

Charge transfer in proton-helium collisions

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An approximate integral form of the close-coupling formalism has been applied to the charge-transfer process in the proton-helium collision problem. Results for the ground-state capture cross section have been obtained with the inclusion of the effect of proton-nucleus interactions and compared with the available experimental and theoretical results. The present values of the capture cross section are in very good agreement with the experimental observations at high as well as intermediate incident energies. At low energies the nature of the experimental curve has been correctly reproduced. Results for the differential capture cross sections in the forward direction and the total elastic cross sections have also been reported.

I. INTRODUCTION

The problem of charge transfer in proton-helium collisions is of special interest to theoretical workers because this problem can be handled with reasonable accuracy and rigor, and reliable experimental results are available for comparison with theory. However, there are only a few calculations on the H^+ -He collision problem based on the wave formalism.¹⁻³ Most of these calculations have been carried out in the Born and impulse approximation. Hence it is worthwhile to develop a suitable method to investigate the problem with rigor.

Ghosh and Basu⁴ and Chaudhuri *et al.*⁵ have used an integral form of the close-coupling equations for the e^\pm -H and e^- -H scattering problem, respectively. This integral form has some advantages over the integro-differential approach in practice. Here in this paper, we have developed the integral form of the close-coupling equations for the H^+ -He system. The attempt to solve the close-coupling equations exactly by partial-wave analysis is impractical because several thousand l values contribute to the total cross sections even at moderate incident energies. Therefore reduction of the three-dimensional coupling equations to a set of one-dimensional equations by partial-wave analysis cannot be achieved and some approximations are required to reduce the close-coupling method to a tractable form. Here we have neglected the principal-value part of the pole term in the kernel. This amounts to the neglect of the virtual excitations and strong distortions. This approximation is expected to be valid in the high-energy region. The infinite set of close-coupling equations has been truncated to set the equations in a tractable form by approximating the total state-function expansion with a truncated state-function expansion for the description of the atomic collision process. Agreement

with the experiment will justify the validity of this truncation. The present approximate form of the close-coupling method when applied to the proton hydrogen system is identical with the approximate form of the Faddeev equations as used by Chaudhuri *et al.*⁵ It has been found that the present formalism provides a good estimate of charge transfer and excitation cross sections even at the intermediate incident-energy range where the Born approximation fails.

We have calculated the electron-capture cross section from 1 keV to 1 MeV and results have been compared with theoretical and experimental findings. We have also presented scattering cross sections for the direct process and the results for the differential capture cross sections in the forward direction.

II. THEORY

We have considered the following transitions:

$$H^+(p) + He(n, 1, 2) \rightarrow H^+(p) + He(n, 1, 2), \quad (1a)$$

$$\rightarrow H(p, 1) + He^+(n, 2), \quad (1b)$$

$$\rightarrow H(p, 2) + He^+(n, 1). \quad (1c)$$

In the initial channel we have the proton (p) incident on the helium atom which is in the ground state. In the final channels we also have two rearrangement channels in addition to the elastic channel. In the rearrangement channel the helium atom is stripped of one of its electrons which is captured by the proton to form a hydrogen atom in ground state.

We now present a brief derivation of the integral form of the close-coupling method. The Schrödinger equation satisfied by the state function Ψ of the system is

$$(H - E)\Psi = 0, \quad (2)$$

where H is the Hamiltonian of the system and is

given by

$$H = T_1 + T_2 + T_p + V_{n1} + V_{n2} + V_{p2} + V_{p1} + V_{12} + V_{pn}. \quad (3)$$

Here T_i is the kinetic-energy operator of the particle i and V_{ij} is the interaction potential between the particle i and j . The state function Ψ may be expanded as

$$\begin{aligned} \Psi(n, 1, 2, p) = & \sum_m [\phi_m(n, 1, 2)F_{m1}(p) + \psi_m(n, 2) \\ & \times w_m(p, 1)F_{m2}(p, 1) \\ & + \psi_m(n, 1)w_m(p, 2)F_{m3}(p, 2)], \quad (4) \end{aligned}$$

where ϕ_m is the wave function of the target helium atom, ψ_m and w_m are the wave functions of the helium ion and hydrogen atom, F_{m1} denotes the motion of proton, while F_{m2} and F_{m3} describe the motion of the hydrogen atom.

Here we consider the helium wave function ϕ_m to be exact and with the Hartree-Fock variational principle we get the following set of coupled integro-differential equations.

$$(E - T_p - E_{\phi_{m'}})F_{m'1}(p) = \sum_m (\hat{X}'_{m'm} + \hat{W}'_{m'm})F_{m1}(p),$$

$$\begin{aligned} (E - T_{(p,1)} - E_{\psi_{m'}} - E_{w_{m'}})F_{m'2}(p, 1) \\ = \sum_m (\hat{X}'_{m'm} + \hat{W}'_{m'm})F_{m2}(p, 1), \quad (5) \end{aligned}$$

$$\begin{aligned} (E - T_{(p,2)} - E_{\psi_{m'}} - E_{w_{m'}})F_{m'3}(p, 2) \\ = \sum_m (\hat{X}'_{m'm} + \hat{W}'_{m'm})F_{m3}(p, 2), \end{aligned}$$

where

$$X'_{m'm} = \int \phi_m^*(V_{p1} + V_{p2} + V_{pn})\phi_m d\tau_1 d\tau_2,$$

$$\hat{W}'_{m'm}F_{m1} = \int \phi_m^*(H - E)\{\psi_m w_m F_{m2} + \psi_m w_m F_{m3}\} d\tau_1 d\tau_2,$$

$$X'_{m'm} = \int \psi_m^* w_m^* \{V_{n2} + V_{12} + V_{p1} + V_{pn}\} \psi_m w_m d\tau_1 d\tau_2,$$

$$\hat{W}'_{m'm}F_{m2} = \int \psi_m^* w_m^* (H - E)\{\phi_m F_{m1} + \psi_m w_m F_{m3}\} d\tau_1 d\tau_2, \quad (6)$$

and $X'_{m'm}$ and $\hat{W}'_{m'm}F_{m3}$ may be similarly defined. E_{ϕ_m} , E_{ψ_m} , and E_{w_m} are the binding energies for the helium, ionized helium, and hydrogen atoms, respectively. Equation (5) can be written in a more compact form as

$$(E - E_{n'a'} - T_{a'})F_{n'a'}(\vec{\mathbf{R}}) = \sum_{n,a} V_{n'a'na} F_{na}(\vec{\mathbf{R}}), \quad (7)$$

where $\hat{V}_{n'a'na}$ is the sum of a direct and exchange operator

$$\hat{V}_{n'a'na} = \hat{X}_{n'a'}\delta_{a'a} + \hat{W}_{n'a'na}(E), \quad (8)$$

where n', n denote states and a', a denote channels.

Following Sloan and Moore⁶ and Ghosh and Basu⁴ we can rewrite Eq. (7) as

$$\langle \vec{\mathbf{k}}' n' a' | Y | \vec{\mathbf{k}} n a \rangle = \langle \vec{\mathbf{k}}' | V_{n'a'na} | \vec{\mathbf{k}} \rangle + \sum_{n'', a''} \int d\vec{\mathbf{k}}'' \frac{\langle \vec{\mathbf{k}}' | V_{n'a'na} | \vec{\mathbf{k}}'' \rangle \langle \vec{\mathbf{k}}'' n'' a'' | Y | \vec{\mathbf{k}} n a \rangle}{E - E_{a''} + i\epsilon}, \quad (9)$$

with

$$\langle \vec{\mathbf{k}}' n' a' | Y | \vec{\mathbf{k}} n a \rangle = \sum_{n'' a''} \langle \vec{\mathbf{k}}' | V_{n'a'n'' a''} | F_{n'' a''}^{(na)}(\vec{\mathbf{R}}) \rangle. \quad (10)$$

We have considered only the ground states of the helium atom, helium ion, and hydrogen atom, so $n = n' = n'' = 1$ and hence we drop this suffix afterwards. We have considered three channels so a, a', a'' can have any value from 1 to 3. The explicit form of the integral equations are

$$\begin{aligned} \langle \vec{\mathbf{k}}' | Y_{11} | \vec{\mathbf{k}} \rangle = & \langle \vec{\mathbf{k}}' | Y_{11}^{(1)} | \vec{\mathbf{k}} \rangle + \int \frac{d\vec{\mathbf{k}}''}{E - E_1'' + i\epsilon} \langle \vec{\mathbf{k}}' | Y_{11}^{(1)} | \vec{\mathbf{k}}'' \rangle \langle \vec{\mathbf{k}}'' | Y_{11} | \vec{\mathbf{k}} \rangle \\ & + \int \frac{d\vec{\mathbf{k}}''}{E - E_2'' + i\epsilon} \langle \vec{\mathbf{k}}' | Y_{12}^{(1)} | \vec{\mathbf{k}}'' \rangle \langle \vec{\mathbf{k}}'' | Y_{21} | \vec{\mathbf{k}} \rangle \\ & + \int \frac{d\vec{\mathbf{k}}''}{E - E_3'' + i\epsilon} \langle \vec{\mathbf{k}}' | Y_{13}^{(1)} | \vec{\mathbf{k}}'' \rangle \langle \vec{\mathbf{k}}'' | Y_{31} | \vec{\mathbf{k}} \rangle, \quad (11a) \end{aligned}$$

$$\begin{aligned} \langle \bar{\mathbf{k}}' | Y_{21} | \bar{\mathbf{k}} \rangle &= \langle \bar{\mathbf{k}}' | Y_{21}^{(1)} | \bar{\mathbf{k}} \rangle + \int \frac{d\bar{\mathbf{k}}''}{E - E_1'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{21}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{11} | \bar{\mathbf{k}} \rangle + \int \frac{d\bar{\mathbf{k}}''}{E - E_2'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{22}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{21} | \bar{\mathbf{k}} \rangle \\ &+ \int \frac{d\bar{\mathbf{k}}''}{E - E_3'' + i\epsilon} \langle \bar{\mathbf{k}} | Y_{23}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{31} | \bar{\mathbf{k}} \rangle, \end{aligned} \quad (11b)$$

$$\begin{aligned} \langle \bar{\mathbf{k}}' | Y_{31} | \bar{\mathbf{k}} \rangle &= \langle \bar{\mathbf{k}}' | Y_{31}^{(1)} | \bar{\mathbf{k}} \rangle + \int \frac{d\bar{\mathbf{k}}''}{E - E_1'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{31}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{11} | \bar{\mathbf{k}} \rangle + \int \frac{d\bar{\mathbf{k}}''}{E - E_2'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{32}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{21} | \bar{\mathbf{k}} \rangle \\ &+ \int \frac{d\bar{\mathbf{k}}''}{E - E_3'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{33}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{31} | \bar{\mathbf{k}} \rangle, \end{aligned} \quad (11c)$$

where

$$\langle \bar{\mathbf{k}}' | Y_{\beta\alpha} | \bar{\mathbf{k}} \rangle \equiv \langle \bar{\mathbf{k}}', 1s, \beta | Y | \bar{\mathbf{k}}, 1s, \alpha \rangle$$

and

$$\langle \bar{\mathbf{k}}' | Y_{\beta\alpha}^{(1)} | \bar{\mathbf{k}} \rangle \equiv \langle \bar{\mathbf{k}}' | V_{1s\beta 1s\alpha} | \bar{\mathbf{k}} \rangle.$$

The three coupled integral equations can be reduced to two coupled integral equations because the antisymmetric combination of (11b) and (11c) is coupled only to itself and can be omitted. The reduced set of equations are

$$\langle \bar{\mathbf{k}}' | Y_{11} | \bar{\mathbf{k}} \rangle = \langle \bar{\mathbf{k}}' | Y_{11}^{(1)} | \bar{\mathbf{k}} \rangle + \int \frac{d\bar{\mathbf{k}}''}{E - E_1'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{11}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{11} | \bar{\mathbf{k}} \rangle + \int \frac{d\bar{\mathbf{k}}''}{E - E_2'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{12}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y^+ | \bar{\mathbf{k}} \rangle, \quad (13)$$

$$\langle \bar{\mathbf{k}}' | Y^+ | \bar{\mathbf{k}} \rangle = 2\langle \bar{\mathbf{k}}' | Y_{21}^{(1)} | \bar{\mathbf{k}} \rangle + 2 \int \frac{d\bar{\mathbf{k}}''}{E - E_1'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{21}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y_{11} | \bar{\mathbf{k}} \rangle + 2 \int \frac{d\bar{\mathbf{k}}''}{E - E_2'' + i\epsilon} \langle \bar{\mathbf{k}}' | Y_{22}^{(1)} | \bar{\mathbf{k}}'' \rangle \langle \bar{\mathbf{k}}'' | Y^+ | \bar{\mathbf{k}} \rangle,$$

where

$$\langle \bar{\mathbf{k}}' | Y^+ | \bar{\mathbf{k}} \rangle = \langle \bar{\mathbf{k}}' | Y_{21} | \bar{\mathbf{k}} \rangle + \langle \bar{\mathbf{k}}' | Y_{31} | \bar{\mathbf{k}} \rangle.$$

Pole terms in (13) can be divided into δ -function and principal-value parts by the relation

$$\frac{1}{E - E'' + i\epsilon} = -i\pi\delta(E - E'') + \frac{\mathbf{P}}{(E - E'')} . \quad (14)$$

Matrix elements for operators $Y_{\beta\alpha}^{(1)}$ and $Y_{\beta\alpha}$ are expressed as follows:

$$\begin{aligned} \langle \bar{\mathbf{k}}' | Y_{\beta\alpha}^{(1)} | \bar{\mathbf{k}} \rangle &= -(1/4\pi^2\mu_\beta) f_{\beta\alpha}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}), \\ \langle \bar{\mathbf{k}}' | Y_{\beta\alpha} | \bar{\mathbf{k}} \rangle &= -(1/4\pi^2\mu_\beta) f_{\beta\alpha}(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}), \end{aligned} \quad (15)$$

where $f_{\beta\alpha}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}})$ represents the corresponding scattering amplitude of the matrix element for the transition operator $Y_{\beta\alpha}^{(1)}$ and $f_{\beta\alpha}(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}})$ is the corresponding scattering amplitude of the operator $Y_{\beta\alpha}$. μ_β is the reduced mass of the channel β . It is important to note that $f_{\beta\alpha}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}})$ reduces to the first Born amplitude on the on-shell. Neglecting the principal-value part and using Eqs. (15) we can rewrite Eqs. (13) as

$$f_{11}(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}) = f_{11}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}) + \frac{i}{4\pi} \left(\int [\bar{\mathbf{k}}_i f_{11}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}'') f_{11}(\hat{\mathbf{k}}'' \cdot \hat{\mathbf{k}}) + \bar{\mathbf{k}}_x f_{12}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}'') f^+(\hat{\mathbf{k}}'' \cdot \hat{\mathbf{k}})] \sin\theta'' d\theta'' d\varphi'' \right), \quad (16)$$

$$f^+(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}) = 2f_{21}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}) + \frac{i}{2\pi} \left(\int [\bar{\mathbf{k}}_i f_{21}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}'') f_{11}(\hat{\mathbf{k}}'' \cdot \hat{\mathbf{k}}) + \bar{\mathbf{k}}_x f_{22}^B(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}'') f^+(\hat{\mathbf{k}}'' \cdot \hat{\mathbf{k}})] \sin\theta'' d\theta'' d\varphi'' \right),$$

where \vec{k}_i is the initial momentum of the incident proton and \vec{k}_x is determined from the energy conservation relation:

$$k_x^2/2\mu_2 = k_i^2/2\mu_1 - E_\phi + E_\psi + E_w. \quad (17)$$

Total direct and exchange cross sections are expressed by the following relations:

$$\sigma_{\text{dir}} = 2\pi(v_f/v_i) \int_{-1}^1 |f_{11}|^2 d\cos\theta, \quad (18)$$

$$\sigma_{\text{ex}} = 2\pi(v_f/v_i) \int_{-1}^1 \frac{1}{2} |f^+|^2 d\cos\theta.$$

III. RESULTS AND DISCUSSION

The coupled integral equations (16) have been solved numerically. In obtaining results, Krylov's quadrature formula⁷ of maximum trigonometric degree of precision has been applied to perform the ϕ integration. The inputs $f_{\beta\alpha}^B$ have been evaluated analytically (Appendix). All numerical computations have been performed with sufficient care so that the cross sections are given with an accuracy of four to five decimal places. In solving the integral equations we have used the Gaussian quadrature method for evaluating the integrals. In heavy-particle collisions the scattering amplitudes are sharply peaked in the forward direction and the angular spread of the scattering amplitudes decreases with the increase of the incident energy. To take care of this feature we have used z as our integration variable instead of θ , where z is related to θ by the following transformation:

$$\frac{k^2}{\lambda^2}(1 - \cos\theta) = \frac{1+z}{1-z}; \quad \lambda = 1.6875.$$

We have calculated total cross sections for the elastic and rearrangement processes for the incident proton energy varying from 1 keV to 1 MeV. We have also calculated the differential cross sections in the forward direction. Convergence of the results for the total cross sections was tested by increasing the number of Gaussian points.

We have used the simplest Hylleraas ground-state wave function of the form

$$\phi(\vec{x}_1, \vec{x}_3) = (z^3/\pi a_0^3) \exp[-(z/a_0)(\vec{x}_1 + \vec{x}_3)],$$

with $z = 1.6875$. Bransden and Sin Fai Lam⁸ calculated the capture cross section for the same process with the two-state impact-parameter formalism for a number of approximate wave functions. Their results show that this Hylleraas-type wave function is sufficient to express the capture cross sections with reasonable accuracy for a range of proton energy $E \geq 30$ keV. Bransden and Sin Fai

Lam⁸ and Mapleton² have noticed that better wave functions for helium enhance the capture cross sections in the low-energy region. Thus our result is expected to be increased in this energy region with a better wave function.

Another point we would like to emphasize is that we have taken the prior form of the interactions in our calculation throughout. Mapleton² has observed that the difference between the values of the cross section using post and prior forms of the interaction is less than 10% in the higher-energy region in the framework of the Born approximation with a Hylleraas wave function. He has observed enhancement in the values of the capture cross section when the post form of the interaction is used instead of the prior form in the low-energy region. It is expected that our result would also increase in the low-energy region with the post

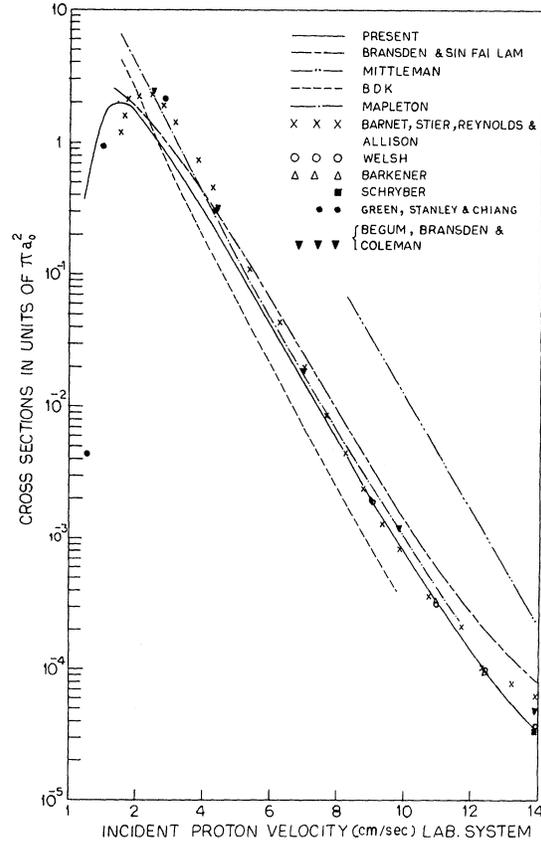


FIG. 1. Present calculations of the ground-state charge-transfer cross section compared with the experimental results of Allison, Stier and Barnett, and Barnett and Reynolds (Ref. 11), Welsh *et al.* (Ref. 12), Berkener *et al.* (Ref. 13), and Schryber (Ref. 14) and with the theoretical curves of Bransden and Sin Fai Lam (Ref. 8), Middleman (Ref. 9), BDK (Ref. 1), Mapleton (Ref. 2), Green *et al.* (Ref. 10), and Begun *et al.* (Ref. 16) in the energy range 1 keV–1 MeV.

form of the interaction.

Figure 1 shows our results for the ground-state charge-transfer cross section along with the corresponding theoretical results due to Mapleton,² Bransden *et al.* (BDK),¹ Bransden and Sin Fai Lam,⁸ Mittleman,⁹ and Green *et al.*¹⁰ Experimental findings¹¹⁻¹⁵ for the total charge-transfer cross section are included in the same figure for comparison. Results of the recent theoretical calculation of Begum *et al.*¹⁶ using the distorted-wave approximation in the impact-parameter formulation are also included in the figure for comparison. Our results are in better agreement with the experimental data in the high-energy region where they have higher cross-section values. Their cross-section values show more or less the same feature as obtained by Mapleton² as well as by ourselves (Table I) in the first Born approximation. The slight upward trend as observed by Barnet *et al.*¹¹ around the incident proton energy 1 MeV has not been found in the recent measurements¹²⁻¹⁵. In the energy region 250 keV–1 MeV our results coincide with the experimental points more closely. First Born results of Mapleton⁷ using a six-parameter wave function show a lower estimate of the total capture cross section. A similar observation was made by Bransden and Sin Fai Lam⁸ in their calculation. This leads us to conclude that our method provides a good fit to the high-energy experimental points. In the energy region 50–250 keV our curve lies below the

experimental findings. The present curve produces the peak in the cross section as observed by Barnet *et al.*¹¹ and this was predicted by Green *et al.*,¹⁰ who have used the two-state approximation as suggested by Bates. However, the position of our peak is slightly shifted towards the lower energies.

The results of the calculation for the elastic cross section for various proton energies together with the capture cross section are presented in Table I. In the calculation of the elastic cross section we have considered the effect of couplings to the rearrangement channels. Calculated first Born elastic and capture cross-section results are also presented for comparison. It may be mentioned that the values of the first Born capture cross section using the present wave function are always greater than the values obtained from our approximation. With increasing energy, the difference between the present charge-transfer results and the corresponding Born results decreases.

In the high-energy region the effect of neglecting the coupling with higher states, virtual excitation, and the strong distortion is not expected to influence the ground-state capture cross section. Sin Fai Lam⁸ observed that the effect of the inclusion of the excited states of hydrogen does not improve the results over the energy range 1–1000 keV. So the discrepancy in the intermediate- and low-energy results can be attributed to the choice

TABLE I. Ground-state total cross sections^a for the elastic and charge-exchange scattering of protons by helium atoms in units of πa_0^2 .

Lab energy (keV)	Close coupling Direct	Born Direct	Close coupling Capture	Born Capture
1	2.6011	81.8212	0.3816	83.4066
5	1.8081	16.3642	1.6982	18.0532
10	1.4922	8.1821	2.0351	8.5918
15	1.2494	5.4547	1.8512	5.5279
18	1.1409	4.5456	1.7011	4.4805
20	1.0799	4.0911	1.6006	3.9485
22	1.0260	3.7191	1.5031	3.5089
24	0.9783	3.4092	1.4114	3.1405
26	0.9355	3.1497	1.3237	2.8257
30	0.8623	2.7274	1.1656	2.3211
35	0.7883	2.3377	0.9967	1.8534
40	0.7284	2.0455	0.8557	1.5069
50	0.6370	1.6364	0.6393	1.0374
100	0.4140	0.8182	0.1855	0.2486
200	0.2589	0.4091	0.2995 (-1)	0.3143 (-1)
395	0.1546	0.2071	0.2611 (-2)	0.2958 (-2)
500	0.1276	0.1636	0.9700 (-3)	0.1088 (-2)
1000	0.7038 (-1)	0.8182 (-1)	0.3773 (-4)	0.4176 (-4)

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

of the wave function, the prior form of interaction, and the neglect of the principal-value part of the pole term which we have considered in this calculation. The choice of a better wave function and the post form of the interaction is expected to increase the value of capture cross sections in this energy region.

In Fig. 2, we have plotted the differential cross section for the charge transfer at 0° scattering angle. No other results have been obtained for comparison. The feature of the curve is similar to that as obtained in the case of the $H^+ - H$ collision problem. Considering the results over the complete range of energy investigated we think this method uniquely provides a correct picture for capture cross sections over a wider range of energy.

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APPENDIX: EVALUATION OF $f_{\beta\alpha}^B$

$f_{\beta\alpha}^B$ can be expressed as (our notations are the same as used by Mapleton²):

$$f_{\beta\alpha}^B = -\frac{\mu_B}{2\pi} \int d\vec{x}_1 d\vec{x}_3 \psi(\vec{x}_1) w(\vec{x}_2) V_{i,f} \phi(\vec{x}_1, \vec{x}_3) \times \exp[i(\vec{A}_1 \cdot \vec{x}_1 + \vec{A}_2 \cdot \vec{x}_2 - \vec{A}_3 \cdot \vec{x}_3)], \quad (\text{A1})$$

where

$$V_i = V_{pn} + V_{p1} + V_{p2},$$

$$V_f = V_{pn} + V_{21} + V_{2n} + V_{p1}.$$

We evaluate the type of integral I defined below by which one can get expression (A1):

$$I = K \int \{ q^2 [(\vec{q} + \vec{A}_1)^2 + l_1^2]^2 [(\vec{q} + \vec{A}_2)^2 + l_2^2]^2 [(\vec{q} + \vec{A}_3)^2 + l_3^2]^2 \}^{-1} d\vec{q}, \quad (\text{A5})$$

where $K = 2^8 \pi l_1 l_2 l_3$. By expanding in partial fractions we get

$$I = K \left(\frac{1}{l_1^4} \int \{ q^2 [(\vec{q} + \vec{A}_2)^2 + l_2^2]^2 [(\vec{q} + \vec{A}_3)^2 + l_3^2]^2 \}^{-1} d\vec{q} - \frac{1}{l_1^4} \int \{ [(\vec{q} + \vec{A}_1)^2 + l_1^2] [(\vec{q} + \vec{A}_2)^2 + l_2^2]^2 [(\vec{q} + \vec{A}_3)^2 + l_3^2]^2 \}^{-1} d\vec{q} - \frac{1}{l_1^2} \int \{ [(\vec{q} + \vec{A}_1)^2 + l_1^2]^2 [(\vec{q} + \vec{A}_2)^2 + l_2^2]^2 [(\vec{q} + \vec{A}_3)^2 + l_3^2]^2 \}^{-1} d\vec{q} \right). \quad (\text{A6})$$

Next we show the evaluation of the third integral of (A6) which is the most difficult one. After simple transformation of the integration variables we can rewrite this third integral as

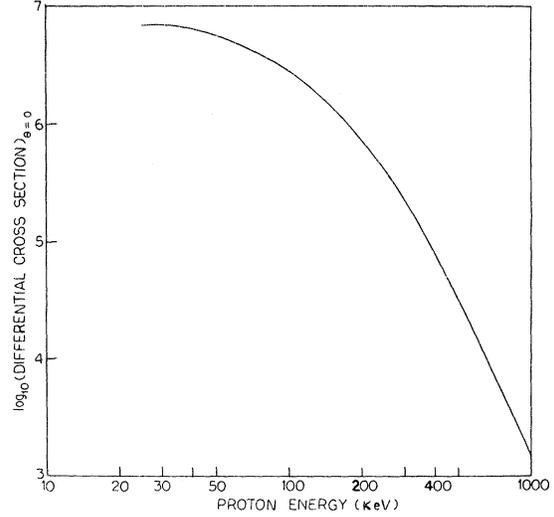


FIG. 2. Results of forward-direction differential cross section presented from 25 keV to 1 MeV (in units of πa_0^2).

$$I = \int \frac{\exp(\vec{A}_1 \cdot \vec{r}_1 + \vec{A}_2 \cdot \vec{r}_2 - \vec{A}_3 \cdot \vec{r}_3)}{|\vec{r}_2 + \vec{r}_1 - \vec{r}_3|} \times e^{-i_1 |\vec{r}_1|} e^{-i_2 |\vec{r}_2|} e^{-i_3 |\vec{r}_3|} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3. \quad (\text{A2})$$

Using the Fourier transforms

$$\frac{1}{|\vec{r}_2 + \vec{r}_1 - \vec{r}_3|} = \frac{1}{2\pi^2} \int e^{i\vec{q} \cdot (\vec{r}_2 + \vec{r}_1 - \vec{r}_3)} \frac{d\vec{q}}{q^2}, \quad (\text{A3})$$

$$e^{-\lambda |\vec{r}|} = \frac{\lambda}{\pi^2} \int \frac{e^{i\vec{p} \cdot \vec{r}}}{(p^2 + \lambda^2)^2} d\vec{p},$$

and the representation

$$\delta(\vec{k} - \vec{k}') = \frac{1}{(2\pi)^3} \int e^{i\vec{p} \cdot (\vec{k} - \vec{k}')} d\vec{p}, \quad (\text{A4})$$

we get

$$-\frac{1}{8l_1 l_2 l_3} \frac{\partial}{\partial l_1} \frac{\partial}{\partial l_2} \frac{\partial}{\partial l_3} J, \quad (\text{A7})$$

where

$$J = \int \{ (q^2 + l_1^2) [(\vec{q} + \vec{A}_2')^2 + l_2^2] [(\vec{q} + \vec{A}_3')^2 + l_3^2] \}^{-1} d\vec{q}. \quad (\text{A8})$$

This can be evaluated with the help of Lewis'¹⁹ method; the result is

$$J = 2\pi^2 N^{-1/2} \tan^{-1}(N^{1/2}/\beta), \quad (\text{A9})$$

where

$$\begin{aligned} N &= \alpha_1 \gamma_1 - \beta^2, \\ \alpha_1 \gamma_1 &= [(\vec{A}_3' - \vec{A}_2')^2 + (l_2 + l_3)^2] [A_2'^2 + (l_2 + l_1)^2] \\ &\quad \times [A_3'^2 + (l_3 + l_1)^2], \end{aligned}$$

$$\begin{aligned} \beta &= l_1 [(\vec{A}_3' - \vec{A}_2')^2 + (l_2 + l_3)^2] + l_3 (l_1^2 + l_2^2 + A_2'^2) \\ &\quad + l_2 (l_1^2 + l_3^2 + A_3'^2), \end{aligned}$$

where

$$\vec{A}_2' = \vec{A}_2 - \vec{A}_1, \quad \vec{A}_3' = \vec{A}_3 - \vec{A}_1.$$

In our case \vec{A}_1 and all its powers are very small quantities ($\vec{A}_1 \approx 10^{-4} \vec{A}_3$). We checked our results with \vec{A}_1 and with $\vec{A}_1 = 0$ and came to the conclusion that \vec{A}_1 can be safely dropped without any damage to the accuracy of the results. In this paper we have presented our result with $\vec{A}_1 = 0$.

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