

## Double-electron capture by protons from helium

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The process of  $H^-$  formation as a result of double-electron capture by protons from helium atoms has been investigated by an approximate integral form of the close-coupling formalism considering three atomic states and indistinguishability of electrons. The cross sections have been presented for incident proton energies ranging from 5 keV to 1 MeV and have been compared with the previous experimental and theoretical results. Our cross sections agree fairly well with the experimental results over the range of energy investigated. The total elastic and single-electron capture cross sections and the differential double-electron capture cross sections in the forward direction also have been reported.

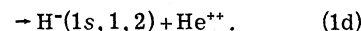
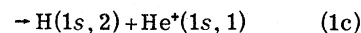
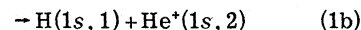
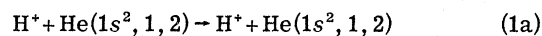
### INTRODUCTION

The single-electron capture process in the proton-helium collision problem has been studied in detail both theoretically<sup>1-12</sup> and experimentally<sup>13-17</sup> by several authors. The process in which a proton captures two electrons from a helium atom resulting in the formation of  $H^-$  has been measured experimentally by Fogel *et al.*,<sup>18</sup> Williams,<sup>19</sup> and Schryber<sup>20</sup> covering the incident proton energy range from 10 to 750 keV. Recently Toburen and Nakai<sup>21</sup> have measured the same cross sections from 75 to 200 keV. In spite of the availability of a large number of experimental results, no reliable theoretical results are available for comparison. Only two theoretical attempts have so far been made in this direction. Gerasimenko<sup>22</sup> has calculated the double-electron capture cross sections by protons from helium atoms using the Born approximation for the high-energy region (150 to 750 keV). His theoretical results are greater than the measured values by two orders of magnitude. Recently, Roy *et al.*<sup>23</sup> have also calculated the same cross sections using the impact-parameter formalism. Their cross-section energy curve, though showing a peak in the low-energy region, differs appreciably from the experimental observations with increase of energy.

The wide discrepancy between the predicted theoretical results and the experimental values has led us to make a fresh theoretical investigation into this problem. In this paper we propose to investigate the above collisional process in an approximate integral form of the close-coupling formalism<sup>11</sup> (CCA). The approximation in the formulation is the neglect of the principal-value part of the pole term in the kernel of the integral equation, required to achieve a tractable form of the close-coupling equation in the wave formalism for the heavy-particle collision problem, since the phase-shift analysis of the problem, where

several thousand  $l$  values contribute to the total cross section, becomes impractical. Our coupled-state calculation includes the contribution of all the  $l$  values. The neglect of the principal-value part amounts to the neglect of the off-shell matrix elements. In the general coupled-channel formalism including excited states, this neglect in the case of excited states means the neglect of virtual excitation. In the entrance channel the principal-value part has strong distorting effects associated with it. Hence the neglect of this effect leads to the neglect of strong distortions. This approximation though expected to be valid in the high-energy region has yielded encouraging results in the intermediate- and low-energy regions for the charge-transfer process.<sup>11, 12, 26</sup>

We have considered the following processes with regard for the indistinguishability of electrons<sup>24</sup>:



In the second and third transitions a hydrogen atom is formed by the capture of the electron numbered 1 or 2, and all atoms are in the ground state. This problem with two active electrons is especially complicated and has associated with it enormous computational difficulties.

We have calculated the double-electron-capture cross sections from 1 keV to 1 MeV, and the results have been compared with other theoretical and experimental findings. We have also presented the results for the coupled channels, namely the elastic and single-electron-capture cross sections and the results for the differential double-electron-capture cross sections in the forward direction.

## THEORY

The state function  $\Psi$  for the proton-helium system is approximated by the expansion

$$\begin{aligned} \Psi = & \phi(n, 1, 2)F_1(p) + \psi(n, 2)\omega(p, 1)F_2(p, 1) \\ & + \psi(n, 1)\omega(p, 2)F_3(p, 2) + \chi(p, 1, 2)F_4(p, 1, 2), \end{aligned} \quad (2)$$

where  $\phi$ ,  $\psi$ ,  $\omega$ , and  $\chi$  are the ground-state wave functions for He, He<sup>+</sup>, H, and H<sup>-</sup>, respectively.  $F_1$  describes the motion of the incident proton,

and  $F_2$  and  $F_3$  denote the motion of the hydrogen atom formed by single electron capture, while  $F_4$  stands for the motion of the H<sup>-</sup> atom. The wave functions used for the ground-state helium atom and H<sup>-</sup> are given by

$$\phi(r_1, r_2) = (Z^3/\pi a_0^3) e^{(-Z/a_0)(r_1+r_2)}, \quad Z = 1.6875 \quad (3a)$$

$$\chi(r_1, r_2) = (Z'^3/\pi a_0^3) e^{(-Z'/a_0)(r_1+r_2)}, \quad Z' = 0.69 \quad (3b)$$

Following Bhadra *et al.*,<sup>11</sup> the CCA equations, neglecting the principal-value parts, for the transitions (1) are (the notation being the same as used by Bhadra *et al.*<sup>11</sup>)

$$f_{11}(\hat{k}' \cdot \hat{k}) = f_{11}^B(\hat{k}' \cdot \hat{k}) + \frac{i}{4\pi} \int [\vec{k}_x f_{11}^B(\hat{k}' \cdot \hat{k}'') f_{11}(\hat{k}'' \cdot \hat{k}) + \vec{k}_x f_{12}^B(\hat{k}' \cdot \hat{k}'') f^*(\hat{k}'' \cdot \hat{k}) + \vec{k}_y f_{14}^B(\hat{k}' \cdot \hat{k}'') f_{41}(\hat{k}'' \cdot \hat{k})] \sin\theta'' d\theta'' d\phi'', \quad (4a)$$

$$f^*(\hat{k}' \cdot \hat{k}) = 2f_{21}^B(\hat{k}' \cdot \hat{k}) + \frac{i}{2\pi} \int [\vec{k}_x f_{21}^B(\hat{k}' \cdot \hat{k}'') f_{11}(\hat{k}'' \cdot \hat{k}) + \frac{1}{2} \vec{k}_x f_{22}^B(\hat{k}' \cdot \hat{k}'') f^*(\hat{k}'' \cdot \hat{k}) + \vec{k}_y f_{24}^B(\hat{k}' \cdot \hat{k}'') f_{41}(\hat{k}'' \cdot \hat{k})] \sin\theta'' d\theta'' d\phi'', \quad (4b)$$

$$f_{41}(\hat{k}' \cdot \hat{k}) = f_{41}^B(\hat{k}' \cdot \hat{k}) + \frac{i}{4\pi} \int [\vec{k}_x f_{41}^B(\hat{k}' \cdot \hat{k}'') f_{11}(\hat{k}'' \cdot \hat{k}) + \vec{k}_x f_{42}^B(\hat{k}' \cdot \hat{k}'') f^*(\hat{k}'' \cdot \hat{k}) + \vec{k}_y f_{44}^B(\hat{k}' \cdot \hat{k}'') f_{41}(\hat{k}'' \cdot \hat{k})] \sin\theta'' d\theta'' d\phi'', \quad (4c)$$

where

$$\begin{aligned} f_{22}^B &= f_{22}^B + f_{23}^B, \\ f^* &= f_{21} + f_{31}. \end{aligned} \quad (5)$$

$f_{22}^B$  is the Born exchange integral which has an appreciable effect on the cross section only at low incident energies.  $\vec{k}_i$  is the incident momentum of the projectile and  $\vec{k}_x$  and  $\vec{k}_y$  are determined from the energy conservation relations

$$k_x^2/2\mu_2 = k_i^2/2\mu_1 - \epsilon_{\text{He}^0} + \epsilon_{\text{He}^+} + \epsilon_{\text{H}}, \quad (6)$$

$$k_y^2/2\mu_3 = k_i^2/2\mu_1 - \epsilon_{\text{He}^0} + \epsilon_{\text{H}^-}, \quad (7)$$

where  $\mu_2$  and  $\mu_3$  are the reduced masses of the final configurations of channels (1, b) and (1, d), respectively, and  $\epsilon_{\text{He}^+}$ ,  $\epsilon_{\text{He}^0}$ ,  $\epsilon_{\text{H}}$ , and  $\epsilon_{\text{H}^-}$  are the corresponding bound-state energies of the respective atoms indicated in subscripts.

## NUMERICAL PROCEDURE AND TEST CALCULATIONS

The Born amplitudes  $f_{11}^B$ ,  $f_{12}^B$ ,  $f_{21}^B$ ,  $f_{22}^B$ , and  $f_{44}^B$  have been analytically evaluated. But the exchange amplitudes  $f_{23}^B$  and  $f_{4i}^B$  or  $f_{4i}^B$  ( $i=1, 2$ ), however, can be expressed as two-dimensional integrals (see the Appendix). In the evaluation of the matrix element the small quantities of the order of  $m/M_n$  ( $m$  being the mass of electron, and  $M_n$ , the mass

of the alpha particle) in the expression of  $A$ 's (see Appendix) have been neglected. We checked our results with and without neglecting this small quantity of the order  $m/M_n$  and came to the conclusion that this approximation does not affect the accuracy in our results.

The wave functions of the H<sup>-</sup> and He atoms used are simple but inaccurate. The use of such inaccurate wave functions causes some error in the cross-section values. We have made an attempt to test the accuracy of the approximate H<sup>-</sup> one-parameter wave function used, by comparing the resulting Born cross-section values with those obtained by employing the more accurate four-parameter H<sup>-</sup> wave function due to Lowdin<sup>25</sup>

$$\begin{aligned} \chi(r_1, r_2) = & (1/4\pi) \{ C_1 e^{-\lambda_1 r_1 - \lambda_1 r_2} + C_2 e^{-\lambda_2 r_1 - \lambda_1 r_2} \\ & + C_3 e^{-\lambda_1 r_1 - \lambda_2 r_2} + C_4 e^{-\lambda_2 r_1 - \lambda_2 r_2} \}, \end{aligned} \quad (8)$$

where

$$\begin{aligned} C_1 &= \alpha_1^2, & \alpha_1 &= 0.30025 \\ C_2 &= \alpha_1 \alpha_2 = C_3, & \alpha_2 &= 1.0001 \\ C_4 &= \alpha_2^2, & \lambda_1 &= 0.4228 \\ & & \lambda_2 &= 0.9794. \end{aligned}$$

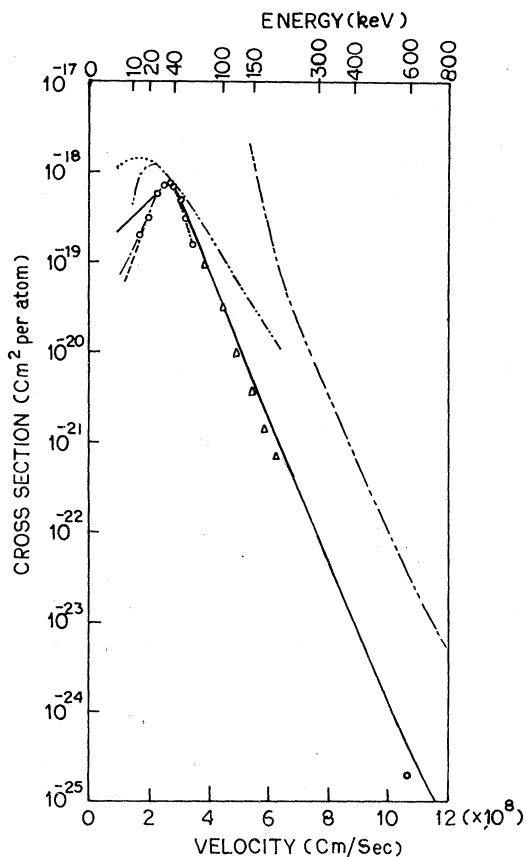


FIG. 1. Total double electron capture in proton-helium collisions. Theoretical: —, present with exchange; ·····, present without exchange; ———, Gerasi-menko; —·—·—·, Roy *et al.*; Experimental: ———, Williams; —·—·—·, Fogel *et al.*; O, Schryber; Δ, Toburen and Nakai.

The disagreement in the two sets of results is found to be within 15% below 100 keV. The variations of the difference in the cross-section values at 5, 15, 26, 40, and 100 keV are 9, 0.7, 10, 11, and 15%, respectively. We presume that our CCA cross-section values with the wave function (8) may be changed accordingly.

The ground-state helium wave function used is also inexact. However, the merits of this wave function have been tested by Bhadra and Sil<sup>26</sup> in detail. Single-capture cross sections both in the CCA and Born approximation have been evaluated with the prior and post forms of interaction using wave function (3a) and the more accurate wave function

$$\begin{aligned} \phi(r_1, r_2) = & (1.6966/\pi)(e^{-1.4r_1} + 0.739e^{-2.6r_1}) \\ & \times (e^{-1.4r_2} + 0.739e^{-2.6r_2}) \end{aligned} \quad (9)$$

due to Byron and Joachain.<sup>27</sup> It was concluded that

the simple Hylleraas wave function with the post form of interaction is adequate for good results in the charge-transfer process. As such, the post form of interaction has been used in the present calculation of amplitudes.

We have used  $z$  as the integration variable instead of  $\theta$ , where they are related by the transformation

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

This takes care of the fact that in heavy-particle collisions scattering amplitudes are sharply peaked in the forward direction and their angular spread decreases with increasing energy. We have converted the set of coupled integral equations into a set of coupled linear simultaneous equations by the Gauss quadrature technique. These equations have been solved by the matrix inversion method. Convergent results have been obtained by successively increasing Gauss points. Numerical calculations have been done with great care allowing a maximum error of 0.01%.

#### RESULTS AND DISCUSSIONS

In Fig. 1 we have shown our calculated results for the formation of  $H^-$  as a result of double electron capture by protons from helium for the incident energies 5 to 750 keV. We have also plotted the experimental findings<sup>18-21</sup> and the theoretical results<sup>22,23</sup> for comparison. Our results for the double-capture cross sections are in good agreement with the measured cross sections of Fogel *et al.*,<sup>18</sup> Williams,<sup>19</sup> Schryber,<sup>20</sup> and Toburen and Nakai.<sup>21</sup> The Born results due to Gerasi-menko<sup>22</sup> are given only for the high-energy region and are more than two orders of magnitude greater than the experimental results. The other theoretical results due to Roy *et al.*<sup>23</sup> also fail to give any quantitative agreement with the experimental findings. We have presented our results both considering the indistinguishability of electrons and neglecting it. The effect of exchange is evident in the low-energy region below 40 keV, where the cross sections are lowered on accounting for indistinguishability. Below 26 keV our calculated values are somewhat higher than those observed experimentally. This discrepancy between the present theoretical values and the experimental findings may be attributed to the absence of the effect of other excited states which are ignored and to the neglect of the principal-value part in our calculation. Our calculated values elsewhere agree well with the observations and show the peak accurately.

In Fig. 2 we have plotted our values of cross sections for single electron capture into the ground-

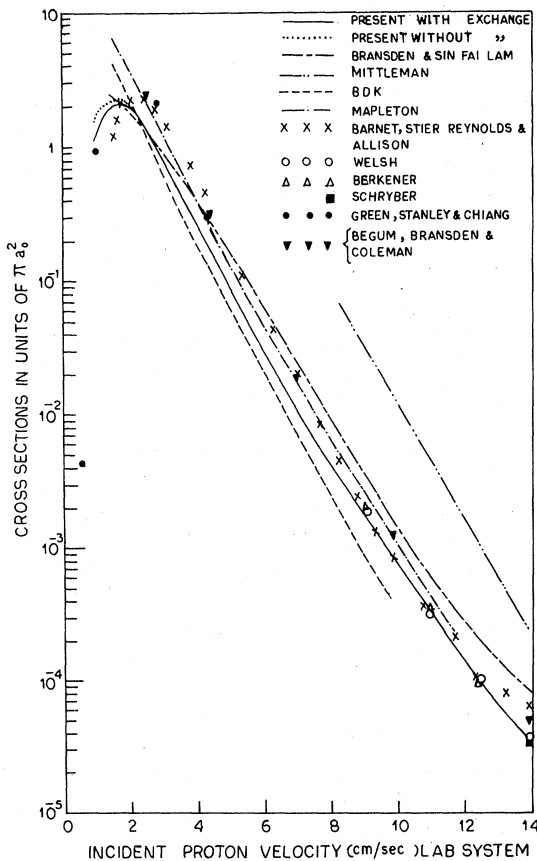


FIG. 2. Total single electron capture in proton-helium collisions. Present calculations with and without exchange as compared with the theoretical curves of Bransden and Sin Failam (Ref. 4), Mittleman (Ref. 10), Mapleton (Ref. 2), Green *et al.* (Ref. 6), Begum *et al.* (Ref. 8), and Bransden *et al.* (Ref. 1), and the experimental curves of Barnett *et al.* (Ref. 13), Welsh (Ref. 14), Berkener (Ref. 15), and Schryber (Ref. 16), in the energy range 1 keV to 1 MeV.

state hydrogen atom. We have also included the theoretical curves due to Mapleton,<sup>2</sup> Bransden *et al.*,<sup>1</sup> Bransden and Sin Failam,<sup>4</sup> Mittleman,<sup>10</sup> Green *et al.*,<sup>6</sup> and Begum *et al.*<sup>8</sup> The experimental findings due to Allison, Stier and Barnett,<sup>13</sup> Barnett and Reynolds,<sup>13</sup> Welsh *et al.*,<sup>14</sup> and Berkener *et al.*<sup>15</sup> are also included for comparison. The single-capture cross-section values are shown both with and without the exchange effect. Consideration of exchange is found to be effective only in the low-energy region below 26 keV, and its inclusion results in the lowering of the capture cross sections. The exchange effect is of little importance<sup>12,28</sup> at intermediate and high energies. This observation can also be easily made<sup>4</sup> if one compares the results of Green *et al.*,<sup>6</sup> who have considered the exchange effect, with those of Bransden and Sin

Failam,<sup>4</sup> who have neglected this indistinguishability. The present single-capture results produce a peak in the low-energy region as observed by Barnett *et al.*<sup>13</sup> and later obtained by Green *et al.*<sup>6</sup> Compared with the more recent theoretical results of Begum *et al.*,<sup>8</sup> our single-capture cross sections are in better agreement with experimental findings in the high-energy region.

In Fig. 3 we have presented the double-electron capture differential cross sections in the forward direction. We found no experimental or theoretical results for comparison. The trend of the curve is more or less of the same nature as that of the single-capture differential cross section in the forward direction for the same collisional process<sup>11,12</sup> but for the present double-capture process the magnitude of the differential cross section is always less than unity in units of  $\pi a_0^2$ .

The cross-section results obtained in all these channels considered are presented in Table I, without accounting for the indistinguishability of electrons. On comparison with previous calculations,<sup>26</sup> where only the elastic and single-capture channels were considered, it is found that the present calculations reproduce, more or less, the elastic and single-capture cross sections formerly obtained. Hence it is apparent that the effect of the double-capture channel on the single-capture and elastic channels is negligible. Roy *et al.* also observed a similar effect. Table II presents the calculated cross sections with the exchange effect.

#### APPENDIX: EVALUATION OF EXCHANGE SCATTERING AMPLITUDE OF MATRIX ELEMENTS

Exchange scattering amplitude  $f_{23}^B$  for ground-state hydrogen atom can be expressed as (our notations are the same as used by Bhadra *et al.*)

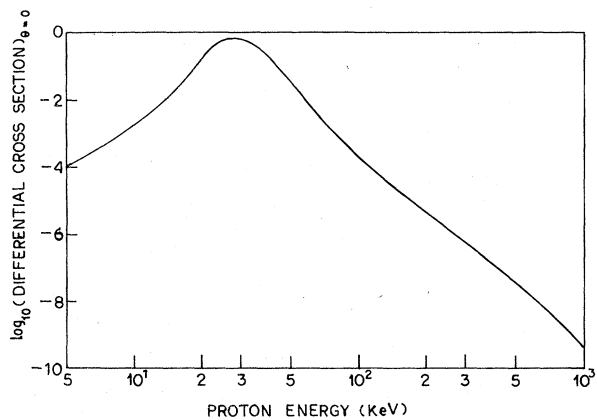


FIG. 3. Differential cross sections for the double-electron capture in the  $0^\circ$  scattering angle presented from 5 keV to 1 MeV (in units of  $\pi a_0^2$ ).

TABLE I. Total cross sections<sup>a</sup> without exchange term for elastic, single-capture, and double-capture processes in proton-helium collisions in units of  $\pi a_0^2$ .

Energy (keV)	Elastic	Single capture	Double capture
5	1.133	1.614	0.1275 <sup>-1</sup>
15	1.043	2.292	0.1529 <sup>-1</sup>
26	0.7529	1.675	0.1113 <sup>-1</sup>
40	0.6139	1.014	0.7342 <sup>-2</sup>
100	0.3874	0.1755	0.3452 <sup>-3</sup>
200	0.2499	0.2407 <sup>-1</sup>	0.1210 <sup>-4</sup>
600	0.1072	0.3596 <sup>-3</sup>	0.4236 <sup>-8</sup>
1000	0.6922 <sup>-1</sup>	0.3524 <sup>-4</sup>	0.6784 <sup>-10</sup>

<sup>a</sup> The superscript in each entry is the exponent of 10 by which the cross-section value should be multiplied.

$$f_{23}^B = -\frac{\mu_2}{2\pi} \int d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 \psi_0(\vec{x}_1) \omega_0(\vec{x}_2) V_f \times \psi_0(\vec{x}_3) \omega_0(|\vec{x}_1 + \vec{x}_2 - \vec{x}_3|), \quad (\text{A1})$$

where  $V_f$  is the post form of interaction.

We evaluate a particular integral  $I$  defined below by which one can get the expression (A1):

$$I = \int \frac{\exp[i(\vec{A}_1 \cdot \vec{x}_1 + \vec{A}_2 \cdot \vec{x}_2 - \vec{A}_3 \cdot \vec{x}_3)]}{|\vec{x}_1 - \vec{x}_3|} \times \exp[-\beta_1 |\vec{x}_1 + \vec{x}_2 - \vec{x}_3| - \beta_2 x_2 - \alpha_2 x_1 - \alpha_1 x_3] \times d\vec{x}_1 d\vec{x}_2 d\vec{x}_3, \quad (\text{A2})$$

which can be written as

$$I = \int J_1 \frac{\exp[i(\vec{A}_1 \cdot \vec{x}_1 - \vec{A}_3 \cdot \vec{x}_3) - \alpha_1 x_3 - \alpha_2 x_1]}{|\vec{k}|}, \quad (\text{A3})$$

where

$$|\vec{k}| = |\vec{x}_1 - \vec{x}_3|, \quad (\text{A4})$$

$$J_1 = \int e^{i\vec{A}_2 \cdot \vec{x}_2} e^{-\beta_1 |\vec{x}_2 + \vec{k}| - \beta_2 x_2} d\vec{x}_2.$$

Using the Fourier transform

$$e^{-\lambda r} = \frac{\lambda}{\pi^2} \int \frac{e^{i\vec{p} \cdot \vec{r}}}{(p^2 + \lambda^2)^2} d\vec{p} \quad (\text{A5})$$

and the representation of  $\delta$  function

$$\delta(\vec{k} - \vec{k}') = \frac{1}{(2\pi)^3} \int e^{i\vec{p} \cdot (\vec{k} - \vec{k}')} d\vec{p}, \quad (\text{A6})$$

we get

$$J_1 = \frac{2}{\pi} \frac{\partial}{\partial \beta_1} \frac{\partial}{\partial \beta_2} \int \frac{e^{i\vec{q} \cdot \vec{k}} d\vec{q}}{(q^2 + \beta_2^2) \{(\vec{A}_2 + \vec{q})^2 + \beta_2^2\}}. \quad (\text{A7})$$

Now using the Feynman integration

$$\frac{1}{ab} = \int_0^1 dx [ax + b(1-x)]^{-2}, \quad (\text{A8})$$

we readily obtain

$$J_1 = \frac{2}{\pi} \frac{\partial}{\partial \beta_1} \frac{\partial}{\partial \beta_2} \int_0^1 dx \int \frac{e^{i\vec{q} \cdot \vec{k}} d\vec{q}}{[(\vec{q} + \vec{\Lambda})^2 + \mu^2]^2}, \quad (\text{A9})$$

where

$$\vec{\Lambda} = (1-x)\vec{A}_2, \quad \mu^2 = x\beta_1^2 + \beta_2^2(1-x) + x(1-x)A_2^2,$$

and then using the standard integral

$$\int \frac{d\vec{k} e^{i\vec{k} \cdot \vec{a}}}{(k^2 + \mu^2)^2} = \frac{\pi^2}{\mu} e^{-\alpha\mu}, \quad (\text{A10})$$

we get

$$J_1 = 2\pi \frac{\partial}{\partial \beta_1} \frac{\partial}{\partial \beta_2} \int_0^1 dx e^{-\vec{\Lambda} \cdot \vec{k}} \frac{1}{\mu} e^{-k\mu}. \quad (\text{A11})$$

Substituting Eq. (A11) in Eq. (A3), we can write

$$I = 2\pi \frac{\partial}{\partial \beta_1} \frac{\partial}{\partial \beta_2} \int_0^1 \int J_2 dx e^{-i(\vec{\Lambda} - \vec{A}_1) \cdot \vec{x}_1} e^{-i\alpha_2 x_1} d\vec{x}_1, \quad (\text{A12})$$

where

$$J_2 = \int e^{i(\vec{\Lambda} - \vec{A}_3) \cdot \vec{x}_3} \times \frac{\exp(-\mu |\vec{x}_1 - \vec{x}_3| - \alpha_1 x_3)}{|\vec{x}_1 - \vec{x}_3|} d\vec{x}_3. \quad (\text{A13})$$

Using the Fourier transform

$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{e^{i\vec{p} \cdot \vec{r}}}{(p^2 + \lambda^2)} d\vec{p}, \quad (\text{A14})$$

and proceeding similarly as done in  $J_1$ , we get

$$J_2 = -2\pi \frac{\partial}{\partial \alpha_1} \int_0^1 dy e^{-\vec{B} \cdot \vec{x}_1} \frac{1}{\nu} e^{-\nu x_1}, \quad (\text{A15})$$

where

$$\vec{B} = (1-y)(\vec{A}_3 - \vec{\Lambda}), \quad \nu^2 = y\mu^2 + \alpha_1^2(1-y) + y(1-y)(\vec{A}_3 - \vec{\Lambda})^2.$$

With Eqs. (A12) and (A15) we can write

TABLE II. Total cross sections<sup>a</sup> with exchange term for elastic, single-capture, and double-capture processes in proton-helium collisions in units of  $\pi a_0^2$ .

Energy (keV)	Elastic	Single capture	Double capture
5	2.0751	1.1680	0.2306 <sup>-2</sup>
26	0.9545	1.6434	0.5718 <sup>-2</sup>

<sup>a</sup> The superscript in each entry is the exponent of 10 by which the cross-section value should be multiplied.

$$I = -4\pi^2 \frac{\partial}{\partial \beta_1} \frac{\partial}{\partial \beta_2} \frac{\partial}{\partial \alpha_1} \int_0^1 dx \int_0^1 dy \int \frac{e^{i(\vec{A}_1 - \vec{A} - \vec{B}) \cdot \vec{x}_1}}{\mu\nu} \times e^{-(\nu + \alpha_2)x_1} d\vec{x}_1. \quad (\text{A16})$$

Again using Eqs. (A5) and (A6) we finally get

$$I = -2^5 \pi^3 \int_0^1 \int_0^1 D_{123} dx dy, \quad (\text{A17})$$

where

$$D_{123} = \frac{\partial}{\partial \beta_1} \frac{\partial}{\partial \beta_2} \frac{\partial}{\partial \alpha_1} \left( \frac{\nu + \alpha_2}{\mu\nu[(\vec{A}_1 - \vec{A} - \vec{B})^2 + (\nu + \alpha_2)^2]^{3/2}} \right).$$

For exchange scattering amplitude we are left with a two-dimensional integral which is numerically evaluated. Using similar technique one can also reduce  $f_{i4}^B$  or  $f_{4i}^B$  ( $i=1, 2$ ) into a two-dimensional integral.

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