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LETTER TO THE EDITOR

Convergent close-coupling calculation of singly differential cross sections in the ionization of atomic hydrogen by electron impact

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Abstract. The convergent close-coupling (CCC) calculations of singly differential cross sections (SDCS) are presented for ionization of atomic hydrogen by electron impact at incident energies of 25, 40, 60, 100, 150 and 250 eV. The SDCS are obtained directly from the T-matrix elements arising in the CCC calculations. The theory is in excellent agreement with the experimental data of Shyn, when normalized to the measurements of the total ionization cross sections by Shah *et al.*

The convergent close-coupling (CCC) method for electron–atom scattering has been recently developed by Bray and Stelbovics (1992a). The CCC method is a non-perturbative approach to the calculation of electron–atom/ion scattering based on the close-coupling (CC) formalism, where the target is represented by a set of square integrable (L^2) states. The number of the L^2 states is increased until convergence in the physical observable of interest is achieved. There are a number of similar approaches generally known as pseudostate methods, see review of Madison and Callaway (1987), and references therein. The CCC method is able to solve a large set of coupled equations using momentum-space techniques (McCarthy and Stelbovics 1983). This allows the method to achieve convergent, basis independent, results for most observables.

Pseudoresonances observed in CC methods with small number of L^2 states, e.g. Callaway and Oza (1984), naturally disappear with an increase in basis size (Bray and Stelbovics 1992b). No averaging technique is necessary to smooth the convergent results. This has also been demonstrated in the J-matrix method, where previously observed pseudoresonances in the calculations of Heller and Yamani (1974) disappear if the number of basis L^2 states used is increased from 10 to 37 (Konovalov and McCarthy 1994).

Since its first introduction the CCC method has been successfully applied to the calculation of various physical observables in electron and positron scattering on hydrogen-like atoms or ions, e.g. Bray (1994) and references therein. Thus, an example which is particularly relevant to this work is the ability to obtain excellent agreement with the measurements of the total ionization cross section (TICS) and spin asymmetry in e–H scattering (Bray and Stelbovics 1993) at all energies.

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Physical observables such as differential and integrated cross sections, total ionization cross section and spin asymmetries may be calculated readily using the CCC method. We now turn to calculating (e, 2e) cross sections using the CC formalism. Following the work of Curran and Walters (1987) we have applied the method successfully to calculating (e, 2e) differential cross sections for electron–hydrogen scattering at 54.4 and 150 eV (Bray *et al* 1994).

In this work we will show how the CC formalism can be used to calculate singly-differential cross sections (SDCS) for ionization phenomena. We work on the electron–hydrogen scattering problem, which is one of the benchmarks of theoretical atomic physics since it contains the full complexity of a Coulomb three-body problem, and the target can be described exactly.

A complete description of the CCC method for hydrogen-like targets can be found in Bray (1994), and therefore only a brief summary is given here. The CCC method solves a coupled set of Lippmann–Schwinger equations in the partial-wave formalism for the K matrix

$$\langle Lk_{nl}ln\|K^{SN}_{J\Pi}\|n_0l_0k_0L_0\rangle = \langle Lk_{nl}ln\|V^{SN}_{J\Pi}\|n_0l_0k_0L_0\rangle + \sum_{l',L'}\sum_{n'=1}^{N_{l'}}\mathcal{P}\int_{k'}\frac{\langle Lk_{nl}ln\|V^{SN}_{J\Pi}\|n'l'k'L'\rangle}{E-\epsilon_{n'l'}-\epsilon_{k'}}\langle L'k'l'n'\|K^{SN}_{J\Pi}\|n_0l_0k_0L_0\rangle \qquad (1)$$

where E is the total energy, $\Pi = (-1)^{l+L} = (-1)^{l'+L'}$ is the parity, l and L are the orbital angular momenta of the target and the projectile electrons, J and S are the total orbital angular momentum and spin of the system. The ϵ_{nl} and $|nl\rangle$ are the channel energies and states obtained upon the diagonalization of the target Hamiltonian H_t in a Laguerre basis of size N_l, with $\langle nl|H_t|n'l'\rangle = \epsilon_{nl}\delta_{nn'}\delta_{ll'}$. The K matrix is related to the T matrix by

$$\langle Lk_{nl}ln\|K^{SN}_{J\Pi}\|n_0l_0k_0L_0\rangle = \sum_{l',L'}\sum_{n'=1}^{N^o_{l'}}\langle Lk_{nl}ln\|T^{SN}_{J\Pi}\|n'l'k_{n'l'}L'\rangle \times (\delta_{l'l_0}\delta_{L'L_0}\delta_{n'n_0} + i\pi k_{n'l'}\langle L'k_{n'l'}l'n'\|K^{SN}_{J\Pi}\|n_0l_0k_0L_0\rangle) \qquad (2)$$

where k_{nl} is defined for $1 \leqslant n \leqslant N^o_l \leqslant N_l$ for which $k_{nl} = \sqrt{2(E-\epsilon_{nl})}$ is real, and $|k_{nl}L\rangle$ is the L-partial wave (plane wave in the case of uncharged targets). In this case the channel nlL is open, and if $E < \epsilon_{nl}$ the channel is closed. For a particular l the number of states that lead to open channels is N^o_l. The appropriate first-order electron–electron and electron–target interaction potentials are denoted by $V^{SN}_{J\Pi}$, see Bray (1994) for details. The superscript N denotes the full set of states. Convergence is obtained at a particular N whenever further increase yields similar results within the required accuracy.

Partial excitation cross sections from the ground state n_0l_0, which will be denoted as 0 from this point on, to each channel are defined as

$$\sigma^N_{nl} = \frac{(2\pi)^4}{4\pi}\frac{k_{nl}}{k_0}\frac{1}{(2l_0+1)}\sum_{LL'JS}\frac{(2S+1)}{4}(2J+1)|\langle Lk_{nl}ln\|T^{SN}_{J\Pi}\|0k_0L'\rangle|^2. \qquad (3)$$

The meaning of σ^N_{nl} is clear for those target states which approximate the actual bound states of the target, i.e. those with negative energy. The sum over all σ_{nl} yields the total

cross section, which may also be obtained via the optical theorem. The TICS σ_i^N may be obtained by

$$\sigma_i^N = \sum_l \sigma_i^{lN} \qquad \sigma_i^{lN} = \sum_{n,\epsilon_{nl}>0} \sigma_{nl}^N. \tag{4}$$

A slightly more accurate method is to subtract the cross sections for negative energy states, projected onto the true discrete spectrum, from the total cross section (Bray and Stelbovics 1993). This method has been used to obtain the TICS from the current CCC calculations, presented in figure 1 and table 1.

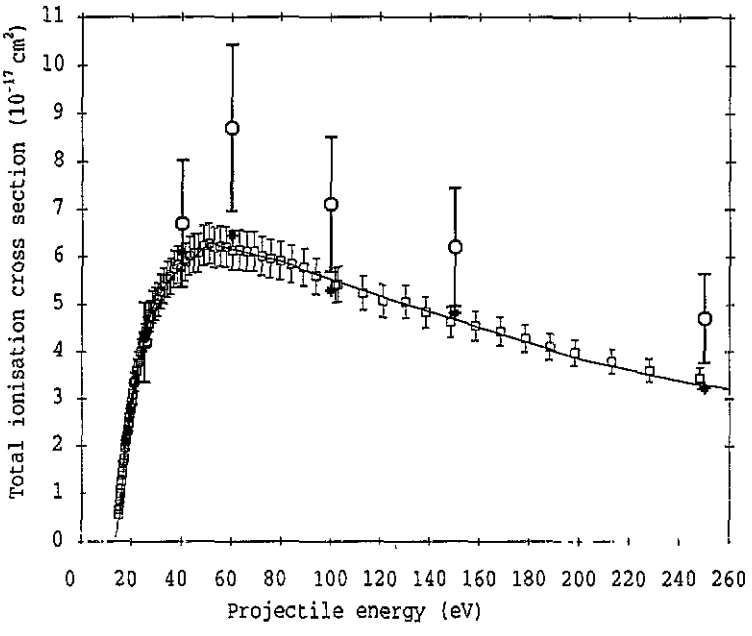

Figure 1. Total ionization cross sections of atomic hydrogen by electron impact. The full curve is due to the CCC calculations of Bray and Stelbovics (1993) and the stars are the present CCC calculations. The experimental points, ○, are due to Shyn (1992) and, □, to Shah *et al* (1987).

In order to extract the singly differential cross sections we use the work of Bransden and Stelbovics (1984) who showed that for each l

$$\sum_{0<\epsilon_{nl}<E_0} |n\rangle\langle n| = \int_0^{E_0} d\varepsilon |\varepsilon\rangle\langle\varepsilon| \approx \sum_{0<\epsilon_{nl}<E_0} w_n |\epsilon_{nl}\rangle\langle\epsilon_{nl}| \tag{5}$$

where $|\epsilon_{nl}\rangle$ are the exact target continuum wavefunctions with energy ϵ_{nl} and w_n are weights which are given by

$$w_j = \tfrac{1}{2}(\epsilon_{j+1} + \epsilon_j) - \tfrac{1}{2}(\epsilon_j + \epsilon_{j-1}) \tag{6}$$

$$w_{\text{first}} = \tfrac{1}{2}(\epsilon_{j_{\text{first}}+1} + \epsilon_{j_{\text{first}}}) \tag{7}$$

$$w_{j_{\text{last}}} = E_0 - \tfrac{1}{2}(\epsilon_{j_{\text{last}}} + \epsilon_{j_{\text{last}}-1}). \tag{8}$$

Table 1. Singly-differential ($d\sigma/d\varepsilon$) and total (σ_i) cross sections for the electron impact ionization of atomic hydrogen calculated using the CCC method (in units of 10^{-17} cm^2 eV^{-1}). Energies of the incident electron and secondary electron are denoted by E and ε. Experimental data of Shah *et al* (1987) and Shyn (1992) are denoted by σ_i^{SEG87} and σ_i^{S92} respectively. The latter we obtained by numerical integration of the corresponding SDCS. All total cross sections are in units of 10^{-17} cm^2.

	E (eV)					
ε	250	150	100	60	40	25
1.0	0.378	0.596	0.521	0.823	0.760	0.857
2.0	0.262	0.422	0.461	0.612	0.658	0.938
3.0	0.214	0.333	0.409	0.485	0.673	0.744
4.0	0.182	0.280	0.359	0.426	0.635	0.554
5.0	0.161	0.239	0.309	0.388	0.547	0.445
5.7	0.149	0.218	0.276	0.362	0.481	0.418
6.0	0.143	0.211	0.262	0.351	0.454	
8.0	0.111	0.162	0.193	0.288	0.321	
10.0	0.847E−01	0.121	0.151	0.227	0.223	
12.0	0.683E−01	0.976E−01	0.121	0.173	0.162	
13.3	0.595E−01	0.846E−01	0.107	0.148	0.151	
15.0	0.493E−01	0.694E−01	0.093	0.121		
20.0	0.314E−01	0.439E−01	0.059	0.070		
23.3	0.240E−01	0.340E−01	0.043	0.061		
25.0	0.208E−01	0.301E−01	0.039			
30.0	0.146E−01	0.222E−01	0.030			
35.0	0.107E−01	0.168E−01	0.022			
40.0	0.798E−02	0.128E−01	0.017			
43.3	0.667E−02	0.108E−01	0.016			
50.0	0.505E−02	0.819E−02				
60.0	0.342E−02	0.598E−02				
65.0	0.285E−02	0.548E−02				
68.3	0.254E−02	0.537E−02				
80.0	0.184E−02					
100.0	0.123E−02					
118.3	0.108E−02					
σ_i	3.22	4.81	5.29	6.45	6.10	4.40
σ_i^{SEG87}	3.43	4.62	5.40	6.13	5.78	4.30
σ_i^{S92}	5.04	6.72	7.67	9.44	7.32	4.41

The labels j_{first} and j_{last} are the first and last j values for energies for each l within the integration region, $0 < \epsilon_{j_{first}}, \epsilon_{j_{first}+1}, \ldots, \epsilon_{j_{last}-1}, \epsilon_{j_{last}} < E_0$. The integration weights w_j satisfy

$$\int_0^{E_0} d\varepsilon = \sum_j w_j = E_0. \tag{9}$$

The sum of σ_{nl}^N in (4) contains the sum $\sum_n |nl\rangle\langle ln|$ via (3). Therefore the l-manifold SDCS are related to the σ_{nl}^N via

$$\int_0^{E_0} d\varepsilon \frac{d\sigma^l(\varepsilon)}{d\varepsilon} = \sum_{n,\epsilon_{nl}>0} \sigma_{nl}^N \approx \sum_n w_n \frac{d\sigma^l(\epsilon_{nl})}{d\varepsilon}. \tag{10}$$

Using the above considerations we define the l-manifold SDCS for a set of $\epsilon_{nl} > 0$ as

$$\frac{d\bar{\sigma}^{lN}(\epsilon_{nl})}{d\varepsilon} = \frac{\sigma_{nl}^{N}}{w_n^l}. \tag{11}$$

In order to extract the SDCS with sufficient accuracy, we require enough open channels with $\epsilon_{nl} > 0$. For an arbitrary ε the $d\bar{\sigma}^{lN}(\varepsilon)/d\varepsilon$ can be found by interpolating between $d\bar{\sigma}^{lN}(\epsilon_{nl})/d\varepsilon$. The singly-differential cross section for a particular ε is found by

$$\frac{d\bar{\sigma}^{N}(\varepsilon)}{d\varepsilon} = \sum_l \frac{d\bar{\sigma}^{lN}(\varepsilon)}{d\varepsilon}. \tag{12}$$

Another important consideration is that the theoretically obtained SDCS ($d\sigma/d\varepsilon$), as well as the l-manifold cross sections ($d\sigma^l/d\varepsilon$), should be symmetric around $E/2$ since the electrons are indistinguishable. In other words, the probability of finding one electron with the energy ε is the same as with $E - \varepsilon$. However, this is not the case for the $d\bar{\sigma}^{lN}(\epsilon_{nl})/d\varepsilon$ since in the CCC formalism the T-matrix elements in (2) have a plane wave for one electron and a square-integrable function for the other. The required symmetry is restored by simple numerical symmetrization

$$\frac{d\sigma^{N}(\varepsilon)}{d\varepsilon} = \sum_l \frac{1}{2}\left(\frac{d\bar{\sigma}^{lN}(\varepsilon)}{d\varepsilon} + \frac{d\bar{\sigma}^{lN}(E-\varepsilon)}{d\varepsilon}\right). \tag{13}$$

The difficult task of measuring the doubly differential cross sections for e–H ionization has been recently performed by Shyn (1992). These measurements have been integrated to obtain singly differential, then integrated again to obtain the corresponding total ionization cross sections (TICS). This method of obtaining TICS results in a relatively large error. On the other hand, the TICS for this system have been measured from 14.6 to 4000 eV with high accuracy by Shah *et al* (1987). The CCC results are in excellent agreement with the latter measurements (Bray and Stelbovics 1993), presented in figure 1. In this figure we have also presented the results of our current calculations using bases different from those used earlier. We see that convergence to a few per cent in the TICS is easily achieved in the CCC method. In the present calculations we have used around 12 states for each target state l, with $l_{max} = 2$. The exponents of the Laguerre basis within each l were varied in order to ensure that approximately half of the states had energies in the region $0 < \epsilon_{nl} < E$.

For the purpose of comparing our SDCS with the measurements of Shyn (1992), we suppose that the TICS of Shah *et al* (1987) are the most accurate. We therefore renormalize the experimental SDCS of Shyn (1992) so that the TICS (σ_i^{S92}) obtained by numerical integration give the same results as those of Shah *et al* (1987) (σ_i^{SEG87}), see table 1. After numerically integrating the SDCS of Shyn (1992) we multiply these by the $\sigma_i^{SEG87}/\sigma_i^{S92}$ factor.

The SDCS are presented in figure 2 for the first half of the secondary electron energy region $0 < \varepsilon < \frac{1}{2}E$. At 25 eV we present an example of the unsymmetrized SDCS (4) where $0 < \varepsilon < E$. Note that at $\frac{1}{2}E$ both the symmetrized and the unsymmetrized cross sections are the same. We find generally excellent agreement with the experiment. Quantitative SDCS are given in table 1. Also presented are the DWBA calculations of Konovalov and McCarthy (1992). These are also in very good agreement with experiment. The DWBA therefore provides a simple picture of the ionization process: 'The slower-moving electron feels the whole charge of the ion while the faster-moving electron feels zero charge at large distances, since the ion is screened by the slow electron'. However in the energy

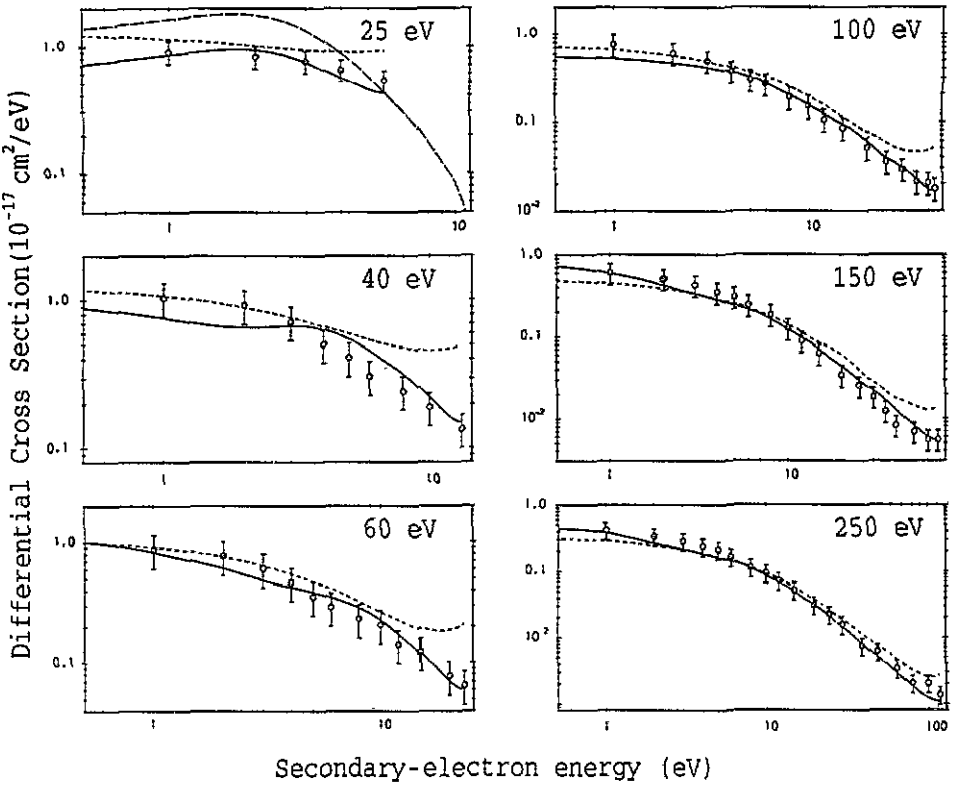

Figure 2. Singly-differential cross sections ($d\sigma/d\epsilon$) for the electron impact ionization of atomic hydrogen. The full curve is the CCC calculation. The long-broken curve denotes an example of the unsymmetrized singly-differential cross section, see text. The short-broken curve denotes the DWBA calculations of Konovalov and McCarthy (1992). The renormalized measurements of Shyn (1992) are denoted by O.

regions where the two outgoing electrons have similar energies, the DWBA calculations are systematically too high.

In conclusion, we have demonstrated that the SDCS may be obtained directly from the close-coupling formalism, so long as large enough basis sizes are used to get a sufficient number of L^2 states with positive energies. To our knowledge, this has been the first time that the close-coupling formalism has been applied to the calculation of SDCS.

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