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Capture into excited states in proton-helium collisions

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An approximate integral form of the close-coupling formalism is used to calculate the cross sections for capture of electrons from helium atoms by protons. Results for the ground-state and excited-2s-state capture cross sections are obtained with the effect of the proton-nucleus interaction included, and compared with experimental and other theoretical results. The effects of the post and prior forms of interaction on the cross sections are studied in detail. The effect of the exchange integral on the capture cross sections is also reported. It is found that the inclusion of the ground-state transition in calculating 2s-state capture cross section enhances the cross section values only in the low-energy region. The present values of the capture cross sections for the ground and excited 2s states are in very good agreement with the experimental observations at high as well as low energies. In the low-energy region the nature of the experimental curve has been correctly reproduced for both cases. Results for the differential capture cross sections in the forward direction and the total elastic cross sections are also reported.

INTRODUCTION

The electron capture by protons passing through helium atoms into the ground state of the hydrogen atom was the subject of theoretical investigation in a recent paper by Bhadra *et al.*[1] The process in which a proton captures an electron from a helium atom to form a hydrogen atom in exicted states has been studied experimentally by several authors,[2–6] but only a few theoretical calculations exist.[7–9] All of the experiments, however, show a shoulderlike trend at low incident energies. Except for some results with the Born and Impulse approximations, the theoretical findings are based mostly on the impact-parameter formalism, and failure of the present methods to predict any shoulderlike structure at low energies has led us to undertake a fresh theoretical investigation of this problem in the wave formalism. We have used an approximate form of the close-coupling formalism[1] (CCA) to calculate the ground- and excited-2s-state capture cross sections from 5 keV to 10 MeV.

THEORY

We have considered the following transitions:

$$H^+ + He(1s^2,1,2) \to H^+ + He(1s^2,1,2), \qquad (1a)$$

$$\to H(1s,1) + He^+(1s,2), \qquad (1b)$$

$$\to H(1s,2) + He^+(1s,1), \qquad (1c)$$

$$\to H(2s,1) + He^+(1s,2), \qquad (1d)$$

$$\to H(2s,2) + He^+(1s,1). \qquad (1e)$$

In the (1b) and (1c) transitions, a hydrogen atom captures electron 1 or 2 in the ground state, while in the (1d) and (1e) transitions a hydrogen atom captures electron 1 or 2 in the 2s state and the rest is in the ground state.

The CCA equations, neglecting the principal-value parts for the transition (1) are (notation is the same as used by Bhadra *et al.*[1])

$$f_{11}(\hat{k}'\cdot\hat{k}) = f^B_{11}(\hat{k}'\cdot\hat{k}) + \frac{i}{4\pi}\left(\int [\vec{k}_i f^B_{11}(\hat{k}'\cdot\hat{k}'')f_{11}(\hat{k}''\cdot\hat{k}) + \vec{k}_x f^B_{12}(\hat{k}'\cdot\hat{k}'')f^+(\hat{k}''\cdot\hat{k}) + \vec{k}_y f^B_{14}(\hat{k}'\cdot\hat{k}'')G^+(\hat{k}''\cdot\hat{k})]\sin\theta''\,d\theta''\,d\phi''\right), \qquad (2a)$$

$$f^+(\hat{k}'\cdot\hat{k}) = 2f^B_{21}(\hat{k}'\cdot\hat{k}) + \frac{i}{2\pi}\left(\int [\vec{k}_i f^B_{21}(\hat{k}'\cdot\hat{k}'')f_{11}(\hat{k}''\cdot\hat{k}) + \tfrac{1}{2}\vec{k}_x f^{+B}_{22}(\hat{k}'\cdot\hat{k}'')f^+(\hat{k}''\cdot\hat{k}) + \tfrac{1}{2}\vec{k}_y f^{+B}_{24}(\hat{k}'\cdot\hat{k}'')G^+(\hat{k}''\cdot\hat{k})]\sin\theta''\,d\theta''\,d\phi''\right), \qquad (2b)$$

$$G^+(\hat{k}'\cdot\hat{k}) = 2f^B_{41}(\hat{k}'\cdot\hat{k}) + \frac{i}{2\pi}\left(\int [\vec{k}_i f^B_{41}(\hat{k}'\cdot\hat{k}'')f_{11}(\hat{k}''\cdot\hat{k}) + \tfrac{1}{2}\vec{k}_x f^{+B}_{42}(\hat{k}'\cdot\hat{k}'')f^+(\hat{k}''\cdot\hat{k}) + \tfrac{1}{2}\vec{k}_x f^{+B}_{44}(\hat{k}'\cdot\hat{k}'')G^+(\hat{k}''\cdot\hat{k})]\sin\theta''\,d\theta''\,d\phi''\right), \qquad (2c)$$

where

$$f^{+B}_{22} = f^B_{22} + f^B_{23}, \quad f^{+B}_{24} = f^B_{24} + f^B_{25}, \quad f^{+B}_{42} = f^B_{42} + f^B_{52}, \quad f^{+B}_{44} = f^B_{44} + f^B_{45}, \qquad (3)$$

and where $\vec{k}_i$ is the initial momentum of the incident proton and $\vec{k}_x$ and $\vec{k}_y$ are determined from the energy conservation relations

$$\frac{k_x^2}{2\mu_2}=\frac{k_i^2}{2\mu_1}-\epsilon_{He}+\epsilon_{He^+}+\epsilon_H\,,$$
$$\frac{k_y^2}{2\mu_2}=\frac{k_i^2}{2\mu_1}-\epsilon_{He}+\epsilon_{He^+}+\epsilon_{H^*}\,, \qquad (4)$$

where ϵ_{He}, ϵ_{He^+}, ϵ_H and ϵ_{H^*} are the bound-state energies of the suffixed atoms (an asterisk indicates the excited 2s state).

RESULTS AND DISCUSSION

The wave function for the helium atom considered is

$$\frac{Z^3}{\pi a_0^3}\exp[-(Z/a_0)(r_1+r_2)],\quad Z=1.6875,$$

and since it is not an exact form, the total cross sections Q_i and Q_f calculated with prior and post forms of interaction,

$$V_i=V_{pn}+V_{p1}+V_{p2},\quad V_f=V_{pn}+V_{21}+V_{2n}+V_{p1},$$

are different. Here we have calculated the cross sections with both forms of interaction V_i and V_f. The exchange scattering amplitudes involve enormous computational time through CCA. Although at high and intermediate energies the exchange integral has negligible effect,[10-12] it appears from our present observation that it has appreciable contribution to the cross section in the low-energy region where the structure lies. We have made two studies on the process. In the first we have considered the electrons to be distinguishable in all channels, which is the same as in the process considered by Sin Fai Lam[8] and Winter and Lin,[9] and in the second we have considered the indistinguishability of electrons only in the ground state capture channel. The 2s and 2p states are strongly coupled, so the omission of the 2p state in our calculation may affect our result.

In Fig. 1 we present our total-cross-section values $\overline{Q}=\frac{1}{2}(Q_i+Q_f)$ for electron capture into the ground state of the hydrogen atom from 5 to 200 keV and compare them with experimental values.[13,14] The average value $\overline{Q}$ is plotted, since it is not known which cross section is the better representation of the exact CCA calculation. Theoretical results[7,15,16,11,12,10] are plotted for com-

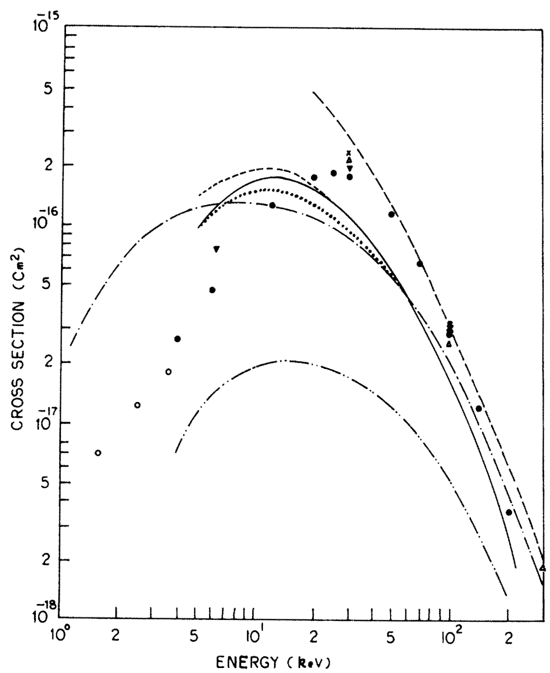

FIG. 1. Total cross sections $\overline{Q}$ for electron capture in the ground state for protons passing through a helium atom. Theoretical: ——, present calculation with exchange; – – –, present calculation without exchange; . . ., Bhadra and Sil (Ref. 10); — — —, Mapleton (Ref. 7); —·—and —··—, Garica *et al*. (Ref. 15); Δ, Begum *et al*. (Ref. 16); ×, Brandsen and Sin Fai Lam (Ref. 12); ∇, Green *et al*. (Ref. 11). Experimental: ○, Stedeford and Hasted (Ref. 13); ●, Stier and Barnett (Ref. 14). Impact energy of H^+ is in keV.

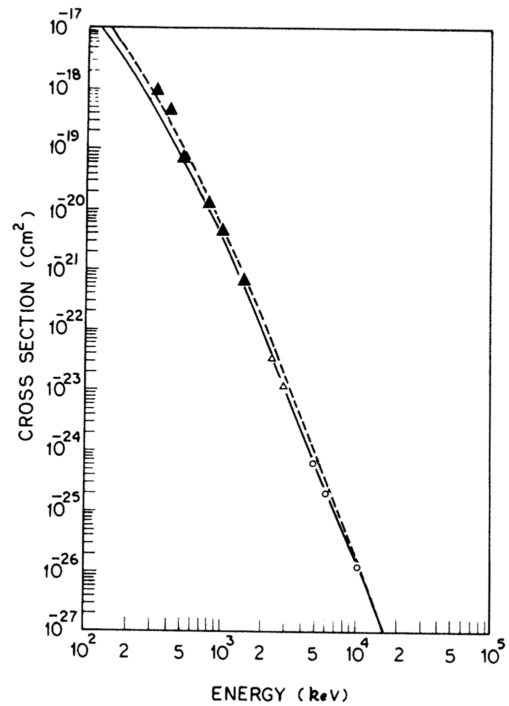

FIG. 2. Electron-capture cross section $\overline{Q}$ in the ground state for protons in helium at high impact energies. ——, present calculation with exchange; – – – Mapleton (Ref. 17); ▲, Toburen *et al*. (Ref. 18); Δ, Welsh *et al*. (Ref. 19); ○, Barkener *et al*. (Ref. 20). Impact energy of H^+ is in keV.

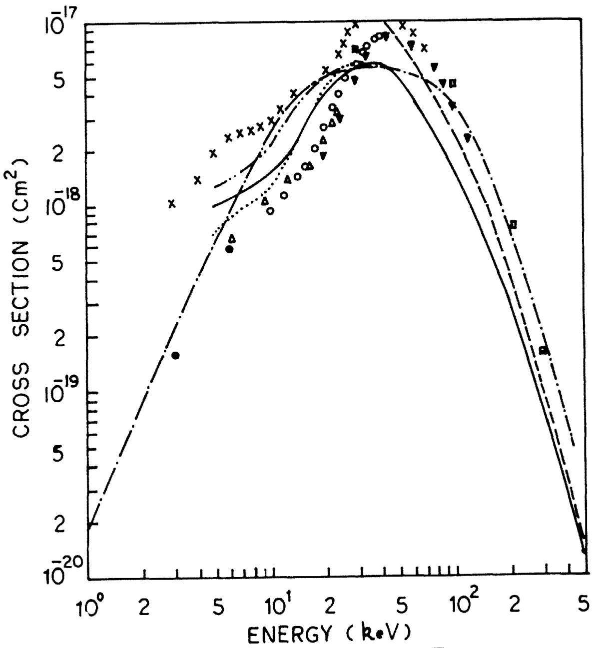

FIG. 3. Electron-capture cross section $\bar{Q}$ in the 2s state of the hydrogen atom for protons passing through helium. Theoretical: ——, present calculation with exchange; —·· —, present calculation without exchange; ··· and — — —, Bhadra and Basu (Ref. 21); —·—, Sin Fai Lam (Ref. 8); □, Winter and Lin (Ref. 9). Experimental: ● (D^+) and ○ (H^+), Jaecks *et al.* (Ref. 2); Δ, Andreev *et al.* (Ref. 3); ×, Dose (Ref. 4); ▼, Hughes *et al.* (Ref. 6). Impact energy of H^+ is in keV.

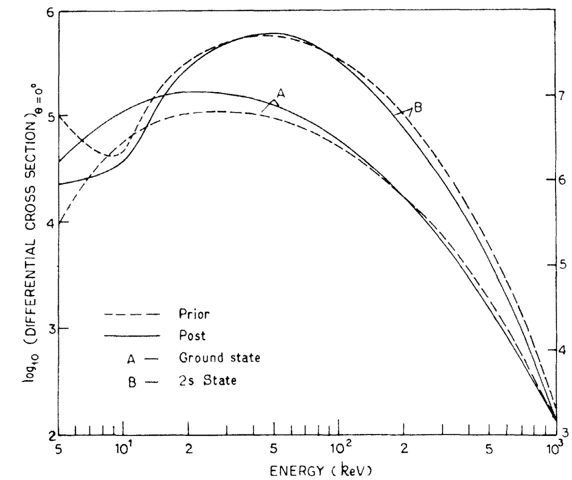

FIG. 4. Forward-direction differential capture cross section in the ground and 2s states of the hydrogen atom for protons passing through helium (in units of πa_0^2). Curve A: right-hand scale; curve B: left-hand scale. Impact energy of H^+ is in keV.

parison. Our results are in very good agreement with the experimental points and show a peak at low energies in the cross-section values, as observed by Stier and Barnett.[14] Our present curve always lies below the experimental points at energies greater than 20 keV. The exchange integral in the ground-state capture, when neglected, shows an increment in the cross-section values at low energies. The present curve, when compared with the $\bar{Q}$ values of Bhadra and Sil,[10] shows that the inclusion of the excited 2s states in the CCA calculation increases the cross-section values at low energies. The discrepancy with experiment in our results over the low- and intermediate-energy range can be attributed to the fact that other higher states of the hydrogen atom, the cascade effects, and also the principal-value part of the

TABLE I. Total cross sections [a] for elastic and charge-exchange scattering of protons by helium atoms (in units of πa_0^2).

Energy (keV)	Elastic	Ground-state capture Q_f	Ground-state capture Q_i	2s-state capture Q_f	2s-state capture Q_i
5	1.5104	1.1283	1.1161	0.1484(−1)	0.1375(−1)
10	1.3011	2.2619	1.7486	0.1853(−1)	0.1787(−1)
15	1.1231	2.2211	1.6828	0.3878(−1)	0.3433(−1)
20	0.9737	1.9567	1.4869	0.5545(−1)	0.4593(−1)
26	0.8387	1.6173	1.2469	0.6652(−1)	0.5267(−1)
40	0.6191	1.0175	0.8370	0.6810(−1)	0.5341(−1)
50	0.5549	0.7308	0.6286	0.5812(−1)	0.4628(−1)
100	0.3869	0.1785	0.1844	0.1935(−1)	0.1888(−1)
200	0.2496	0.2441(−1)	0.3014(−1)	0.3063(−1)	0.3810(−2)
395	0.1506	0.2082(−2)	0.2676(−2)	0.2876(−3)	0.3780(−3)
560	0.1247	0.7971(−3)	0.1002(−2)	0.1115(−3)	0.1457(−3)
625	0.1037	0.3064(−3)	0.3716(−3)	0.4373(−4)	0.5477(−4)
1000	0.6922(−1)	0.3552(−4)	0.3910(−4)	0.5141(−5)	0.5707(−5)
5000	0.1558(−1)	0.8599(−8)	0.6186(−8)	0.1149(−8)	0.8526(−9)
10 000	0.7962(−2)	0.1765(−9)	0.1167(−9)	0.2231(−10)	0.1540(−10)

[a] Number in parentheses in each entry is the exponent of 10 by which the cross-section value should be multiplied.

TABLE II. Percentage of the post-prior discrepancy in the charge-exchange cross-section values in the proton-helium collision process.

Energy (keV)	Method	% of post-prior discrepancy Ground-state cap.	2s-state cap.
40	CCA	17.92	21.57
39.5	Born	12.57	14.94
395	CCA	22.16	23.92
	Born	18.03	18.36
1000	CCA	9.16	9.93
	Born	7.21	8.51

pole term have been neglected in our calculation.

In Fig. 2 we have plotted our high-energy results $\overline{Q}$, along with the Born calculation of Mapleton[17] and experimental results.[18-20] Our curve coincides with Born results at 10 MeV, and at other energies it passes through most of the observed values, indicating a better fit with experiment than that of Mapleton. It may be supposed from our results in this high-energy range that effects of higher states of the hydrogen atom and ionized helium are negligible.

Figure 3 shows our electron-capture total cross sections $\overline{Q}$ in the excited 2s states of the hydrogen atom, taking into account the influence of the ground-state capture both with and without the exchange effect, along with previous theoretical calculations[21,8,9] and the experimental observations.[2-4,6] Our present calculation agrees fairly well with the experimental observations, and it reaches its maximum at 40 keV, as observed experimentally[2,3]; also, the shoulderlike trend of the experimental line[2-4] has been correctly reproduced. Another point worth mentioning is that in contrast to Sin Fai Lam's calculation[8] our curve lies below the Born calculation,[21] and finally coincides with it at high energies. The present curve, without the exchange effect in the ground state, though, gives values comparable at low energies with those of Sin Fai Lam,[8] but at 5 keV they differ appreciably. This disagreement in the result may be due to the neglect of the principal-value part in our calculation. When curve[21] C (without the ground-state capture channel) for the total cross section $\overline{Q}$ is compared with the present curve, we find that the inclusion of the ground-state capture transition enhances this 2s capture cross section in the low-energy region. The present curve also shows that the inclusion of the exchange integral term in the ground-state capture transition lowers the values of the capture cross sections at the low incident energies, and the exchange effect effectively vanishes at about 26 keV.

The forward-direction differential cross sections for the capture of electrons in the ground and 2s states of the hydrogen atom with post and prior forms of interaction are shown in Fig. 4. No other calculation of the differential cross section is available for comparison. At about 12 keV we find a point of inflection in the differential curve of the 2s capture cross section.

In Table I we have given our CCA calculations for elastic, ground-state capture, and 2s-state capture cross sections with post and prior forms of interaction from 5 keV to 10 MeV, considering the exchange integral in the ground-state capture transition. The differences in cross-section values with prior and post forms ($i-f$) for CCA ground-state capture is always less than 25%, while that for the excited 2s state of the hydrogen atom is always less than 22%. Similar behaviors were found by Mapleton[7] for $i-f$ in Born cross-section values. For a brief comparison of the overall magnitudes of the post-prior discrepancy between Mapleton's results[7] and ours, we show in Table II the percentage of the post-prior discrepancy in the two methods of calculation. It is found that the percentages of $i-f$ in the Born results are always less than those of the CCA results. It can also be noted that CCA $Q_{i,f}$ values approach Born $Q_{i,f}$ values in the high-energy region.

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