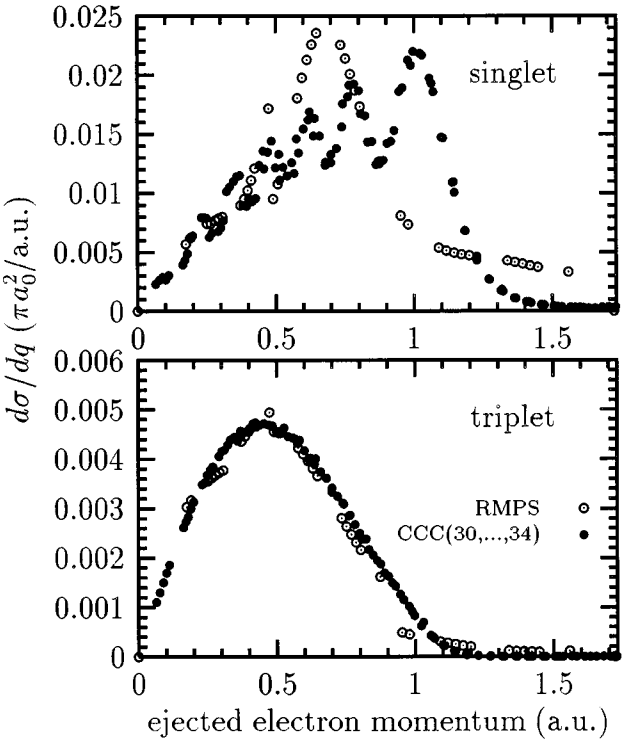

FIG. 3. Single-differential ionization cross section $d\sigma/dq$ for the Temkin-Poet model of e-H scattering as a function of the ''ejected'' electron momentum at an incident electron energy of 54.4 eV. See text for details.

target) energy of $E=1.5$ a.u.; ϵ and q are the energy and linear momentum of the ejected electron, respectively. The RMPS results correspond to the estimates obtained by using the results for excitation of three open pseudostates in the 13 calculations whose sums were closest to the final result for the total ionization cross section. Furthermore, the final curves were renormalized to ensure the reproduction of the total ionization cross section after numerical integration. The CCC results were obtained by performing 30- to 34-state calculations and are presented together to indicate the surprising structure of the cross section and the very slow rate of convergence with increasing basis size in the singlet channel. These states were obtained by diagonalizing the target Hamiltonian with $\lambda=2\alpha=2.5$ and basis sizes $N=45,\ldots,49$. All open and just a few closed channels were included in the calculations. Even though there is some discrepancy between the CCC and RMPS results for this channel, the integrals (dq) are much the same (cf. Fig. 2). This is another example of the strength of a unitary formalism. Convergence in the elastic T-matrix element implies convergence in both the elastic and the total cross section (optical theorem). Convergence in the nonbreakup cross section then implies convergence in the total ionization cross section without the requirement of convergence in the individual contributions to this channel [18].

The results for the triplet spin channel exhibit a much better convergence pattern. For this case, convergence with basis size is very rapid and hence the CCC and RMPS results are in very good agreement. Note the fact that the triplet single-differential cross section essentially vanishes at $q=\sqrt{E}\approx 1.2$ a.u., the point that corresponds to both of the outgoing electrons having the same energy. In fact, by performing a series of CCC(N) calculations we found that the cross section at this point diminishes further with increasing N. In an exact treatment of this problem with true continuum states, a final triplet state with two electrons having zero orbital angular momentum and the same energy is Pauli forbidden. Consequently, our results indicate that, at least in the case of scattering from the ground state, the Pauli principle for the two-electron continuum is accurately implemented using just a few states in the multichannel expansion, despite the different treatment of the two electrons.

This asymmetric treatment of the two outgoing electrons, one by a plane wave and the other one by a pseudostate, is the reason for the lack of symmetry about $E/2$ of the raw CCC results for the single-differential cross section $d\sigma/d\epsilon=1/q(d\sigma/dq)$ for the e-He system at 100 eV [17]. Here, in a much simplified model, this is also the case in both the singlet and triplet channels. Thus the TP model, too, suggests that the unitary close-coupling formalism treats the two electrons as distinguishable. For this reason, Bray and Fursa [17] suggested that the close-coupling single-differential ionization cross section to be compared with experiment is $d\sigma/d\epsilon(\epsilon)+d\sigma/d\epsilon(E-\epsilon)$.

In conclusion, we have demonstrated that the RMPS method can yield reliable total-cross-section results for elastic scattering, excitation, and ionization for the Temkin-Poet model. The advantages of the R-matrix method as an efficient way to obtain results for a large number of collision energies can be preserved by averaging the outcome of several rather small calculations. In addition, we have given the results in this model for the raw single-differential ionization cross sections at a single energy of 54.4 eV, which we hope will stimulate debate and calculations with the many other

techniques that have already been applied to this model. There is no doubt that the TP model has been of great benefit in testing general electron-impact scattering theories when applied to discrete transitions. We believe it to also be an ideal testing ground for general methods of calculating electron-impact ionization processes.

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[1] A. Temkin, Phys. Rev. **126**, 130 (1962).
[2] R. Poet, J. Phys. B **11**, 3081 (1978).
[3] R. Poet, J. Phys. B **13**, 2995 (1980).
[4] R. Poet, J. Phys. B **14**, 91 (1981).
[5] J. Callaway and D. H. Oza, Phys. Rev. A **29**, 2416 (1984).
[6] P. G. Burke, C. J. Noble, and M. P. Scott, Proc. R. Soc. London Ser. A **410**, 289 (1987).
[7] M. Le Dourneuf, J. M. Launay, and P. G. Burke, J. Phys. B **23**, L559 (1990).
[8] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **69**, 53 (1992).
[9] S. Watanabe, Y. Hosoda, and D. Kato, J. Phys. B **26**, L495 (1993); D. Kato and S. Watanabe, Phys. Rev. Lett. **74**, 2443 (1995).
[10] D. A. Konovalov and I. E. McCarthy, J. Phys. B **27**, L407 (1994).
[11] K. Meyer, C. H. Greene, and I. Bray, Phys. Rev. A **52**, 1334 (1995).
[12] K. Bartschat, E. T. Hudson, P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B **29**, 115 (1996).
[13] I. Bray and A. T. Stelbovics, At. Data Nucl. Data Tables **58**, 67 (1994).
[14] I. Bray and A. T. Stelbovics, Adv. At. Mol. Phys. **35**, 209 (1995).
[15] D. V. Fursa and I. Bray, Phys. Rev. A **52**, 1279 (1995).
[16] D. A. Konovalov, I. Bray, and I. E. McCarthy, J. Phys. B **27**, L413 (1994).
[17] I. Bray and D. V. Fursa, J. Phys. B **28**, L435 (1995).
[18] I. Bray, Phys. Rev. Lett. **73**, 1088 (1994).