Calculation of the Total Ionization Cross Section and Spin Asymmetry in Electron-Hydrogen Scattering from Threshold to 500 eV

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We present the total ionization cross section and spin asymmetry at projectile energies ranging from threshold to 500 eV for electron-impact excitation of atomic hydrogen. They are calculated using the convergent close-coupling formalism of Bray and Stelbovics [Phys. Rev. A **46**, 6995 (1992)]. Both observables are found to be in complete quantitative agreement with measurements over almost the entire energy range. This is the only electron-atom scattering theory that is able to achieve this result to date.

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The calculation of accurate total ionization cross sections is one aspect which a complete theory of electron-hydrogen scattering must encompass. The experimental situation is that the cross section is known to high accuracy (statistical errors of order 3%) over the energy range from 14.6 eV to 4 keV through the pulsed crossed-beam measurements of Shah, Elliott, and Gilbody [1]. Their experiment supersedes the earlier studies of Fite and Brackmann [2] and Rothe *et al.* [3]. The recent experiment of Shyn [4] yields results that are 25% higher than those of Shah, Elliott, and Gilbody. However, these total ionization cross section estimates have relatively large uncertainties. They are derived by performing a double integration over extrapolated energy and angles of the measured doubly differential cross sections, which are themselves only accurate to 20%.

On the theoretical side, calculations of the total ionization cross section have been surprisingly poor over the last fifty odd years. All models have struggled to reproduce the ionization cross section observed in the experiments in the region of 20 to 100 eV. It is here (the intermediate-energy region) that the cross section takes its largest values. For energies above 500 eV it has been assumed that the Born approximation gives accurate answers, which is amply confirmed by the experiment of Shah, Elliott, and Gilbody [1]. A characteristic common to this approximation and its variants for hydrogen (see, for example, Rudge [5]) is that the cross sections are overestimated by 20%–40% in the intermediate-energy region. The explanation for this is simply that the approximation of the three-body wave function for the ionization region by the product of a plane and Coulomb wave or screened Coulomb waves is inadequate. Recently a proper treatment of the boundary condition and its implementation to give an approximate solution for the ionization part of the three-body wave function has been given by Brauner, Briggs, and Klar [6]. However, this form is best suited to higher energies.

An alternative route to obtaining a suitable representation of the three-body wave function for ionization is to employ a close-coupling formulation in which allowance for scattering to target continuum states is made. In such a model the total ionization cross section is obtained by using the optical theorem to get the total cross section, and subtracting the integrated cross sections from the scattering to the discrete states. For target states expanded in a basis of L^2 functions, all but the lowest lying states are poor approximations to the true target states. Nevertheless, the part of Hilbert space representing the higher discrete and continuum target states will be completely described as the basis is extended to completeness. Estimations of the total ionization cross sections using such expansions have been given by Gallaher [7], Callaway and Oza [8], and Callaway [9] for energies up to 54 eV. They tend to underestimate the ionization cross section and there is no attempt made to test the convergence of their expansions with an increasing number of basis expansions. A further estimate of total ionization cross sections has been made with the intermediate-energy R-matrix theory (IERM) [10]. This model overshoots the experiment by 10% to 20%.

In this Letter we present results for our convergent close-coupling (CCC) method whose application was demonstrated in a simplified model [11], and in the full electron-hydrogen scattering problem [12], where elastic and inelastic scattering to the $n = 2$ levels were discussed. In the former work we demonstrated that the method does yield correct cross sections in the Poet-Temkin model [13, 14], and that pseudoresonances are simply an indication of an inadequate representation of the target. In the latter paper we applied the CCC method to the full e-H scattering problem in order to

see if the long-standing discrepancies between experiment and various theories for the $2p$ angular correlation parameters could be resolved. Unfortunately, this did not prove to be the case; our (converged) results were in good agreement with the other theories, and so, not experiment. It was therefore of considerable interest to us to calculate the total ionization cross section using the CCC method because this cross section is known to a much higher degree of accuracy than are the angular correlation measurements.

The complete description of the CCC method is given by Bray and Stelbovics [12]. The full three-body Schrödinger equation is solved via the close-coupling formalism by solving the momentum-space Lippmann-Schwinger equation expanded in partial waves of total orbital angular momentum. The complete set of target states is obtained by diagonalizing the target Hamiltonian in an orthogonal Laguerre basis. This basis has the advantage that for each partial wave l, the basis size N_l may be of arbitrary size, i.e., linear dependence problems are not evident as they are in the Slater-type basis. The resulting wave functions $|\phi_n^{N_l}\rangle$ (with corresponding energies $\epsilon_n^{N_l}$) are all square integrable, and hence no special treatment of the continuum is necessary. Our basis functions are essentially Sturmians as introduced by Rotenburg [15]. Their application to atomic scattering problems is discussed by Rotenburg [16].

In Ref. [12] we demonstrated how to solve the resulting momentum-space close-coupling equations using real arithmetic and symmetric kernels. This achieves considerable saving of computer memory and so allows for the treatment of a large number of target states.

In order to extract the total ionization cross section σ_i^S from the channel cross sections for a projectile of linear momentum k_0 incident on an atom in ground state ϕ_0 $\sigma^S(k_n, \phi_n, \phi_0, k_0)$, we invoke the optical theorem to get the total cross section σ_t^S, and write

$$\sigma_i^S = \sigma_t^S - \sum_{n:\epsilon_n<0} \sigma^S(k_n, \phi_n, \phi_0, k_0), \tag{1}$$

where ϕ_n are the exact target discrete states with corresponding energies ϵ_n, and S is the total spin. In the CCC formalism we compute

$$\sigma_i^{SN} = \sigma_t^{SN} - \sum_{m:\epsilon_m^N<0} \sigma^{SN}(k_m, \phi_m^N, \phi_0, k_0) \times \sum_{n:\epsilon_n<0} |\langle\phi_n|\phi_m^N\rangle|^2, \tag{2}$$

where we use N to denote the total number of target states in the L^2 basis. The sum over the n overlap terms between the exact bound states $|\phi_n\rangle$ and negative energy Laguerre basis state $|\phi_m^N\rangle$ is used to project the cross sections onto the exact discrete subspace. This sum is only significantly less than unity for m such that $\epsilon_{m+1}^N > 0$. A similar form was also employed by Callaway and Oza [8]. For sufficiently large N these overlaps play no role in determining σ_i^{SN}, but we find they speed up the rate of convergence as a function of N. We require that N be sufficiently large so that $|\phi_0^N\rangle = |\phi_0\rangle$, which we take to be the ground state of hydrogen, and that σ_i^{SN} has reached convergence.

Writing $S = 0$ for singlet, and $S = 1$ for triplet scattering, the spin averaged total ionization cross section σ_i and spin asymmetry A_i are given by

$$\sigma_i = (\sigma_i^0 + 3\sigma_i^1)/4, \quad A_i = (\sigma_i^0 - \sigma_i^1)/\sigma_i. \tag{3}$$

Calculations of these parameters with the CCC method have been undertaken at a large number of energies chosen to adequately cover the energy range from threshold to 500 eV. As in Ref. [12], to demonstrate convergence at each energy we performed three distinct calculations. We started with the smallest calculation that had $10s$, $9p$, and $8d$ target states. This calculation we denote by 52CC since the close-coupling equations couple up to 52 $(10 \times 1 + 9 \times 2 + 8 \times 3)$ channels. To check for convergence as a function of basis size N_l we then performed a 70CC calculation which contained $13s$, $12p$, and $11d$ target states. Finally, to check for convergence as a function of target state l, we performed an 80CC calculation which had $10s$, $9p$, $8d$, and $7f$ target states. The 70CC and 80CC calculations are the largest that we are able to perform on our local IBM RS6000/530 computers.

We found that in the intermediate-energy range, where the cross section is at its largest, all three calculations of the total ionization cross section are within 5% of each other. At higher energies the 52CC and 70CC gave identical results indicating that convergence as a function of basis size N_l is readily obtained, but the 80CC is a little higher indicating that larger target l are more important at higher energies. At the lower energies we found that the size of N_l was more important. This is consistent with our results [11] in the Poet-Temkin model, where we showed that pseudoresonances manifest themselves in this energy region. These disappear as the basis size is increased.

In Fig. 1 we present the results of our CCC calculations of the total ionization cross sections. For energies below 50 eV the results are from the 70CC calculations; those above are from 80CC runs. We see remarkable quantitative agreement with the measurements of Shah, Elliott, and Gilbody [1] across most of the energy range. We tend to undershoot the cross section in the threshold region up to 4 eV above the ionization threshold. The ionization cross sections are only accurate to within 30% in this region. This is not an unexpected result. It is merely a reflection of the interesting physics in the Wannier [17] region. At these low energies the ionized electrons are strongly correlated. Thus any expansion, such as in the close-coupling method where the two-electron wave function is represented as a sum of separable terms in the two electron coordinates, will need to be very extended. More suitable forms of expansion (see, for example, Read [18])

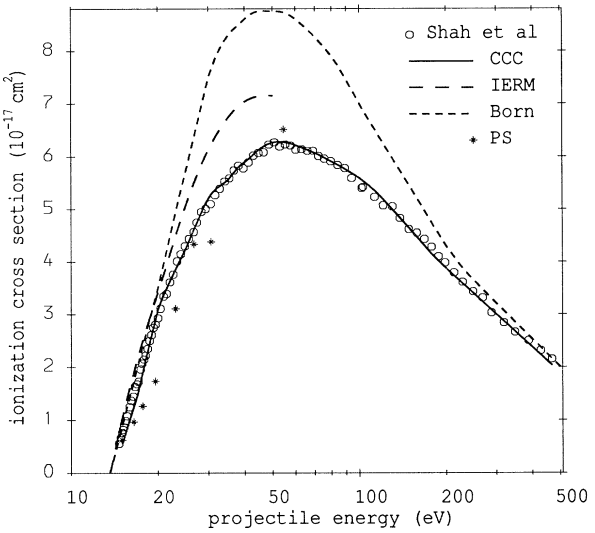

FIG. 1. The total ionization cross section calculated using the convergent close-coupling (CCC) method. The measurements of Shah, Elliott, and Gilbody [1] are denoted by o. The IERM results are due to Scholz, Walters, and Burke [10], the pseudostate (PS) results are due to Callaway and Oza [8], and the Born approximation is due to Peach [1].

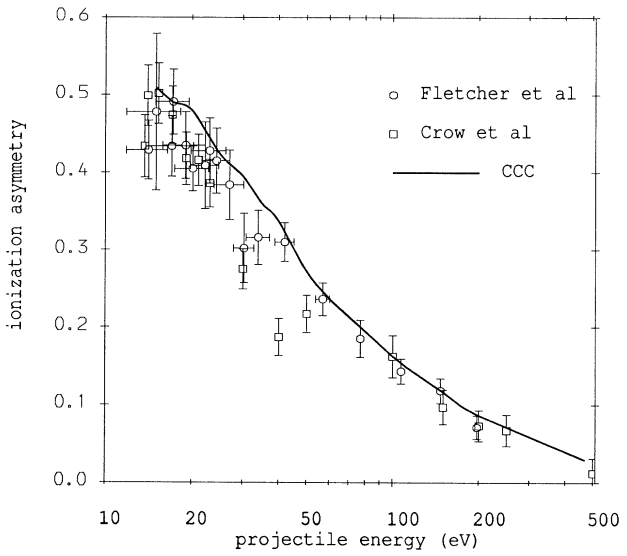

FIG. 2. The ionization spin asymmetry calculated using the convergent close-coupling (CCC) method. The measurements denoted by o and □ are due to Fletcher *et al.* [19] and Crowe *et al.* [20], respectively.

might need to be adopted to take account of this correlation. We find it encouraging that these difficulties for the CCC method are confined to such a small energy region. Our results are also a few percent too low at the very high energies where the Born approximation (we used the values of Peach given in Fig. 7 of Ref. [1]) is valid, indicating that even higher l states than f states are necessary at these energies to achieve an accuracy of order 1%. Comparison with the IERM theory of Scholz, Walters, and Burke [10] and the pseudostate method of Callaway and Oza [8] indicates how difficult it has been for theories to get the ionization cross section right. The latter of these calculations is the most similar to the ones undertaken here. It utilizes $5s$, $4p$, and $2d$ states, i.e., it may be denoted by 19CC in our notation. Though it is a considerably smaller calculation than ours, it provided a good indication that an L^2 approach to electron-atom scattering was feasible as early as 1979.

The ionization spin asymmetry of the CCC method is shown in Fig. 2. As in Fig. 1 the results below 50 eV are due to the 70CC calculation, above 50 eV, the 80CC calculation. We see good agreement with the measurements of Fletcher *et al.* [19] and Crowe *et al.* [20]. The latter work compares the asymmetries with a number of other theories. The only one of these that gets good agreement with experiment over most of the energy range is due to Bray, Madison, and McCarthy [21]. However, this turns out to be a fortuitous result as the associated total ionization cross section is even worse than the Born of Fig. 1 (see Ref. [22]), and so we do not present it here. There are more detailed measurements of the ionization asymmetry (twenty data points within 2 eV range of threshold) by Guo *et al.* [23], which we do not attempt to study here, due to the difficulties associated with this energy region as discussed above.

In conclusion, we have demonstrated that the convergent CCC model [12] of electron-hydrogen scattering yields exceptionally good total ionization cross sections and spin asymmetries for all energies excluding a small region of a few electron volts near the ionization threshold. It is the only electron-atom scattering theory that is able to achieve such a result to date, and provides us with the strongest confirmation yet of the validity of the CCC approach.

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[1] M. B. Shah, D. S. Elliott, and H. B. Gilbody, J. Phys. B **20**, 3501 (1987).
[2] W. L. Fite and R. T. Brackmann, Phys. Rev. **112**, 1141 (1958).
[3] E. W. Rothe, L. L. Marinio, R. H. Neynaber, and S. M. Trujillo, Phys. Rev. **125**, 582 (1962).
[4] T. W. Shyn, Phys. Rev. A **45**, 2951 (1992).
[5] M. R. H. Rudge, Rev. Mod. Phys. **40**, 564 (1968).
[6] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[7] D. F. Gallaher, J. Phys. B **7**, 362 (1974).
[8] J. Callaway and D. H. Oza, Phys. Lett. **72A**, 207 (1979).

[9] J. Callaway, Phys. Rev. A **44**, 2192 (1991).
[10] T. T. Scholz, H. R. J. Walters, and P. G. Burke, J. Phys. B **23**, L467 (1990).
[11] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **69**, 53 (1992).
[12] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[13] R. Poet, J. Phys. B **11**, 3081 (1978).
[14] A. Temkin, Phys. Rev. **126**, 130 (1962).
[15] M. Rotenburg, Ann. Phys. (N.Y.) **19**, 262 (1962).
[16] M. Rotenburg, Adv. At. Mol. Phys. **6**, 233 (1970).
[17] G. H. Wannier, Phys. Rev. **90**, 817 (1953).
[18] F. H. Read, in *Electron Impact Ionization*, edited by T. D. Märk and G. H. Dunn (Springer, Berlin, 1985), p. 42.
[19] G. D. Fletcher, M. J. Alguard, T. J. Gay, V. W. Hughes, P. F. Wainwright, M. S. Lubell, and W. Raith, Phys. Rev. A **31**, 2854 (1985).
[20] D. M. Crowe, X. Q. Guo, M. S. Lubell, J. Slevin, and M. Eminyan, J. Phys. B **23**, L325 (1990).
[21] I. Bray, D. H. Madison, and I. E. McCarthy, Phys. Rev. A **41**, 5916 (1990).
[22] I. Bray, D. A. Konovalov, and I. E. McCarthy, Phys. Rev. A **43**, 5878 (1991).
[23] X. Q. Guo, D. M. Crowe, M. S. Lubell, F. C. Tang, A. Vasilakis, J. Slevin, and M. Eminyan, Phys. Rev. Lett. **65**, 1857 (1990).