Rearrangement Collisions. II. Electron Excitation of He(2^3P)†

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A systematic study is made of various first-order approximations to the T matrix for a rearrangement collision. Detailed calculations are performed for the process of excitation of the 2^3P level of helium by electron impact. Comparison is drawn between the various theoretical cross sections obtained and the experimental data. The polarization of the emitted radiation is also studied.

I. INTRODUCTION

THE excitation of triplet states of helium by electron impact are among the simplest rearrangement collisions where theoretical calculations from first principles might be compared to experiments. In a previous paper,[1] we investigated the dynamical problem, e.g., the ambiguities associated with the various possible T matrix formulations of rearrangement processes. We performed explicit calculations in the case of electron excitation of the 2^3S level of helium and found that, as far as that reaction was concerned, the projection-operator formalism for the T matrix was a significant improvement over the Born-Oppenheimer approximation.

In order to pursue further the study of the dynamical problem, we have investigated in this paper the excitation of the 2^3P state of helium by electron impact. In Sec. II, we briefly recall the relevant theoretical formulas. Our results are presented and discussed in Sec. III, where they are also compared with previous theoretical calculations and the existing experimental data.

II. THEORY

Let us label the three electrons involved in the reaction with suffixes 0, 1, 2. If we single out the (0) particle as the incoming one, then the unsymmetrized state is given by

$$\lambda_i(0)=\chi_i(0)\alpha(0)\frac{1}{\sqrt{2}}[\alpha(1)\beta(2)-\alpha(2)\beta(1)], \quad (1)$$

where

$$\chi_i(0)=e^{i\mathbf{p}_1\cdot\mathbf{r}_0}\phi_0(r_1,r_2) \quad (2)$$

is the initial free wave and where ϕ_0 is the spatial part of the ground-state wave function of helium. The quantities $\alpha(n)$ ($\beta(n)$) are the usual spin-up (down) functions of the nth electron.

In the same way, the unsymmetrized final state with particle (1) singled out as the outgoing one is

$$\lambda_f(1)=\chi_f(1)\frac{1}{\sqrt{6}}[\alpha(1)\alpha(0)\beta(2) +\alpha(1)\beta(0)\alpha(2)-2\beta(1)\alpha(0)\alpha(2)], \quad (3)$$

where

$$\chi_f(1)=e^{i\mathbf{p}_f\cdot\mathbf{r}_1}\phi_1(\mathbf{r}_0,\mathbf{r}_2) \quad (4)$$

is the final free wave and ϕ_1 is the spatial part of the 2^3P state of helium. The spin part represents an orthonormal doublet state symmetric in the interchange of particles (0) and (2).

After meeting the symmetrization requirements and performing the spin algebra, one gets for the differential cross section in atomic units[1]:

$$\frac{d\sigma}{d\Omega}=\frac{3}{4\pi^2}\frac{p_f}{p_i}|T_{fi}|^2, \quad (5)$$

where the initial and final momenta p_i and p_f are related by

$$p_f^2=p_i^2-\epsilon \quad (6)$$

and where $\epsilon=1.541$ is the experimental value of the excitation energy of the 2^3P state (in atomic units). The quantity T_{fi} refers to the reduced T matrix from which the spin dependence has been removed.[1]

We now perform the calculation of the various approximate forms of the T matrix which were considered in Ref. 1 in the framework of the free wave approximation (e.g., the replacement of the exact scattering wave functions by their unperturbed values). The interaction potential in the initial channel is given by

$$V_i(0)=-\frac{2}{r_0}+\frac{1}{r_{01}}+\frac{1}{r_{02}} \quad (7)$$

whereas in the final channel

$$V_f(1)=-\frac{2}{r_1}+\frac{1}{r_{01}}+\frac{1}{r_{12}}. \quad (8)$$

Therefore, the eight approximate T matrices which we

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[1] C. J. Joachain and M. H. Mittleman, Phys. Rev. 140, A432 (1965).

consider are[1]

$$T_1=\langle\chi_f(1)V_f(1)\chi_i(0)\rangle, \quad (9)$$

$$T_2=\langle\chi_f(1)V_i(0)\chi_i(0)\rangle, \quad (10)$$

$$T_3=\langle\chi_f(1)\hat{V}_f(1)\chi_i(0)\rangle, \quad (11)$$

$$T_4=\langle\chi_f(1)\hat{V}_i(0)\chi_i(0)\rangle, \quad (12)$$

$$T_5=\langle\chi_f(1)[\pi_f(1),V_f(1)]\chi_i(0)\rangle, \quad (13)$$

$$T_6=\langle\chi_f(1)[V_i(0),\pi_i(0)]\chi_i(0)\rangle, \quad (14)$$

$$T_7=\langle\chi_f(1)[\pi_f(1),H]\chi_i(0)\rangle, \quad (15)$$

$$T_8=\langle\chi_f(1)[H,\pi_i(0)]\chi_i(0)\rangle. \quad (16)$$

In these formulas, we have defined

$$\hat{V}_f(1)=V_f(1)+\frac{2}{r_1}-\frac{1}{r_{10}}+\frac{1}{r_{12}}, \quad (17)$$

and

$$\hat{V}_i(0)=V_i(0)+\frac{2}{r_0}-\frac{1}{r_{10}}+\frac{1}{r_{02}}, \quad (18)$$

whereas $\pi_i(0)$ and $\pi_f(1)$ are projection operators respectively on the initial and final state, and H is the total Hamiltonian of the system.

We have evaluated the eight forms $T_i(i=1, 2, \cdots, 8)$ and the corresponding cross sections by using simple variational wave functions to describe the relevant bound states of helium. For the ground state we use the Hylleraas one-parameter wave function

$$\phi_0(r_1,r_2)=\alpha^3/\pi e^{-\alpha(r_1+r_2)}, \quad (19)$$

with $\alpha=27/16$, whereas for the 2^3P state we took a two-parameter Eckart wave function

$$\phi_{1,M}(\mathbf{r}_0,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[u(r_0)v_M(\mathbf{r}_2)-u(r_2)v_M(\mathbf{r}_0)], \quad (20)$$

where

$$u(r)=\beta^{3/2}/\pi^{1/2}e^{-\beta r}, \quad (21)$$

and

$$v_M(\mathbf{r})=\gamma^{5/2}/(32\pi)^{1/2}re^{-\gamma r/2} \times\begin{cases}\cos\theta, & M=0\\ (2^{-1/2}\sin\theta)e^{\pm i\phi}, & M=\pm1;\end{cases} \quad (22)$$

M being the magnetic quantum number with the direction of quantization taken as the incident electron momentum. The variational parameters β and γ are given[2] respectively by $\beta=1.99$ and $\gamma=1.09$. The only complicated integral appearing in the calculations is the expression

$$I=\langle\chi_f(1)(1/r_{01})\chi_i(0)\rangle \quad (23)$$

which was performed numerically after reducing it to a one-dimensional integral. Since our expression for I disagrees with a previous work,[3] we give a brief survey of our calculational method in the Appendix.

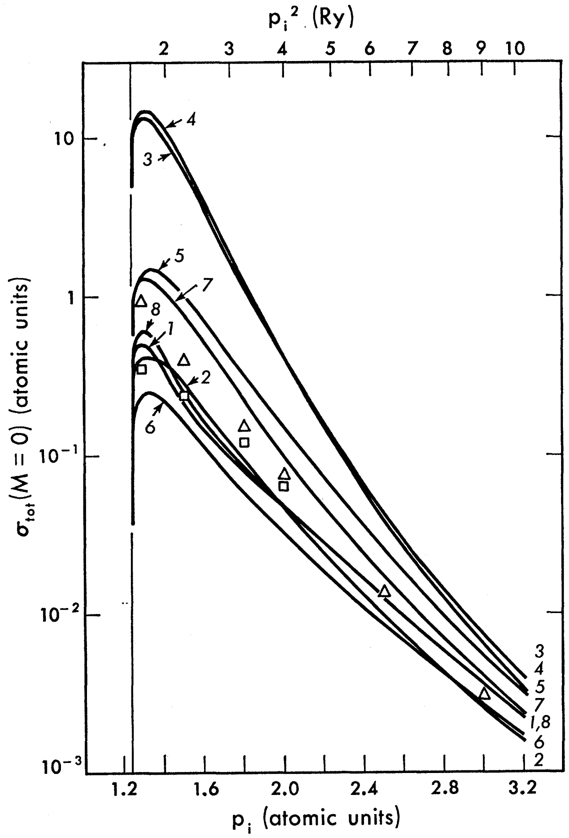

FIG. 1. Total cross section for excitation of the 2^3P ($M=0$) state of helium in atomic units ($a^2\equiv0.279\times10^{-16}$ cm^2) versus magnitude of the incident electron momentum p_i in atomic units (lower scale) or incident electron energy p_i^2 in rydbergs (upper scale). △ Born-Oppenheimer approximation, Massey-Moiseiwitsch (Ref. 3); □ distorted-wave approximation, Massey-Moiseiwitsch (Ref. 3).

III. RESULTS AND DISCUSSION

In Fig. 1 we display the total cross section $\sigma_{tot}(M=0)$ for excitation of the 2^3P state with $M=0$. As expected, curves 3 and 4 containing spurious exchange contributions from large distances grossly overestimate the cross section. The Born-Oppenheimer curves 1 and 2 exhibit a satisfactory post-prior behavior, as do the projection-operator curves 5–7 and 6–8, respectively. We have also shown several points of the Born-Oppenheimer calculation of Massey and Moiseiwitsch[3] and of their distorted-wave treatment.

In Fig. 2, we show the total cross section $\sigma_{tot}(M=\pm1)$ for excitation of the 2^3P states with $M=\pm1$, which again we compare with the previous theoretical calculations of Massey and Moiseiwitsch.[3]

[2] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms* (Academic Press Inc., New York, 1957), p. 158.

[3] H. S. W. Massey and B. L. Moiseiwitsch, Proc. Roy. Soc. (London) A258, 147 (1960).

The total cross section

$$\sigma_{tot}=\sigma_{tot}(M=0)+2\sigma_{tot}(M=\pm 1) \qquad (24)$$

for excitation of the 2^3P state is shown in Fig. 3, where it is compared with the presently available experiments.

An analysis of the experimental data for electrons with energies less then 45 eV has been made by Frost and Phelps[4] collected data from the observations of Lies,[5] Thieme,[6] Maier-Leibnitz,[7] Dorrenstein,[8] and Schulz.[9] The curve obtained by Frost and Phelps[4] (quoted in the work of Massey and Moiseiwitsch[3]) rises to a maximum of $\sigma_{tot}\cong 0.07\ a^2$ at an incident electron energy around 22.5 eV and gives $\sigma_{tot}\cong 0.045\ a^2$ at 39 eV (see Fig. 3). Recently, Holt and Krotkov[10] have measured the sum of the 2^3S and 2^3P cross sections in the energy range 19.8–23.2 eV. They also estimated the 2^3P cross section by subtracting from the sum an estimated 2^3S cross section (obtained by averaging differential cross sections measured by Schulz and Philbrick[11] and Chamberlain and Heideman[12]). Only relative cross sections were measured in the Holt and Krotkov[10] experiment. The absolute values quoted were obtained by making measurements relative to the peak of the 2^3S cross section. Assuming a value of $(0.11\pm 0.03)\ a^2$ for this peak, Holt and Krotkov found that the 2^3P cross section rises from threshold to $(0.11\pm 0.04)\ a^2$ at 23.2 eV. This value is substantially larger than the maximum obtained by Frost and Phelps[4] (see Fig. 3).

At higher energies, Gabriel and Heddle[13] have studied the shape of the excitation functions for the n^3P levels

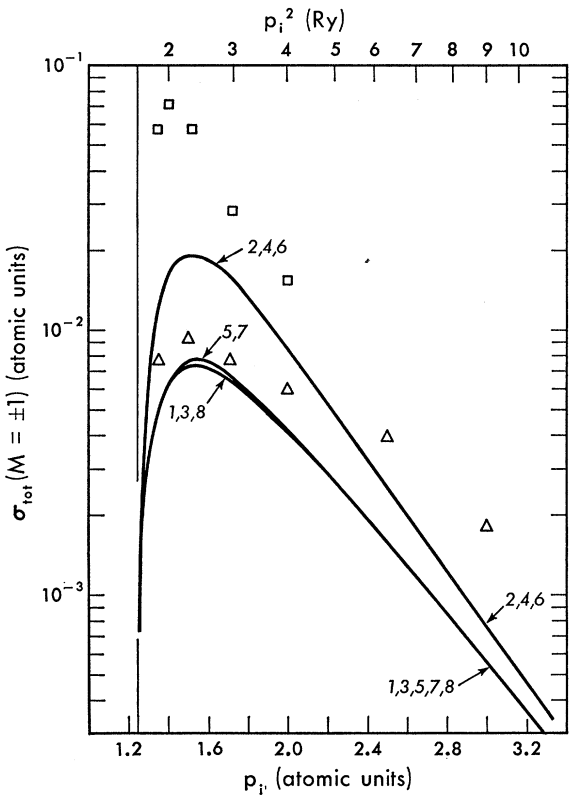

FIG. 2. Total cross section for excitation of the 2^3P $(M=\pm 1)$ state of helium in atomic units (a^2) versus magnitude of the incident electron momentum p_i in atomic units (lower scale) or incident electron energy p_i^2 in rydbergs (upper scale). △ Born-Oppenheimer approximation, Massey-Moiseiwitsch (Ref. 3); □ distorted-wave approximation, Massey-Moiseiwitsch (Ref. 3).

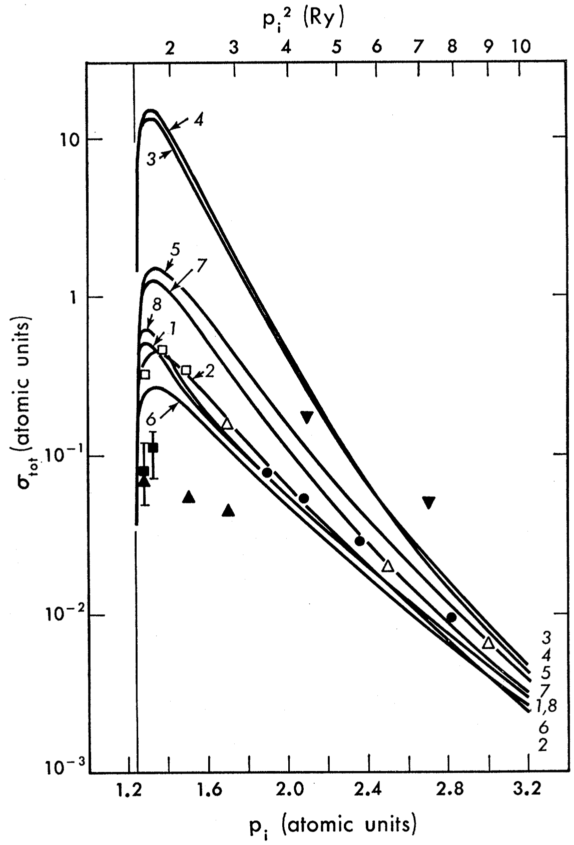

FIG. 3. Total cross section for excitation of the 2^3P state of helium in atomic units (a^2) versus magnitude of the incident electron momentum p_i in atomic units (lower scale) or incident electron energy p_i^2 in rydbergs (upper scale). ▲ Experimental points, Frost and Phelps (Ref. 4), ■ experimental points, Holt and Krotkov (Ref. 10), ● experimental points, Gabriel and Heddle (Ref. 13), ▼ experimental points, St. John *et al.* (Ref. 14), △ Born-Oppenheimer approximation, Massey and Moiseiwitsch (Ref. 3), □ distorted-wave approximation, Massey and Moiseiwitsch (Ref. 3).

[4] L. S. Frost and A. V. Phelps, Westinghouse Laboratory Research Report No. 6-94439-6-R3, 1957 (unpublished).
[5] J. M. Lees, Proc. Roy. Soc. (London) **A137**, 173 (1932).
[6] O. Thieme, Z. Physik **78**, 412 (1932).
[7] H. Maier-Leibnitz, Ann. Physik. **95**, 499 (1935).
[8] R. Dorrenstein, Physica **9**, 447 (1942).
[9] G. J. Schulz, Phys. Rev. **112**, 150 (1958).
[10] H. K. Holt and R. Krotkov, Phys. Rev. **144**, 82 (1966).
[11] G. J. Schulz and J. W. Philbrick, Phys. Rev. Letters **13**, 477 (1964).
[12] G. E. Chamberlain and H. G. M. Heideman, Phys. Rev. Letters **15**, 337 (1965).
[13] A. H. Gabriel and D. W. O. Heddle, Proc. Roy. Soc. (London) **A258**, 124 (1960).

TABLE I. Percentage polarization P of $2^3P_2 \rightarrow 2^3S_1$ radiation after excitation by electron impact.

Magnitude of the incoming electron momentum p_i (a.u.)	Energy of the incoming electron p_i^2 (Ry)	P From the various "first-order" approximations $T_i(i=1,\cdots,8)$ to the T matrix [Eqs. (9)–(16)] 1	2	3	4	5	6	7	8	Distorted-wave approximation[a]
1.24 (threshold)	1.54	44.6	44.6	44.6	44.6	44.6	44.6	44.6	44.6	44.6
1.27	1.61	44.4	43.7	44.5	44.5	44.6	43.0	44.5	44.4	35.5
1.30	1.69	44.1	42.8	44.6	44.5	44.4	41.6	44.4	44.2	
1.36	1.85	43.3	41.1	44.5	44.4	44.3	38.7	44.2	43.5	27.2
1.40	1.96	42.6	40.0	44.5	44.5	44.1	36.9	44.0	42.9	
1.45	2.10	41.4	38.8	44.6	44.4	44.0	34.9	41.8	42.3	
1.50	2.25	41.1	37.6	44.3	44.4	43.8	33.1	43.6	41.5	25.3

[a] See Ref. 3.

($n=3$, 4, 5), while at an energy of 108 eV absolute measurements were carried out. They have also estimated the cross section for 3^3P excitation in the energy range 30–400 eV using observed values of Thieme[6] corrected for cascade effects. The data suggest that these measurements can be extrapolated to $n=2$ by assuming that $\sigma_{\text{tot}}(n)\sim n^{-3}$. Thus Gabriel and Heddle[13] quote $\sigma_{\text{tot}}=0.26\times10^{-18}$ cm^2 (i.e., $\sigma_{\text{tot}}=9.3\times10^{-3}\ a^2$) as an absolute value for the excitation of the 2^3P level at 108 eV. Other "experimental" points can be obtained by this extrapolation procedure from their estimated cross sections for the 3^3P level in the range 30–400 eV. We have displayed several of these in Fig. 3. Also shown in Fig. 3 are the results (extrapolated to $n=2$) of recent absolute measurements performed at 60 and 100 eV by St. John *et al.*[14] for the excitation of the 3^3P level. It is worth noting that the values obtained by St. John *et al.*, are much larger than those of Gabriel and Heddle.[13]

Comparison of our various theoretical curves with these experimental data shows that all the "first-order" formulations we have used overestimate the total cross section at low energies (curve 6 being the best one), whereas at higher energies curves 1, 2, 6, and 8 are in reasonable agreement with the Gabriel and Heddle[13] experiments. A disturbing fact, however, is the behavior of curves 5 and 7. This seems to indicate that our first-order formulas (13) or (15) are not accurate enough to take into account the considerable amount of distortion occurring in the outgoing P-state channel. On the contrary, since in the ingoing channel the helium atom is in its ground state the distortion is less marked and the first-order formulas (14) and (16) leading respectively to curves 6 and 8 are probably more reliable.[15] Among those two last curves, 6 is presumably more trustworthy than 8, since the appearance of kinetic-energy operators in H (formula 16) emphasizes the errors in the approximate bound state wave functions.

We also display in Fig. 3 several points of the Born-Oppenheimer calculation of Massey and Moiseiwitsch,[3] and of their distorted-wave treatment.[16]

Finally, in Table I, we give the percentage polarization[3]

$$p=\frac{100[\sigma_{\text{tot}}(M=0)-\sigma_{\text{tot}}(M=\pm1)]}{(47/21)\sigma_{\text{tot}}(M=0)+(73/21)\sigma_{\text{tot}}(M=\pm1)} \quad (25)$$

of the light emitted in the $2^3P_2\rightarrow 2^3S_1$ transition after impact excitation, in a direction at right angles to the incoming electron beam. We have compared the values obtained from our eight approximations to the T matrix [Eqs. (9)–(16)] with the distorted-wave calculation of Massey and Moiseiwitsch,[3] for incoming electron energies ranging from threshold to about 30 eV (i.e., $p_i=1.5$ a.u.). If we accept the distorted-wave results as the most reliable points of comparison, then formulation 6 proves again superior to our other "first-order" ones, yielding a percentage polarization which decreases from 44.6% at threshold to 33.1% at $p_i=1.5$ a.u.

APPENDIX

We want to evaluate the quantity

$$I_M=\langle\chi_f(1)\left|\frac{1}{r_{01}}\right|\chi_i(0)\rangle, \quad (A1)$$

or, explicitly

$$I_M=\int e^{-i\mathbf{p}_f\cdot\mathbf{r}_1}\phi_{1,M}(\mathbf{r}_0,\mathbf{r}_2)\frac{1}{r_{01}}e^{i\mathbf{p}_i\cdot\mathbf{r}_0}\times\phi_0(r_1,r_2)d\mathbf{r}_0d\mathbf{r}_1d\mathbf{r}_2, \quad (A2)$$

where $\phi_0(r_1,r_2)$ and $\phi_{1,M}(\mathbf{r}_0,\mathbf{r}_2)$ are given respectively by Eqs. (19) and (20). After performing the integration over the $\mathbf{r}_2$ coordinates, we get

$$I_M=-\frac{\alpha^3\beta^{3/2}\gamma^{5/2}}{\pi(\alpha+\beta)^3}J_M, \quad (A3)$$

[14] R. M. St. John, F. L. Miller, and C. C. Lin, Phys. Rev. **134**, A888 (1964).

[15] The same argument holds for the excitation of the 2^3S state. In the light of the present calculations, the qualitative argument suggested in Ref. 1 and favoring curve 5 should be discarded, therefore leaving curve 6 as the most reliable one.

[16] It is interesting to note that improving the ground-state wave function of helium does not lead to any significant change in the distorted-wave calculation [see C. N. Lashmore-Davies, Proc. Roy. Soc. (London) **86**, 783 (1965)].

where

$$J_{(M=0)}=\int e^{-i\mathbf{p}_f\cdot\mathbf{r}_1}r_0e^{-\frac{1}{2}\gamma r_0}\times\cos\theta_0\frac{1}{r_{01}}e^{i\mathbf{p}_i\cdot\mathbf{r}_0}e^{-\alpha r_1}d\mathbf{r}_0d\mathbf{r}_1, \quad (A4)$$

and

$$J_{(M=\pm1)}=\frac{1}{\sqrt{2}}\int e^{-i\mathbf{p}_f\cdot\mathbf{r}_1}r_0e^{-\frac{1}{2}\gamma r_0}\times\sin\theta_0e^{\mp i\phi_0}\frac{1}{r_{01}}e^{i\mathbf{p}_i\cdot\mathbf{r}_0}e^{-\alpha r_1}d\mathbf{r}_0d\mathbf{r}_1. \quad (A5)$$

Using the well-known relation

$$\frac{1}{r_{01}}=\frac{1}{2\pi^2}\lim_{\epsilon\to0+}\int\frac{e^{i\mathbf{K}\cdot(\mathbf{r}_1-\mathbf{r}_0)}}{K^2-i\epsilon}d\mathbf{K} \quad (A6)$$

and doing the $\mathbf{r}_0$ and $\mathbf{r}_1$ integrations in momentum space, we obtain

$$J_M=-i64\alpha\gamma\int\frac{\mathbf{A}_M\cdot(\mathbf{K}-\mathbf{p}_i)}{K^2-i\epsilon}\times\frac{1}{[\alpha^2+|\mathbf{K}-\mathbf{p}_f|^2]^2[\frac{1}{4}\gamma^2+|\mathbf{p}_i-\mathbf{K}|^2]^3}, \quad (A7)$$

where the axis of quantization is defined along the incident momentum (which we choose to coincide with the z direction) such that

$$\mathbf{A}_0=\hat{p}_i, \quad (A8)$$

and

$$\mathbf{A}_{\pm1}=(1/\sqrt{2})(\hat{a}_x\pm i\hat{a}_y). \quad (A9)$$

Here $\hat{p}_i$ is the unit vector along $\mathbf{p}_i$, whereas $\hat{a}_x$ and $\hat{a}_y$ are unit vectors respectively in the x and y directions. Now, setting

$$a=\alpha^2+|\mathbf{K}-\mathbf{p}_f|^2 \quad (A10)$$

and

$$b=\tfrac{1}{4}\gamma^2+|\mathbf{p}_i-\mathbf{K}|^2 \quad (A11)$$

and using the Feynman integral representation[17]

$$a^{-2}b^{-3}=\int_0^1\frac{12t(1-t)}{[at+b(1-t)]^5}dt, \quad (A12)$$

we get from (A7)

$$J_M=-i768\alpha\gamma\int_0^1 t(1-t)^2dt\times\int\frac{\mathbf{A}_M\cdot(\mathbf{K}-\mathbf{p}_i)}{K^2-i\epsilon}\frac{1}{[|\mathbf{K}-\mathbf{\Lambda}|^2+\Gamma^2]^5}d\mathbf{K}, \quad (A13)$$

[17] R. P. Feynman, Phys. Rev. **76**, 769 (1949).

with

$$\mathbf{\Lambda}=\mathbf{p}_i(1-t)+\mathbf{p}_ft, \quad (A14)$$

and

$$\Gamma^2=\alpha^2t+\tfrac{1}{4}\gamma^2(1-t)+(\mathbf{p}_i-\mathbf{p}_f)^2t(1-t). \quad (A15)$$

The $\mathbf{K}$ integration can be done by starting from the known integral[18]

$$\lim_{\epsilon\to0+}\int\frac{d\mathbf{K}}{[K^2-i\epsilon][|\mathbf{K}-\mathbf{\Lambda}|^2+\Gamma^2]^2}=\frac{\pi^2}{\Gamma(\Lambda^2+\Gamma^2)}, \quad (A16)$$

and using the fact that

$$\mathbf{A}_M\cdot\mathbf{K}\to(\mathbf{A}_M\cdot\mathbf{\Lambda})(\mathbf{\Lambda}\cdot\mathbf{K})/\Lambda^2. \quad (A17)$$

This yields

$$\int\frac{\mathbf{A}_M\cdot(\mathbf{K}-\mathbf{p}_i)}{K^2-i\epsilon}\frac{1}{[|\mathbf{K}-\mathbf{\Lambda}|^2+\Gamma^2]^5}d\mathbf{K}=\frac{\pi^2}{64\Gamma^7}\left[\mathbf{A}_M\cdot\mathbf{\Lambda}\frac{5\Lambda^4+14\Lambda^2\Gamma^2+(35/3)\Gamma^4}{(\Lambda^2+\Gamma^2)^3}-\mathbf{A}_M\cdot\mathbf{p}_i\frac{5\Lambda^6+21\Lambda^4\Gamma^2+35\Lambda^2\Gamma^4+35\Gamma^6}{(\Lambda^2+\Gamma^2)^4}\right], \quad (A18)$$

and therefore, using Eqs. (A3), (A8), (A9), (A13), and (A14), we get

$$I_{M=0}(\theta)=i\frac{12\pi\alpha^4\beta^{3/2}\gamma^{7/2}}{(\alpha+\beta)^3}\int_0^1\frac{t(1-t)^2}{\Gamma^7}\times\left\{\frac{5\Lambda^4+14\Lambda^2\Gamma^2+(35/3)\Gamma^4}{(\Lambda^2+\Gamma^2)^3}[p_f\mu t+p_i(1-t)]-p_i\frac{5\Lambda^6+21\Lambda^4\Gamma^2+35\Lambda^2\Gamma^4+35\Gamma^6}{(\Lambda^2+\Gamma^2)^4}\right\}dt, \quad (A19)$$

and

$$I_{M=\pm1}(\theta,\phi)=i\frac{12\pi\alpha^4\beta^{3/2}\gamma^{7/2}}{\sqrt{2}(\alpha+\beta)^3}e^{\pm i\phi}\int_0^1\frac{t^2(1-t)^2}{\Gamma^7}\times\frac{5\Lambda^4+14\Lambda^2\Gamma^2+(35/3)\Gamma^4}{(\Lambda^2+\Gamma^2)^3}\times p_f(1-\mu^2)^{1/2}dt, \quad (A20)$$

where

$$\mu=\cos\theta=\mathbf{p}_i\cdot\mathbf{p}_f/p_ip_f, \quad (A21)$$

and where the angle ϕ is measured in the xy plane from the x direction $\hat{a}_x$.

The one-dimensional integrals appearing in the expressions (A19) and (A20), as well as the subsequent angular integrations leading to the total cross sections, have been evaluated numerically.

[18] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 1083.