THE FORMATION OF POSITRONIUM
IN HYDROGEN AND HELIUM GASES

A Thesis

submitted in Partial Fulfillment of the Requirements

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by

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SUMMARY

The formation of positronium by the process of electron capture by positrons passing through hydrogen has been studied theoretically. For formation in the ground state, the cross section has a maximum value equal to 4.9 times the area of the hydrogen atom, when the incoming positron has about the same velocity as the bound electron in hydrogen. Above this velocity, the cross section falls off rapidly, going asymptotically as v^{-12} .

Various approximations have been made in analogous problems, including some work on helium.

ACKNOWLEDGMENTS

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Historical Introduction

In 1951, M. Deutsch (2) was able to show that a group of positrons, injected in a gas, did not all behave the same way before annihilation; that different decay periods were observed, and that some of these periods did not vary if the pressure in the gas was allowed to change. This phenomenon was explained by assuming another phase in the positron history: its existence in a bound state with an electron, just before annihilation. The system escapes the influence of the surroundings and can undergo annihilation with its mean life essentially independent of ambiant pressure.

This system has been called positronium, and it is very similar to the hydrogen atom. Its reduced mass is one half that of hydrogen, and its Bohr radius twice as large. If we introduce this new Bohr radius in the quantum mechanical expression for the wave function and energy levels of an hydrogen atom, we get the proper equivalent term for positronium, that is:

$$U_{n\ell m} = -\left\{\left(\frac{1}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}\right\}^{1/2} e^{-\frac{1}{2}\rho}\rho^{\ell} L^{2\ell+1}_{n+\ell}(\rho)\, Y_{\ell m}(\theta,\varphi)$$

$$\rho = r/na_0$$

$$E_n = \frac{-e^2}{4a_0 n^2}$$

The ionisation potential is 6.8 ev., or half of the hydrogen value.

Depending on whether the spins are parallel or anti-parallel in the atom, it is called ortho-positronium or para-positronium. The first one has a mean life of $\sim 10^{-7}$ sec., and decays in three gamma rays, while the second lives $\sim 10^{-10}$ sec., where only two gamma rays are emitted.

When positrons are sent into a gas, a certain fraction of them end up bound with an electron in a positronium atom.

The process is a complex one involving several steps. If the positron has a relatively high velocity initially, it will lose energy in the usual manner by ionization and excitation of the gas atoms. As its velocity falls into the region of atomic electron velocities, it will perhaps capture an electron to form positronium. This neutral atom will make further collisions, losing energy, and perhaps the electron will be stripped off. The positron continues losing energy and capturing and losing electrons, until it reaches a velocity at which it is energetically impossible to lose or capture an electron. A certain fraction of positrons reaching this energy will be bound in positronium atoms. The rest will be free. The fraction forming positronium can be estimated by relatively crude arguments (see Deutsch (2)).

The aim of the present work was to find out the cross-section of different gases for the initial electron capture process. No attempt was made to evaluate the complex process which leads to a certain number of positrons eventually existing in the gas as positronium atoms of very low energies.

Atomic hydrogen was the first gas considered. The cross-section was evaluated completely in the Born approximation. Some approximations were obtained for the capture cross-section in helium, but the complete calculation was too involved.

Positrons in Atomic Hydrogen

The process of electron capture and positronium formation will be studied by means of a Born approximation. The cross-section for capture into a given final state then appears as follows:

$$\frac{d\sigma_f}{d\Omega} = \left(\frac{\mu_f}{2\pi\hbar^2}\right)^{1/2}\left(\frac{v_f}{v_0}\right)|I_f|^2$$

where $\mu_f = 2m$ is the final reduced mass of the system, (assuming the proton is infinitely heavy relative to the positron and electron),

(v_f/v_0) is the ratio of final and initial velocity,

and I_f is the perturbation matrix element:

$$I_f = \int e^{-i\bar{k}_f\cdot\bar{R}'}\,\Psi_f^*(r')\,V(R,r')\,e^{i\bar{k}_0\cdot\bar{R}}\,\Psi_0(r)\,d\bar{r}\,d\bar{R}$$

$V(r',R)$ is the interaction Hamiltonian.

Figure I shows the system of coordinates used in the calculation.

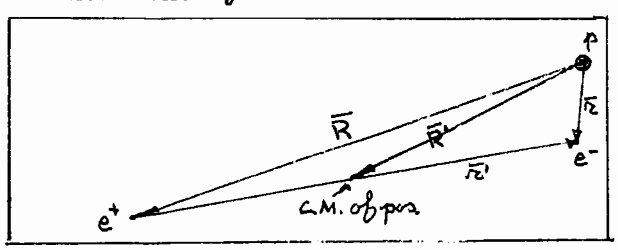


Figure I

Before the collision, the electron is bound around the proton, and the incoming positron feels an interaction potential:

$$V_i = \frac{e^2}{R} - \frac{e^2}{r'}$$

from the H atom.

The wave function describing the initial state is:

$$\Psi_0(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

for an hydrogen atom in its ground state. The term $e^{i\bar{k}_0 \cdot \bar{R}}$, in the matrix element, represents the relative motion of the two systems involved, if we neglect the polarisation created in the atom by the incident positron.

$$|k_0| = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

(E is the initial energy of the positron relative to the hydrogen atom).

For ground state capture, the final wave function is

$$\Psi_f = \frac{1}{\sqrt{\pi(2a_0)^3}} e^{-r/2a_0}$$

for the positronium atom. The factor $e^{i\bar{k}_f \cdot \bar{R}'}$ describes the motion of the positronium atom relative to the proton. The final wave number is

$$|k_f| = \left(\frac{4mE_f}{\hbar^2}\right)^{1/2}$$

(the mass now being 2m).

Because the collision is a rearrangement collision, the interaction is different in the final state:

$$V_f = \frac{e^2}{R} - \frac{e^2}{r}$$

However, as is shown in Appendix A of Jackson and Schiff (3), the perturbation matrix element I_f is the same, whether one employs V_i or V_f

Conservation of energy requirements are that:

$$k_0^2 - \frac{k_f^2}{2} = 1/2a_0^2$$

For convenience, we introduce the new variables:

$$\bar{C} = \bar{k_0} - \bar{k_f}/2$$
$$\bar{B} = \bar{k_0} - \bar{k_f}$$

and use $\bar{r}$ and $\bar{r}'$ as independent variables, instead of $\bar{r}$ and $\bar{R}$. Then, the matrix element becomes:

$$I_f = \int e^{-i\bar{C}\cdot\bar{r}'} \Psi_f(r') \left[\frac{e^2}{|\bar{r}-\bar{r}'|} - \frac{e^2}{r}\right] e^{i\bar{B}\cdot\bar{r}} \Psi_0(r)\, d\bar{r}\, d\bar{r}'.$$

So far, the spins of the electron and positron have been ignored. In the final state, the bound system of electron and positron can be in either a triplet or a singlet spin state. Since the interaction is not dependent on spins, the two spin states will be populated according to their statistical weights. Thus, of the total number of atoms formed, three-fourths will be ortho-positronium atoms (triplet spin state), and the remaining fourth, para-positronium atoms (singlet spin state).

We first determine the ground state capture cross-section, using an approximation introduced by Brinkman and Kramers (1).

This approximation considers only the electron-positron interaction in evaluating the matrix element, (neglecting nucleus-positron interaction). The details of the calculation are similar to those given in Appendix A of Jackson and Schiff (3). This matrix element called I_{BK} is $I_{BK} = -\frac{\sqrt{8}\,\pi e^2 a_0^2}{E^3}\frac{1}{\Delta^3}$

where $\Delta = \left[1.5 - (2 - 1/E)^{1/2}\cos\theta\right]$

$E = k_0^2 a_0^2$ = Initial energy of positron in units of 13.6 ev.

θ = scattering angle.

The differential cross-section is:

$$\frac{d\sigma_{BK}}{d\Omega} = \frac{4a_0^2\,(2-1/E)^{1/2}}{E^6}\,\frac{1}{\Delta^6}$$

When integrating over angles, we get the total cross-section:

$$\frac{\sigma_{BK}}{\pi a_0^2} = \frac{1.6}{E^6}\,(P^5 - Q^5) \qquad P = \left(1.5 - (2-1/E)^{1/2}\right)^{-1}$$

$$Q = \left(1.5 - (2-1/E)^{1/2}\right)^{-1}$$

The graphs in the four following pages illustrate the theory.

Figure II represents the total cross-section in the B.K. approximation. As expected, it has a threshold at a value of positron energy equal to the difference between the hydrogen atom and the positronium atom ground state energies, i.e. 6.8 ev. The cross-section peaks quite sharply around 12-13 ev., and then falls

Figure II

$H\,1s \rightarrow pos\,1s$

Total cross-section

$\frac{\sigma_{BK}}{\pi a_0^2}$ vs E

For $E \rightarrow \infty$
$\frac{\sigma_{BK}}{\pi a_0^2} \rightarrow \frac{3.44 \times 10^5}{E^6}$

Total area, 72.5

For every graph $E = k_i^2 a_0^2$ is the energy in units of 13.6 ev.

The total area under the curve is given in units of

(1.2×10^{-15} ev. cm.^{2})

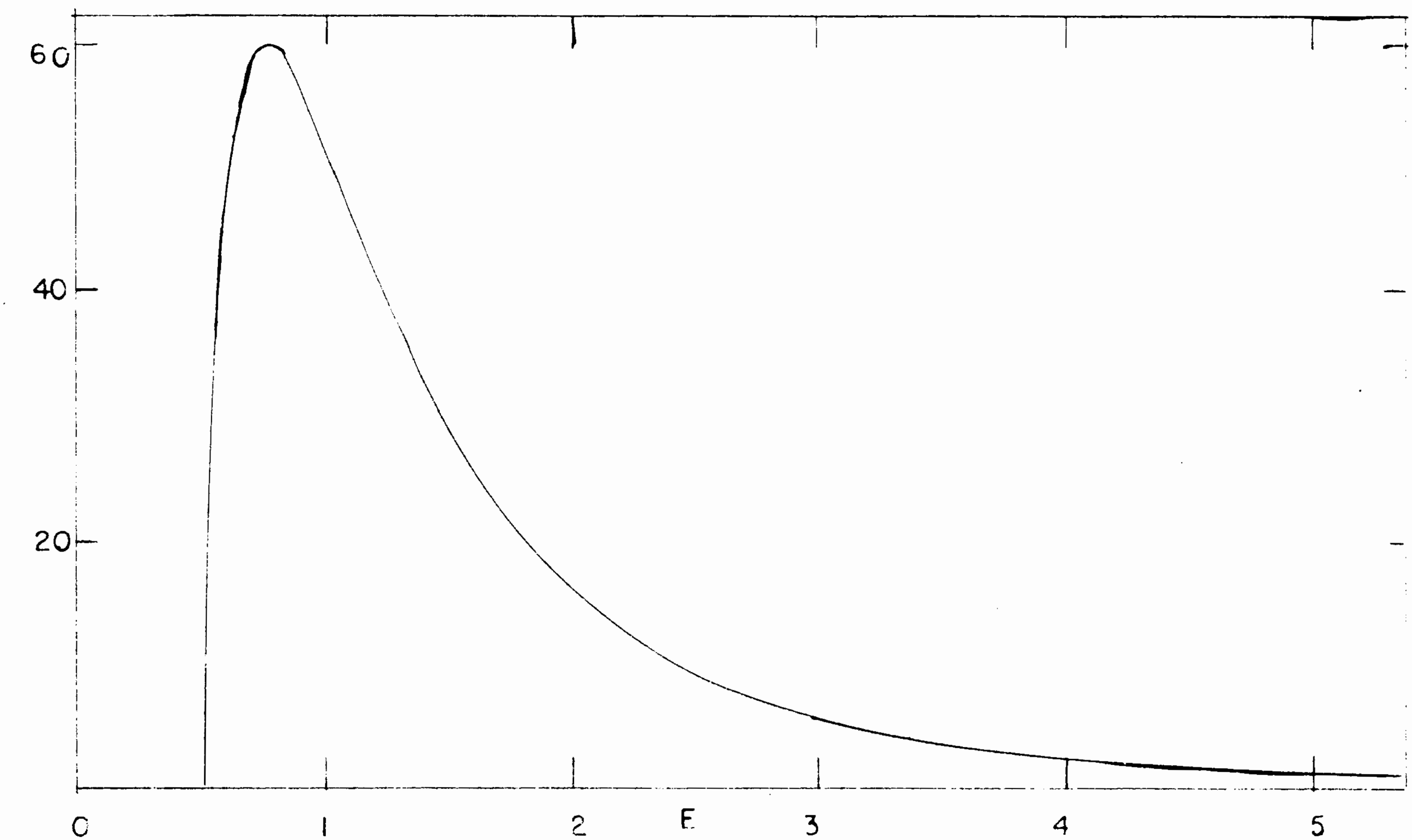

60
40
20
0
1
2
E
3
4
5

Figure III

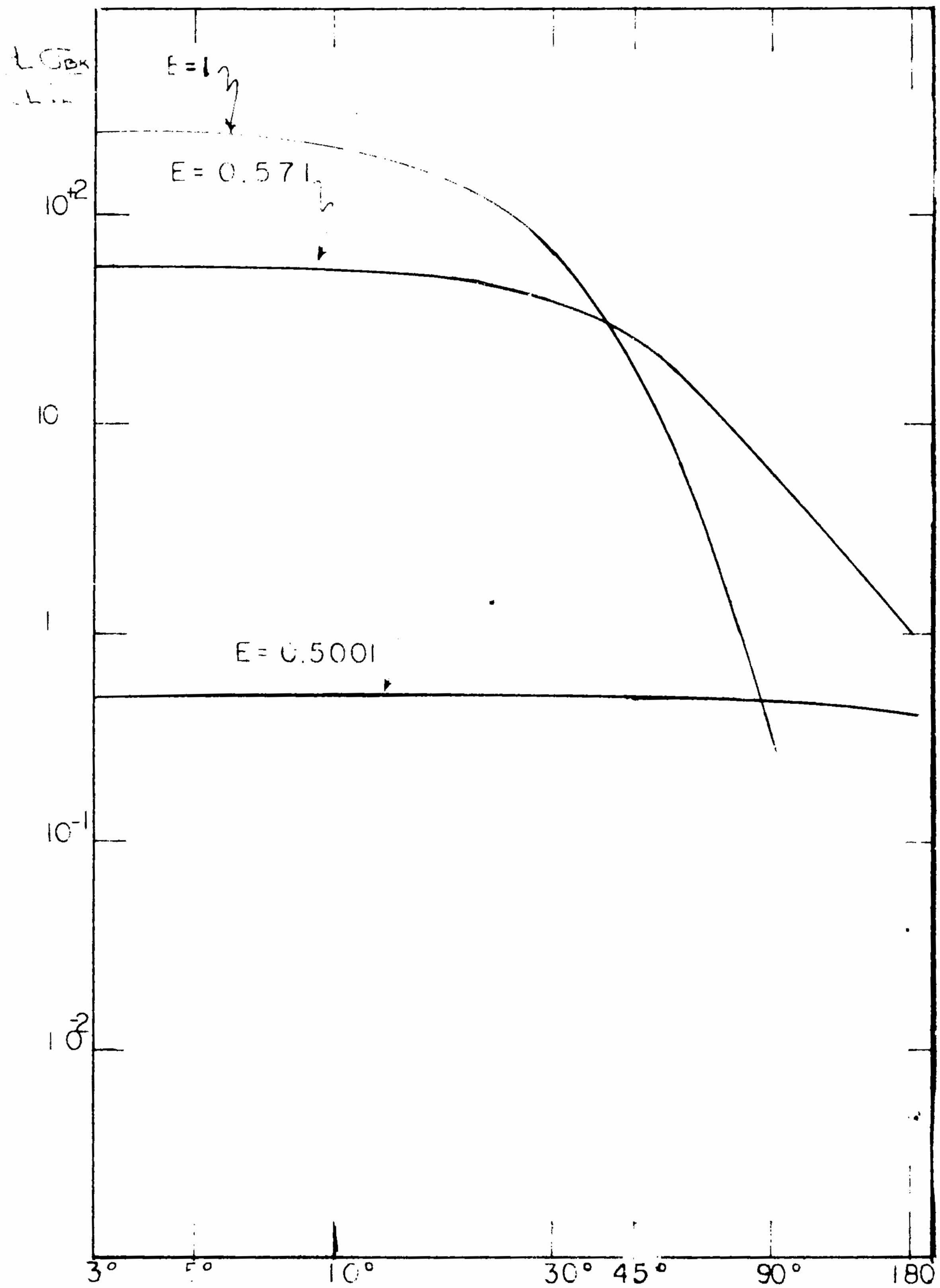
$H_{1s} \rightarrow p_{\infty}\, 1s$

Differential cross-section

$\frac{d\sigma_{BK}}{d\Omega}$ in units of a_0^2

vs θ

for E 0.5001, 0.571, 1.0



E = 1
E = 0.571
E = 0.5001
10^{+2}
10
1
10^{-1}
10^{-2}
3°
10°
30°
45°
90°
180

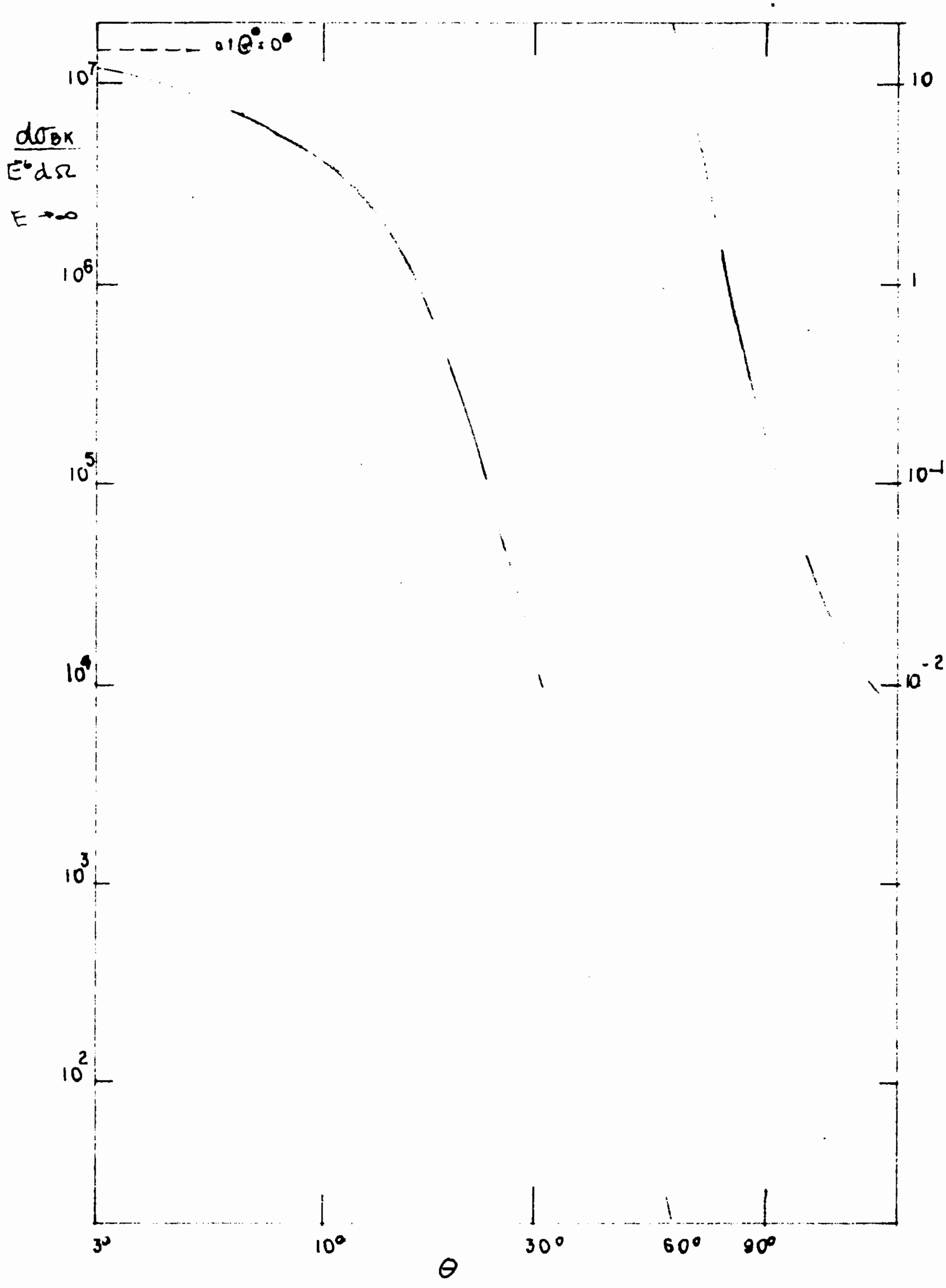
Figure IV

$H_{1s} \rightarrow pos\ 1s$

Differential cross-section

$$\frac{d\sigma_{BK}}{d\Omega} \times \frac{E^6}{a_0^2} \sim \theta$$

for $E \rightarrow \infty$



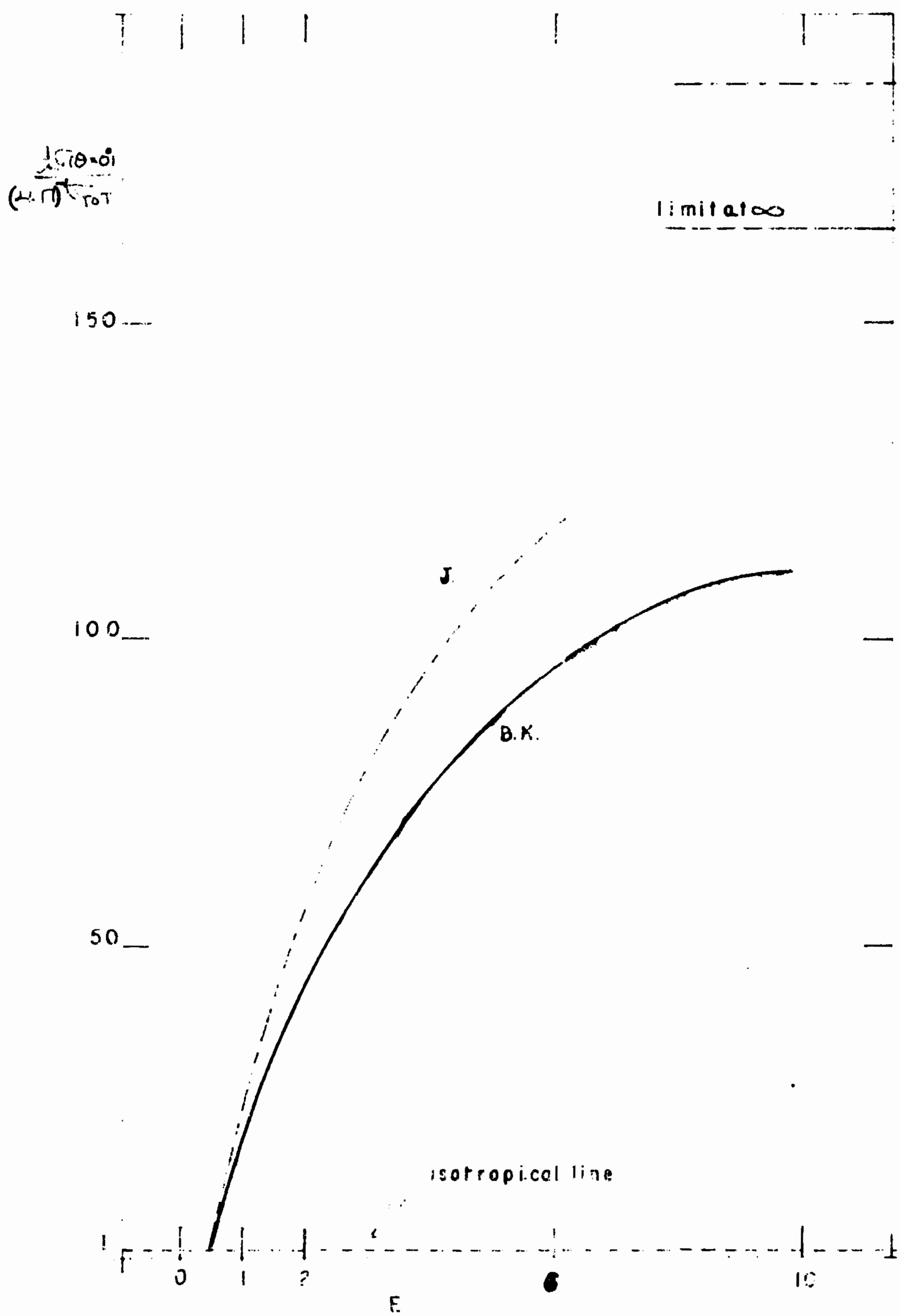
at θ = 0°
10^7
$\frac{d\sigma_{BK}}{E^6 d\Omega}$
$E \to \infty$
10^6
10^5
10^4
10^3
10^2
10
1
10^{-1}
10^{-2}
3°
10°
30°
60°
90°
θ

Figure V

$H_{1s} \rightarrow p_{os1s}$

Measure of Anisotropy

$$\frac{4\pi}{\sigma_{TOT}}\left(\frac{d\sigma}{d\Omega}\right)_{\theta^{\circ}=0^{\circ}} \text{ vs } E$$


limit at ∞
150
100
50
J
B.K.
isotropical line
0
1
2
6
10
E

off rapidly as the sixth power of energy.

It should be emphasized that this result is for atomic hydrogen gas. For H_2 gas, molecular effects will change curve in the low energy region.

Figures III and IV the differential cross-sections for different energies.

The angular distribution is seen to be essentially independent of angle for energies close to threshold. It becomes more and more peaked in the forward direction as E increases.

To afford a better study of this effect, we define as "anisotropy" the "Ratio of actual cross-section at 0° over cross-section at 0° if the same total number of emitted particles was emitted isotropically", that is:

$$\frac{4\pi}{\sigma_{TOT}}\left(\frac{d\sigma}{d\Omega}\right)_{\theta=0^\circ}$$

For our case, this is shown in Figure V. Thus, one can see whether he is justified in considering only the cross-section at small angles in a particular calculation.

The capture cross-section was then evaluated, taking into account the nucleus-positron interaction in the matrix element, according to a method developed by Jackson and Schiff (3).

The following Fourier transform is used,

$$\frac{1}{|\bar{r}-\bar{r}'|} = \frac{1}{2\pi^2}\int\frac{d\bar{k}}{k^2}\exp\left[i\,\bar{k}\cdot(r-r')\right]$$

and the nucleus-positron part of the matrix element reads:

$$I = \frac{4\sqrt{2}\,e^2}{\pi a_0^5}\int \frac{d\bar{k}}{k^2}\,\frac{1}{\left[(\bar{B}-\bar{k})^2+a_0^{-2}\right]^2}\,\frac{1}{\left[(\bar{C}-\bar{k})^2+(2a_0)^{-2}\right]^2}$$

To evaluate this, we use the Feynman Integral:

$$(ab)^{-2} = \int_0^1 \frac{6x(1-x)\,dx}{\left[ax+b(1-x)\right]^4}$$

with

$$a = 1/2\left[(\bar{B}-\bar{k})^2+a_0^{-2}\right]$$

$$b = \left[(\bar{C}-\bar{k})^2+(2a_0)^{-2}\right]$$

we find $ax+b(1-x) = \Delta + k^2\mu - 2\bar{k}\cdot\bar{q}$.

with $\Delta = C^2+(2a_0)^{-2}$ $\qquad \mu = 1-x/2$

$$\bar{q} = \bar{B}x/2 + \bar{C}(1-x)$$

and $B^2/2 = C^2-(2a_0)^{-2}$

from conservation of energy.

We now use the formula

$$6\int \frac{d\bar{k}}{k^2(k^2-2\bar{k}\cdot\bar{s}+p)^4} = \pi^2\left\{\frac{2}{p^3(p-s^2)^{1/2}}+\frac{1}{p^2(p-s^2)^{3/2}}+\frac{3/4}{p(p-s^2)^{5/2}}\right\}$$

where we put

$$p = \Delta/\mu \qquad \bar{s} = \bar{q}/\mu$$

$$(p-s^2) = \frac{ax^2+bx+c}{(2-x)^2} \qquad a = -E/a_0^2 \qquad b = E/a_0^2 \qquad c = 1/a_0^2$$

With these substitutions, and after integration over "x" of integrals of the form $\int \frac{x^n\,dx}{(ax^2+bx+c)^{m/2}}$

we get the needed matrix element.

The complete matrix element, (summing both terms), is now:

$$I_J = \frac{\sqrt{2}\,\pi e^2 a_0^2}{E^3}\left[\frac{G}{\Delta^3} + \frac{H}{\Delta^2} + \frac{K}{\Delta}\right]$$

$$G = \Phi(0.5 - 2/E) + (2/E - 2)$$

$$H = 6\Phi - 24/(4+E)$$

$$K = -6\Phi + 8(5E^2+5E+12)/(4+E)^2$$

$$\Phi = (2/\sqrt{E})\ tg^{-1}(\sqrt{E}/2)$$

$$\Delta = 1.5 - (2 - 1/E)^{1/2}\cos\theta.$$

$$\frac{d\sigma_J}{d\Omega} = \frac{a_0^2\,(2-1/E)^{1/2}}{E^6}\left[\frac{G^2}{\Delta^6} + \frac{2GH}{\Delta^5} + \frac{(H^2+2GK)}{\Delta^4} + \frac{2HK}{\Delta^3} + \frac{K^2}{\Delta^2}\right]$$

$$\frac{\sigma_{J\,TOT}}{\pi a_0^2} = \frac{1}{E^6}\left\{0.4\,G^2(P^5-Q^5) + GH(P^4-Q^4) + \frac{2}{3}(H^2+2GK)(P^3-Q^3) + 2HK(P^2-Q^2) + 2K^2(P-Q)\right\}$$

$$P = \left[1.5 - (2-1/E)^{1/2}\cos\theta\right]^{-1}$$

$$Q = \left[1.5 + (2-1/E)^{1/2}\cos\theta\right]^{-1}$$

The graphs on the four following pages illustrate the behaviour of these cross-sections, and their comparison with the Brinkman-Kramer results.

In Figure VI, the shape of the σ_J curve appears to be very similar to the previous one, but the numerical values are about ten times smaller. This implies that the repulsion of the positron greatly decreases the probability of positronium formation.

Figure VII is the ratio of the two cross-sections σ_{BK}/σ_J . As $E \to \infty$ the ratio approaches a limiting value of about 1.57. This means that the two parts of the interaction are always effective, and should be retained in any calculation.

This importance of both terms can also be brought in evidence if we look at the matrix element appearance at high energy.

$\mathcal{G}$ goes to -2 $\quad H \to 0 \quad K \to 40$

and
$$\frac{d\sigma_J}{d\Omega} \xrightarrow[E\to\infty]{} \frac{\sqrt{2}\,a_0^2}{E^6}\left\{\frac{4}{\Delta^6} - \frac{160}{\Delta^4} + \frac{1600}{\Delta^2}\right\}$$

The first term in r.h.s. is identical with $\dfrac{d\sigma_{BK}}{d\Omega}$.

Grouping the two last terms, we have

$$\frac{\sigma_J}{\pi a_0^2} \xrightarrow[E\to\infty]{} \frac{3.44\times10^5}{E^6} - \frac{1.26\times10^5}{E^6}$$

where again the first term is the B.K. term ($E \to \infty$).

In Figures VIII and IX, the J differential cross-section shows a remarkable difference from the B.K. one. First of all,

Figure VI

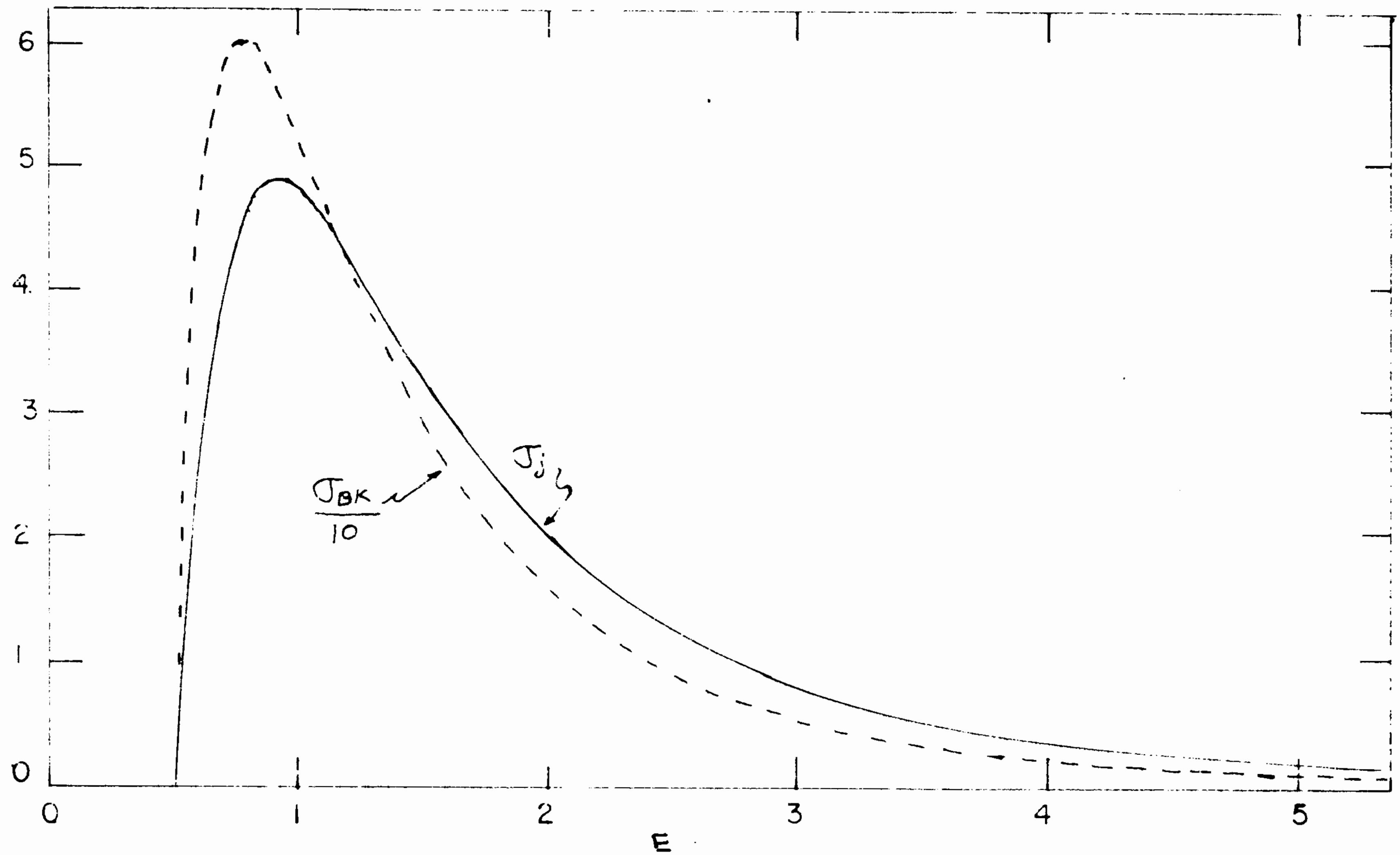
H1s $\longrightarrow$ pos 1s

Total cross-section

$$\frac{\sigma_J}{\pi a_0^2} \text{ vs } E \qquad \Bigg| \; \text{for } E \to \infty \quad \frac{\sigma_J}{\pi a_0^2} \to \frac{2.18 \times 10^5}{E^6}$$

Total area, 7.75

$$\frac{\sigma_{Bk}}{\pi a_0^2} \times \frac{1}{10}$$ appears also in ——.——.——.



0
1
2
3
4
5
6
E
$\frac{\sigma_{BK}}{10}$
σ_j

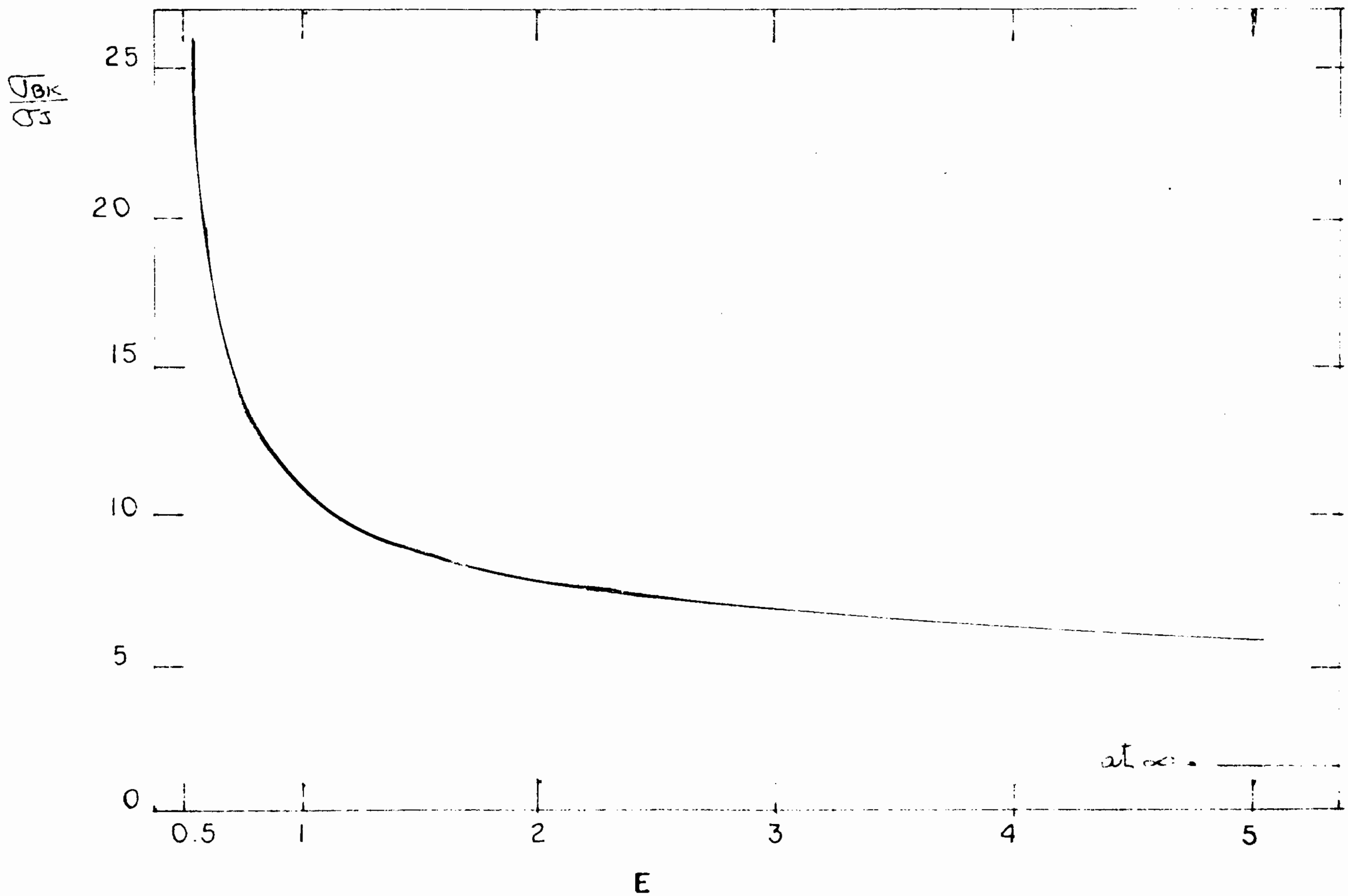
<u>Figure VII</u>

$H_{1s} \rightarrow p_{os}\ 1s$

Ratio of $\sqrt{B_K}/\sqrt{J}$

vs E

Limit at ∞ is 1.57



$\frac{\sigma_{BK}}{\sigma_J}$
25
20
15
10
5
0
0.5
1
2
3
4
5
E
at ∞:

Figure VIII

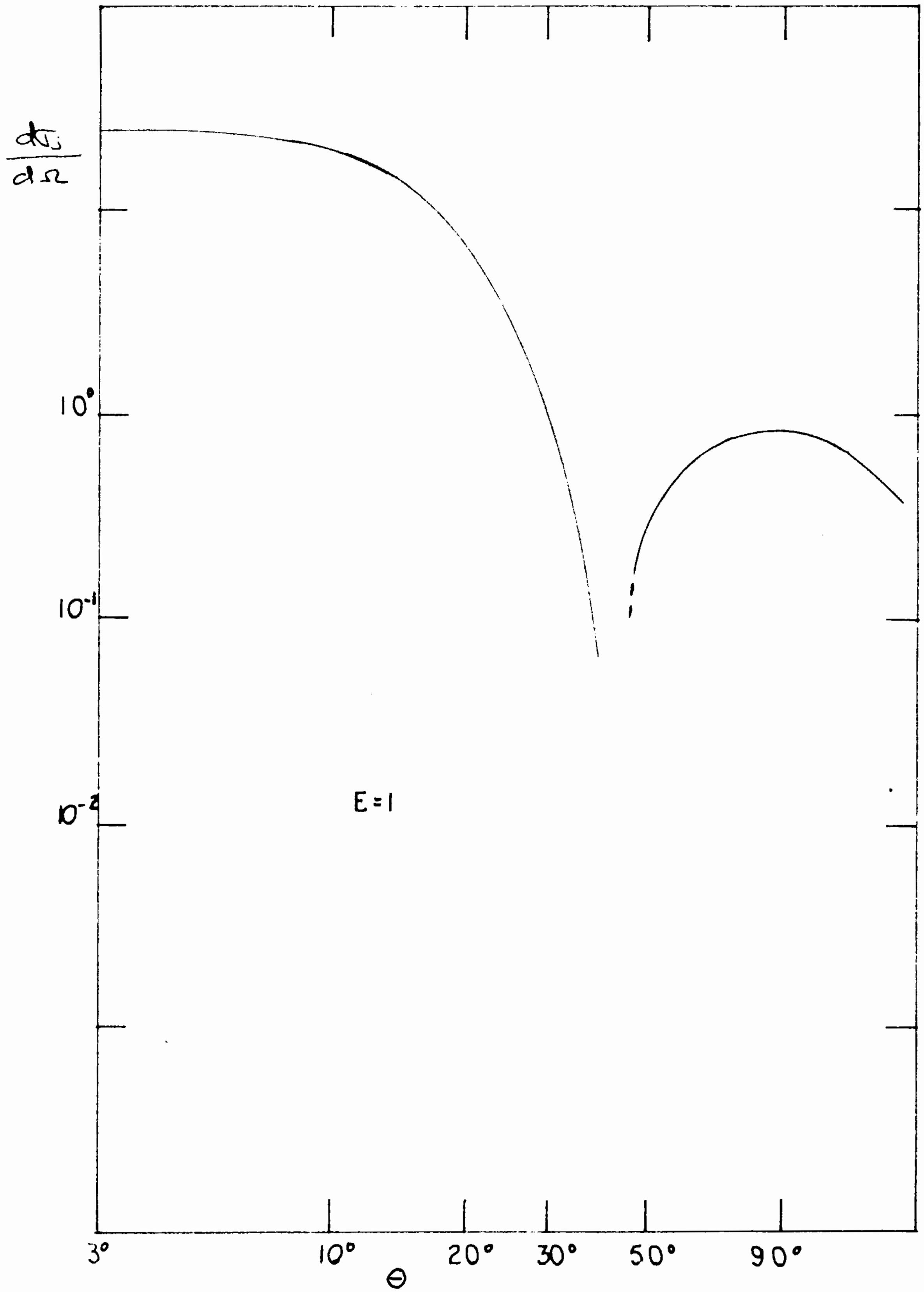
H1s → pos 1s

Differential cross-section

$\frac{d\sigma_J}{d\Omega}$ in units of a_0^2

vs θ

for E=1



$\frac{d\sigma_j}{d\Omega}$
10^0
10^{-1}
10^{-2}
E=1
3°
10°
20°
30°
50°
90°
Θ

Figure IX

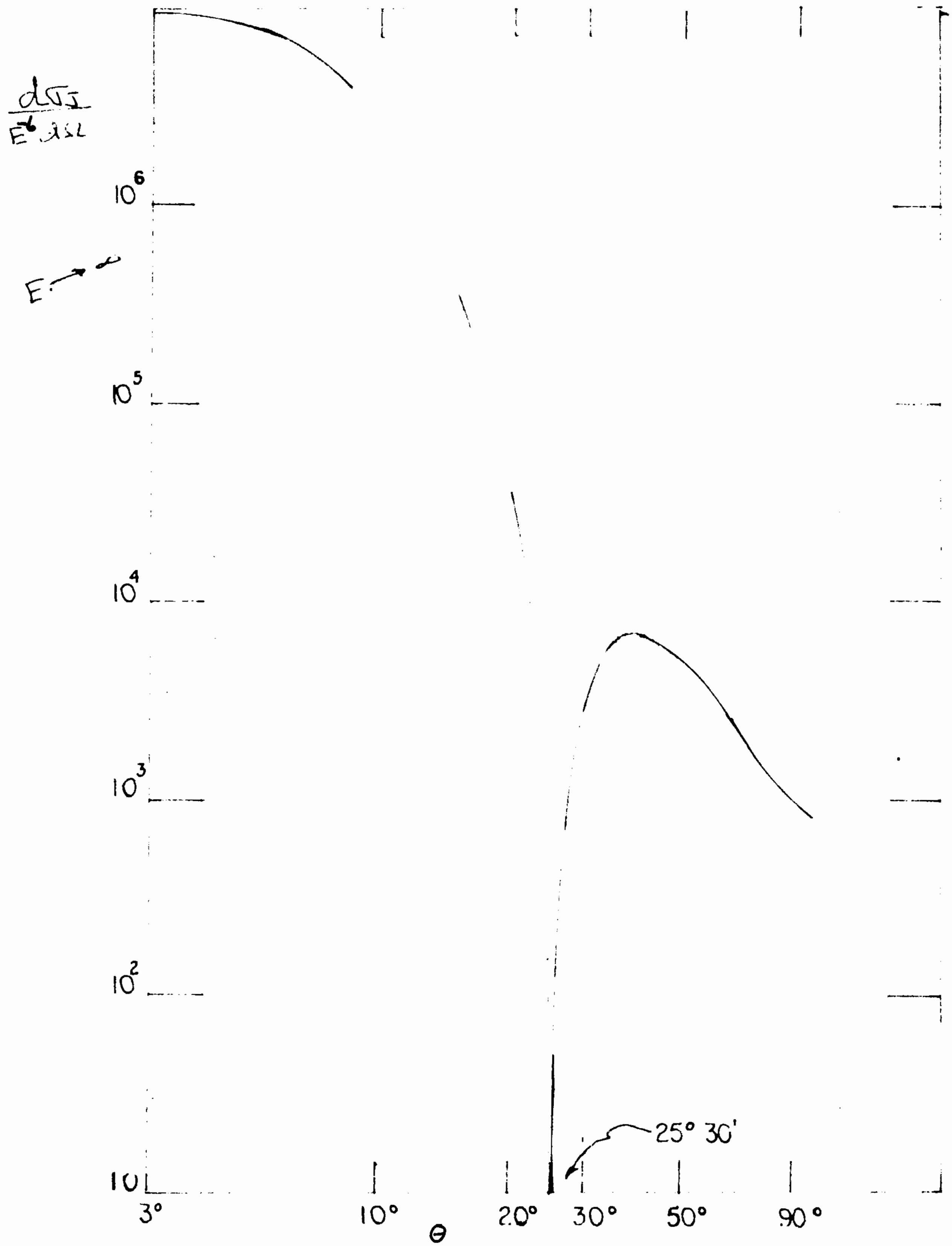
H1s → pos 1s

Bifferential cross-section

$\frac{d\sigma_J}{d\Omega} \times E^6$ in units of a_0^2

vs θ

for E ⟶ ∞



$\frac{d\sigma_I}{E^6\, d\Omega}$
10^6
$E \to \infty$
10^5
10^4
10^3
10^2
10
25° 30'
3°
10°
20°
30°
50°
90°
θ

it vanishes at a certain angle. This can be attributed to interference between the two parts of the matrix element. In the high energy limit, there is a root at $\theta = 25°, 30'$ (θ is the scattering angle). At lower energies, it is hard to determine the roots exactly, as we deal with a 6^{th} order equation in θ.

Figure VIII represents an attempt at doing it graphically for E = 1. Quite a number of points were taken, and there is a gap in the curve, at an angle higher than in the previous case.

By the same effect, the differential cross-section at high angles is in the mean much more important than in the B.K. case. A small table will illustrate that:

	$E = 1$ $\quad d\sigma_{\theta=0°}/d\sigma_{\theta=90°}$	$E = \infty$ $\quad d\sigma_{\theta=0°}/d\sigma_{\theta=90°}$
BK	780	4×10^7
J	21	10^4

Unfortunately, because of the actual definition of the "anisotropy", this is not visible in the corresponding figure, which appears as a dotted line in Figure V.

Before leaving the ground state capture problem, we mention a proposal of Schiff (6) that good results can be obtained by using a screened potential for the incident ion-electron interaction in order to include at least partially the effect of the incident ion-nucleus interaction in a B.K. type of calculation, and so avoid the more complex computations involved when the complete interaction is used. Schiff has applied this idea to the capture of electrons by protons in hydrogen. His result is in moderate agreement with that obtained by the use of the complete interaction.

To test Schiff's idea further, the corresponding calculation was made for positrons in hydrogen. The details are presented in Appendix I and Figure XIII. There is no agreement between the results using the screened potential and those employing the complete interaction, the cross-section differing by a factor of 2 or 3 in the region of interest.

Captures into excited states

The possibility of formation of positronium in $2s$ and $2p$ excited states from hydrogen ground state was then investigated.

The final wave functions involved here are:

$$\Psi_{f\,2s} = \frac{1}{16\sqrt{\pi}\,a_0^{3/2}}\left(2 - r/2a_0\right) e^{-r/4a_0}$$

$$\Psi_{f\,2p} = \frac{r\,e^{-r/4a_0}}{16\sqrt{\pi}\,(a_0)^{3/2}}\cos\theta$$

where the subscripts on Ψ are the quantum numbers n and l .

The degenerate energy level is $E = -e^2/16a_0$ and conservation of energy requirements are that $k_0^2 - \frac{k_f^2}{2} = 7/8a_0^2$

The calculation proceeds in the same manner as for formation in the ground state. Only the end results will be stated here.

The I_{BK} matrix element is considered first:

$$I_{BK\,2s} = -\frac{e^2 \pi a_0^2}{E^3}\left[\frac{1}{\Delta^3} - \frac{1}{8E\Delta^4}\right]$$

$$I_{BK\,2p} = -\frac{i e^2 \pi a_0^2}{2E^4}\left[\frac{C\cos\theta}{\Delta^4}\right]$$

$$\Delta = \left\{1.5 - \left(2 - \frac{7}{4E}\right)^{1/2}\cos\theta - 3/8E\right\}$$

$$\frac{\sigma_{BK\,2s}}{\pi a_0^2} = \frac{1}{E^6}\left\{\frac{1}{5}(Q^5 - P^5) - \frac{1}{24E}(Q^6 - P^6) + \frac{1}{448E^2}(Q^7 - P^7)\right\}$$

$$\frac{\sigma_{BK\,2p}}{\pi a_0^2} = \frac{1}{E^6}\left\{\frac{1}{24E}(Q^6 - P^6) - \frac{1}{448E^2}(Q^7 - P^7)\right\}$$

$$P = \left\{1.5 + \left(2 - \frac{7}{4E}\right)^{1/2} - \frac{3}{8E}\right\}^{-1}$$

$$Q = \left\{1.5 - \left(2 - \frac{7}{4E}\right)^{1/2} - \frac{3}{8E}\right\}^{-1}$$

As expected, the threshold is somewhat higher, namely at $E = 0.875$. The two curves have the usual shape (Figure X), with σ_{2s} slightly higher than σ_{2p} .

It is of interest to note that one can express $\sigma_{BK\,2p}$ in function of $\sigma_{BK\,2s}$ by:

$$\frac{\sigma_{BK\,2s}}{\pi a_0^2} = \frac{1}{5E^6}\left[Q^5 - P^5\right] - \frac{\sigma_{BK\,2p}}{\pi a_0^2}$$

and further that for $E \to \infty$ the total cross-section for the degenerate levels is:

$$\sigma_{BK\,2} = (\sigma_{BK\,2s} + \sigma_{BK\,2p}) = \frac{1}{8}\sigma_{BK\,1}$$

This is a special case of the general result that $\sigma_{BK\,n} = \frac{1}{n^3}\sigma_{BK\,1}$ for $E \to \infty$.

The equivalent J calculation in $2s$ case involves a matrix element of the form

$$I_J = \frac{2e^2}{\pi a_0^5}\int \frac{d\bar{k}}{k^2}\left\{\frac{1}{\left[(\bar{B}-\bar{k})^2 + a_0^{-2}\right]^2}\right\} \times \left\{\frac{1}{\left[(\bar{C}-\bar{k})^2 + (4a_0)^{-2}\right]^2} - \frac{1}{8a_0^2\left[(C-k)^2 + (4a_0)^{-2}\right]^3}\right\}$$

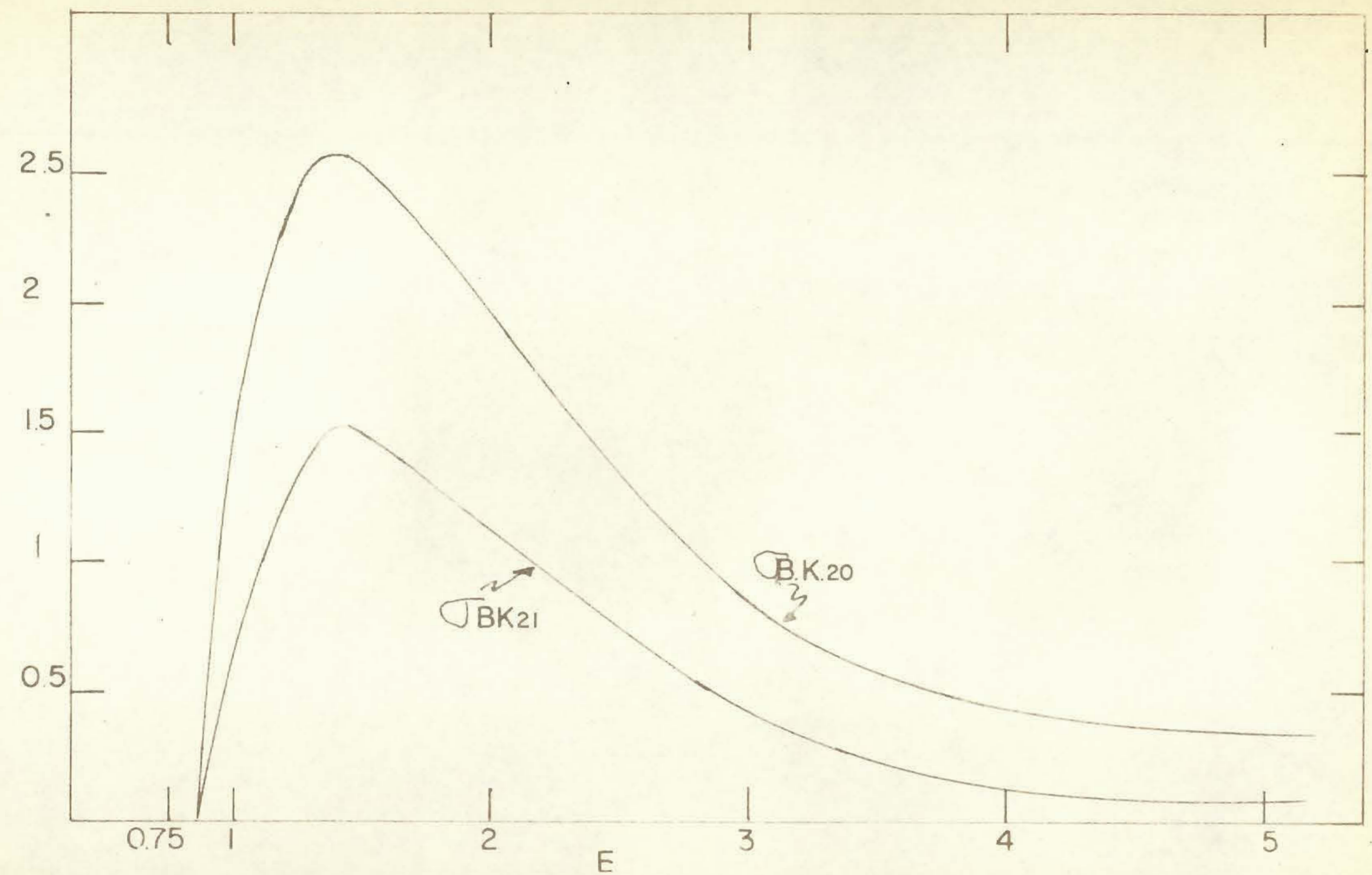
we use $$(a^3 b^2)^{-1} = 12\int_0^1 \frac{x^2(1-x)\,dx}{\left[ax + b(1-x)\right]^5}$$

Figure X

$H_{1s} \rightarrow p_{os}\ 2s, 2p$

Total cross-section

$\frac{\sqrt{BK}}{\pi a_0^2}$ vs E



2.5
2
1.5
1
0.5
0.75
1
2
3
4
5
E
σBK21
σB.K.20

Also $$\int_0^1 \frac{24\, d\bar{k}}{k^2(k^2-2\bar{k}\cdot s+p)^5} = \pi^2 \left\{ \frac{6}{p^4(p-s^2)^{1/2}} + \frac{3}{p^3(p-s^2)^{3/2}} + \frac{9/4}{p^2(p-s^2)^{5/2}} + \frac{15/8}{p(p-s^2)^{7/2}} \right\}$$

$$p = \Delta/\mu = \frac{2}{(2-x)}\left[C^2 + (2a_0)^{-2}\right]$$

$$(p-s^2) = \frac{ax^2+bx+c}{(2-x)^2} \qquad a = -E/a_0^2 \qquad b = (E+3/4)/a_0^2 \qquad c = (2a_0)^{-2}$$

The expressions for I_J, $d\sigma_J/d\Omega$, σ_J are too complicated to be written here, but they are of the same form as in the ground state case.

For E =1 the total cross-section gives

$$\frac{\sigma_J}{\pi a_0^2} = 0.34$$

The ratio $\sigma_{BK2s}/\sigma_{BK1s}$ is about 0.04 at this value of energy, whereas the $\sigma_{J_2}/\sigma_{J_1}$ is 0.2.

Massey and Mohr (4) give a graph of this cross-section, which they evaluated by a spherical harmonic expansion method. According to the graph, their value for E = 1 seems to be about five times smaller than that quoted here. No reason has been found for this disagreement.

Formation of Positronium in Helium

The next purpose was to obtain some results in experimentally available gases. Molecular hydrogen soon revealed itself an extremely complicated case, because of the number of particles involved (5). The helium atom case was hardly easier, (4 particles involved). The trouble in this case is more in the interminable length of the calculation than in the mathematics itself. General formulae and some approximations are given in the following pages.

Figure XI shows the new sets of coordinates:

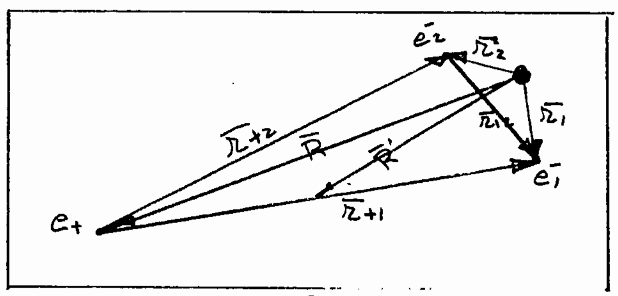


Fig XI

The matrix element for the Born approximation is now:

$$I = \int e^{-i\bar{k}_f\cdot\bar{R}'}\,\Psi_f(r_{+1}, r_{+2})\,V(R, r_{+2}, r_{+1})\,e^{i\bar{k}_0\cdot\bar{R}}\,\Psi_0(r_1, r_2)\,d\bar{R}\,d\bar{r}_1\,d\bar{r}_2$$

The initial interaction potential is:

$$V_i = \left(\frac{2e^2}{R} - \frac{e^2}{r_{+2}} - \frac{e^2}{r_{+1}}\right)$$

A variational principle as given in Schiff (5) will give us the approximate wave function for the helium atom:

$$\Psi_0 = \frac{\beta^3}{\pi a_0^3} e^{-\frac{\beta}{a_0}(r_1+r_2)} \qquad \beta^2 = 2.85 \qquad E = -\frac{\beta^2 e^2}{a_0}$$

If we consider for the final state an ionized atom in its ground state:

$$\Psi_f = \Psi_{(\text{ion. He})} \times \Psi_{\text{pos}} = \frac{2\sqrt{2}}{\sqrt{\pi}\, a_0^{3/2}} e^{-\frac{2r_2}{a_0}} \times \frac{e^{-\frac{r_{+1}}{2a_0}}}{\sqrt{8\pi a_0^3}}$$

Conservation of energy requirements are that:

$$k_0^2 - \frac{k_f^2}{2} = 1.2/a_0^2$$

We use again variables $\bar{B}$ and $\bar{C}$ and $\bar{r}_{+1}, \bar{r}_1, \bar{r}_2$ instead of $\bar{R}, r_{+1}, r_{+2}$,

The presence of two electrons multiplies the cross-section by a factor of two. The positronium systems are distributed in spins, according to the following remarks:

The initial spin of the system is one half, as only the positron contributes to it. Since spin is conserved throughout the collision, the final spin must be one half. Thus, the positronium spin ($S=0$ or 1) must combine with the remaining helium electron ($S=1/2$) to give a resultant total spin of one half. In writing down the final spin wave function, one has to be careful in order as to conserve the symmetry property under exchange of the two electrons in the helium atom. When this is done properly, one finds that the triplet factor is 1.5, the singlet one 0.5. The sum is two, as expected. The cross-section presented below is that for a single helium electron.

The matrix element appears as

$$I = \int \exp(-i\,\bar{C}\cdot r_{+1}) \left[\frac{e^{-\frac{r_{+1}}{2a_0}}}{\sqrt{8\pi a_0^3}}\right]\left[\frac{2\sqrt{2}\,e^{-\frac{2r_2}{a_0}}}{\sqrt{\pi a_0^3}}\right]$$
$$\left[\frac{2e^2}{|\bar{r}_1 - \bar{r}_{+1}|} - \frac{e^2}{|\bar{r}_{+1} - \bar{r}_1 + \bar{r}_2|} - \frac{e^2}{|\bar{r}_{+1}|}\right] \exp(i\,\bar{B}\cdot r_1)$$
$$\left[\beta^3/\pi a_0^3\, e^{-\frac{\beta}{a_0}(r_1 + r_2)}\right] d\bar{r}_1\, d\bar{r}_2\, d\bar{r}_{+1}$$

We now separate I in two parts.

$$I = I_a + I_b + I_c$$

where I_a contains the positron nucleus interaction

(analogous to I_J)

I_b, the positron-stolen electron interaction

(analogous to I_{Bk})

I_c the positron-left electron interaction.

We shall treat each of them separately.

$$I_b = -\frac{41.4\,\pi a_0^2}{E^3}\left[\frac{1}{\left[M - N\cos\theta - \frac{0.35}{E}\right]}\;\frac{1}{\left[M - N\cos\theta + \frac{0.225}{E}\right]^2}\right]$$

$$M = 1.5$$

$$N = \left(2 - \frac{2.4}{E}\right)^{1/2}$$

$$\frac{\sigma_{BK}}{\pi a_0^2} = \frac{1.708 \times 10^3}{E} \Big\{ (g_- - g_+) + 4(\ln g_+ - \ln g_-)$$

$$+ 6 \left(g_+^{-1} - g_-^{-1} \right) + 2\left(g_-^{-2} - g_+^{-2} \right) + 1/3 \left(g_-^{-3} - g_+^{-3} \right) \Big\}$$

$$g_\pm = 1 + \frac{0.575}{E\, \Delta_\pm}$$

$$\Delta_\pm = \left[1.5 \pm \left(2 - \frac{2.4}{E} \right)^{1/2} \cos\theta - \frac{0.35}{E} \right]$$

For I_a

$$I_a = \frac{41.4 e^2}{\pi a_0^5} \int \frac{d\bar{k}}{k^2} \frac{1}{\left[(\bar{c} - \bar{k})^2 + (2a_0)^{-2} \right]^2} \frac{1}{\left[(\bar{B} - \bar{k})^2 + \left(\frac{a_0}{B} \right)^{-2} \right]^2}$$

The calculations are similar to the I_3 case in hydrogen, except that

$$ax + b(1-x) = \Delta - 2\,\bar{k}\cdot\bar{g} + k^2\mu + \epsilon x$$

$$\epsilon = \frac{0.575}{a_0^2}$$

Figure XII

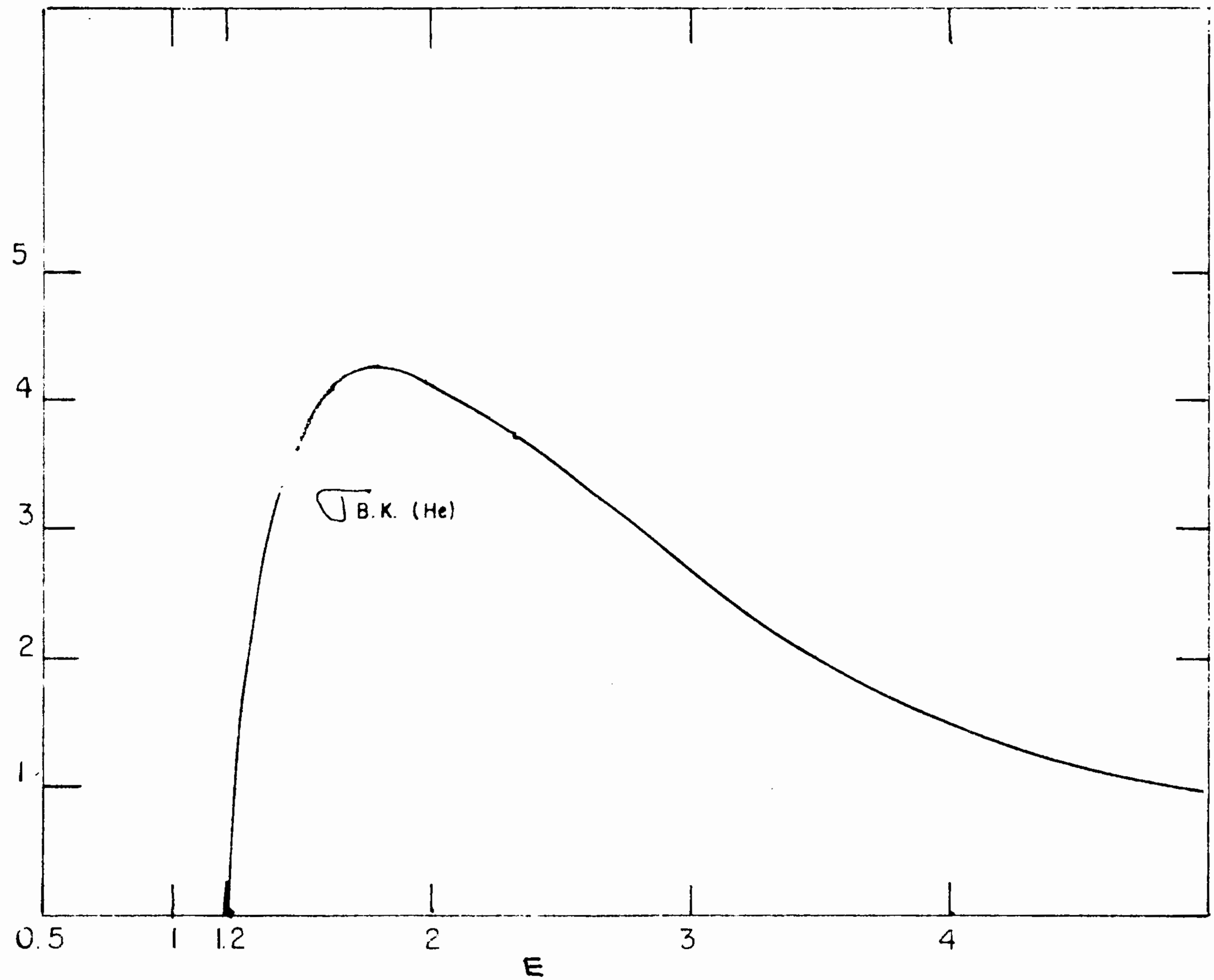
He 1s → pos 1s

Total cross-section

$$\frac{\sigma_{BK}}{\pi a_0^2} \text{ vs } E$$

for E → ∞ $\frac{\sigma_{BK}}{\pi a_0^2} \rightarrow \frac{4.62 \times 10^6}{E^6}$

Total area 23.5


5
4
3
2
1
0.5
1
1.2
2
3
4
E
σ B.K. (He)

$$\bar{s} = \bar{q}/\mu \qquad p = \frac{\Delta + \epsilon x}{\mu}$$

$$(p - s^2) = \frac{a x^2 + b x + c}{(2 - x)^2}$$

$$a = \frac{-1}{a_0^2}\left[E + 2\epsilon\right]$$
$$b = \frac{1}{a_0^2}\left[E + 3\right]$$
$$c = (a_0)^{-2}$$

For I_c

$$I_c = \frac{-6.13 e^2}{\pi a_0^9} \int \frac{d\bar{k}}{k^2} \frac{1}{\left[(\bar{c} - \bar{k})^2 + (2a_0)^{-2}\right]} \frac{1}{\left[(\bar{B} - \bar{k})^2 + (\beta/a_0)^{-2}\right]} \frac{1}{\left[k^2 + \left(\frac{2+\beta}{a_0}\right)^2\right]^2}$$

The convenient formula here is

$$(a^2 b^2 c^2)^{-1} = 120 \int_0^1 x(1-x)\,dx \int_0^1 \frac{dy\,(1-y)}{\left[axy + by(1-x) + c(1-y)\right]^6}$$

The rest of the integration in these two cases presents no analytical difficulties, but involves extremely long calculation.

Integration of functions of the type

$$\int \frac{x^n\, dx}{(\Delta + \epsilon x)^m \mathcal{X}^{1/2}} \qquad \mathcal{X} = ax^2 + bx + c$$

are troublesome because they lead to arcsin of complicated functions of Δ . Because of the fact that Δ contains in itself the angle between incident and ejected particles, the integration of the total cross-section after squaring of the matrix element would be analytically extremely involved, and probably possible only numerically.

In the limit of large E some simplifying approximations are possible. We can expand the factor $(\Delta + \epsilon x)^{-m}$ in inverse powers of Δ which is proportional to E:

$$(\Delta + \epsilon x)^{-n} = \Delta^{-n}\left(1 - n\epsilon x \Delta^{-1} + \right)$$

To examine the magnitude of the terms, we inspect the ratio of the minimum value of Δ for a given energy, and the maximum value of $\epsilon x \lessgtr \epsilon = 0.575$

For $E \geqslant 50 \qquad \Delta/\epsilon \simeq 0.15 E$

Below this value of E, we cannot neglect ϵx

Keeping the first term in the expansion, we obtain

$$I_a = \frac{1.51 \times 10^3 \, e \pi a_0^2}{E^3} \left\{ \frac{1}{\left(1.5 - \left(2 - \frac{2.4}{E}\right)^{1/2} \cos\theta - \frac{0.35}{E}\right)} \right\}$$

Another method of approximation deals with the original form of the matrix element before the introduction of the Feynman integrals.

If $E \gg 1$, $\bar{B} > 1$, $\bar{C} > 1$ the integrand is large only at certain regions in the $\bar{k}$ space, namely when $\bar{B} \sim \bar{k}$, $\bar{C} \sim k$
Therefore we may write approximately:

$$I_a \simeq \frac{1}{B^2\left[(\bar{B}-\bar{C})^2 + (2a_0)^{-2}\right]^2} \int \frac{d\bar{\kappa}}{\left[\kappa^2 + (B/a_0)^2\right]^2} + \frac{1}{C^2\left[(B-C)^2 + \frac{B^2}{a_0^2}\right]^2} \int \frac{d\bar{\kappa}}{\left[\kappa^2 + (2a_0)^{-2}\right]^2}$$

provided that the regions where the integrals come from do not overlap. This condition is seen to be fulfilled if $E \gg 10.8$

When integrated, this limitating value of I_a is seen to agree exactly with the result given above, so that the two schemes of approximation are equivalent.

We now use the second method of approximation in I_c and see that it falls off with energy as E^{-4} whereas I_a and I_b go like E^{-3}. At high energies, we can therefore neglect it.

It is probable that I_c is small at all energies, since it represents the interaction of the positron with the electron that is left behind. The principal effect of this interaction would be to weaken somewhat the positron-nucleus interaction, i.e. I_c would tend to cancel some part of I_a.

Using the asymptotic forms of I_a and I_b, neglecting I_c , we find that the total cross-section for $E \rightarrow \infty$ is $\sigma_J/\pi a_0^2 \rightarrow 2.15 \times 10^6/E^6$

when the equivalent

$\sigma_{BK}/\pi a_0^2 \rightarrow 4.62 \times 10^6/E^6$

Both appear to be larger than the equivalent hydrogen cross-sections:

$$\frac{\sigma_{BK}(He)}{\sigma_{BK}(H)} = 13.4 \; ; \qquad \frac{\sigma_J(He)}{\sigma_J(H)} = 10$$

A few numerical calculations were then carried out at $E=2.4$. By taking into account I_a and I_b , the differential cross-section in forward direction $(\theta = 0^\circ)$ was found to be $d\sigma_J/d\Omega = 2.67\ a_0^2$

The ratio $d\sigma_{B.K}/d\sigma_J = 6.6$

A rough numerical integration to take account of I_c gives a $\dfrac{d\sigma_{TOT}}{d\Omega} = 2.35\ a_0^2$

differing of the $d\sigma_J/d\Omega$ by about 15%.

The ratio $d\sigma_{BK}/d\sigma_{TOT}$ now climbs up to 7.5.

Figure XIII

H 1s → pos 1s

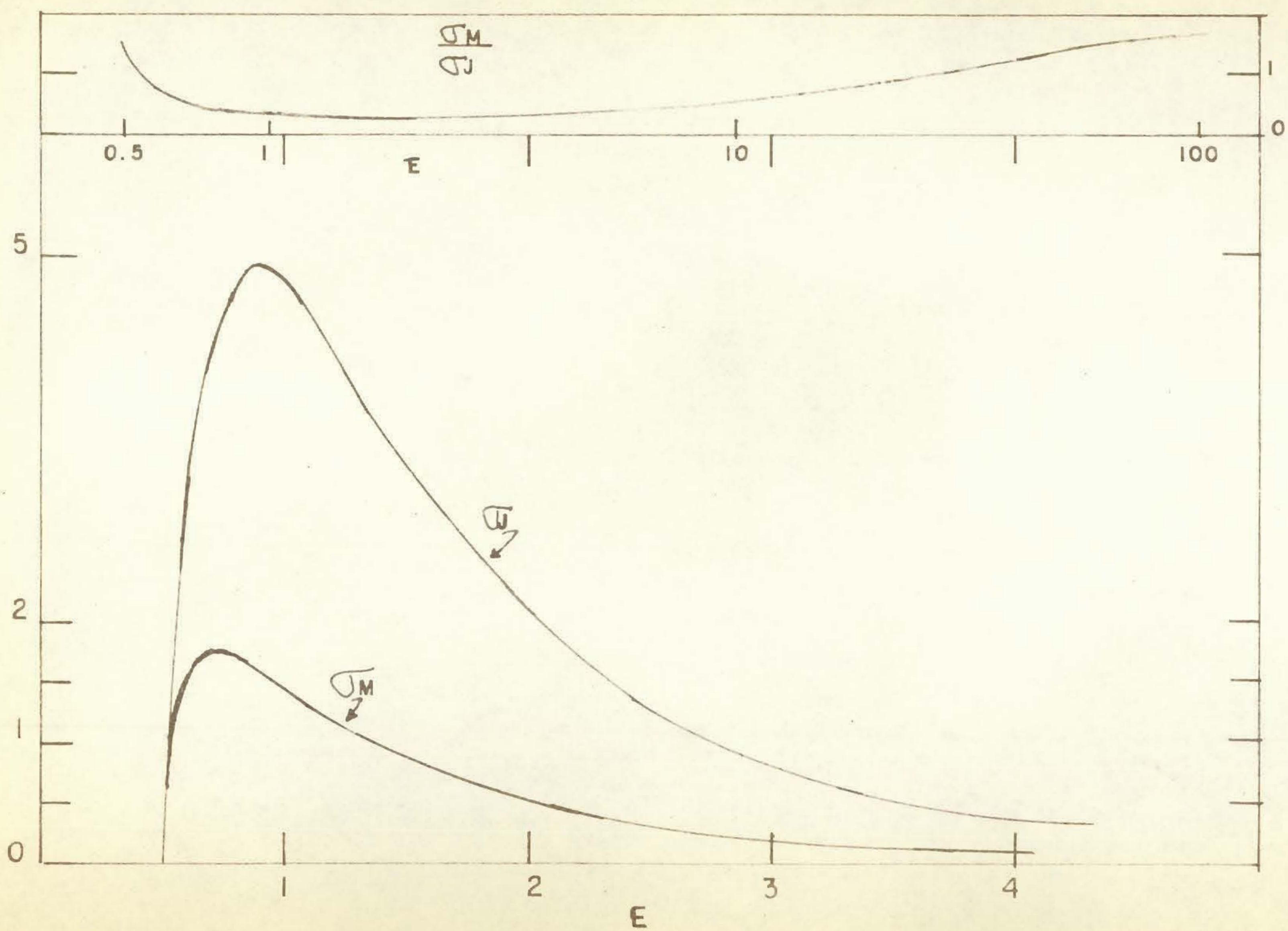
Total cross-section

$$\frac{\sigma_M}{\pi a_0^2} \text{ vs } E$$

for E $\longrightarrow \infty$ $\quad \sigma_M \rightarrow \sigma_{BK}$

$\dfrac{\sigma_J}{\pi a_0^2}$ appears also for comparison

In the top of the graph, $\dfrac{\sigma_M}{\sigma_J}$ with E on a log. scale.



$\frac{\sigma_M}{\sigma_J}$
1
0
0.5
1
E
10
100
5
2
1
0
σ_J
σ_M
1
2
3
4
E

APPENDIX I:

Use of an Averaged Potential as the Perturbation

An attempt was made to include the nucleus-positron interaction in some sort of approximate manner in a B.K. type calculation: we replace the usual (sum of two terms) perturbation potential obtained by averaging the proton charge distribution around the electron in the H atom.

Instead of $e^2/R - e^2/r'$

we replace e^2/R by $e^2 \int \Psi_0^*(r) \frac{1}{|\bar{r} - \bar{r}'|} \Psi_0(r)\, d\bar{\tau} = V(r')$

We call $H'_{eff} = V(r') - e^2/r'$

$$= e^2 \left[\exp\left(-\frac{2r'}{a_0}\right)\left(\frac{1}{r'} + \frac{1}{a_0}\right)\right]$$

The matrix element is then:

$$I = \underline{2\sqrt{2}\,\pi a_0^2} \left[\frac{1}{(c^2 + (2a_0)^{-2})}\right]\left[\frac{1}{(c^2 + \frac{25}{4a_0^2})^2} + \frac{5}{a_0}\frac{1}{(c^2 + \frac{25}{4a_0^2})}\right]$$

$$\bar{C} = \bar{k}_0 - \bar{k}_f$$

and the total cross-section

$$\frac{\sigma_M}{\pi a_0^2} = \frac{4}{9E}\left\{\frac{25}{E^6}\left(Q^3S^3 - P^3R^3\right) + \frac{55}{2E^5}\left(Q^3S^2 - P^3R^2\right)\right.$$

$$+\frac{311}{12E^4}\left(Q^3S - P^3R\right) - \frac{311}{54E^3}\left(Q^3 - P^3\right)$$

$$\left.+\frac{311}{216E^2}\left(Q^2 - P^2\right) - \frac{311}{648E}\left(Q - P\right) + \frac{311}{3888}\ln\frac{QR}{SP}\right\}$$

$$Q = 1/M+N \qquad P = 1/M-N,\ R = 1/M-N+O$$

$$S = 1/M+N+O$$

$$M = .65 \qquad N = \left(2 - 1/E\right)^{1/2}$$

$$O = 6/E$$

At present, it is not clear where this type of approximation fits into the consistent theory of collision processes. In particular, it is uncertain whether σ_M offers any improvement over the straight forward calculation.

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ERRATA

1. In page 4, first equation, read:

$$\frac{d\sigma_f}{d\Omega} = \left(\frac{\mu_f}{2\pi\hbar^2}\right)^2 \frac{v_f}{v_0} \left| I_f \right|^2$$

2. In page 19, third equation, read:

$$I_b = -\frac{10.3\,\pi a_0^2}{E^3}\left[\left(M - N\cos\theta - \frac{0.35}{E}\right)\left(M - N\cos\theta + 0.\frac{225}{E}\right)^2\right]^{-1}$$

3. In page 20, third equation, read:

$$\Delta_\pm = \frac{E}{a_0^2}\left[1.5 \pm \left(2 - \frac{2.4}{E}\right)^{1/2} - \frac{0.35}{E}\right]$$

4. In Figure XII, divide the ordinates by 16.