Electron-impact ionization of atomic hydrogen at 2 eV above threshold

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The convergent close-coupling method is applied to the calculation of fully differential cross sections for ionization of atomic hydrogen by 15.6 eV electrons. We find that even at this low energy the method is able to yield predictive results with small uncertainty. The reason for the success of the method is investigated and explained.

34.80.Bm, 34.80.Dp

At the base of all electron-atom scattering and ionization problems is the fundamental, yet unsolved, three-body problem of an electron interacting with atomic hydrogen. This problem occupies a special place in the set of unsolved problems of interest to physicists due to its fundamental nature in the realm of atomic physics. It represents a class of Coulomb three-body problems which includes electron interaction with the single positive ion of helium, and hence the problem of helium double photoionization. For these reasons one of the Centennial Symposia of the 1999 meeting of the American Physical Society is devoted to the study of such problems.

For heavier atoms the complexity of the Coulomb three-body problem may be masked by the collective behavior of the many target electrons. Similarly, for high incident electron energies the complicated role played by the long-ranged Coulomb interaction is also somewhat hidden. The problem exhibits all of its complexities at energies a little above the ionization threshold. Here we have the possibility of exciting a countably infinite number of the hydrogen discrete states as well as the three-body continuum of two very slow strongly interacting electrons. In this Letter we consider the e-H problem at the incident electron energy of 15.6 eV, i.e. only 2 eV above the ionization threshold.

To solve the e-H problem means to correctly predict all of the possible scattering amplitudes for both the discrete \( f_n^S(k) \) and continuum \( f^S(k_A,k_B) \) transitions for a total spin \( S \). For the discrete transitions close-coupling methods have proved to be the most successful, particularly at low energies. These rely on expanding the total wave function in a set of orthonormal states. From the landmark work of Yamani and Reinhardt [1], followed by Broad [2], Stelbovics [3] and others, it became clear that the set of orthonormal states obtained by diagonalizing the target Hamiltonian in a Laguerre basis formed an unusual equivalent-quadrature rule. Thus-obtained states provide a finite \( N \) quadrature rule that incorporates both the infinite set of true target discrete states and the target continuum. This is an immensely powerful result and forms the basis of the convergent close-coupling (CCC) method for the calculation of electron-atom scattering [4–6]. The idea relies on simply increasing \( N \) until convergence in the parameter of interest is obtained to an acceptable accuracy, just like with standard numerical quadrature. This approach has proved very successful for the discrete transitions at all energies. In the rare case of substantial discrepancy with experiment [4] subsequent new measurements were found to be in agreement with the CCC theory [7].

Obtaining reliable scattering amplitudes \( f_n^S(k) \) for the discrete transitions is a good start, but what about ionization? The expansion-states \( \phi_n \) have both negative and positive energies \( \epsilon_n \). By summing the cross sections, obtained upon solution of the close-coupling equations, for just the positive energy states yields excellent agreement with the measurements of the e-H total ionization cross section [8–10]. Though this is the least detailed ionization process it is an encouraging first step. The question is: do the scattering amplitudes \( f_n^S(k) \) for \( \epsilon_n > 0 \) contain all of the detailed ionization information?

The work of Bray and Fursa [11] attempted to provide a correct interpretation of the already calculated positive-energy-state scattering amplitudes, with some confronting and controversial results. It was shown that the ionization amplitudes may be defined from the \( f_n^S(k) \) by

\[
f^S(k_A,k_B) = \langle k_B|^{(-)}\phi_B\rangle f_B^S(k_A), \tag{1}
\]

where \( k_B^{(-)} \) is a Coulomb wave (in the case of H target) of energy \( k_B^2/2 = \epsilon_B \), and where \( k_A^2/2 + k_B^2/2 = E \), the total (excess) energy. This definition is in fact a simplification of the pioneering work of Curran and Walters [12]. The overlap has the effect of changing the unitary normalization of \( \phi_B \) to that of the true continuum, as well as introducing a one-electron Coulomb phase. The controversy [13] arises not from the above definition, but from the subsequent use of (1) to define the triply differential cross section (TDCS) by

\[
\frac{d^3\sigma^S(k_A,k_B)}{d\Omega_A d\Omega_B dE_A} = |f^S(k_A,k_B)|^2 + |f^S(k_B,k_A)|^2. \tag{2}
\]
The second term above looks like an exchange term, but it is not. The close-coupling equations are solved separately for each total spin $S$. Thus, the amplitudes $f^S_A(k)$, and hence $f^S_A(k_A, k_B)$ are already a coherent combination of their own direct and exchange amplitudes as determined by $S$. The two terms have very different origin, see (1). The amplitude $f^S_A(k_A)$ arises from the excitation of the state $\phi_n$ with $\epsilon_A = \epsilon_B$, with the boundary condition that the “$k_A$” electron exits as a plane wave totally shielded from the ion by the other electron in (bound) state $\phi_B$. If $\epsilon_B < k^2_A/2$ then this is the physically sound shielding approximation, but then the boundary conditions for the amplitude $f^S_A(k_B)$ are unphysical (low-energy outgoing plane wave shielded by a higher energy bound state). Yet, these two theoretically distinguishable amplitudes correspond to the same ionization process since $E = \epsilon_A + \epsilon_B$. For $E' = \epsilon_A + \epsilon_B + \Delta E$ these amplitudes still arise, but would correspond to different ionization processes.

From (2) we see that close-coupling yields twice as many amplitudes as we may expect from formal ionization theory. A careful numerical study of the problem led to the suggestion that with increasing $N$ the second term in (2) converges to zero [14]. This brings about consistency with formal ionization theory. However, for finite $N$ a consistent interpretation of the close-coupling approach to ionization requires the use of both terms. A further consequence of the numerical study [14] is that the close-coupling method is unable to obtain convergence in the singly differential cross section (SDCS) whenever the true SDCS at equal energy sharing is substantial. Nevertheless, it was argued, that if the true SDCS was known then accurate ionization cross sections could still be predicted.

The concept of convergence with increasing $N = \sum_{l \leq l_{\text{max}}} N_l$ involves both the increase of $l_{\text{max}}$ and $N_l$. We will denote the CCC calculations by $\text{CCC}(N_0, l_{\text{max}})$ with $N_l = N_0 - l$. To examine the rate of convergence we perform two vastly different calculations $\text{CCC}(20,5)$ and $\text{CCC}(13,4)$, which require approximately 2Gb and 500Mb of computer core memory, respectively. In both cases the Laguerre exponential fall-off parameter was set $\lambda_l \approx 0.6$ with the variation performed to ensure that for each $l$ there was a state $\phi_{nl}$ with energy $\epsilon_{nl} = 1\, \text{eV}$.

The first test of the calculations is the comparison of the total ionization cross sections (TICS) and its spin asymmetry $A_I$ with the highly accurate measurement [15] of TICS $1.08 \times (10^{-17}\, \text{cm}^2)$ and the $A_I \approx 0.5$ measurements [16,17]. The $\text{CCC}(20,5)$ and $\text{CCC}(13,4)$ results for the TICS, $A_I$ are 1.18, 0.50 and 0.91, 0.51, respectively. Thus, we see that both calculations attribute approximately the correct amount of electron flux to the two spin ionization channels.

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Next, in Fig. 1, we consider the energy distribution within the ionization channels, i.e. the SDCS

$$\frac{d\sigma^S}{dE} = \int d\Omega_A d\Omega_B |f^S(k_A, k_B)|^2. \quad (3)$$

FIG. 1. The singly differential cross sections arising in the $\text{CCC}(N_0, l_{\text{max}})$ (see text) calculations. The step function labeled by $\text{CCC}(\infty, 5)$ is an integral preserving estimate.

The spin-averaged SDCS is presented. We see that there is no convergence in the $\text{CCC}(20,5)$ and $\text{CCC}(13,4)$ SDCS, though the integral of both is much the same. The step function $\text{CCC}(\infty, 5)$ is an estimate of what the CCC-calculated SDCS would converge to for $N_0 = \infty$ (there are no problems in obtaining convergence with increasing $l_{\text{max}}$). In other words, we assume that at this low energy the true SDCS is approximately flat. The SDCS symmetrically on either side of 1 eV correspond to the same ionization process and is why we have the two terms in (2). For the asymmetric energy-sharing only one term contributes significantly, but both are significant at equal energy sharing. Before looking at the angular distributions determined by (2) it is clear from Fig. 1 that their magnitude will be wrong. In order that integration of (2) over the angular variables yielded the estimated SDCS of 1.08 $(10^{-17}\, \text{cm}^2/\text{eV})$ we will multiply the CCC $E_A = E_B = 1\, \text{eV}$ TDCS by $1.08/(0.2 \times 2) = 2.7$.

In Figs. 2, 3, and 4 we present the TDCS calculated by the two CCC models and compare these with experiment and the previously overall best agreement yielding theory, the distorted-wave Born approximation (DWBA) of Jones, Madison, and Srivastava [18]. The relative measurements were initially presented by Brauner et al. [19], but were remeasured and put on the absolute scale, with estimated 35% uncertainty, by Röder et al. [20]. The DWBA calculations [18] work relatively well at this low energy since they utilise the effective charge formalism of Rudge [21] in the distorting potentials. For an example of a more common DWBA approach and the 3C theory see Rouet, Tweed, and Langlois [22] and Brauner et al. [19], respectively.

In the TDCS figures we use the convenient, for the coplanar geometry, convention that the negative scattering angles are on the opposite side of the incident beam (z-axis). For best visual comparison with the rescaled
CCC calculations we have multiplied all of the experimental values by the single constant of 0.45. Having done so, we see excellent agreement between the two CCC calculations and experiment, which is of considerable improvement on the comparison with the DWBA calculation. The quality of the agreement gives us confidence that the rescaling of the experiment has brought it into consistency with the estimated SDCS value of 1.08 \(\times 10^{-17}\) cm\(^2\)/eV. Should the true SDCS prove to be a little convex then the experimental rescaling should be done by a factor a little greater than 0.45. Perhaps the experimentally determined normalization is an indication that this may indeed be so.

Let us turn specifically to the case \(\theta_{AB} = 80^\circ\) given in Fig. 3. Though no experiment is available for this case we present it because it shows a greater difference between the two CCC calculations, but is still experimentally accessible. In fact, smaller \(\theta_{AB}\) geometries yield even greater differences. Such geometries, first suggested by Whelan, Allan, and Walters [23], are an excellent test

FIG. 2. The coplanar, “fixed \(\theta_A\) (Ehrhardt) geometry”, triply differential cross sections for electron-impact ionization of atomic hydrogen with two 1 eV outgoing electrons. Absolute experiment of Röder et al. [20] has been scaled by a factor of 0.45 for best visual fit to the rescaled CCC data, see text. The DWBA calculations are due to Jones, Madison, and Srivastava [18].

FIG. 3. Same as for Fig. 2, except for the “fixed \(\theta_{AB}\) (Whelan) geometry".
of the CCC theory because the cross sections fall rapidly with decreasing $\theta_A$. We see that the bigger calculation yields the smaller cross section. This is an important indication of how well the CCC theory is working. For the other presented cases the fact that the shapes of the two calculations are much the same, even though one requires four times as much computational resources as the other, suggests rapid shape convergence for the largest cross sections. On the other hand, almost identical overall magnitude suggests that convergence to the true correct SDCS is extremely slow.

calculated SDCS. The CCC theory does not solve the e-H Coulomb three-body problem, but curiously, has pushed the uncertainty to just that of determining the shape of the SDCS.

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\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig4.png}
\caption{Same as for Fig. 2, except for the "symmetric (Pochat) geometry". See text for definition of CCC(mix).}
\end{figure}

So how is it that the CCC theory yields such good TDCS angular distributions? To help answer this question let us have a look in more detail at Fig. 4. Given the good agreement between CCC(13,4) and CCC(20,5) TDCS one would imagine that one may readily interchange the partial wave amplitudes of (1) $\langle kl | \phi_{nl} | f_{nl} \rangle$ in the two calculations. The curve labeled by CCC(mix) was generated by taking the 1 eV $l = 1$ partial wave amplitude of the CCC(20,5) calculation and using it with the remaining CCC(13,4) amplitudes. Whereas one may reasonably expect the CCC(mix) calculated TDCS to be between the other two, it differs substantially when the two electrons emerge close together. This is an indication of the importance of treating all partial waves in a consistent manner. The Laguerre basis choice $N_l = N_0 - l$ with similar $\lambda_l$ results in much the same integration rule over the true continuum for each $l$. In other words, the number of positive energy states and their separation is similar for each $l$. We also use the same set of states for each partial wave of total orbital angular momentum $J$. Thus, for each $J$, the error in the energy distribution is also very similar for each $l$, and this is why the CCC($N_0, l_{\text{max}}$) calculations yield good TDCS angular distributions whose magnitude is in error by a single constant.

Concluding, it seems that the CCC theory is able to yield accurate TDCS angular distributions for all kinematical conditions, with the error in the magnitudes being determined simply from the error in the CCC-

\begin{thebibliography}{10}
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