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LETTER TO THE EDITOR

Comparison of convergent electron–hydrogen calculations

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Abstract. Integrated cross sections for the $n = 1$ and 2 states of atomic hydrogen are calculated by the convergent-close-coupling method for a range of closely spaced energies just above the $n = 2$ threshold. The cross sections are compared with those calculated by a pseudo-state calculation, and two other methods that also converge, in principle, to the exact result. These are the intermediate-energy R-matrix method and the convergent J-matrix method. Experimental data are described very well by all of these theories.

Three types of calculation that converge, in principle, to the exact solution of the electron–atom scattering problem are applied to the electron–hydrogen problem at energies just above the $n = 2$ excitation threshold.

The intermediate-energy R-matrix (IERM) method (Burke *et al* 1987) has recently been applied to this problem by Odgers *et al* (1995). In this method the Schrödinger equation for the interaction of two electrons and a proton is solved inside a spherical box, chosen so that exchange can be neglected in the external region. The solution is matched to external solutions with appropriate boundary conditions. Loss of flux into the continuum is accounted for by describing the motion of the atomic electron in terms of the same one-electron bound and continuum basis as is used to describe the motion of the scattering electron. R-matrix methods are convenient for calculating a range of closely spaced energies, once the internal solution has been computed.

Odgers *et al* display the effect of the target continuum in their calculation by comparing it with a 15-state R-matrix calculation by Fon *et al* (1995), which has essentially converged to the limit of a close-coupling calculation that couples only discrete channels. Just above the $n = 2$ threshold the effect of the continuum is a substantial reduction in the integrated cross sections for $n = 2$ excitations.

The J-matrix (JM) method (Broad and Reinhardt 1976) has been applied to hydrogen in a similar energy region by Konovalov and McCarthy (1994). In this method the Schrödinger equation for the scattering problem is solved in a square-integrable basis, for which both the atomic and scattering electron are represented by finite sets of Laguerre functions. Cross sections converge as the basis size is increased. Calculation of cross sections for a range of closely spaced energies involves little more computational labour than for a single energy.

The IERM results presented by Odgers *et al* (1995) and JM cross sections for $n = 2$ excitations differ, usually by up to 20% (Odgers *et al* 1995) in the energy range below

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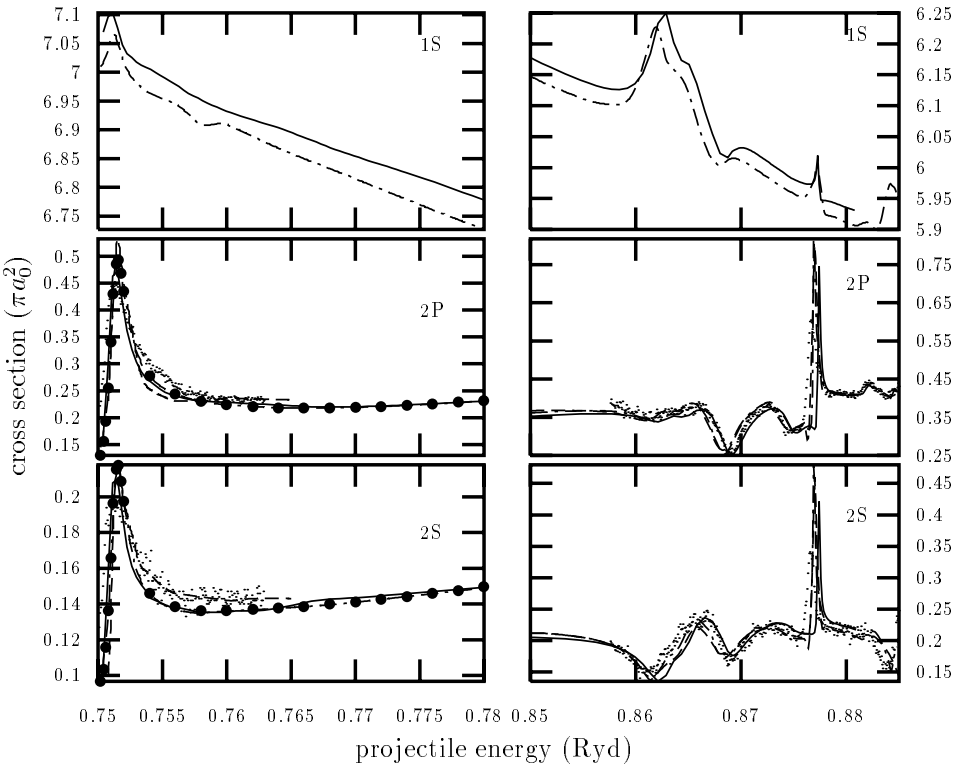

Figure 1. Integrated cross sections for electron impact excitation of the indicated states of atomic hydrogen. The curves are: ——, CCC (present); — · —, PS (Callaway 1982); – – –, JM (Konovalov and McCarthy 1994); corrected (see the text) •, IERM (Odgers *et al* 1995). The experiment of Williams (1988) is represented by the small dots.

0.78 Rydbergs. There is a similar discrepancy between the IERM calculations and a coupled-pseudostate calculation (PS) by Callaway (1982). The latter method is basis dependent but Callaway's calculation uses a basis that gives quite close agreement with the experimental data of Williams (1988).

The rather large discrepancies between these calculations made it interesting to try another method that converges, in principle, to the correct solution. This is the convergent-close-coupling (CCC) method of Bray and Stelbovics (1992), which solves the close-coupling equations for a finite set of square-integrable states that diagonalize the hydrogen-atom problem in a Laguerre basis. This method can be implemented to convergence in the form of coupled Lippmann–Schwinger integral equations in momentum space. It has produced remarkable agreement with a range of detailed experiments for spin-dependent and spin-independent quantities and fully differential and partially integrated ionization cross sections. The method is, in principle, simple. For a particular energy it can be implemented on a desktop workstation. More modern computing technology, utilizing clusters of workstations, makes calculations for a large range of closely spaced energies equally simple. This has hitherto been one of the advantages of IERM or JM.

In the present CCC calculations convergence at the 5% level has been achieved with a basis described by the number of target states for each orbital angular momentum, namely

8s, 6p, 4d, 2f and 1g. A constant value $\lambda = 1$ for the exponential fall-off factor (Bray and Stelbovics 1992) has been taken for all states. During the course of this work we have been informed by the authors that the earlier presentation of the IERM cross section results was incorrect, and have been kindly provided with the preliminary corrected data below 0.78 Rydbergs. The full corrected data set will be published in due course.

Figure 1 compares CCC with PS, and where possible with JM and the corrected IERM, for the 1s, 2s and 2p integrated cross sections in the energy ranges 0.75–0.78 Ryd and 0.85–0.885 Ryd. The theories are in good agreement with each other and the experimental data of Williams (1988). The earlier discrepancies found by Odgers *et al* (1995) have been clearly resolved, leading to a much more satisfactory situation from the theoretical point of view. Another use for a convergent calculation is to test methods that may be simpler, or more widely applicable, but still take into account all channels *ab initio*. Such a method is the coupled-channels-optical method, whose equivalent local implementation (Lower *et al* 1987) has been applied to the present problem by McCarthy and Shang (1992). For this method the $n = 2$ integrated cross sections differ only in minor detail from the CCC results.

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References

Bray I and Stelbovics A T 1992 *Phys. Rev.* A **46** 6995–7011
Broad J T and Reinhardt W P 1976 *J. Phys. B: At. Mol. Phys.* **9** 1491–502
Burke P G, Noble C J and Scott M P 1987 *Proc. R. Soc.* A **410** 289–310
Callaway J 1982 *Phys. Rev.* A **26** 109–208
Fon W C, Ratnavelu K and Aggarwal K M 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 2973–84
Konovalov D A and McCarthy I E 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** L741–7
Lower J, McCarthy I E and Weigold E 1987 *J. Phys. B: At. Mol. Phys.* **20** 4571–84
McCarthy I E and Shang B 1992 *Phys. Rev.* A **46** 3959–62
Odgers B R, Scott M P and Burke P G 1995 *J. Phys. B: At. Mol. Opt. Phys.* **8** 2973–84
Williams J F 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2107–16