RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 50, NUMBER 4 OCTOBER 1994

Calculation of triple-differential cross sections in electron scattering on atomic hydrogen

Igor Bray,* Dmitry A. Konovalov, and Ian E. McCarthy
Electronic Structure of Materials Centre, The Flinders University of South Australia, G.P.O. Box 2100, Adelaide 5001, Australia

Andris T. Stelbovics
Centre for Atomic, Molecular and Surface Physics, School of Mathematical and Physical Sciences, Murdoch University, Perth 6150, Australia

(Received 4 March 1994)

We present calculations of triple-differential cross sections (TDCS) for electrons scattering on the ground state of atomic hydrogen at incident energies of 54.4 and 150 eV. The convergent close-coupling method is used. For this target the method is fully *ab initio*. The total wave function is expanded in an ever increasing Laguerre basis until convergence in the TDCS has been obtained. We generally find good agreement with experiment, though some small quantitative discrepancies remain.

PACS number(s): 34.80.Dp

The recent development of the convergent close-coupling (CCC) method for e-H scattering by Bray and Stelbovics [1] has taken the close-coupling formalism to its logical conclusion. Rather than expanding the total wave function in a complete set of exact target discrete and continuous states, the expansion functions are obtained by diagonalizing the target Hamiltonian in a large Laguerre basis which can be extended to completeness. This ensures that the generated states are all square-integrable, allowing for the application of standard close-coupling techniques, and making the CCC method equally applicable at all projectile energies. The utility of the method relies on being able to obtain convergence in the observable of interest as the size of the basis is increased. Since the method is based on the close-coupling formalism it provides complete calculations in the sense that all transitions such as elastic, inelastic, ionization, and total cross sections are calculated simultaneously.

The CCC method has been widely applied to various problems in atomic physics. For example, it is able to provide quantitative agreement with the Poet-Temkin model [2,3] of e-H scattering, where only states of zero orbital angular momentum are considered [4]. This validated the use of square-integrable states and showed that pseudoresonances, typically associated with the use of square-integrable expansions, disappeared as the basis size was increased. A similar conclusion was drawn by Scholz [5] using the intermediate energy R-matrix method, and by Konovalov and McCarthy [6] using the J-matrix method. Another most important achievement of the method, which is particularly relevant to this work, is the quantitative agreement with the measurements of the total ionization cross section and spin asymmetry in e-H scattering [7].

The method has also been generalized to incorporate hydrogenlike targets, atoms, or ions [8]. This provided for a more sensitive application of the method due to the availability of spin-resolved measurements [9] at a wide range of energies in e-Na scattering. The CCC theory [8] is the only one that is able to obtain almost complete quantitative agreement with these measurements. In these calculations the effects of exchange and continuum were found to be very large, and were handled very accurately by the CCC formalism. More recently, the CCC method has been applied to e-He scattering at 30 eV [10], where it is the only one that is able to achieve quantitative agreement with the $n=1,2,3$ differential cross sections.

In our view the CCC method is the most generally successful reliable method for the description of electron scattering on helium and hydrogenlike targets at all projectile energies, and for any transition of interest. For the single-electron targets (H, He^+, ...), where the target wave functions are known exactly, the nonrelativistic electron scattering problem may be solved numerically to a required accuracy without approximation.

In this work we expand the application of the method to the calculation of $(e,2e)$ differential cross sections. The extension is very straightforward and in principle leads to an *ab initio* method for the calculation of $(e,2e)$ processes for hydrogenlike targets whose validity is independent of projectile energy. Here we restrict ourselves to atomic hydrogen as the target.

Close-coupling methods have already been applied to the calculation of $(e,2e)$ reactions by Curran and Walters [11] and Curran, Whelan, and Walters [12]. They used a small set of square-integrable pseudostates, which were chosen to give a good description of scattering to low-lying discrete states [13]. The usage of an orthogonal Laguerre basis allows us to test the convergence by simply increasing the basis size, without encountering any linear dependence problems associated with nonorthogonal bases.

The $(e,2e)$ problem for atomic hydrogen has attracted a great deal of attention. Brauner, Briggs, and Klar [14] used an approximate final-state wave function, which has the correct Coulomb three-body boundary conditions. This yielded generally good agreement with experiment at high energies, but had considerable difficulties in describing both shape and magnitude at the lower energies. Jones *et al.* [15] have followed a similar approach by including short-range effects in the incident wave function and using a different electron-electron correlation factor for the outgoing electrons, while

*e-mail: igor@esm.ph.flinders.edu.au

still maintaining the three-body boundary condition. This resulted in some improvement in the magnitude of the calculated cross sections. The close-coupling approach to electron-hydrogen scattering relies on being able to achieve convergence in the full expansion of the target discrete and continuous spectrum. In this work we provide an outline of such an approach.

The total wave function $|\Psi^{S(+)}\rangle$, where S is the total spin, and the notation $(+)$ indicates incoming plane-wave and outgoing spherical-wave boundary conditions, may be written as [1]

$$|\Psi^{S(+)}\rangle \simeq |0\boldsymbol{k}_0\rangle + \sum_{l,n}^{l_{\max},N_l} \int d\boldsymbol{k} \frac{|nl\boldsymbol{k}\rangle\langle kln|T^S|0\boldsymbol{k}_0\rangle}{E^{(+)}-\epsilon_{nl}-k^2/2}, \quad (1)$$

where $|\boldsymbol{k}_0\rangle$ is a plane wave denoting the the incident projectile with momentum $\boldsymbol{k}_0$, $|0\rangle$ indicates the incident target state, E is the total energy, and the $|nl\rangle$ states with corresponding energy ϵ_{nl} are obtained from the diagonalization of the target Hamiltonian. The sense of Eq. (1) is that the equality is achieved only in the limit $l_{\max},N_l\rightarrow\infty$. As the left-hand side of the T^S matrix contains only square-integrable states, which are associated with discrete energies (and hence momenta), one cannot apply it directly to the calculation of $(e,2e)$ differential cross sections. Instead one needs an interpolative method for arbitrary allowed momenta $\boldsymbol{k}_a$, $\boldsymbol{k}_b$. We define the required T matrix by

$$\langle \boldsymbol{k}_a\chi^{(-)}(\boldsymbol{k}_b)|T^S|0\boldsymbol{k}_0\rangle = \langle \boldsymbol{k}_a\chi^{(-)}(\boldsymbol{k}_b)|I_2V^S|\Psi^{S(+)}\rangle, \quad (2)$$

where V^S is given by [1]

$$V^S = V_1 + V_{12} - E\,\theta I_1 + (-1)^S[H - E(1-\theta)]P_r, \quad (3)$$

and is used to obtain the T matrix in Eq. (1). Here H is the total Hamiltonian, P_r is the space-exchange operator, V_1 is the Coulomb potential in projectile space, and V_{12} is the electron-electron potential. Any nonzero constant θ leads to a unique T matrix [1]. The operators I_1 and I_2 are the identity operators in the designated space. For the outgoing electrons $\boldsymbol{k}_a$ and $\chi^{(-)}(\boldsymbol{k}_b)$ we use a plane and a Coulomb wave, respectively. In the case of target eigenstates $|f\rangle$ (discrete or continuous) the T matrix (2) reduces to the usual result

$$\langle \boldsymbol{k}_a f|T^S|0\boldsymbol{k}_0\rangle = \langle \boldsymbol{k}_a f|(\ _1 + \checkmark_{12})[1+(-1)^S P_r]|\Psi^{S(+)}\rangle. \quad (4)$$

In our discretization of the target space we replace I_2 in Eq. (2) by the projection onto the target-space identity operator $I_2^N = \Sigma_{l,n}^N |nl\rangle\langle ln|$, which ensures that a square-integrable representation of $|\chi^{(-)}(\mathbf{k}_b)\rangle$ is used. We use $N = \Sigma_{l=0}^{l_{\max}} N_l$ to denote the full set of states. The T matrix in Eq. (2) may be readily evaluated once the time-consuming part of the calculation, solution of (1), has been completed using a partial-wave expansion [1]. We note that if $\langle\chi^{(-)}(\boldsymbol{k}_b)|$ in (2) is replaced by any of the coupled states $\langle ln|$, then the original $\langle kln|T^S|0\boldsymbol{k}_0\rangle$ used in (1) is obtained.

Now we turn to the consideration of convergence in the results as the basis size N is increased. A major difference between scattering and $(e,2e)$ calculations is that in the former case the target states in the required T matrix elements have small orbital angular momentum l. Often taking $l \leq l_{\max} = 3$ in the coupled set of states is sufficient for convergence in the required scattering T matrix. However, in $(e,2e)$ calculations this is rarely so. We require as many target-space l as are necessary to adequately describe the slowest of the outgoing electrons (the orbital angular momentum L of the fast electron may be arbitrarily large). Depending on the kinematics, l may readily exceed 10 (not to be confused with $l_{\max}$). There are no problems with existence of integrals for $0 \leq l \leq l_{\max}$ due to the projection operator I_2^N. For l larger than $l_{\max}$ in the partial-wave expansion of $\langle\chi^{(-)}(\boldsymbol{k}_b)|$ we only calculate the direct contribution, dropping the square-integrable representation of I_2. In this way we circumvent the problem of nonexistent integrals (see last paragraph on page 344 of Curran and Walters [11] for more detail). For higher energies, in the present very-asymmetric kinematics, direct scattering is dominant and is included for all l necessary to describe the slower of the two outgoing electrons. The exclusion of exchange for larger l may be tested by varying $l_{\max}$ in the close-coupling formalism, and based on these tests the $l_{\max}=4$ choice is adequate for the calculations in this paper.

There is another aspect of convergence that has to be tested. Given an $l_{\max}$ we must ensure that our results are stable, as the basis sizes N_l are increased within each l. We find that an optimal way of achieving this is by choosing the basis parameter λ_l for each N_l [8] such that one of the resulting states has the same energy as the slow electron. Taking an initial $\lambda_l \approx 1$, typically after ten iterations, the required energy for one of the states may be achieved to six-figure accuracy, with the final λ_l having only varied from the initial one by no more that 10%. This way we find that taking a few more than ten states within each l is sufficient to obtain convergence in the presented calculations. This reduces the problem of convergence to just a variation of $l_{\max}$.

In this paper we provide calculations for 150 and 54.4 eV electron-impact ionization of atomic hydrogen. At the former energy there are relative measurements (normalized experimentally) of the triply differential cross sections (TDCS) for three angles of the fast electron and three energies of the slow electron [16]. Using a nine-state pseudostate calculation, Curran, Whelan, and Walters [12] demonstrated the large effect of the second term in (1), which brought about very good, but not quite perfect, agreement with experiment. They demonstrated a significant difference between the magnitudes of their results and those of Brauner, Briggs, and Klar [14], and requested further theoretical and experimental work in order to resolve the remaining discrepancies. We are able to provide accurate results at this energy by performing much larger calculations than those of Curran, Whelan, and Walters, demonstrating convergence in the close-coupling formalism.

At the 54.4-eV projectile energy there are unnormalized relative measurements of the TDCS for four angles of the fast electron and one energy of the slow electron [17]. Here Jones *et al.* [15], following the work of Brauner, Briggs, and Klar [14] and Brauner *et al.* [17] demonstrated that simply adding the three-body Coulomb boundary condition to the distorted-wave Born approximation (DWBA) results in a very large effect bringing about qualitative agreement with experiment. Klar, Konovalov, and McCarthy [18] showed

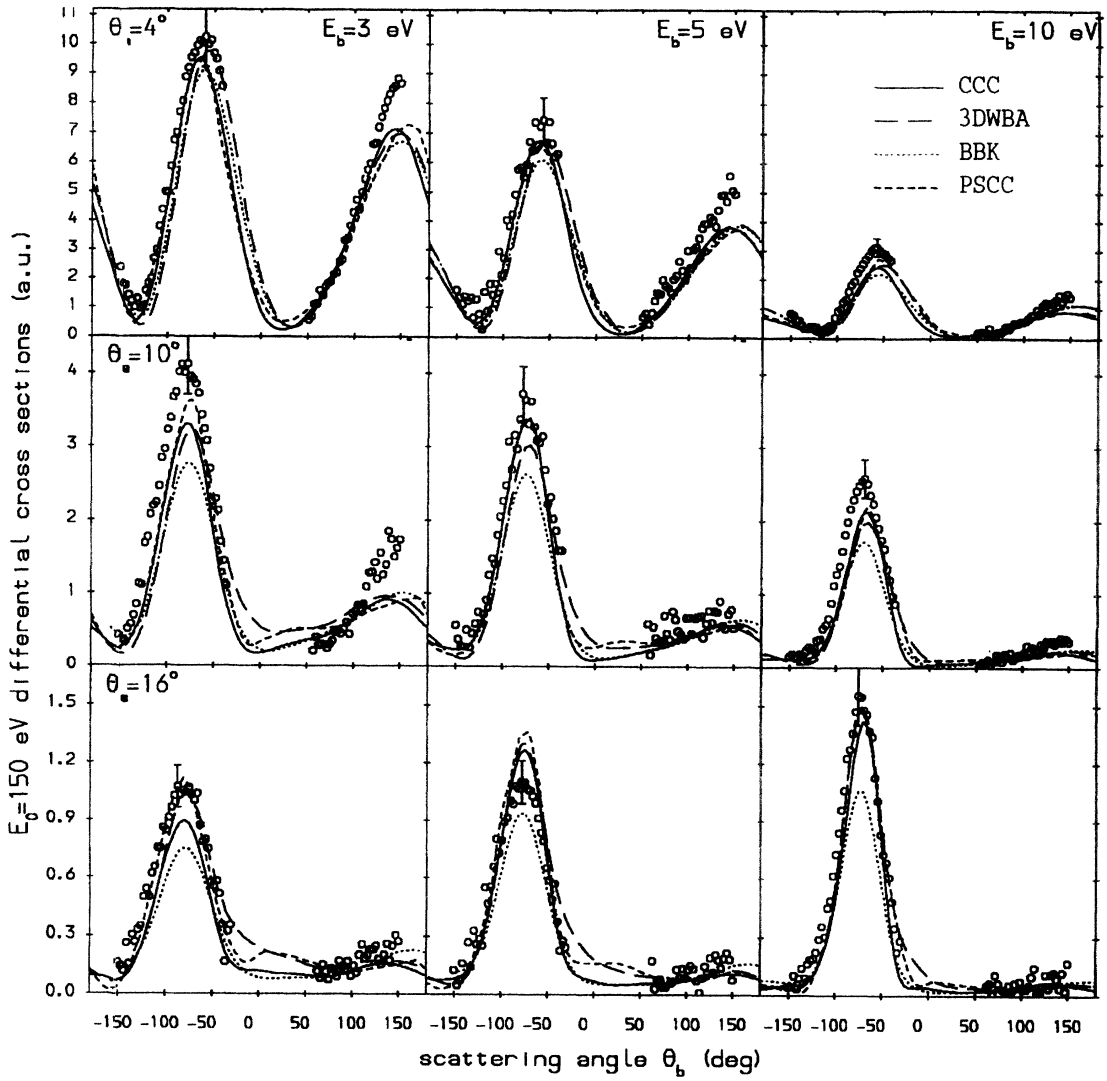

FIG. 1. Triply differential cross sections of e-H ionization at incident electron energy $E_0 = 150$ eV. The absolute measurements are due to Ehrhardt *et al.* [16]. The present calculations (CCC) have been obtained by coupling $13s$, $12p$, $11d$, and $10f$ states. The calculations denoted by 3DWBA, BBK, and PSCC are due to Jones *et al.* [15], Brauner, Briggs, and Klar [14], and Curran, Whelan, and Walters [12], respectively. Quantitative results may be obtained from the first author.

that it is not necessary to satisfy the final-state boundary condition if the initial-state boundary condition is satisfied. We are able to show that the very important electron-electron correlation may be readily treated via the close-coupling formalism.

In Fig. 1 we present our CCC calculations for a projectile energy of 150 eV. These have been obtained by coupling $13s$, $12p$, $11d$, and $10f$ states ($l_{\max}=3$). In describing the slow and fast electrons we used $l \leq 15$ and $L \leq 70$, respectively. We have established convergence by performing a sequence of smaller calculations. Our results (CCC) are compared with the experiment of Ehrhardt *et al.* [16] and calculations of Jones *et al.* [15] (3DWBA), Brauner, Briggs, and Klar [14] (BBK), and the close coupling with pseudostates calculation of Curran, Whelan, and Walters [12] (PSCC). We see that there is generally good qualitative agreement between all theories and experiment. Since the target is atomic hydrogen, we would expect complete quantitative agreement with our CCC calculations, as is the case for the total ionization cross section and spin asymmetry [7]. However, we see that this is not so. Comparison of the CCC and PSCC results shows that the latter were very nearly convergent. In our view any larger calculations than those presented would not yield significantly different results. The good agreement of the 3DWBA calculation with experiment and the CCC and PSCC calculations shows the improvement over the BBK in obtaining better magnitudes.

The 54.4-eV results are presented in Fig. 2. The measurements of Brauner *et al.* [17] are not absolute, though the normalization is the same for all four angles θ_a. As our calculations are able to reproduce the total ionization cross section [7], we are confident in the accuracy of the magnitude of our calculation, and so have normalized the experiment by best visual fit to the CCC calculations. These have been generated using $13s$, $12p$, $11d$, $10f$, and $9g$ states ($l_{\max}=4$). This is a 55-state calculation that generates as

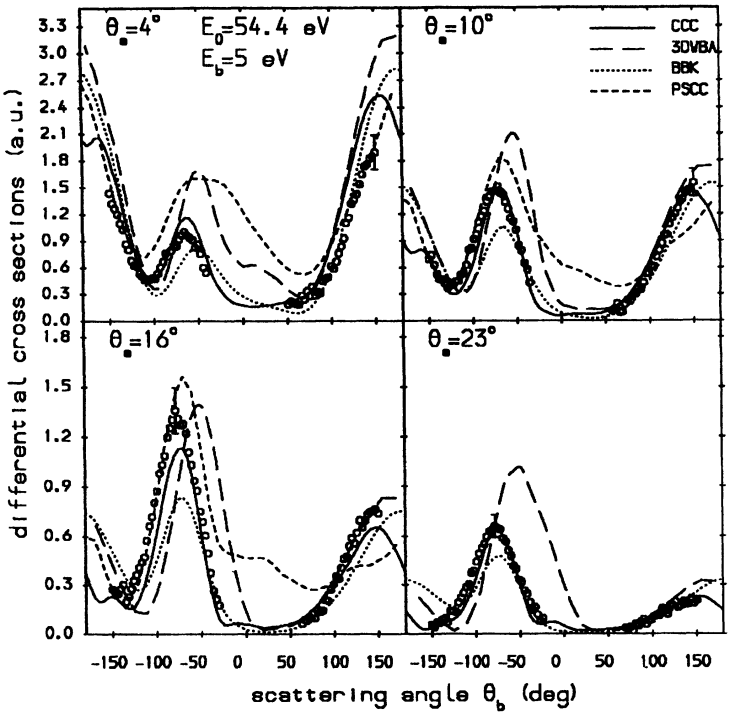

FIG. 2. Triply differential cross sections of e-H ionization at incident electron energy $E_0=54.4$ eV. The relative measurements of Brauner *et al.* [17] have been normalized using best visual fit to the CCC theory using a single multiplicative constant. The present calculations (CCC) have been obtained by coupling $13s$, $12p$, $11d$, $10f$, and $9g$ states. The calculations denoted by 3DWBA, BBK, and PSCC are due to Jones *et al.* [15], Brauner *et al.* [17], and Curran and Walters [11], respectively.

many as 155 channels, and using techniques outlined in Ref. [8] may be performed on a desktop workstation with 256M of core memory. The smaller projectile energy allows us to take $L \leq 40$. The agreement with experiment is very good, and is of the same quality as that at 150 eV, which is not the case for the other presented theories. The very large electron-electron correlation effects, as demonstrated by Jones *et al.* [15], are even better treated within the close-coupling formalism. The difference between the PSCC and CCC results indicates that the nine states used by Curran and Walters [11] are insufficient at this energy. Though the 3DWBA results are not in as good agreement with experiment as CCC they have considerably better magnitudes than the BBK results.

In conclusion, we found that we are able to obtain good agreement with the TDCS at 54.4- and 150-eV projectile energies. It is a little disappointing that we are unable to obtain complete quantitative agreement with the presented measurements, particularly at 150 eV, where convergence in the multichannel expansion is readily achieved, and the measurements have been put on an absolute scale [16]. Further experimental investigation would be very helpful. The application of the CCC method to the calculation of $(e,2e)$ TDCS at lower projectile energies is currently being undertaken, where early indications are that the larger electron-electron correlation effects will require bigger $l_{\max}$ in our calculations.

We are grateful to S. Jones, D. H. Madison, J. Röder, and J. Berakdar for communicating their data in electronic form. We would like to acknowledge support from the Australian Research Council and The Flinders University of South Australia.

[1] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[2] A. Temkin, Phys. Rev. **126**, 130 (1962).
[3] R. Poet, J. Phys. B **11**, 3081 (1978).
[4] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **69**, 53 (1992).
[5] T. T. Scholz, J. Phys. B **24**, 2127 (1991).
[6] D. A. Konovalov and I. E. McCarthy, J. Phys. B **27**, L407 (1994).
[7] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **70**, 746 (1993).
[8] I. Bray, Phys. Rev. A **49**, 1066 (1994).
[9] M. H. Kelley *et al.*, in *Correlation and Polarization in Electronic and Atomic Collisions and (e,2e) Reactions* (Institute of Physics, Adelaide, 1991), p. 23.
[10] I. Bray, D. V. Fursa, and I. E. McCarthy, J. Phys. B **27**, L421 (1994).
[11] E. P. Curran and H. R. J. Walters, J. Phys. B **20**, 337 (1987).
[12] E. P. Curran, C. T. Whelan, and H. R. J. Walters, J. Phys. B **24**, L19 (1991).
[13] W. C. Fon, K. A. Berrington, P. G. Burke, and A. E. Kingston, J. Phys. B **14**, 1041 (1981).
[14] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[15] S. Jones, D. H. Madison, A. Franz, and P. L. Altick, J. Phys. B **22**, 2265 (1989).
[16] H. Ehrhardt, K. Jung, G. Knoth, and P. Schlemmer, Z. Phys. D **1**, 3 (1986).
[17] M. Brauner *et al.*, J. Phys. B **24**, 657 (1991).
[18] M. Klar, D. A. Konovalov, and I. E. McCarthy, J. Phys. B **26**, L711 (1993).