Excitation of hydrogen atoms by electron impact at intermediate energies

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The cross sections for the $1s$-$2s$ and $1s$-$2p$ transitions in atomic hydrogen have been calculated for electron impact energies in the range 12–20 eV using a pseudostate expansion.

This note supplements a previous discussion[1] of electron-hydrogen scattering in the intermediate energy range by reporting our results for the $1s$-$2s$ and $1s$-$2p$ excitation cross sections in the range from 12 to 20 eV using the algebraic variational method[2,3] and a pseudostate expansion. Our earlier paper presented results for elastic scattering from 10 to 30 eV, and for $1s$-$2s$ and $1s$-$2p$ excitation from 10 to 12 eV. The calculations reported in that paper have been extended by computations for states of total angular momentum $L=3$. These states do not make a significant contribution to the elastic scattering (~1%), but are of considerable importance in the excitation of the $2p$ state. The contributions from states of $L \geqslant 4$ have simply been estimated using the partial-wave Born approximation with exchange. The results would be changed by not more than 6% if the contributions for $L \geqslant 4$ were obtained from close-coupling calculations[4] instead of the Born-exchange approximation. We have terminated the present calculation at 20 eV since for energies greater than this, the Born-approximation contribution for $L \geqslant 4$ to the $2p$ excitation cross section becomes large, and the results correspondingly unreliable.

Our calculations are based on an eleven-state expansion, including the exact $1s$, $2s$, $2p$, and $3d$ states plus seven pseudostates (three of s-type, three of p-type, and one d-type). The pseudochannels are allowed to be open; however, the parameters of the pseudostates are varied to some extent to avoid spurious resonances associated with the opening of pseudochannels. Details of our method including parameters of the basis functions can be found in Ref. 1.

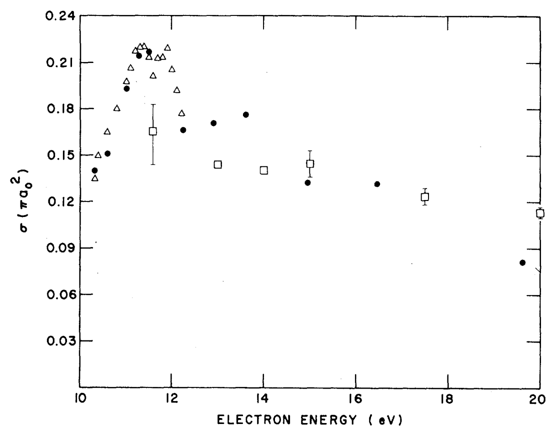

FIG. 1. Cross section for $1s$-$2s$ excitation (units, πa_0^2). The present results are indicated by solid circles, ●. Some experimental points as determined from published graphs are shown as open squares, □ (Ref. 7) and triangles, △ (Ref. 6).

Tables I and II contain the partial and total cross sections for the $1s$-$2s$ and $1s$-$2p$ transitions, respectively.[5] The accuracy of the results is not as great as that obtained in the case of elastic scattering. The elastic cross section is dominated by large contributions from the $L=0$, $S=1$ and $L=1$, $S=1$ states. These contributions do

TABLE I. $1s$-$2s$ excitation cross sections (units of πa_0^2) in the range $k^2=0.90$–1.44 (a.u.). Factors of $\frac{1}{4}(2S+1)$ are included.

k^2	$L=0$ $S=0$	$L=0$ $S=1$	$L=1$ $S=0$	$L=1$ $S=1$	$L=2$ $S=0$	$L=2$ $S=1$	$L=3$ $S=0$	$L=3$ $S=1$	$L\geq 4$ Born Exchange	Total
0.90	0.045	0.0021	0.013	0.034	0.051	0.008	0.004	0.009	0.000	0.166
0.95	0.043	0.0026	0.009	0.048	0.043	0.011	0.006	0.008	0.000	0.171
1.00	0.038	0.0029	0.013	0.048	0.047	0.013	0.008	0.006	0.000	0.176
1.10	0.029	0.0033	0.011	0.035	0.024	0.016	0.010	0.004	0.000	0.133
1.21	0.027	0.0034	0.017	0.035	0.018	0.017	0.012	0.003	0.000	0.132
1.44	0.014	0.0038	0.016	0.022	0.004	0.013	0.007	0.000	0.001	0.081

TABLE II. $1s$-$2p$ excitation cross sections (units of πa_0^2) in the range $k^2=0.90$–1.44. Factors of $\frac{1}{4}(2S+1)$ are included.

k^2	$L=0$ $S=0$	$L=0$ $S=1$	$L=1$ $S=0$	$L=1$ $S=1$	$L=2$ $S=0$	$L=2$ $S=1$	$L=3$ $S=0$	$L=3$ $S=1$	$L\geq4$ Born Exchange	Total
0.90	0.019	0.0016	0.071	0.038	0.137	0.015	0.013	0.061	0.013	0.369
0.95	0.028	0.0024	0.056	0.037	0.143	0.016	0.018	0.075	0.028	0.404
1.00	0.020	0.0031	0.070	0.025	0.198	0.023	0.023	0.082	0.049	0.493
1.10	0.027	0.0044	0.051	0.023	0.122	0.025	0.032	0.096	0.104	0.484
1.21	0.022	0.0059	0.053	0.020	0.137	0.028	0.043	0.102	0.176	0.587
1.44	0.018	0.0078	0.039	0.013	0.080	0.035	0.045	0.109	0.335	0.682

not depend strongly on either the parameters of the pseudostates or on the type of variational procedure employed [Kohn, inverse Kohn, OMN (optimized minimum norm), OAF (optimized, anomaly free)]. The smaller excitation cross sections show greater scatter. The results from different variational approaches differ by as much as ±10% in some instances. We have averaged the cross sections from the methods used in obtaining the results presented in the tables; however, obvious anomalies were excluded. Other uncertainties result from the choice of pseudostates. Results at $k^2=1.0$ were obtained from a different set of pseudostates (variant 2 of Table II of Ref. 1) in order to avoid a threshold, and the cross sections at this energy seem somewhat too high.

Our calculated cross sections are shown in Figs. 1 and 2 where they are compared with experimental results due to Kochsmeider *et al.*[6] and Kauppila *et al.*[7] for the $1s$-$2s$ transition and of McGowan *et al.*[8] and Williams and Willis[9] for the $1s$-$2p$ transition. Our results in the 10–12 eV range, as reported in Ref. 1, are also included in the figures. It is seen that there is a substantial but by no means perfect, degree of agreement between our calculations and the experimental results. We believe that the degree of agreement is sufficient to indicate that the pseudostate approach can work rather well in a region of energies in which other methods fail. Finally, we note that our results are in good agreement with the previous pseudostate calculations of Geltman and Burke[10] and in general agreement with those of Burke and Webb[11] ($1s$, $2s$, $2p$ plus two open pseudostates) where the energy ranges overlap. They are substantially lower than the cross sections obtained in the three-state close-coupling approximation.[4]

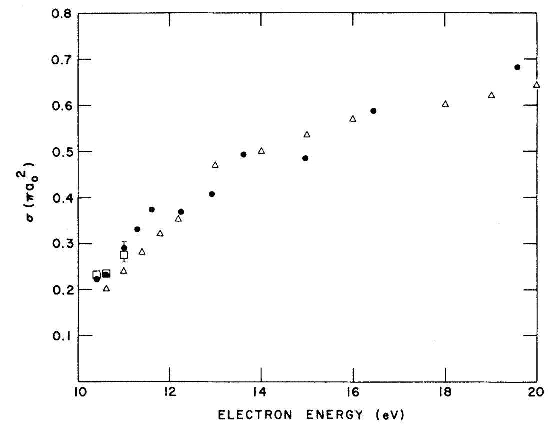

FIG. 2. Cross section for $1s$-$2p$ excitation (units πa_0^2). The present results are indicated by solid circles, ●. Some experimental points as determined from published graphs are shown as open squares, □ (Ref. 9) and triangles, △ (Ref. 8).

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[1]J. Callaway and J. W. Wooten, Phys. Rev. A 9, 1924 (1974). We take this opportunity to correct some typographical errors in that paper. S_{il} above Eq. (12b) should be s_{ip}; l in Eq. (12b) should be l_i, l in Table II should be l_a; (16) and (17) at the bottom of column 1 of p. 1927 should be (17) and (18); $L\leq3$ in column 2 of p. 1929 should be $L\geq3$; the exponents of Eq. (12a) are listed in Table V, not Table IV, and S. Ormonde's name is misspelled in Ref. 20.

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[4]P. G. Burke, H. M. Schey, and K. Smith, Phys. Rev. 129, 1258 (1963).

[5]Additional tables of complex transition amplitudes can

be obtained from the authors, or from ASIS/NAPS (NAPS document No. 02526; 5 pages of supplementary material). Order from National Auxiliary Publication Service, c/o Microfiche Publications, 440 Park Avenue South, New York, NY 10016. Remit in advance for each NAPS accession number $1.50 for microfiche or $5.00 for photocopies up to 30 pgs. Make checks payable to Microfiche Publications.

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