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ELECTRON SCATTERING FROM HYDROGEN ATOMS AND H-LIKE IONS

K.A. BERRINGTON

Department of Applied Mathematics and Theoretical Physics, Queen's University, GB-Belfast BT7 1NN, Great-Britain

Résumé - Cette revue pour l'"Atomic Data Workshop" de Meudon (1-2 septembre 1989) est une mise à jour de l'atelier précédent (St. Catherine's College Oxford, 1987) pour ce qui est des données sur la diffusion des électrons par les atomes d'hydrogène et les ions hydrogénoïdes. Pour l'hydrogène, le nouveau calcul "Intermediate Energy R-Matrix" (IERM) de Scholz et al. devient la source recommandée de taux d'excitation pour les transitions $1s-2s$ et $1s-2p$; pour les ions hydrogénoïdes multichargés, les formules semi-empiriques de Sampson et Zhang sont recommandées.

Abstract - This review, for the "Atomic Data Workshop" held at Meudon 1-2 September 1989, provides an update on the last Workshop (at St Catherine's College Oxford, 1987) for data on electron scattering from hydrogen atoms and H-like ions. For hydrogen, the new "Intermediate Energy R-Matrix" (IERM) calculation by Scholz et al becomes the recommended source of excitation rates for the $1s - 2s$ and $1s - 2p$ transitions; for highly charged H-like ions Sampson and Zhang's semiempirical formulae are recommended.

1 - UPDATE SUMMARY, 1987-1989

Since the last Atomic Data Workshop held at St Catherine's College Oxford [1] there have been a number of publications describing new work on electron scattering from hydrogen atoms and H-like ions [2-12]. We concentrate here primarily on integrated cross sections and excitation rate coefficients, and these are summarised in the following subsections.

1.1 Electron-hydrogen scattering

- (a) Callaway [2] extended his pseudo-state calculations using the algebraic variational method to calculate $1s - 2s$ and $1s - 2p$ cross sections between the $n = 3$ and 4 thresholds of hydrogen.
- (b) Pathak et al [3,4] used the R-matrix method to analyse H^- resonances to the n -th hydrogenic threshold.
- (c) Bransden et al [5] used the Schwinger variational method to calculate $1s - 2s$ cross sections at intermediate energies.
- (d) Giovanardi and Palla [6] calculated low temperature electron excitation rate coefficients for $n = 1,2$ to $n = 2,3$ transitions using cross sections from Callaway et al.
- (e) Williams [7] provided experimental data on resonances between the $n = 2$ and $n = 3$ thresholds.
- (f) Scholz et al and Scott et al [8,9,10] developed an Intermediate Energy R-Matrix method (IERM) to calculate $1s-1s$, $1s-2s$ and $1s-2p$ cross sections at intermediate energies, and calculated the corresponding effective collision strength, which we reproduce in subsection 3.1.

1.2 Electron excitation of H-like ions

(g) Lengyel et al [11] analysed Feshbach resonances in the $1s - 2p$ transitions in He^+ .
 (h) Sampson and Zhang [12] derived simple semiempirical formulae for collision strengths and rate coefficients for $n - n'$ transitions in highly charged hydrogenic ions. They claim better than 25% accuracy for H-like ions with $Z \geq 10$ for the conditions of major interest for plasma modelling. The corresponding formulae for electron impact ionization cross sections and rate coefficients are also given with the effects of lowering of the continuum included.

2 - THE INTERMEDIATE ENERGY R-MATRIX METHOD (IERM)

The IERM method is fully described in [8,9,10]; essentially both the valence electron and the scattering electron is expanded in an R-matrix basis (rather than just the scattering electron as in the "traditional" R-matrix approach). Because the basis functions are finite on the boundary (unlike bound state orbitals which tend to decay rapidly at the boundary), the method can give a good representation of correlation effects at both small and large distances. Thus loss of flux to highly excited and ionisation channels can be accounted for. Clearly the method also offers a natural route to describe electron impact ionisation, since two continuum electrons are accounted for in the expansion of the total wavefunction.

For more complex atoms, where the target states require a configuration-interaction (CI) wavefunctions for an accurate representation, the method can be used to systematically improve the target state description by including R-matrix basis functions (which form a complete orthonormal set in the inner region) with no orthogonalization problems caused by extra correlation-type orbitals which are usually introduced in conventional bound-state codes.

These features of the IERM method make possible the systematic investigation of intermediate energy scattering to arbitrarily high accuracy; the limitation is computer power. Calculations on atomic systems other than hydrogen are only feasible on the next generation of parallel super-computers.

3 - RECOMMENDATIONS

3.1 Electron-hydrogen collision rates

The new IERM rates for $1s-2s$ and $1s-2p$ by Scholz et al [9] are therefore now recommended, and they presented their data in the form of an analytic fit for the effective collision strength (Υ) in the range 5000 - 500 000 K:

$$\Upsilon_{1s-2s}(X) = 0.045168 \ln(28.056X) \exp(-7.2945X) \\ + 0.24805 + 0.10044X - 0.011143X^2 - 0.0013432X^3 + 0.00037570X^4$$

where $X = kT$ in Rydbergs; and

$$\Upsilon_{1s-2p}(X) \\ = 0.36177 + 1.3891X + 0.50866X^2 - 0.38011X^3 + 0.10158X^4 - 0.010072X^5.$$

For electron excitation of the $n = 3$ states of hydrogen, the recommendation of the last Atomic Data Workshop report [1] remains: Callaway [13] and Callaway et al [14], or the derived rates of Giovanardi and Palla [6].

3.2 Electron collision rates for H-like ions

In the last Atomic Data Workshop report [1], Hayes compared intermediate-energy

collision strengths for $e^- - \text{He}^+$ for transitions up to the $n = 5$ levels in order to assess the accuracy of various approximations. Bearing in mind the inadequacy of their results at intermediate energies which Hayes showed, Hummer and Storey [15] remain the recommended source of rate coefficients for excitation of $n = 3$ states in He^+ . Also there is no change to the recommendation of Zygelman and Dalgarno [15] for electron and proton collision rates among the $n = 2$ fine-structure levels of He^+ , C^{5+} , Mg^{11+} , S^{15+} and Ar^{17+} .

The Sampson and Zhang [12] semiempirical formulae are now recommended for electron collision rates for highly charged H-like ions.

4 - CONCLUSION

It is clear that further theoretical work is needed on intermediate energy scattering for H-like ions in order to improve the accuracy of rate coefficients over a useful temperature range. Experimental determinations of cross sections are also needed as a check on the theory.

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