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Letter to the editor: J. Phys. B: At. Mol. Opt. Phys.

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LETTER TO THE EDITOR

Electron impact ionization of atomic hydrogen from the 1S and 2S states

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Abstract. We present results from R-Matrix with Pseudo-States (RMPS) and Convergent Close-Coupling (CCC) calculations for electron impact total ionization of the 1S and 2S states of atomic hydrogen in the energy region from threshold to 100 eV. Particular attention is given to the near threshold region. We find the results for energies more than 2 eV above threshold to be in excellent agreement with the available experimental data.

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The calculation of accurate ionization cross sections is of vital importance for many applications in the physics of fusion, lasers, stars, and upper atmospheres. In addition, the theoretical treatment of electron impact ionization of atomic hydrogen, as a pure three-body Coulomb problem with exactly known target wavefunctions, continues to attract the interest of the theoretical physics community (see, for example, Macek *et al* 1995).

In this Letter, we report the results of recent work using the R-Matrix with Pseudo-States (RMPS) (Bartschat *et al* 1996) and Convergent Close-Coupling (CCC) (Bray and Stelbovics 1992a,b) methods for the e-H collision problem. These calculations are the natural extension of our previous work (Bartschat and Bray 1996) on the Temkin-Poet S-wave model (Temkin 1962, Poet 1978). We demonstrate below that the RMPS method, too, provides highly accurate total ionization results for a realistic collision system, as did the CCC method before (Bray and Stelbovics 1993). In addition, both the RMPS and CCC methods yield accurate results for incident projectile energies more than approximately 2 eV above the ionization threshold, a considerable improvement on the initial CCC work.

The basic ideas behind the RMPS and CCC methods have been summarized elsewhere and will not be repeated here. Details can be found in Bartschat *et al* (1996) for the RMPS and in Bray and Stelbovics (1995,1996) for the CCC approach. A few points, however, specific to our ionization calculations, will be mentioned here.

To begin with, ionization cross sections in both methods are obtained by summing, for a given incident projectile energy, the excitation cross sections from the initial state (1S or 2S in this work) to final (positive-energy) continuum states which are represented by a set of square-integrable pseudo-states. In addition, the relatively small number of bound states in the RMPS calculation requires a correction plus averaging procedure. It needs to be applied to diminish the effect of pseudo-resonances and to avoid an overestimate of the discrete excitation cross sections by estimating the contribution to the ionization cross section from the bound pseudo-states with $\bar{n} = 4$. This procedure, as applied in the present case, will be described below.

In the RMPS calculations reported here, the (analytically known) physical 1s, 2s, 2p, 3s, 3p, and 3d orbitals were included in the R-matrix expansion to ensure a correct non-relativistic representation of the bound spectrum up to principal quantum number $n = 3$. In addition, pseudo-orbitals $n\bar{\ell}$ were constructed, to approximate the effect of higher discrete states as well as 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 pseudo-states were then obtained through diagonalization of the target Hamiltonian. A similar procedure is applied in the CCC method, where *all* states are constructed by diagonalizing the target hamiltonian in a Laguerre basis. If the basis is sufficiently large, the lower eigenfunctions and eigenvalues will converge pointwise to the

physical solutions, while the higher ones provide both an approximation to the higher discrete states and a square-integrable representation of the target continuum.

As pointed out before (Bartschat *et al* 1996, Bartschat and Bray 1996), the value of the range parameter α is, in principle, arbitrary, but the *rate of convergence* of the results will depend on its choice. Also, different choices of α or a different number of Laguerre basis states with a fixed value of α result in different distributions of the pseudo-thresholds.

In the CCC method generally a fixed α is taken, but the basis size is increased until convergence is obtained. This value may be varied by 10% or so to ensure that no pseudo-threshold lies too closely to the total energy, thereby reducing pseudo-resonance phenomena. This is possible, since the CCC calculations are performed by solving the standard close-coupling equations in momentum space for each collision energy separately, thereby allowing for a large number of states to be included in the close-coupling expansion, and having no restriction on the energy range of applicability.

The R-matrix method, on the other hand, is designed to solve the scattering problem for a large number of collision energies almost simultaneously, with the most essential modification to other methods being the separation of coordinate space into two regions, $r \leq a$ and $r > a$. The R-matrix radius a is chosen in such a way that exchange effects between the projectile and the target electrons can be neglected in the external region. In this region, the standard coupled equations (without exchange) are solved for each collision energy and matched, at the boundary $r = a$, to the solution in the internal region. Here the total wavefunction is expanded in terms of a set of *energy-independent basis functions*, which are obtained through diagonalization of the total (target plus projectile) Hamiltonian inside the R-matrix box. While this one-time effort in the internal region is advantageous if solutions for many collision energies are required, the size of the matrices to be diagonalized puts practical limits on the number of states that can be included and the highest collision energy that can be treated.

As we have demonstrated in the solutions of the S-wave model (Bartschat and Bray 1996), most of the RMPS pseudo-resonance problems associated with a relatively small number of pseudo-states in an individual calculation can be remedied by performing several RMPS calculations with different α values while keeping a fixed basis size. Effectively, this corresponds to different box sizes into which all physical and pseudo-states have to be squeezed. It is also important to note that such box-averaging only needs to be performed for partial waves with low angular momenta and is most important for collision energies near the ionization threshold. Hence, it is by no means necessary to repeat the full RMPS calculation many times.

In the RMPS calculations reported here, we chose an R-matrix radius of 55 a_0 and α values between 0.51 and 0.77. This range of α's insured that the eight S states, seven P states, five D states, and three F states included in the close-coupling expansion fit into

the box, with one pseudo-state per angular momentum being bound. The full calculation for collision energies up to 100 eV was performed with 60 continuum orbitals per angular momentum and $\alpha = 0.65$, while all other calculations were performed for partial waves with total orbital angular momentum $L \leq 4$ and only 40 continuum orbitals per angular momentum. Exchange between the projectile and the target electrons was included up to $L \leq 12$, while no-exchange calculations were performed up to $L = 30$. Note that all RMPS calculations were carried out on a single 64Mb DEC-Alpha desktop workstation, mainly to demonstrate the applicability of the RMPS method for realistic ionization problems. By increasing the computer resources even moderately, the accuracy of the RMPS results presented here (the average of 15 individual runs) could certainly be increased significantly.

Since separate CCC calculations are performed at each energy, the target expansion states may be chosen to suit the energy range and observable of interest. At very low energies, for example, only a few states are usually necessary for convergence, as has been demonstrated by standard close-coupling methods over many decades. Near, but above, the ionization threshold, one needs large and long-ranged bases for each target-space orbital angular momentum ℓ to ensure a good representation of the target continuum in the small energy range with open ionization channels. Furthermore, since here we are interested in obtaining very small cross sections accurately, we include in our expansions the higher lying discrete states whose cross section is commensurate with the total ionization cross section. The CCC results presented here combine a set of calculations on a fine projectile energy mesh (14 to 24 eV relative to the 1S state in steps of 0.2 eV) that were performed with the threshold investigation in mind, as well as those performed at a coarser mesh chosen to cover an energy range up to 1 keV. In the threshold region we set the basis sizes $N_\ell = 15 - \ell$ for $\ell = 0, 1, 2, 3$ with $\alpha_\ell \approx 0.25$, resulting in a total of 54 states (approximately 32 with negative and 22 with positive energy). Note that allowing for a small variation in α with incident energy may result in a slightly different distribution between negative and positive energy states. At higher energies two sets of calculations were performed. One had $N_\ell = 14 - \ell$ for $\ell = 0, 1, 2, 3$ with $\alpha_\ell \approx 0.5$ and the other $N_\ell = 12 - \ell$ for $\ell = 0, 1, 2, 3, 4$ with $\alpha_\ell \approx 0.5$. In both cases, approximately 20 of the 50 states had a negative energy. Where necessary, we shall denote these two calculations by CCC_3 and CCC_4, respectively; comparison of the results gives a very good indication of convergence. These CCC calculations were performed in parallel on up to 24 machines with 256 Mb of core memory each.

Finally, as mentioned above, it is important in the RMPS calculations to estimate the contribution to the ionization cross sections from the bound pseudo-states with $\bar{n} = 4$. Extending the idea outlined by Callaway and Oza (1984), this estimate was obtained as follows. At the ionization threshold, the excitation cross section for the $\bar{n} = 4$ states provides a reasonable estimate for excitation of all physical bound states

with $n > 3$. For very high incident energies, on the other hand, the sum of the excitation cross sections to all these states should approximate the Born limit. For excitation from the 1S ground state, this corresponds to 1.08 times the excitation cross sections for the $n = 3$ states. Assuming that the Born value is reached from the threshold value via a $1/\epsilon^2$ power law, where ϵ is the excess energy shared by the two outgoing electrons, one can thus obtain a correction to the raw ionization result (i.e., the sum of the excitation cross sections for positive-energy states). Detailed tests showed that this correction is, indeed, usually positive, i.e., this approach overcomes the standard problem of projection methods that often underestimate the ionization cross section near threshold (Callaway and Oza 1984, Meyer *et al* 1995, Bartschat and Bray 1996). Note that this problem is much less critical in the CCC calculations, since the larger number of physical discrete states diminishes the size of the correction tremendously.

The method outlined above was applied for ionization from the ground state, for each partial wave symmetry with total orbital angular momentum L, total spin S, and total parity π separately. Potential problems lie in the fact that the Born limit may not be valid yet starting with $n = 4$, and this is certainly true for ionization from the 2S state. In the latter case, we assumed that the ratio found at threshold remains constant over the entire energy range of interest. This is qualitatively supported by comparing with the results from the CCC calculations with more physical states included. Also, in all cases, only 35% of the excitation cross section for the $4\bar{\mathrm{F}}$ state was counted towards discrete excitation. While the importance of the F states is generally small for ionization from the ground state, this is not the case for the 2S initial state (see below). Consequently, larger RMPS calculations, beyond the computer resources available for the present project, would need to be performed to increase the reliability of the latter results.

In figure 1, we present our results for the total ionization cross section σ_{I} for electron impact on the 1S ground state of atomic hydrogen, from threshold (13.6 eV) to 100 eV incident energy E. These results are compared with the measurements of Shah *et al* (1987). The agreement between the two theoretical predictions and the experimental data is excellent over the entire energy range. CCC results for even higher energies have been presented elsewhere (Bray and Stelbovics 1993), and the agreement between experiment and theory continues to be excellent to 1 keV.

We also present results for the ionization spin asymmetry A_{I} defined as

$$A_{\mathrm{I}} = \frac{1}{P_e P_{\mathrm{A}}} \frac{N_{\uparrow\downarrow} - N_{\uparrow\uparrow}}{N_{\uparrow\downarrow} + N_{\uparrow\uparrow}} = \frac{\sigma_{\mathrm{I}}^{\mathrm{s}} - \sigma_{\mathrm{I}}^{\mathrm{t}}}{\sigma_{\mathrm{I}}^{\mathrm{s}} + 3\sigma_{\mathrm{I}}^{\mathrm{t}}}, \tag{1}$$

where $N_{\uparrow\downarrow}$ ($N_{\uparrow\uparrow}$) are the count rates for ionization with anti-parallel (parallel) projectile (P_e) and target (P_{A}) spin polarizations, while $\sigma_{\mathrm{I}}^{\mathrm{s}}$ ($\sigma_{\mathrm{I}}^{\mathrm{t}}$) is the contribution from the singlet (triplet) total spin channel, with $\sigma_{\mathrm{I}}^{\mathrm{s}} + 3\sigma_{\mathrm{I}}^{\mathrm{t}} = \sigma_{\mathrm{I}}$. The agreement between the results from the two independent calculations is once again very good. There are some minor discrepancies between these predictions and two sets of experimental data (Fletcher *et al* 1985, Crowe *et al* 1990), but we also note some scatter in the experimental data.

It is worth noting that the correct prediction of these quantities has been a great challenge to theorists for a very long time. Bray and Stelbovics (1993) first demonstrated the ability to do this using the CCC method; comparison with some previous theories may be found in that work. Since that time Kato and Watanabe (1995) reproduced the total ionization cross section by applying the hyperspherical close-coupling (HSCC) method, though they did not present the spin asymmetry. In addition Macek *et al* (1995), using the hidden crossing theory, obtained good results near the threshold region.

In figure 2, we present the results on an extended energy scale between 0 and 10 eV excess energy ϵ, and we also plot $\sigma_{\mathrm{I}}/\epsilon$ to emphasize the behaviour near threshold. Here we also compare with the data obtained by McGowan and Clarke (1968). Very good agreement with the experimental data is obtained above 2 eV excess energy, while some apparently unphysical structures appear in the highly sensitive parameter $\sigma_{\mathrm{I}}/\epsilon$ between 0 and 2 eV excess energy. These are the remaining effects of the pseudo-resonances that, in principle, could be further diminished by increasing the number of states and/or calculations to be averaged over. In any case, the present results appear to be at least as accurate as those obtained with the HSCC approach (Kato and Watanabe 1995), although the latter method might seem to be more suitable in the threshold region.

In figure 3, we compare the contributions from excitation of pseudo-states with different orbital angular momentum ℓ to the total ionization cross section in the RMPS and CCC approaches. Convergence with the maximum target orbital angular momentum ℓ is assisted by the built-in unitarity of the close-coupling formalism (for details, see Bray 1994). It ensures convergence in the total ionization cross section without requiring convergence in the individual ℓ-dependent contributions. This is the reason for the oscillations seen in the CCC contributions to the total ionization cross section. Turning to ionization of the ground state, the agreement between the RMPS and CCC results is very good, with the biggest relative deviation being in the F state contribution, where the RMPS estimate of the ionization contribution from the $4\bar{\mathrm{F}}$ state is not expected to be as accurate as for the lower angular momenta. (Note that the CCC results for the S and F contributions are very similar.) Even though there are some differences in the individual contributions, unitarity ensures that the sum is in very good agreement.

The effect of unitarity can be seen much more clearly in the case of ionization of the 2S metastable state. Here we see that the RMPS, CCC_3 and CCC_4 results for the total ionization cross section are all in good agreement with each other and also with the measurements of Defrance *et al* (1981). Agreement of the two CCC calculations suggests convergence in the expansion of the target space with just the inclusion of F states. Note, however, that in the peak region around 15 eV incident energy the largest contribution to the ionization cross section originates from F states! Though the partial contributions

from the CCC_4 calculations are not shown (for clarity of presentation), the introduction of G states greatly diminishes the presented F and D state contributions. These findings are identical to those for electron impact ionization of the 3S and 3P states of sodium (Bray 1994). They indicate that the calculation of differential ionization cross sections at these energies will be particularly difficult, due to slow convergence with increasing target angular momentum ℓ.

In conclusion, we have presented RMPS and CCC results for electron impact ionization of atomic hydrogen from the 1S and 2S initial states. Excellent agreement between the predictions from the two approaches and the available experimental data was obtained, even for the critical ratio of cross section over excess energy if the latter is greater than about 2 eV. This indicates that they are as accurate as, for example, the HSCC approaches which were thought to be better suited to the study of threshold behaviour (Kato and Watanabe 1995). It is also very likely that even better accuracy could be obtained by increasing the computational resources.

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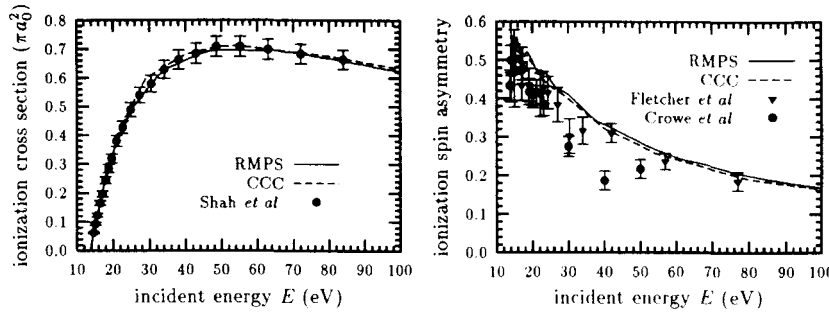

Figure 1. Total cross section σ_1 (left) and spin asymmetry A_1 (right) for electron impact ionization of H(1S) as a function of the projectile energy E. See text for details of the theories.

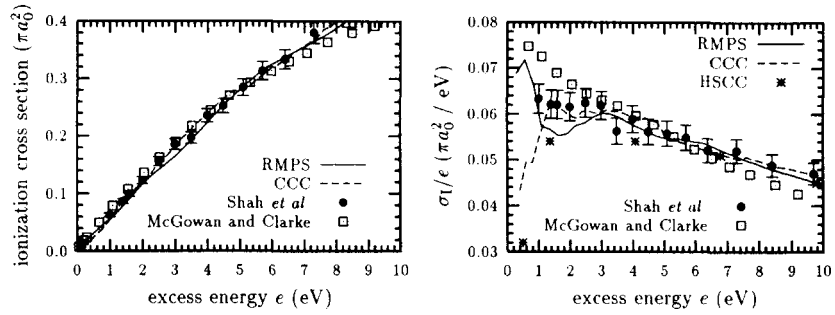

Figure 2. Total cross section σ_1 (left) and ratio of cross section over excess energy (right) for electron impact ionization of H(1S) as a function of the excess energy e. See text for details of the theories.

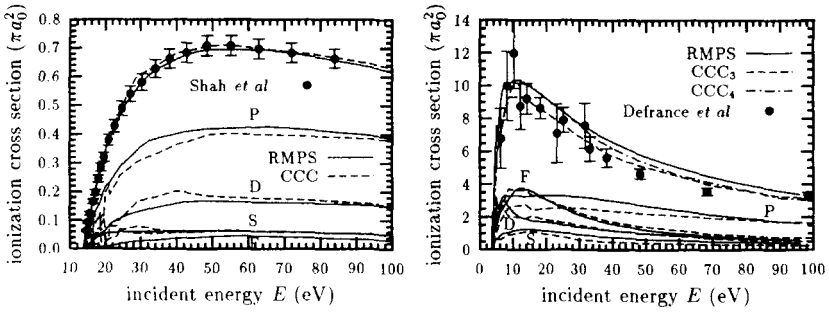

Figure 3. Contributions to the total electron ionization cross section of H(1S) (left) and H(2S) (right) from excitation of pseudo-states with the indicated angular momenta as a function of the projectile energy E. See text for details of the theories.

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