Calculation of proton-impact excitation of the $n=4$ level of atomic hydrogen

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Differential and integrated cross sections summed over all angular momentum sublevels are calculated for the process $H^{+}+H(n=1)\rightarrow H^{+}+H(n=4)$ in the incident-proton energy range 15–400 keV, employing the Glauber approximation. The integrated cross sections are in very good agreement in curve shape with the available experimental measurement. Results are also presented for the integrated Glauber cross sections for $1s$-$4d$ and $1s$-$4f$ excitations of hydrogen by proton impact and are compared with available theoretical results.

The theoretical study of the fundamental ion-atom collision process involving a proton and a hydrogen atom has so far received a lot of interest because it can provide a meaningful test of the validity of the approximations underlying a theoretical approach when compared with the experimental observations. For excitation of the $n=2$ and 3 levels of hydrogen by proton impact, cross sections integrated over the scattering angle have been calculated by a number of authors.[1–6] The only measurement by Park *et al.*[7] in the intermediate- through high-energy region does not, however, distinguish between the sublevels. Comparison between theory and experiment shows that quite good agreement with the shape of the curves of the observed cross sections is given by the Glauber and distortion calculations.[7] For excitation to $n=4$ states, however, the only existing calculation employing a second-order–diagonalization (SOD) method[4] showed very poor agreement with the measurement.[7] This calls for further theoretical studies of the $n=4$ excitations, whereby the reliability of the experimental data can also be judged.

Since the knowledge of the differential cross sections for a collision phenomenon can provide a better understanding of the physical process concerned, a number of recent theoretical studies[8–10] have been undertaken for the calculation of angular differential cross sections in fundamental ion-atom collisions. Moreover, the difficulties associated with the measurement of such cross sections have recently been removed[11,12] and comparison between calculated and observed angular differential cross sections have become possible. For proton-impact excitation of the $n=2$ levels of hydrogen, the observed data[11] are in excellent agreement with the Glauber calculations.[2]

In the present work we study the direct collisional excitation of the $n=4$ levels of hydrogen by the impact of protons using the Glauber approximation (GA) and present the differential and total cross sections summed over all sublevels. We also present the integrated cross sections for each of the individual sublevel excitations.

The Glauber scattering amplitude[13] for the $1s$-nlm excitation of hydrogen by charged particle impact has been reduced to computable forms by several authors.[5,6,14,15] Since we are presently interested in the excitation of a relatively low-lying level ($n=4$), the closed-form expression obtainable from the work of Thomas and Franco[5] (see also Ref. 6) is the most suitable here, and we employ the same in our calculation.

Our results of the center-of-mass Glauber differential cross sections for excitation of the $n=4$ states of hydrogen summed over all sublevels are presented graphically in Figs. 1 and 2 for 30-, 50-, and 100-keV protons. We also calculate and include in these figures the cross sections in the first Born approximation (FBA).

As regards the relative magnitudes of the individual sublevel excitation cross sections (not presented here), the predominating contribution in the forward direction comes from the optically allowed p-state transitions. With increasing angle, however, the $1s$-$4p$ differential cross sections decrease at a faster rate than the $1s$-$4s$ cross sections and eventually fall below the latter results. At relatively larger scattering angles, the $1s$-$4s$ excitation makes the highest contribution, as manifested from the differential cross sections. The $1s$-$4s$ and $1s$-$4d$ cross sections are comparable in magnitudes at small scattering angles and contribute a total of more than 10% to the net $n=4$ differential cross sections summed over all sublevels. The differential cross sections for $1s$-$4f$ excitation are, however, always small, never amounting to more than 0.1% of the above sum.

Comparison between the Glauber and FBA differential cross sections for $n=4$ excitations (cf. Figs. 1 and 2) shows that at high energies the two results agree in absolute magnitude as well as in angular dependence for small-angle scattering. With increasing angle, however, the FBA results fall more sharply than the GA results. It may here be recalled that a

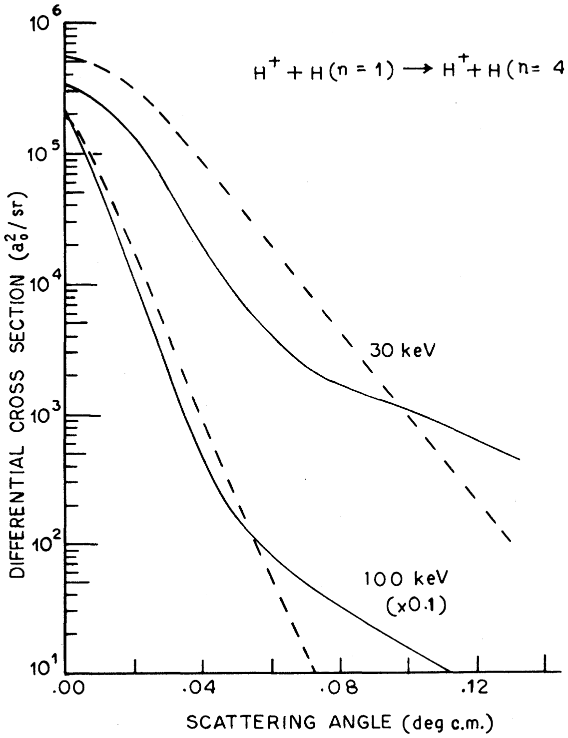

FIG. 1. Center-of-mass differential cross sections for excitation of $n=4$ levels of hydrogen by 30- and 100-keV protons. ——, Glauber approximation; – – –, first Born approximation.

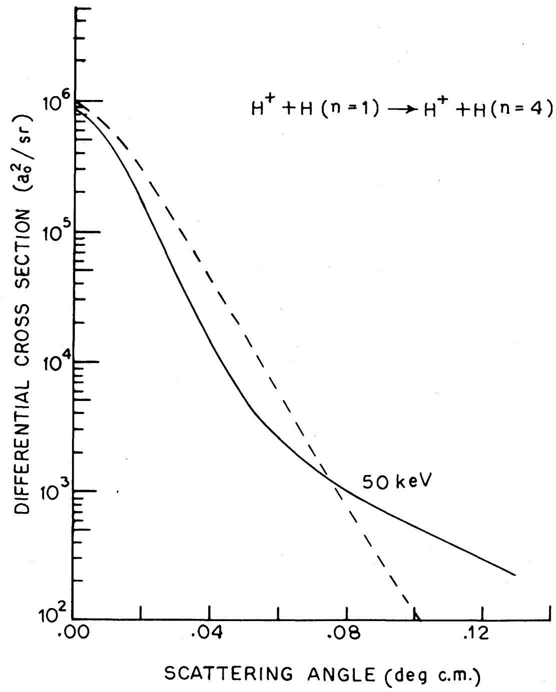

FIG. 2. Same as Fig. 1, but for 50-keV protons.

similar relative behavior of the FBA and GA cross sections has earlier been obtained for $n=2$ excitations of hydrogen as well, where the Glauber results show excellent agreement with the experimental measurements.[11] It would be interesting to compare our present calculated curve shapes for $n=4$ excitations with the experimental measurements.

In Table I we compare our integrated GA and FBA cross sections with the SOD results of Baye and Heenen[4] for each of the $1s$-$4l$ ($l=0$–3) excitations of hydrogen in the incident-proton energy range of 15–400 keV. Whereas the optically allowed $1s$-$4p$ transition makes the predominating contribution to the total $n=4$ integrated cross sections summed over all sublevels, the contribution of the $1s$-$4f$ transition is negligible. Each of the $1s$-$4s$ and $1s$-$4d$ excitations contribute about 10% to the above sum. The oscillations occurring in the curve of integrated $1s$-$4s$ Glauber cross sections when plotted against energy[6] are, however, absent from the $1s$-$4d$ result, as also

TABLE I. Integrated cross sections ($10^{-3}\pi a_0^2$) for the processes $H^+ + H(1s) \rightarrow H^+ + H(4l)$.

Energy		$1s \rightarrow 4s$			$1s \rightarrow 4p$			$1s \rightarrow 4d$			$1s \rightarrow 4f$	
(keV)	GA	FBA	SOD	GA	FBA	SOD	GA	FBA	SOD	GA	FBA	SOD
15	4.69	32.4	· · ·	16.6	117	· · ·	5.95	19.1	· · ·	0.181	0.380	· · ·
25	5.41	23.4	43.4	35.0	109	105	8.36	18.6	93.4	0.238	0.338	28.4
40	6.96	16.7	· · ·	50.2	100	· · ·	8.69	15.5	· · ·	0.219	0.256	· · ·
50	7.21	14.1	30.8	57.3	94.5	77.1	8.32	13.7	50.8	0.195	0.216	8.24
60	7.10	· · ·	· · ·	58.5	· · ·	· · ·	7.80	· · ·	· · ·	0.171	· · ·	· · ·
75	6.71	10.1	· · ·	57.5	77.2	· · ·	7.05	10.4	· · ·	0.160	0.153	· · ·
100	5.87	7.59	15.5	54.2	67.2	56.7	5.91	8.35	21.7	0.114	0.118	1.73
200	3.60	3.94	6.69	40.1	44.0	18.6	3.49	4.62	7.97	0.060	0.060	0.323
400	1.97	2.01	2.84	26.0	27.2	10.1	1.90	2.43	2.96	0.030	0.030	0.070

TABLE II. Integrated cross sections (10^{-17} cm^2) for the process $H^+ + H(n=1) \rightarrow H^+ + H(n=4)$. The last column gives experimental data normalized to GA results at 200 keV.

Energy (keV)	GA	FBA	SOD	Experiment Park *et al.* (1976)	Normalized
15	0.240	1.48	...	...	...
25	0.429	1.33	2.37	0.78	0.41
40	0.579	1.14	...	...	...
50	0.640	1.07	1.46	1.13	0.59
60	0.645	0.975	...	...	...
75	0.626	0.861	...	1.21	0.63
100	0.579	0.730	0.838	...	...
145	...	...	...	0.92	0.48
200	0.414	0.461	0.295	0.77	0.41
400	0.262	0.278	0.279	...	...

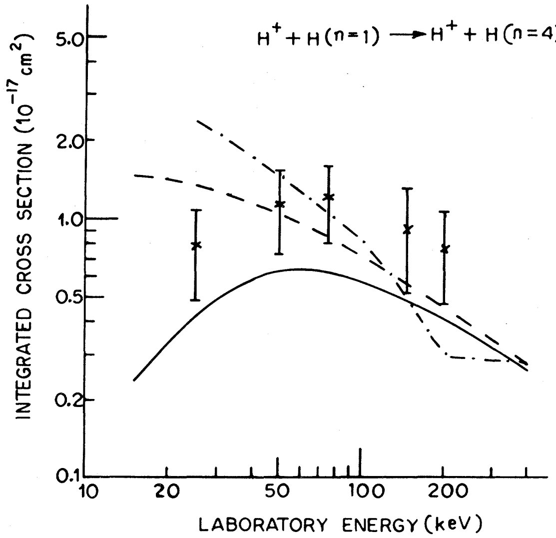

FIG. 3. Integrated cross sections for excitation of $n=4$ levels of hydrogen by proton impact. ——, Glauber approximation; – – –, first Born approximation: —·—·, second-order diagonalization method (Baye and Heenen, 1973); ×, experiment (Park *et al.*, 1976).

from the results of the other two sublevel excitations. Whereas the FBA and GA cross sections for individual sublevel excitations either converge or approach each other at high energies, the SOD results, except for the case of $1s$-$4p$ excitation, largely overestimate the results of the other two calculations.

The present integrated GA and FBA cross sections summed over all sublevel excitations are compared in Table II with the SOD results and the experiment.[7] The FBA results approach the Glauber values at high energies. The SOD predictions are, however, greater than the other two results at lower energies. As regards quantitative agreement with the experiment, the GA cross sections are seen to appreciably underestimate the observed values, whereas the FBA and SOD results appear to fare better at least in the energy range of 50–100 keV.

The actual picture regarding the relative success of various calculations over the entire energy range, however, emerges when we compare the above results graphically (cf. Fig. 3). Neither of the FBA or SOD calculations can predict the observed energy dependence of the cross sections. The Glauber calculation, on the other hand, can almost exactly predict the shape of the curve of the observed cross sections throughout the energy range considered in spite of its underestimation of the latter results. But, as discussed by Park *et al.*,[7] only the relative shape of the observed cross-section curve is reasonably accurate. The absolute cross sections were obtained by normalizing the data to the FBA results for $n=2$ excitation at 200-keV proton energy. On considering the good agreement of the Glauber and the observed cross sections for $n=2$ and 3 excitations, Park *et al.* further suggested that it might have been better to normalize the data to the Glauber values. We have done this at 200 keV. The results are shown in the last column of Table II, which immediately shows the agreement of the Glauber and the measured cross sections.

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