Charge transfer in proton-hydrogen collisions by the Faddeev approach. II

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A tractable form of the Faddeev equations as used by Chaudhuri *et al*. has been applied to the proton-hydrogen collision problem, retaining $1s$ and $2s$ states of the hydrogen atom in the expansion. To judge the effect of the proton interaction on the capture cross sections, calculations have been carried out with and without the inclusion of this interaction. The results for the $1s$-$2s$ capture and excitation cross sections are presented together with the elastic and ground-state capture cross sections. The present results have been compared with experimental findings and other theoretical results.

I. INTRODUCTION

In our previous communication[1] (henceforth denoted as paper I), an approximate form[2] of the Faddeev equations was applied to the investigation of the proton-hydrogen collision problem. This tractable form has also been used by different workers[2-4] to study e^+-H collision problems. This method can include the effects of direct and rearrangement channels and also couplings to higher excited states. Moreover, this form preserves the important constraint of unitarity below the breakup threshold. In paper I, we neglected the effect of coupling to higher excited states. It is well known[5-7] that the proton-proton interaction plays an important role in determining the behavior of the capture cross sections in the framework of first Born approximation. On the other hand, the neglect of this interaction is justifiable since it can be removed by canonical transformation.[7] Several workers[8] have investigated this problem from different angles to ascertain the exact physical picture. In view of this fact, we, in paper I, calculated the capture cross sections with and without the proton-proton interaction. There it was found that all the experimental points[9] and the theoretical results[10-13] lie between the two sets of our results, one without proton-proton interaction and the other with this interaction at low and intermediate energies. At high incident proton energies, our results with the ion-nucleus interaction ignored approach Brinkman and Kramers[5] (BK) values, whereas our results retaining this interaction tend to the results obtained by Jackson and Schiff[7] (JS).

Being encouraged by these results, we have extended our previous formalism to the same system by retaining the $1s$ and $2s$ states of hydrogen atom in this paper. It should be noted that there are very few coupled-state calculations on the ion-atom collision problem using the wave formalism; most of the existing coupled-state calculations are based on the impact-parameter treatment. To avoid enormous analytical complication, we have neglected the $2p$ states of the hydrogen atom in our calculations at present. We have obtained the elastic and ground-state capture cross sections along with the results of $1s$-$2s$ capture and excitation cross sections.

II. THEORY

The following direct and rearrangement processes have been considered:

$$\mathrm{H}^+(1)+\mathrm{H}_{1s}(2,3)\to\mathrm{H}^+(1)+\mathrm{H}_{1s}(2,3) \tag{2.1a}$$

$$\to\mathrm{H}^+(1)+\mathrm{H}_{2s}(2,3) \tag{2.1b}$$

$$\to\mathrm{H}^+_{1s}(1,2)+\mathrm{H}^+(3) \tag{2.1c}$$

$$\to\mathrm{H}^+_{2s}(1,2)+\mathrm{H}^+(3)\,. \tag{2.1d}$$

The particles 1 and 3 are protons and 2, the electron. The on-shell three-body transition amplitudes[1,2] from the bound state α with initial momentum $\vec{k}$ to the bound state β with the final momentum $\vec{k}'$ are given (the notations are the same as used in Refs. 1 and 2),

$$\langle\beta\vec{k}'n'|Y|\alpha\vec{k}n\rangle=\langle\beta\vec{k}'n'|Y^{(1)}|\alpha\vec{k}n\rangle-i\pi\sum_{\gamma}\sum_{n''=1}^{N_\gamma}\int d\vec{k}''\langle\beta\vec{k}'n'|Y^{(1)}|\gamma\vec{k}''n''\rangle\delta(E-E'')\langle\gamma\vec{k}''n''|Y|\alpha\vec{k}n\rangle\,. \tag{2.2}$$

The proton-proton bound states are not possible; therefore two values of the channel γ are considered. Retaining only the first-order term, the on-shell form[1,2] of the operators $Y^{(1)}_{\beta\alpha}$ from the high-energy consideration are approximated as

$$Y^{(1)}_{11}\simeq V_{12}+V_{13}\,,\quad Y^{(1)}_{13}\simeq V_{12}+V_{13}\,,\quad Y^{(1)}_{31}\simeq V_{23}+V_{13}\,,\quad Y^{(1)}_{33}\simeq V_{23}+V_{13}\,.$$

Here we retain the $1s$ and $2s$ states in the summation over n'' in Eq. (2.2). Therefore the explicit form of Eq. (2.2) becomes

$$\begin{aligned}\langle \vec{k}'1s|Y_{11}|\vec{k}1s\rangle = \langle \vec{k}'1s|Y_{11}^{(1)}|\vec{k}1s\rangle - i\pi\Big(&\int d\vec{k}''\langle \vec{k}'1s|Y_{11}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'1s|Y_{11}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'1s|Y_{13}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{31}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'1s|Y_{13}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{31}|\vec{k}1s\rangle\Big)\,,\end{aligned} \tag{2.3}$$

$$\begin{aligned}\langle \vec{k}'2s|Y_{11}|\vec{k}1s\rangle = \langle \vec{k}'2s|Y_{11}^{(1)}|\vec{k}1s\rangle - i\pi\Big(&\int d\vec{k}''\langle \vec{k}'2s|Y_{11}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'2s|Y_{11}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'2s|Y_{13}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{31}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'2s|Y_{13}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{31}|\vec{k}1s\rangle\Big)\,,\end{aligned} \tag{2.4}$$

$$\begin{aligned}\langle \vec{k}'1s|Y_{31}|\vec{k}1s\rangle = \langle \vec{k}'1s|Y_{31}^{(1)}|\vec{k}1s\rangle - i\pi\Big(&\int d\vec{k}''\langle \vec{k}'1s|Y_{31}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'1s|Y_{31}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'1s|Y_{33}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{31}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'1s|Y_{33}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{31}|\vec{k}1s\rangle\Big)\,,\end{aligned} \tag{2.5}$$

$$\begin{aligned}\langle \vec{k}'2s|Y_{31}|\vec{k}1s\rangle = \langle \vec{k}'2s|Y_{31}^{(1)}|\vec{k}1s\rangle - i\pi\Big(&\int d\vec{k}''\langle \vec{k}'2s|Y_{31}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'2s|Y_{31}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{11}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'2s|Y_{33}^{(1)}|\vec{k}''1s\rangle\,\delta(E-E'')\langle \vec{k}''1s|Y_{31}|\vec{k}1s\rangle\\ &+\int d\vec{k}''\langle \vec{k}'2s|Y_{33}^{(1)}|\vec{k}''2s\rangle\,\delta(E-E'')\langle \vec{k}''2s|Y_{31}|\vec{k}1s\rangle\Big)\,.\end{aligned} \tag{2.6}$$

Proceeding the same way as in paper I, we have obtained two sets of two coupled equations:

$$F^{\pm}_{1s,1s} = g^{\pm}_{1s,1s} + \frac{ik}{4\pi}\int [g^{\pm}_{1s,1s}(\theta,\theta'',\varphi'')F^{\pm}_{1s,1s}(\theta'') + g^{\pm}_{1s,1s}(\theta,\theta'',\varphi)F^{\pm}_{2s,1s}(\theta'')]\sin\theta''\,d\theta''\,d\varphi''\,, \tag{2.7a}$$

$$F^{\pm}_{2s,1s} = g^{\pm}_{2s,1s} + \frac{ik}{4\pi}\int [g^{\pm}_{2s,1s}(\theta,\theta'',\varphi'')F^{\pm}_{1s,1s}(\theta'') + g^{\pm}_{2s,2s}(\theta,\theta'',\varphi'')F^{\pm}_{2s,1s}(\theta'')]\sin\theta''\,d\theta''\,d\varphi''\,, \tag{2.7b}$$

where

$$F^{\pm}_{1s,1s} = f_{11}(1s,1s) \pm f_{31}(1s,1s)\,,$$
$$F^{\pm}_{2s,1s} = f_{11}(2s,1s) \pm f_{31}(2s,1s)\,,$$
$$g^{\pm}_{1s,1s} = f^{B}_{11}(1s,1s) \pm f^{B}_{31}(1s,1s)\,,$$
$$g^{\pm}_{2s,1s} = f^{B}_{11}(2s,1s) \pm f^{B}_{31}(2s,1s)\,,$$
$$g^{\pm}_{2s,2s} = f^{B}_{11}(2s,2s) \pm f^{B}_{31}(2s,2s)\,,$$

with

$$f_{\beta\alpha}(\hat{K}',\hat{K}) = -4\pi^2\langle \vec{k}'n'|Y_{\beta\alpha}|\vec{k}n\rangle\,,$$

$$f^{B}_{\beta\alpha}(\hat{K}',\hat{K}) = -4\pi^2\langle \vec{k}'n'|Y^{(1)}_{\beta\alpha}|\vec{k}n\rangle\,.$$

The $g^{\pm}$ have been obtained analytically with and without the inclusion of the proton-proton interaction. The total cross section for the particular s-s transition is obtained from the relation

$$Q = 2\pi\int_0^{\pi}|f_{\beta\alpha}|^2\sin\theta\,d\theta\,.$$

It is seen that the major contribution to the total cross section comes from the forward direction, and hence for actual calculation we have given a suitable transformation so that a slight change in the forward direction is taken into account.

III. RESULTS AND DISCUSSION

The integral equations are solved numerically. The numerical procedure is given in the Appendix.

Figure 1 represents our two curves for the total ($1s$-$1s$ and $1s$-$2s$) capture cross section, one with the proton-proton interaction [denoted as $\mathrm{CGS_{II}(JS)}$] and the other without the interaction [denoted as $\mathrm{CGS_{II}(BK)}$] along with the two sets of the results for the ground-state capture cross section of paper I [denoted as $\mathrm{CGS_{I}(JS)}$ and $\mathrm{CGS_{I}(BK)}$] from 1 to 120 keV. Recent experimental findings[9] are given for comparison. A noticeable difference between the $\mathrm{CGS_{II}(JS)}$ and $\mathrm{CGS_{I}(JS)}$ values has been observed from 1 to 70 keV, the difference being a maximum at 1 keV. Aside from the slight change in the energy range 6 to 40 keV, the values of $\mathrm{CGS_{II}(BK)}$ and $\mathrm{CGS_{I}(BK)}$ are almost the same. With these changes the difference between our two sets of results has been narrowed down in comparison with the two sets of results obtained in paper I in the low-energy range. The slope of the $\mathrm{CGS_{II}(JS)}$ curve is slightly different from that given by the experimental findings, whereas the slope of $\mathrm{CGS_{II}(BK)}$ is similar to the latter. The $\mathrm{CGS_{II}(JS)}$ curve lies below the experimental findings,[9] whereas the $\mathrm{CGS_{II}(BK)}$ curve is always above. For a comparison with the observed values, one should consider the contribution from all the higher states, of which the $2p$-state contribution is most important. If one adds the experimentally known values for the $2p$ capture cross section to the $\mathrm{CGS_{II}(JS)}$ and $\mathrm{CGS_{II}(BK)}$ values, the added results for the case of $\mathrm{CGS_{II}(JS)}$ come closer to the measured values, whereas the corresponding results for $\mathrm{CGS_{II}(BK)}$ are further away from the experimental findings. However, there still remain appreciable discrepancies in the energy range 5 to 50 keV [in the case of $\mathrm{CGS_{II}(JS)}$]. One of the reasons for this discrepancy may be the neglect of the effect of $2p$-state coupling on the ground-state capture cross section. It is expected that the effect of coupling with the $2p$ states and other higher states on the ground-state capture cross section is negligible at high energies. As the incident energy increases, the present results and the results of paper I become very close to each other (see also Table I). Here also $\mathrm{CGS_{II}(JS)}$ and $\mathrm{CGS_{II}(BK)}$ are approaching the JS and BK values, respectively, with the increase of incident energy.

Figure 2 contains our two curves for the $1s$-$2s$ capture cross section, PR(JS) (with JS as input) and PR(BK) (with BK as input) along with the corresponding JS and BK curves. The $1s$, $2s$, $2p$, and $1s$, $2s$, $2p$, $3s$, $3p$ close-coupling results obtained by Cheshire *et al.*[14] using the impact-parameter treatment, are also included in the same figure. The experimental findings due to Bayfield[15] and due to Morgan *et al.*[16] have been given for comparison. The results obtained neglecting the proton-proton interaction [PR(BK)] show better agreement with the experimental findings than those obtained by retaining the proton-proton interaction [PR(JS)]. Fluctuations occur in the PR(JS) curve as in both the curves due to Cheshire, although the nature of the PR(JS) curve is somewhat different from those obtained by Cheshire *et al.* On the other hand PR(BK) does not show any fluctuations. The strong fluctuation obtained in PR(JS) may be smoothed out by including a larger number of states, as noticed by Cheshire *et al.* As the energy increases the PR(BK) result approaches the BK value, whereas the PR(JS) result tends towards the JS value (Table II). In view of the $2s$-$2p$ strong coupling, it is expected that the inclusion of the $2p$ states will considerably influence the behavior of the $1s$-$2s$ capture cross section. For a comparison with the experimental findings, we have to consider the cascade contribution.

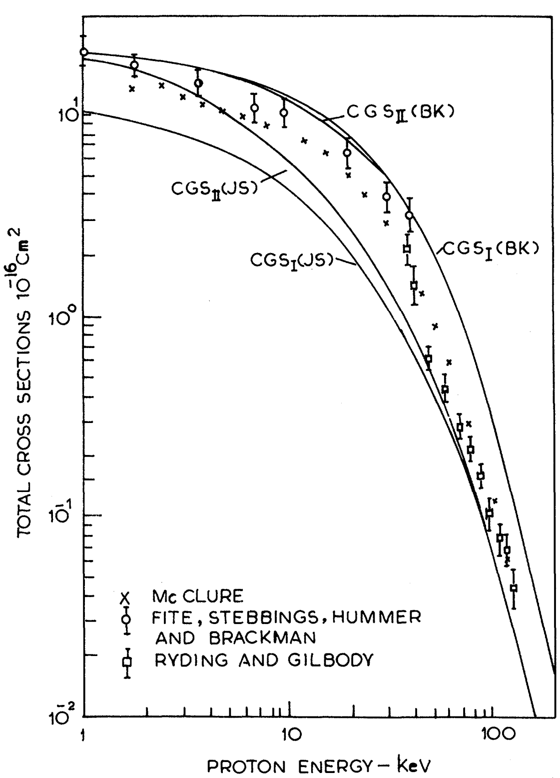

FIG. 1. Present calculations for the total capture cross section $\mathrm{CGS_{II}(BK)}$ and $\mathrm{CGS_{II}(JS)}$ are compared with the experimental results and $\mathrm{CGS_{I}(BK)}$ and $\mathrm{CGS_{I}(JS)}$ results.

TABLE I. Ground-state capture cross section (in units of πa_0^2). (The number in parentheses in each entry is the power of 10 by which the amplitude value should be multiplied.)

Energy (keV)	BK	CGS$_1$(BK)[a]	Present[b] (with BK as input)	(JS)	CGS$_1$ (JS)[a]	Present[c] (with JS as input)
1	1.217(.3)	2.352(1)	2.352(1)	1.440(2)	1.191(1)	2.216(1)
2	5.794(2)	2.124(1)	2.124(1)	6.902(1)	1.015(1)	1.844(1)
4	2.629(2)		1.842(1)	3.175(1)		1.341(1)
10	7.943(1)	1.398(1)	1.337(1)	9.975	4.869(0)	6.451
15	4.240(1)	1.130(1)	1.062(1)	5.490	3.405(0)	4.074
20	2.570(1)	9.119(0)	8.535	3.426	2.451(0)	2.756
30	1.148(1)	5.853(0)	5.557	1.615	1.351(−1)	1.417
50	3.368	2.40	2.383	5.198(−1)	4.89(−1)	4.883(−1)
100	3.994(−1)	3.51(−1)	3.620(−1)	7.338(−2)	7.34(−2)	7.189(−2)
200	2.629(−2)	2.43(−2)	2.513(−2)	5.988(−3)	6.02(−3)	5.932(−3)
300	4.159(−3)		3.998(−3)	1.081(−3)		1.071(−3)
1000	7.930(−6)	7.57(−6)	7.682(−6)	2.932(−6)	2.88(−6)	2.897(−6)
2000	1.563(−7)	1.51(−6)	1.520(−7)	6.746(−8)	6.63(−8)	6.670(−8)
5000	7.411(−10)		7.240(−10)	3.738(−10)		3.698(−10)

[a] The results of paper I.
[b] Without proton-proton interaction.
[c] With proton-proton interaction.

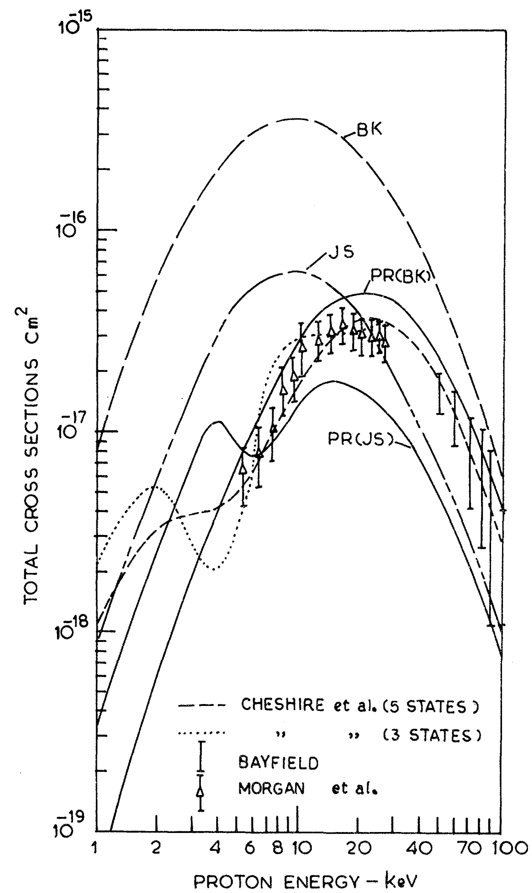

FIG. 2. 1*s*-2*s* capture cross-section curves PR(BK) and PR(JS) are compared with BK and JS curves, the curves obtained by Cheshire *et al.*, and the experimental results.

However, in the case of the 2*s* capture cross section, this contribution has been estimated by Morgan *et al.*[16] to be negligible.

Figure 3 shows our two sets of results PR(JS) and PR(BK) for the 1*s*-2*s* excitation cross section along with the corresponding results of the first Born (FBA) and Glauber approximations.[17] The results of Cheshire *et al.* using the 1*s*, 2*s*, 2*p*, 3*s*, 3*p* close-coupling approximation and the experimental findings[16] are plotted for comparison. The data of Morgan *et al.* present the observed 1*s*-2*s* excitation cross section values including the cascade

TABLE II. 1*s*-2*s* capture cross sections (in units of πa_0^2). (The number in parentheses in each entry is the exponent of 10 by which the cross-section value should be multiplied.)

Energy (keV)	BK	PR(BK)	JS	PR(JS)
1	1.014(−1)	3.654(−4)	1.064(−2)	3.836(−4)
2	6.747(−1)	8.134(−3)	6.612(−2)	2.770(−2)
4	2.733(−1)	4.602(−2)	3.766(−1)	1.281(−1)
6	3.654	1.213(−1)	6.309(−1)	8.595(−2)
10	4.204	3.369(−1)	7.298(−1)	1.654(−1)
15	3.559	5.094(−1)	5.775(−1)	2.048(−1)
20	2.753	5.642(−1)	4.193(−1)	1.899(−1)
30	1.582	5.081(−1)	2.241(−1)	1.299(−1)
50	5.605(−1)	2.817(−1)	7.871(−2)	5.492(−2)
100	7.132(−2)	4.997(−2)	1.184(−2)	9.253(−3)
200	4.412(−3)	2.505(−3)	9.241(−4)	7.851(−4)
300	6.562(−4)	5.412(−4)	1.615(−4)	1.405(−4)
1000	1.083(−6)	9.823(−7)	3.951(−7)	3.661(−7)
2000	2.051(−8)	1.934(−8)	8.782(−9)	8.332(−9)
5000	9.450(−11)	8.915(−11)	4.743(−11)	4.563(−11)

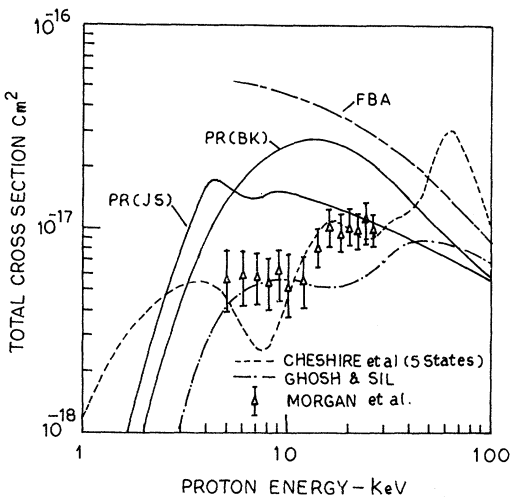

FIG. 3. 1s-2s excitation cross section is presented along with the results of the first Born approximation (FBA), the Glauber approximation, the curve obtained by Cheshire, and experimental points.

TABLE III. 1s-2s excitation cross sections (in units of πa_0^2). (The number in parentheses in each entry is the exponent of 10 by which the cross-section value should be multiplied.)

Energy (keV)	FBA	PR(BK)	PR(JS)
1	9.775(−2)	3.648(−4)	9.866(−4)
2	3.067(−1)	1.039(−2)	2.973(−2)
4	5.321(−1)	1.005(−1)	2.033(−1)
6	5.805(−1)	2.055(−1)	1.663(−1)
10	5.363(−1)	2.990(−1)	1.666(−1)
15	4.502(−1)	3.111(−1)	1.512(−1)
20	3.804(−1)	2.841(−1)	1.342(−1)
30	2.865(−1)	2.093(−1)	1.135(−1)
50	1.899(−1)	1.184(−1)	9.312(−2)
100	1.025(−1)	6.622(−2)	6.543(−2)
200	5.331(−2)	4.081(−2)	4.081(−2)
300	3.592(−2)	2.971(−2)	2.972(−2)
1000	1.099(−2)	1.032(−2)	1.029(−2)
2000	5.513(−3)	5.343(−3)	5.334(−3)
5000	2.211(−3)	2.184(−3)	2.185(−3)

contribution which is quite appreciable for this process. Morgan *et al.* have estimated this contribution to be 10% on the basis of simple Born calculations. In all the theoretical estimates, however, the cascade contribution has been neglected. Because of the great importance of the $2p$-state coupling, reasonable results for the $1s$-$2s$ excitation cross section are expected only after the inclusion of the $2p$ states.

The present results in the low-energy region do not completely settle the controversy regarding the role of ion-nucleus interaction in the ion-atom scattering. The results for the $1s$-$2s$ capture cross section are expected to change appreciably with the inclusion of the $2p$ states in the close-coupling scheme. The present inelastic-scattering results are of purely academic interest. In the high-energy region the effect of coupling with higher excited states and the off-shell contributions would not change the ground-state capture cross section appreciably. At high energies our $\mathrm{CGS_{II}}$(JS) results are in better agreement with the experimental results than $\mathrm{CGS_{II}}$(BK) and the ion-nucleus interaction does not seem to be negligible. The inclusion of the $2p$ states in the close-coupling scheme will be considered in a future work.

APPENDIX

We describe the numerical procedure for the solution of the integral equation.

We have two separate sets of integral equations (each consists of two coupled integral equations). An integration over φ'' is performed to reduce the above set of equations to single-variable integral equations. Special care has been taken to evaluate the integral over φ'' where we have followed the numerical procedure given by Krylov and Kruglikova.[18] The one-dimensional integral equations are then converted to simultaneous equations by using the Gaussian quadrature method to evaluate the integrals. The simultaneous equations are next solved numerically by matrix method. The convergence of the results is tested by increasing the number of Gaussian quadrature points.

It is well known that in ion-atom collisions the scattering amplitudes are strongly peaked in the forward direction and fall off very rapidly with increase in scattering angle. In fact, the scattering amplitude is practically negligible when the angle is $>M_e/M_p$ (ratio of the electron mass to the proton mass). Hence we have taken a suitable transformation which appropriately incorporates this feature. The transformation is given by the relation

$$z = 1 - \frac{2\lambda_{1s}^2}{\lambda_{1s}^2 + k_{1s}^2(1-\cos\theta)} .$$

Instead of θ, z has been used as the variable in the Gaussian quadrature. The BK and JS cross sections are obtained, by using the above substitution, as a check on the program.

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