Matematisk-fysiske Meddelelser
udgivet af
Det Kongelige Danske Videnskabernes Selskab
Bind **31**, nr. 13

Mat. Fys. Medd. Dan. Vid. Selsk. **31**, no. 13 (1959)

COULOMB DEFLECTION EFFECTS ON IONIZATION AND PAIR-PRODUCTION PHENOMENA

BY

JENS BANG AND JOHANNES M. HANSTEEN

København 1959
i kommission hos Ejnar Munksgaard

CONTENTS

Synopsis

The process of K-ionization of atoms by heavy, charged particles is analysed by a semi-classical, time-dependent perturbation method. Non-relativistic wave functions are used for the atomic electrons. The deflection of the bombarding particle in the Coulomb field of the target nucleus is shown to play an important part in the calculation of cross sections in the low-energy region of the projectile. Numerical calculations of K-ionization cross sections for protons turn out to be in good agreement with recent light-target experiments. An estimate is made of the effect of using relativistic electron wave functions in the present perturbation treatment. The method developed is further applied to the pair-production process caused by slow protons impinging on a heavy target element.

Printed in Denmark
Bianco Lunos Bogtrykkeri A-S

1. Introduction

The ejection of atomic electrons by impingement of heavy, charged particles (protons, deuterons, α-particles) is followed by the emission of the characteristic x-radiation of the target. Recent measurements have given more accurate information about this effect[1–4]. The experimental cross sections turned out to deviate greatly from the values given by the existing theory.

The theory of the excitation of atoms by slow, heavy, charged particles has been considered by Mott[5], Bethe[6] and Henneberg[7]. The last-mentioned author has performed extensive calculations of the K-shell ionization cross sections. He used the Born approximation, i. e. plane waves for the incoming particles and Coulomb wave functions with respect to the nucleus for the electrons, treating the interaction between the projectile and the electron to first order. A partial justification for this procedure was given by Henneberg[7], and also by Mott along somewhat different lines[5]. This question will be treated in detail in sections 2 and 3.

If we accept the above assumption of Henneberg, the differential cross section for ejection of a K-electron with the final energy E_f is given by

$$\frac{d\sigma_K}{dE_f} = \frac{4\pi}{\hbar^2} Z_1^2 e^4 \frac{M_1}{E_1} \int_{q_0}^{\infty} \frac{dq}{q^3} J \tag{1.1}$$

$$J = \sum_f \left| \int e^{i\underline{q}\underline{r}} \psi_i(\underline{r}) \psi_f^*(\underline{r}) \, d\underline{r} \right|^2 . \tag{1.2}$$

Here, Z_1, M_1 and E_1 are the charge, mass and energy of the bombarding particle; q is the momentum change of the projectile, q_0 its minimum value. The electron wave functions are denoted by ψ. The summation in (1.2) is extended over all final electron states.

Henneberg used non-relativistic Coulomb wave functions in (1.2). As it became clear that there was considerable discrepancy between the theory and the experiments, Jamnik and Zupančič[8] repeated the calculations with relativistic wave functions for the electron. The relativistic increase of the electron density near the origin resulted in an enlargement of the cross section for heavy elements. For elements in the middle of the periodic table, however, the relativistic corrections were small[1].

The deviations mentioned above may be due in part to the fact that the approximation of Henneberg does not take into account the Coulomb repulsion between the impinging particle and the nucleus. The most recent observations seem to support this idea[2, 3, 4]. The repulsion prevents particles of low energy from getting close to the nucleus and may thus be expected to give rise to a cross section smaller than predicted by the above-mentioned theory. It is the purpose of the present work to investigate the energy region where this repulsion effect can be expected to be of importance.

Later in the work it will be shown that the decisive parameter in this connection is $\xi = dq_0$, where d is half the distance of closest approach in a head-on collison and q_0 is, as before, the minimum momentum transfer of the bombarding particle. For values $\xi \gtrsim 1$, ionization cross sections much smaller than the predictions of the earlier calculations may be expected. Only in the limit $\xi \ll 1$ can the Coulomb repulsion be neglected and the plane-wave procedure be considered valid.

It is just in the low-energy region, where the great divergences from the earlier calculations are found, that a classical treatment of the projectile is justified. The condition for such a treatment is (cf. § 1.3 of ref. 10)

$$\varkappa = \frac{2 Z_1 Z_2 e^2}{\hbar v_1} \gg 1, \tag{1.3}$$

where Z_2 is the charge of the target nucleus and v_1 the velocity of the incoming particle. This enables us to take the Coulomb repulsion into account by choosing an appropriate path for the projectile.

Stephens and Staub[11, 12] recently reported measurements of the cross section for pair production by slow protons impinging on a tantalum target. They found values smaller by a factor of over a hundred than the predictions of first-order Born-approximation calculations[13]. This too may be due to the deflection of the proton in the Coulomb field of the nucleus. The phenomenon is briefly considered in the last section of this work.

[1] A summary of both the experimental and the theoretical aspects of x-ray production by heavy, charged particles is given by Merzbacher and Lewis in Handbuch der Physik **34** (1958) 166.

2. Approximations Used in the Treatment of *K*-ionization by Heavy Particles

The character of the process of *K*-ionization by heavy, charged particles depends on the relations between the four inverse lengths k, α, $\frac{1}{d}$, and q_0. Here, $\hbar k$ is the momentum of the ejected electron and $\alpha = \frac{Z_2 e^2 m}{\hbar^2}$ the inverse *K*-shell radius. The parameter $1/d$ is the inverse of half the distance of closest approach in a head-on collision, $d = \frac{Z_1 Z_2 e^2}{2 E_1}$ (cf. sec. 1). For the minimum momentum transfer q_0 of the bombarding particle we have, provided $\frac{\Delta E}{E_1} \ll 1$,

$$\left.\begin{aligned} q_0 &= \frac{\Delta E}{\hbar v_1} \\ \Delta E &= E_f + E_B \end{aligned}\right\}, \tag{2.1}$$

where E_f is the kinetic energy of the ejected electron and $|E_B| = \frac{Z_2^2 e^4 m}{2\hbar^2}$ is the binding energy of the *K*-electron.

It is of interest to notice that the relative values of d^{-1}, q_0, and α are largely determined by the parameter $\varkappa$. Thus, if we define ξ_0 as the value of $\xi = d q_0$ for $\Delta E = E_B$, we have

$$d\alpha = \frac{1}{4 Z_1} \frac{m}{M_1} \varkappa^2, \tag{2.2}$$

$$\xi_0 = \left(\frac{1}{4 Z_1}\right)^2 \frac{m}{M_1} \varkappa^3 \tag{2.3}$$

and

$$\frac{d\alpha}{\xi_0} = \left(\frac{\alpha}{q_0}\right)_{\max} = \frac{4 Z_1}{\varkappa}. \tag{2.4}$$

For the above-mentioned quantities one has the following four possibilities—corresponding, in the order mentioned, to increasing energy of the projectile—:

1) $$\frac{1}{q_0} < \frac{1}{\alpha} < d, \quad \varkappa > 2\sqrt{\frac{M_1}{m} Z_1}\ . \tag{2.5}$$

This corresponds to a projectile which is unable to force its way into the K-shell. If $\frac{Z_1}{\alpha} < d$, we even get $\Delta E > E_1$, so that ionization is impossible.

2) $$\frac{1}{q_0} < d < \frac{1}{\alpha}, \quad 2\sqrt{\frac{M_1}{m}} Z_1 > \varkappa > 4 Z_1; \; (\xi > 1). \tag{2.6}$$

For such energies the projectile is able to penetrate the K-shell, but the ionization probability is very strongly affected by the Coulomb deflection.

3) $$d < \frac{1}{q_0} < \frac{1}{\alpha}, \quad \varkappa > 4 Z_1; \; (\xi < 1). \tag{2.7}$$

In this domain the Coulomb deflection still plays a part. (It is shown in the present work that the earlier calculations (cf. refs. 7 and 18) are in principle correct for $\xi \to 0$.)

4) $$d < \frac{1}{\alpha} < \frac{1}{q_0}, \quad \varkappa \ll 4 Z_1. \tag{2.8}$$

Here the ionization process cannot be handled by semi-classical methods. The relevant treatment is the one given by Bethe in his article on the passage of heavy, charged particles through matter, cf. ref. 6.

In the present treatment we consider especially the energy domains 2) and 3). We shall therefore assume in the following that

$$\frac{\alpha}{q_0} \ll 1. \tag{2.9}$$

As will be seen later, the calculations are considerably simplified when

$$\frac{k}{q_0} \ll 1. \tag{2.10}$$

The condition for this inequality to hold true is nearly the same as the condition for (2.9) (cf. eqs. (2.5), (2.6) and (2.7)), namely

$$\varkappa \gg 4 Z_1, \tag{2.11}$$

which is seen from the inequality

$$\frac{k}{q_0} = \frac{2\, m k v_1}{\hbar\,(\alpha^2 + k^2)} < \frac{2\, m k v_1}{\hbar\, 2\, \alpha k} = \frac{2\, Z_1}{\varkappa}. \tag{2.12}$$

Later it is shown that the majority of the secondary electrons are ejected with energies much smaller than the K binding energy, i. e.

$$k \ll \alpha. \tag{2.13}$$

TABLE 2.1

Element	Z_2	E_1 (keV)	$\varkappa$	ξ_0	$d\alpha$
Fe	25	140[3] 1300[3]	21.8 7.2	0.28 0.0094	0.051 0.0052
Mo	42	240[3] 1600[2] 2400[1]	26.8 10.5 8.6	0.56 0.033 0.018	0.084 0.013 0.0083
Pb	82	1920[1]	18.6	0.21	0.046

[1] See ref. 1. [2] See ref. 2. [3] See ref. 4.

Besides, it should be noted that for the following perturbation treatment to be valid it is a necessary condition that the charge of the projectile is much smaller than that of the target nucleus, i.e. $Z_1 \ll Z_2$.

Table 2.1 shows the various parameter values for some of the cases experimentally investigated by proton bombardment.

3. First-order, Time-dependent Perturbation Treatment of the K-ionization

We want to deal with the ionization process in such a way that the Coulomb deflection can be taken into account. This may be done by a semi-classical perturbation treatment. We express the problem in impact

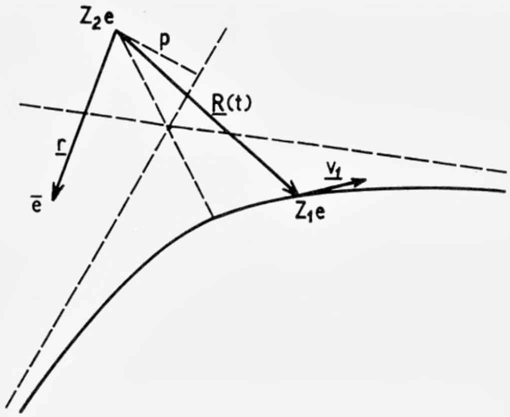

Fig. 3.1. Classical picture of the impact process.

parameter form and treat the interaction between the projectile and the electron as the perturbation.

The differential cross section for the ejection of an atomic electron with the final energy E_f is given by the general expression

$$\frac{d\sigma}{dE_f} = \frac{2\pi}{\hbar^2}\int_0^\infty p\,dp\left|\int_{-\infty}^{\infty} dt e^{i\omega t}\langle f|V(r,t)|i\rangle\right|^2. \tag{3.1}$$

Here, p is the impact parameter and $\omega = \Delta E/\hbar$. In the following we shall consider interactions of the Coulomb type

$$V = \frac{Z_1 e^2}{|\underline{r} - \underline{R}(t)|}; \tag{3.2}$$

$\underline{r}$ is here the position vector of the electron and $\underline{R}(t)$ that of the incoming particle.

a. The cross section for straight-line paths of the incoming particles

(i) *A general theorem*

We first consider the case where the projectiles follow straight-line paths, that is, we disregard the Coulomb repulsion of the bombarding particles by the nucleus. The cross sections thus obtained are exactly the same as those

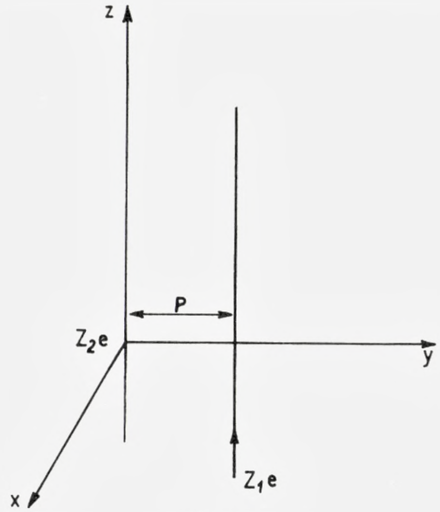

Fig. 3.2.

found if one employs the previously mentioned plane-wave method, disregarding the deflection of the bombarding particles by collision with the electrons (cf. also ref. 14). This is shown mathematically in Appendix I, but can also be seen from the fact that the cross section (1.1) for a bombarding particle with a given velocity v_1 is independent of its mass. The mass may therefore be infinitely great, and thus the particle may be treated in a classical way.

We place our coordinate system with its origin at the nuclear centre of mass and its z-axis in the direction of the incoming particle. This particle moves in the y–z plane as illustrated in fig. 3.2. As shown in Appendix I, the cross section is then given by

$$\left.\begin{aligned} \frac{d\sigma}{dE_f} &= 4\pi Z_1^2 \frac{M_1}{E_1}\frac{e^4}{\hbar^2}\int_0^\infty p\,dp\,|\mathrm{M}_p|^2 \\ \mathrm{M}_p &= \int d\tau\, \psi_i \psi_f^* e^{iq_0 z} K_0(q_0\varrho). \end{aligned}\right\} \tag{3.3}$$

K_0 is the modified Bessel function of the third kind and zeroth order, and

$$\varrho^2 = x^2 + (p-y)^2. \tag{3.4}$$

(ii) The matrix element for emission of K-electrons

From eqs. (3.3) we are now able to derive the cross section for K-electron emission for a fixed value of the impact parameter, $(d\sigma_K/dE_f)_p$. For the electrons we use non-relativistic Coulomb eigenfunctions in the form given by Alder and Winther[15].

The details of the evaluation of this matrix element are given in Appendix II, b. By a rather lengthy procedure one reaches the following result:

$$\left.\begin{aligned} \mathrm{M}_p(l,m) &= i^{-m}\frac{\Gamma(2l+3)}{\Gamma\left(l+\frac{3}{2}\right)}\left[(2l+1)\frac{(l-m)!}{(l+m)!}\right]^{1/2} \\ &\times \frac{\pi}{2} N_i N_f^{l,k} k^l \int_0^\infty dt\, t^{m+1} J_m(pt)\, s^{l-m-2}\, C_{l-m}^{m+\frac{1}{2}}\left(\frac{q_0}{s}\right) \\ &\times (\alpha + i(s-k))^{-(2l+3)} F_2\{\}. \end{aligned}\right\} \tag{3.5}$$

In (3.5), N_i and $N_f^{l,k}$ are energy normalization constants; l and m denote the angular momentum quantum numbers of the final state in the continuum; s is defined by

$$s^2 = q_0^2 + t^2; \;\; 0 \leq t \langle \infty ,$$

and $C_{l-m}^{m+\frac{1}{2}}$ is a Gegenbauer polynomial.

$$F_2\{\} = F_2\left\{2\,l+3,\; l+1,\, l+1+i\eta,\; 2\,l+2,\; 2\,l+2;\; \frac{2\,is}{\alpha+i\,(s-k)},\; \frac{-2\,ik}{\alpha+i\,(s-k)}\right\} \tag{3.6}$$

is an Appell function, which is a hypergeometric function of two variables. In sub-section (ii) of Appendix II, b it is shown that

$$\left.\begin{aligned} F_2\{\} &= \frac{1}{l+1}\left(\frac{\alpha-i\,(s+k)}{\alpha+i\,(s-k)}\right)^{-(l+1)}\left(\frac{\alpha+i\,(s+k)}{\alpha+i\,(s-k)}\right)^{-(l+1+i\eta)} \\ &\times \frac{1}{\alpha-i\,(s+k)}\left\{(-i\eta)\,(\alpha-ik)\;{}_2F_1\left(l+1,\; l+1+i\eta,\;\; 2\,l+2;\; \frac{4\,sk}{\alpha^2+(s+k)^2}\right)\right. \\ &\left.+\,(l+1+i\eta)\,\alpha\,\frac{\alpha+i\,(s-k)}{\alpha+i\,(s+k)}\;{}_2F_1\left(l+1,\; l+2+i\eta,\;\; 2\,l+2;\; \frac{4\,sk}{\alpha^2+(s+k)^2}\right)\right\}. \end{aligned}\right\} \tag{3.7}$$

Here, $\eta = -\dfrac{Z_2\,e^2}{\hbar v} = -\dfrac{\alpha}{k}$ (minus sign because we are dealing with negatrons); v is the final electron velocity, and ${}_2F_1\,(\;)$ are ordinary hypergeometric functions.

Up to this point in the development no approximations have been introduced.

In the following we shall restrict ourselves to cases where the inequalities (2.9) and (2.10) are fulfilled. Under these conditions, the contributions to the matrix element $\mathrm{M}_p\,(l,\, m)$ in eq. (3.5) from l-values larger than zero become negligible. The $F_2\{\}$ function is then considerably simplified. As sketched in sub-section (ii) of Appendix II, b, we arrive at the result

$$\left.\begin{aligned} G\,(k) &\equiv (\alpha+i\,(s-k))^{-3}\,F_2\{\} \\ &= \frac{i}{2\,s}\,Im\left\{\frac{(\alpha+i\,(s-k))^{i\eta-1}}{(\alpha+i\,(s+k))^{i\eta+1}}\right\}. \end{aligned}\right\} \tag{3.8}$$

An expansion of G in powers of k/s and α/s gives

$$G = \frac{1}{s^3}\left\{\frac{\alpha}{s}\left(1-\frac{\eta k}{\alpha}\right)+\left(\frac{\alpha}{s}\right)^3\frac{2}{3}\left(-19+5\,\frac{k^2}{\alpha^2}\right)+ - - - \right\}. \tag{3.9}$$

Since

$$\int_0^\infty t^{m+1} J_m\,(p\,t)\,(t^2+q_0^2)^{-\mu-1} = \frac{p^\mu\, q_0^{m-\mu}\, 2^{-\mu}}{\Gamma\,(\mu+1)}\,K_{m-\mu}\,(p\,q_0) \tag{3.10}$$

(see ref. 16, 7.14.2, eq. (59), hereafter quoted as H. T. F.), we have from eqs. (3.5) and (3.9)

$$M_p(0,0) \simeq \frac{\alpha}{2} N_i N_f^{0,k} \frac{1}{q_0^4} (p q_0)^2 K_2(p q_0) \tag{3.11}$$

and consequently

$$\left(\frac{d\sigma_K}{dE_f}\right)_p = Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \frac{Z_2^2}{2\, a_0^2} |N_i|^2 |N_f^{0,k}|^2 \frac{1}{q_0^8} (p q_0)^4 (K_2(p q_0))^2, \tag{3.12}$$

where a_0 is the Bohr radius.

Fig. 3.3 shows the variation of $|M_p(0,0)|^2$ with the impact parameter. The greatest contributions to the ionization probability are seen to come from impact parameters for which $p \sim \frac{1}{q_0}$.

The expression (3.12) contains only the leading term in a development in powers of $\frac{\alpha}{q_0}$. From (3.10) it may be shown, however, that also higher terms in the cross section (corresponding for instance to higher terms in (3.9) or to higher l-values) exhibit a similar dependence on p.

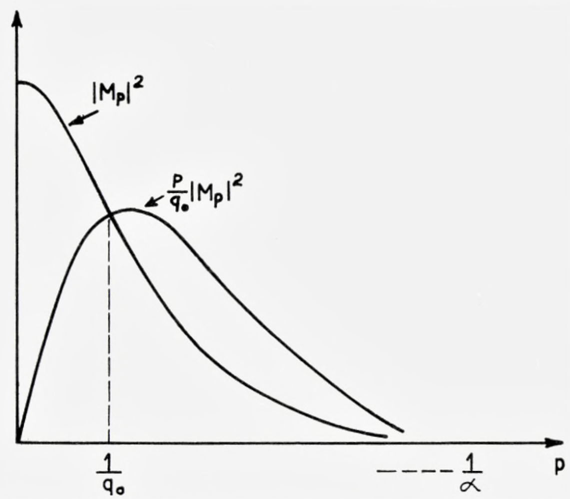

Fig. 3.3. The probability of ejection of a K-electron as a function of the impact parameter p for straight-line orbits. The area under the curve $\frac{p}{q_0}|M_p|^2$ shows the contributions to the total cross section from the various p-values. It is assumed that $\frac{1}{q_0} \ll \frac{1}{\alpha}$. The calculations are valid only for $p \ll \frac{1}{\alpha}$.

Since the Coulomb deflection becomes large for impact parameters of the order of or smaller than the distance of closest approach $d\left(=\frac{Z_1 Z_2 e^2}{2 E_1}\right)$, this deflection must be expected to be of importance when d is not very much smaller than $\frac{1}{q_0}$.

Up till now we have assumed $\alpha \ll q_0$, corresponding to the cases considered in eqs. (2.6) and (2.7). In the opposite case of $q_0 \lesssim \alpha$, the expansions employed above are no longer valid, and, moreover, the semi-classical methods break down, cf. eqs. (2.8). The velocity of the projectile is in this case larger than that of the K-electron; therefore we may apply considerations from the stopping-power calculations extensively treated by Bethe in ref. 6.

The total cross section for emission of K-electrons with the final energy E_f is given by

$$\left(\frac{d\sigma_K}{dE_f}\right)_{\text{str. } l.} = 2\pi \int_0^\infty p\, dp \left(\frac{d\sigma_K}{dE_f}\right)_p.$$

Using an integral formula given by Lommel (cf. ref. 17, p. 136), we deduce

$$\left(\frac{d\sigma_K}{dE_f}\right)_{\text{str. } l.} = \frac{2^5}{5} \pi Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \frac{Z_2^2}{a_0^2} |N_i|^2 |N_f^{0,k}|^2 \frac{1}{q_0^{10}}. \tag{3.13}$$

This is exactly the same formula as the one derived by Huus et al.[18] by means of the Born approximation.

Eq. (3.12) also enables us to calculate the cross section for K-ionization by particles scattered through a small angle, $\theta \ll 1$, since this cross section is expected to be the same as that for a straight-line path with corresponding impact parameter. (See fig. 3.5 and the explanatory text to that figure.) We have

$$\left(\frac{d\sigma_K}{d\Omega}\right)_{\text{str. } l.} = \frac{d\sigma_R}{d\Omega}\left(\frac{d\sigma_K}{dE_f}\right)_p = f_1 \frac{\left(\xi \operatorname{cotg}\frac{\theta}{2}\right)^4}{\sin^4\frac{\theta}{2}} \left(K_2\left(\xi \operatorname{cotg}\frac{\theta}{2}\right)\right)^2; \tag{3.14}$$

$d\sigma_R/d\Omega$ is the differential cross section for Rutherford scattering, and

$$f_1 = \frac{d^2}{4} Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \frac{Z_2^2}{2 a_0} |N_i|^2 |N_f^{o,k}|^2 \frac{1}{q_0^8}. \tag{3.15}$$

The cross sections (3.13) and (3.14) have been labelled with the index str. *l.* because they are derived on the basis of a straight-line calculation. The expressions are expected to be valid in the limit $\xi \to 0$.

In fig. 3.5, $\left(\frac{d\sigma_K}{d\Omega}\right)_{\text{str.}\,l.}$ is given for $\xi = 0.2$. In the same figure it is shown how the angular dependence is influenced by the Coulomb deflection, as calculated below.

b. Cross sections for hyperbolic paths

(i) *General procedure*

In the following we shall calculate the cross section for emission of secondary K-electrons, taking into account the deflection of the projectile. We shall confine ourselves to the monopole term in the potential, assuming that term to be the dominating one for $\alpha \ll q_0$ as in the case of the straight-line integrals. We then have

$$\left.\begin{aligned} \frac{d\sigma_K}{dE_f} &= \frac{2\pi}{\hbar^2} d^2 Z_1^2 e^4 \int_1^\infty \varepsilon\, d\varepsilon \\ &\times \left| \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle \psi_f \left| \begin{Bmatrix} \dfrac{1}{R(t)}, & r < R \\ \dfrac{1}{r}, & r > R \end{Bmatrix} \right| \psi_s \rangle \right|^2, \end{aligned}\right\} \quad (3.16)$$

where ε is the eccentricity of the hyperbolic path of the incoming particle. For this path we use a parametric representation previously employed by, among others, TER-MARTIROSYAN[19]:

$$\left.\begin{aligned} x &= d(\cosh w + \varepsilon) \\ y &= d\sqrt{\varepsilon^2 - 1}\, \sinh w \\ z &= 0 \\ R &= d(\varepsilon \cosh w + 1) \\ t &= \frac{d}{v_1}(\varepsilon \sin h w + w). \end{aligned}\right\} \quad (3.17)$$

Inserting for the electronic wave functions in eq. (3.16) the integral representations given by ALDER and WINTHER[15], we get

$$\left.\begin{aligned}\frac{d\sigma_K}{dE_f} &= \frac{2\pi}{\hbar^2} d^2 Z_1^2 e^4 \left|N_i\right|^2 \left|N_f^{0,k}\right|^2 \int_1^\infty \varepsilon\, d\varepsilon \\ &\times \left| \int_{-\infty}^{\infty} dt\, e^{i\omega t} \left\{ \frac{1}{\Gamma(1-i\eta)\,\Gamma(1+i\eta)} \int_0^1 du \left(\frac{u}{1-u}\right)^{i\eta} \right.\right. \\ &\times \left.\left. \left[\int_0^R \frac{dr}{R} r^2 e^{-rb} + \int_R^\infty dr\, r\, e^{-rb} \right] \right\} \right|^2 .\end{aligned}\right\} \tag{3.18}$$

Here,

$$b = \alpha - ik + 2\, iku. \tag{3.19}$$

The integration over r is easily carried out, yielding for the factor in square brackets in (3.18)

$$I_R = \frac{2}{Rb^3} - \frac{e^{-bR}}{b^2}\left(1 + \frac{2}{Rb}\right). \tag{3.20}$$

The integration over time is more complicated. Using (3.17), we have

$$\left.\begin{aligned}I_b = v_1 \int_{-\infty}^{\infty} dt\, e^{i\omega t} I_R = \int_{-\infty}^{\infty} dw \left\{ \frac{2}{b^3} - \frac{e^{-bd(\varepsilon\cosh w + 1)}}{b^2} \left(d(\varepsilon\cosh w + 1) + \frac{2}{b} \right) \right\} \\ \times e^{i\xi(\varepsilon\sinh w + w)}.\end{aligned}\right\} \tag{3.21}$$

As shown in Appendix II, c, the integration leads to

$$\left.\begin{aligned}I_b = 4\, b^{-3} e^{-\frac{\pi}{2}\xi} K_{i\xi}(\varepsilon\xi) - 2\, b^{-2}(d + 2\, b^{-1})\, e^{-bd} \left(\frac{bd+i\xi}{bd-i\xi}\right)^{\frac{i\xi}{2}} \\ \times K_{i\xi}\left(\varepsilon\sqrt{b^2 d^2 + \xi^2}\right) - d\, b^{-2} e^{-bd} \varepsilon \left\{ \left(\frac{bd+i\xi}{bd-i\xi}\right)^{\frac{i\xi+1}{2}} K_{i\xi+1}\left(\varepsilon\sqrt{b^2 d^2+\xi^2}\right) \right. \\ \left. + \left(\frac{bd+i\xi}{bd-i\xi}\right)^{\frac{i\xi-1}{2}} K_{i\xi-1}\left(\varepsilon\sqrt{b^2 d^2+\xi^2}\right) \right\}\end{aligned}\right\} \tag{3.22}$$

or

$$\left.\begin{aligned}I_b = 2\, b^{-3} \left\{ 2\, e^{-\frac{\pi}{2}\xi} K_{i\xi}(\varepsilon\xi) - e^{-bd} \left(\frac{bd+i\xi}{bd-i\xi}\right)^{\frac{i\xi}{2}} \right. \\ \times \left. \left[\left(2 + \frac{b^2 d^2}{bd - i\xi}\right) K_{i\xi}\left(\varepsilon\sqrt{b^2 d^2+\xi^2}\right) + \frac{\varepsilon\, b^2 d^2}{\sqrt{b^2 d^2 + \xi^2}} K_{i\xi-1}\left(\varepsilon\sqrt{b^2 d^2+\xi^2}\right) \right] \right\}.\end{aligned}\right\} \tag{3.23}$$

Up to this point the development is exact.

According to a multiplication theorem for the Bessel functions (H.T.F. 7.15, eq. (19) we have

$$\frac{K_\nu\left(\varepsilon\sqrt{b^2 d^2+\xi^2}\right)}{\left(\sqrt{b^2 d^2+\xi^2}\right)^\nu} = \sum_{n=0}^{\infty}\left(-\frac{\varepsilon b^2 d^2}{2}\right)^n \frac{1}{\xi^{\nu+n}} \frac{K_{\nu+n}(\varepsilon\xi)}{n!}. \tag{3.24}$$

As

$$\frac{|b|\,d}{\xi} \simeq \frac{\alpha}{q_0}$$

and

$$|b|d \simeq d\alpha,$$

this expansion is fast converging, provided the inequality (2.9) is fulfilled.

Applying (3.24) to (3.23), we deduce

$$\left.\begin{aligned} I_b = 2\,e^{-\frac{\pi}{2}\xi}\,b^{-3}\Bigg\{&2\,K_{i\xi}(\varepsilon\,\xi) - e^{-bd}\left(1-\frac{bd}{i\xi}\right)^{-i\xi} \\ \times\Bigg[&\left(2+\frac{b^2 d^2}{bd-i\xi}\right)K_{i\xi}(\varepsilon\,\xi) - \frac{b^4 d^4}{bd-i\xi}\,\frac{\varepsilon}{2\,\xi}\,K_{-i\xi+1}(\varepsilon\,\xi) \\ +&\left(-2+\frac{b^2 d^2}{bd-i\xi}\right)b^4 d^4\,\frac{\varepsilon^2}{8\,\xi^2}\,K_{-i\xi+2}(\varepsilon\,\xi) + - - - - \Bigg]\Bigg\}, \end{aligned}\right\} \tag{3.25}$$

where we have written explicitly terms arising from the expansion (3.24) with $n \leq 2$.

Since

$$\left(1-\frac{bd}{i\xi}\right)^{-i\xi} = e^{-i\xi\, ln\left(1-\frac{bd}{i\xi}\right)}$$

$$\simeq e^{bd}\left\{1+\frac{i\xi}{2}\left(\frac{bd}{i\xi}\right)^2+\frac{i\xi}{3}\left(\frac{bd}{i\xi}\right)^3+\left(\frac{i\xi}{4}-\frac{\xi^2}{8}\right)\left(\frac{bd}{i\xi}\right)^4+ - - - - \right\},$$

we obtain by inserting this expression into (3.25) and taking into account that $|b|\,d \simeq d\alpha \ll 1$

$$b^3 \cdot I_b \simeq 2\,e^{-\frac{\pi}{2}\xi}\sum_{n=0}^{\infty} k'_n\,\varepsilon^n\,K_{-i\xi+n}(\varepsilon\,\xi), \tag{3.26}$$

where

$$\left.\begin{aligned}
k_0' &= -\frac{b^3\,d^3}{3\,\xi^2} + \frac{b^4\,d^4}{\xi^2}\left(\frac{i}{2\,\xi} - \frac{1}{4}\right)\\
k_1' &= i\,\frac{b^4\,d^4}{2\,\xi^2}\\
k_2' &= \frac{b^4\,d^4}{4\,\xi^2}\\
k_3' &= -\frac{b^6\,d^6}{12\,\xi^3}\\
&-\ -\ -\ -\ -\ -\\
k_n' &= \frac{n-1}{2^{n-1}\,n\,!}\left(-\frac{b^2\,d^2}{\xi}\right)^n \text{ (valid for } n \geq 2).
\end{aligned}\right\} \tag{3.26, a}$$

We can now carry out the u-integration (see eq. (3.18)) by using an integral representation of the ordinary hypergeometric function (H.T.F. 2.12, eq. (1)). In the general case the result of the u-integration is given by

$$\int_0^1 \left(\frac{u}{1-u}\right)^{i\eta} b^n\,du = (\alpha - ik)^n\;{}_2F_1\left(3 - 2\,n,\; 1 + i\eta,\; 2;\; \frac{2\,ik}{ik-\alpha}\right);\; (n \geq 2). \tag{3.27}$$

For the majority of the ejected electrons, $k \ll \alpha$ (cf. eq. (3.13)). This enables us to perform a confluence, thus getting

$$I_\varepsilon = 2\,e^{-\frac{\pi}{2}\xi} \sum_{n=0}^{\infty} k_n\,\varepsilon^n\,K_{-i\xi+n}(\varepsilon\,\xi) \tag{3.28}$$

with

$$\left.\begin{aligned}
k_0 &= \left(-\frac{d^3}{\xi^2}\right)\left(\left(\frac{1}{3} + \frac{d\alpha}{2}\right) - i\,\frac{d\alpha}{\xi}\right)\\
k_1 &= i\,\alpha\,\frac{d^4}{\xi^2}\\
k_2 &= \frac{\alpha}{2}\,\frac{d^4}{\xi^2}\\
k_3 &= -\frac{1}{36}\,\frac{d^6}{\xi^3}\,19\,\alpha^3\\
&-\ -\ -\ -\ -\ -\ -\ -\ -\\
k_n &= \frac{1}{\alpha^3}\,\frac{n-1}{2^{n-1}\,n\,!}\,\Phi\,(3 - 2\,n,\; 2;\; -2)\left(-\frac{d^2\,\alpha^2}{\xi}\right)^n;\; n \geq 2.
\end{aligned}\right\} \tag{3.28, a}$$

Φ is here the confluent hypergeometric function.

As $\frac{d\alpha}{\xi_0} = \frac{4 Z_1}{\varkappa}$, we see that for sufficiently high values of $\varkappa$, (3.28) may to a good approximation be written as

$$I_\varepsilon = 2\, e^{-\frac{\pi}{2}\xi} \left\{ \left[-\frac{d^3}{3\,\xi^2} + \alpha \frac{d^4}{\xi^2}\left(\frac{i}{\xi} + \frac{\varepsilon^2 - 1}{2}\right)\right] K_{i\,\xi}(\varepsilon\,\xi) + \alpha \frac{d^4}{\xi^3}\,\varepsilon\, K_{-i\,\xi+1}(\varepsilon\,\xi)\right\}. \quad (3.29)$$

This equation will be useful in the following discussion of the angular distribution.

(ii) *Angular distributions of the scattered projectiles after ionization*

Equations (3.28) and (3.29) for I_ε give a direct expression for the dependence of the cross section on ε, i.e. on the deflection of the incident particle.

First we let the hyperbolic path of the incoming particle degenerate into a straight line, i.e. we put $\varepsilon \gg 1$ in eqs. (3.17), which corresponds to keeping the impact parameter fixed, but letting $d \to 0$. Eq. (3.28) is then replaced by

$$I_{\text{str.}\,l.} = 2 \sum_{n=2}^{\infty} k_n \varepsilon^n K_n(\varepsilon\,\xi), \quad (3.30)$$

where $k_2, k_3, \ldots.$ are given by (3.28, a). This result is obtained in a straightforward manner by application of the integral formulae given in Appendix II, c. The terms in (3.30) correspond exactly to the terms in the straight-line monopole expansion, the first of which is given by (3.11), since for $\varepsilon \gg 1$ we have $\varepsilon\xi \simeq p q_0$.

It is also useful to consider the opposite extreme case $\varepsilon = \varepsilon_c \simeq 1$. This corresponds to ionization by particles scattered in the backward direction. Putting

$$K_{-i\,\xi+1}(\varepsilon\xi) = -\frac{i}{\varepsilon} K_{i\,\xi}(\varepsilon\xi) - K'_{i\,\xi}(\varepsilon\xi)$$

in (3.29), we have

$$I_\varepsilon = 2\, e^{-\frac{\pi}{2}\xi} \frac{d^3}{\xi^2} \left\{ \left(-\frac{1}{3}\right) K_{i\xi}(\varepsilon\xi) - \varepsilon \frac{d\alpha}{\xi} K'_{i\xi}(\varepsilon\xi)\right\}. \quad (3.31)$$

We shall furthermore evaluate (3.31) for the case of $\xi \ll 1$. Here we may use the approximate expressions

$$\left.\begin{aligned} K_{i\,\xi}(\varepsilon_c\,\xi) &\simeq -\ln(\varepsilon_c\,\xi) \\ K'_{i\,\xi}(\varepsilon_c\,\xi) &\simeq -\frac{1}{\varepsilon_c\,\xi}. \end{aligned}\right\} \quad (3.32)$$

From (3.31) we then obtain

$$\left.\begin{aligned} I_\varepsilon &\simeq 2\, e^{-\frac{\pi}{2}\xi} \frac{d^2}{\xi^2} \left\{ \frac{d}{3} \ln(\varepsilon_c \xi) + \frac{d^2 \alpha}{\xi^2} \right\} \\ &= 2\, e^{-\frac{\pi}{2}\xi} \frac{1}{q_0^2} \left\{ \frac{\alpha}{q_0^2} + \frac{d}{3} \ln(\varepsilon_c \xi) \right\}. \end{aligned}\right\} \tag{3.33}$$

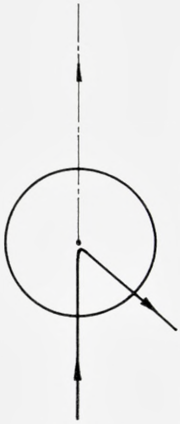

Fig. 3.4.

The dominating term in this formula corresponds to the main term in the matrix element for a particle moving on a straight-line path with the impact parameter zero. This is immediately seen from eq. (3.12), considering that

$$\lim_{pq_0 \to 0} \left((pq_0)^2 K_2(pq_0) \right) = 2.$$

From a physical point of view this was to be expected since the monopole effect considered does not depend on the direction of the outgoing particle. Moreover, for $\xi \ll 1$ the region of deflection ($\sim d$) is small compared with q_0^{-1}, the quantity characterizing the interaction with the electron. Thus, the approach to the straight-line excitation probability, for $\xi \ll 1$, is to be expected not only for backward scattering but for any scattering angle.

Quite generally we define

$$y = \frac{I_\varepsilon}{e^{-\frac{\pi}{2}\xi} \cdot I_{\text{str. } l.}} \tag{3.34}$$

since, in many cases, the main deflection effect is contained in the factor $\exp\left\{-\frac{\pi}{2}\xi\right\}$. For particles scattered in the backward direction ($\varepsilon = \varepsilon_c \simeq 1$) with sufficiently large $\varkappa$ and $\xi \ll 1$ it is easily seen from (3.33) that

$$\left.\begin{aligned} y &= 1 + \frac{4}{3} Z_1 \frac{M_1}{m} \left(\frac{\xi}{\varkappa}\right)^2 \ln(\varepsilon_c \xi) \\ &\text{or} \\ y &= 1 + \frac{1}{12} Z_1 \frac{M_1}{m} \left(\frac{\Delta E}{E_1}\right)^2 \ln(\varepsilon_c \xi). \end{aligned}\right\} \tag{3.35}$$

For $\varepsilon \gg 1$ and $\xi \gtrsim 1$ we have

$$y \simeq \frac{K_{-i\xi+2}(\varepsilon \xi)}{K_2(\varepsilon \xi)} \simeq 1 - \frac{\xi}{2\varepsilon} \tag{3.36}$$

(see p. 204 of ref. 20).

The case $\xi \gg 1$, $\varepsilon \simeq 1$ may in principle also be handled by the aid of asymptotic formulae for $K_{i\xi}(\xi)$, $\xi \gg 1$. Such formulae are found in Chapter 8 of ref. 17. We stress the fact that these considerations are valid only for sufficiently high values of $\varkappa$. For smaller $\varkappa$, more terms in (3.28) must be taken into account. The results of the above analysis may be used to modify the angular distribution found from the straight-line approach in (3, a, (ii)). Choosing $\xi = 0.2$ and a $\varkappa$-value of 25, we obtain for α-particles a result which in fig. 3.5 is compared with the corresponding curve for $(d\sigma_K/d\Omega)_{\text{str.}\,l.}$

(iii) *Total cross sections*

The total cross section for emission of a K-electron with definite energy can be obtained from (3.28) by an integration over the eccentricity. Using one of LOMMEL's integral formulae (ref. 17, Chapter 5), one obtains after an elementary but rather tedious integration

$$\left.\begin{aligned} I &= \int_1^\infty d\varepsilon \cdot \varepsilon \,|\, I_\varepsilon|^2 \\ &= 4\, e^{-\pi\xi}\left(\frac{d^3}{\xi^2}\right)^2 \left\{A\,(K_{i\xi}(\xi))^2 + B\,\xi\, K_{i\xi}(\xi)\, K'_{i\xi}(\xi) + C\,(K'_{i\xi}(\xi))^2\right\}. \end{aligned}\right\} \quad (3.37)$$

A, B, and C are polynomials whose number of terms depends on the number included in (3.28).

The convergence of the expressions for A, B, and C depends, as seen from (3.28), on the parameters $d\alpha$ and ξ, which in their turn may be expressed in terms of $\varkappa$ (cf. eqs. (2.2) and (2.3)). For sufficiently large $\varkappa\,(\varkappa \gtrsim 30$ for protons) a rather good approximation may be obtained if one neglects terms in (3.28) of higher order than $n = 2$. For the coefficients A, B, and C one then finds

$$\left.\begin{aligned} A &= -\frac{4}{9}\frac{d\alpha}{\xi^2} + \frac{8}{5}\left(\frac{d\alpha}{\xi^2}\right)^2 \\ B &= \frac{1}{9}\frac{d\alpha}{\xi^2} - \frac{8}{5}\left(\frac{d\alpha}{\xi^2}\right)^2 \\ C &= \frac{1}{18} - \frac{4}{9}\frac{d\alpha}{\xi^2} + \frac{8}{5}\left(\frac{d\alpha}{\xi^2}\right)^2 \\ &\left(\frac{d\alpha}{\xi_0^2} = 64\, Z_1^3 \frac{M_1}{m}\frac{1}{\varkappa^4}\right). \end{aligned}\right\} \quad (3.38)$$

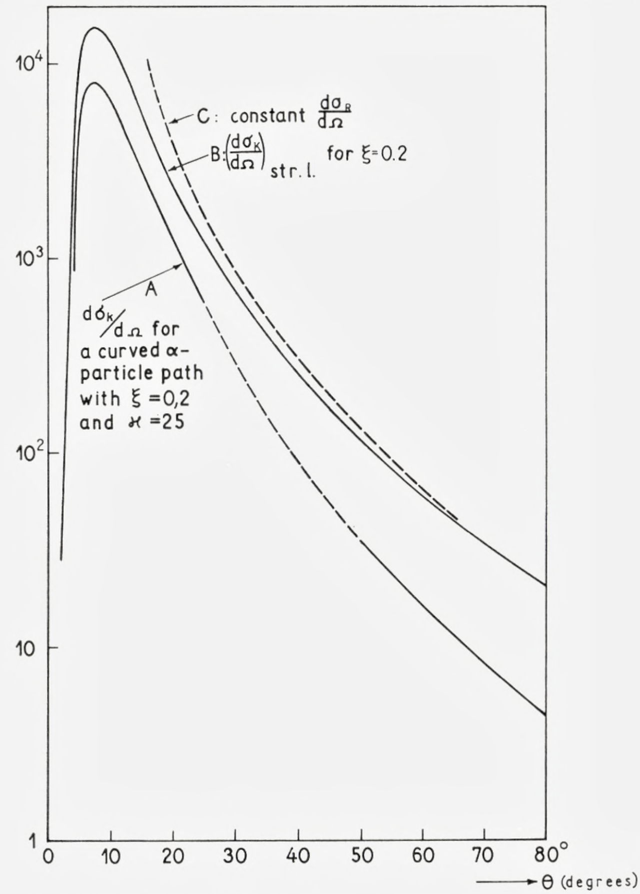

Fig. 3.5. The angular distribution, $\frac{d\sigma_K}{d\Omega}$, of α-particles after K-ionization (curve A) compared with the corresponding curve for straight-line orbits, $\left(\frac{d\sigma_K}{d\Omega}\right)_{str.\,l.}$ (curve B). The ordinate is in arbitrary units.

The angles for the straight-line curve are determined from the relation $\varepsilon^2 = 1 + \frac{p^2}{d^2}$ between the eccentricity $\varepsilon = \frac{1}{\sin\frac{\theta}{2}}$ and the impact parameter p. Thus, $pq_0 = \xi \operatorname{cotg}\frac{\theta}{2}$.

The dotted curve C is proportional to the Rutherford-scattering cross section $\frac{d\sigma_R}{d\Omega} = \frac{\varepsilon^4}{4}d^2$ and has been normalized so as to approach $\left(\frac{d\sigma_K}{d\Omega}\right)_{str.\,l.}$ for small p.

The curve denoted $d\sigma_K/d\Omega$ includes Coulomb-deflection effects (cf. the text). Consequently, the ratio between the curves A and B in the region of small angles is given by the factor $e^{-\pi\xi}$.

The dotted part of curve A represents the region in which the approximation formulae for the Hankel functions break down.

For smaller values of $\varkappa$, higher terms in (3.28) may have a significant effect. However, for $\varkappa \leq 30$ one may utilize the fact that the third term in eq. (3.37) (the one including C) is greatly dominating. For A and B the approximation (3.38) is then sufficient, but for C one must take into account terms in (3.28) in which $n > 2$. The general expression for C is given by

$$\left.\begin{aligned} C &= \frac{1}{18} - \frac{4}{9}\frac{d\alpha}{\xi^2} + \frac{1}{\xi^2}\sum_{m=0}^{\infty} a_m \left(\frac{d^2\alpha^2}{\xi^2}\right)^{m+1} \\ \text{with}\quad a_m &= \frac{(-1)^m}{2(m+5)} \sum_{i+j=m} 2(i+1)\,2(j+1) \\ &\times \Phi(-1-2i, 2; -2)\,\Phi(-1-2j, 2; -2). \end{aligned}\right\} \qquad (3.39)$$

Thus,

$$a_0 = \frac{8}{5}, \quad a_1 = -\frac{152}{9}, \quad a_2 = \frac{8}{5}\frac{4061}{63}, \quad \ldots. \qquad (3.39, \text{a})$$

It should be noted that the term $\frac{8}{5}\left(\frac{d\alpha}{\xi^2}\right)^2$ in C (eqs. (3.38) and (3.39)) corresponds to the dominating term obtained from the straight-line calculations (cf. eq. (3.13)), provided we use the approximate expressions (3.32) for the Bessel functions in (3.37).

The general expression for the cross section for ejection of K-electrons is given by

$$\frac{d\sigma_K}{dE_f} = \frac{2\pi}{\hbar^2} d^2 Z_1^2 e^4 |N_i|^2 |N_f^{0,k}|^2 \frac{1}{v_1^2} I, \qquad (3.40)$$

which can also be written in the form

$$\frac{d\sigma_K}{dE_f} = e^{-\pi\xi} (d\sigma_K/dE_f)_{\text{str.}\,l.} (1 - f(\varkappa, \xi)), \qquad (3.41)$$

where $(d\sigma_K/dE_f)_{\text{str.}\,l.}$ is the dominating term in the cross section for straight-line paths given by eq. (3.13). The correction factor $f(\varkappa, \xi)$ can then be found from (3.38) and (3.39).

As the coefficients k_n in (3.28) are calculated under the condition $k \ll \alpha$, the most consistent procedure is to use $f(\varkappa, \xi_0)$ when calculations are made on the basis of (3.41).

However, in the cases considered, the difference between $f(\varkappa, \xi_0)$ and $f(\varkappa, \xi)$ is of no importance. In the domain of large $\varkappa$-values the main correction to the cross section arises from the factor $e^{-\pi\xi}$, in which one should insert the value of ξ appropriate to the electron energy considered.

c. Symmetrization of the cross sections

The above semi-classical treatment of the K-ionization process depends on the condition $\varkappa \gg 4 Z_1$ and in addition requires $\Delta E \ll E_1$. If the value of $\Delta E/E_1$ is not very small compared with unity, one may obtain a significant improvement of the semi-classical expressions by choosing symmetrized values for the parameters d and ξ which enter in these expressions.

The problem is analogous to the one considered in the case of Coulomb excitation of nuclei, and the symmetrizing procedure may be justified in the same way as for that process, cf. ref. 21, sec. II, B 6.

The symmetrized parameters d and ξ are given by

$$d^S = \frac{Z_1 Z_2 e^2}{M_1 v_1 v_2} \tag{3.42}$$

$$\xi^S = \frac{Z_1 Z_2 e^2}{\hbar}\left(\frac{1}{v_2} - \frac{1}{v_1}\right) \tag{3.43}$$

or

$$d^S = d\left(1 - \frac{\Delta E}{E_1}\right)^{-\frac{1}{2}} \tag{3.44}$$

$$\xi^S = \xi \frac{2 E_1}{\Delta E}\left(\left(1 - \frac{\Delta E}{E_1}\right)^{-\frac{1}{2}} - 1\right). \tag{3.45}$$

Here, v_2 is the velocity of the projectile after the impact. We also define ξ_0^S and d_0^S by putting $\Delta E = E_B$ in the symmetrized equations.

d. The effects of screening and finite nuclear size

The screening of the Coulomb field of the nucleus by the atomic electrons may interfere in two different manners.

a) The incoming particle is moving in a screened Coulomb field rather than an unscreened one. The orbit described in (3.17) is therefore not quite correct. On the other hand, we are only concerned with those energies of the incoming particles for which $d \ll {}^1/_\alpha$. This means that the motion in the region of considerable screening is already nearly unperturbed by the field of the nucleus. The screening effect is thus negligible.

b) The electron—in the bound as well as in the free state—is moving in the screened Coulomb field. This case is treated in the following ways:

1) The electron gets additional energy from the repulsion by the other electrons. Although this energy is relatively small as compared with the K binding energy, it is of some significance owing to the great dependence of the cross section on ξ. However, we may take this effect into account by using the experimental ionization energies in the expression for $\Delta E = E_B + E_f$ rather than the theoretical, unscreened ones.

2) The change of the wave functions by the screening potential falls into two parts:

α) The so-called internal screening effect is taken into account by the use of the screened nuclear charge $Z_2^{\mathrm{eff}} \simeq Z_2 - 0.3$ rather than Z_2 in the expressions for $d\sigma_K/dE_f$. This is obviously a small correction.

β) The effect of the outer part of the screening is a rather smooth change of the potential, appreciable only for distances larger than $\frac{a_0}{2\,Z_2^{1/3}}$ (see Chapter 2 of ref. 22). Clearly, such a change is rather negligible for the initial states, where the wave functions extend only to distances of about $\frac{a_0}{Z_2}$.

For the final-state wave functions we may again argue that in the inner region, which determines the transition matrix element, the wave function is approximately equal to that for a free Coulomb field, except for the normalization factor. However, to the extent to which the penetration through the screened part of the field can be treated in the WKB approximation, the normalization in the inner region is determined directly from that chosen in the asymptotic region and does not depend on the potential in the intermediate region. Thus, the use of pure Coulomb wave functions for the continuous states seems to be rather well justified. From such an argument, one expects the normalization factor to be affected by a factor of the order of $\theta^{\frac{1}{4}}$, where θ is the ratio of the observed to the unscreened binding energy. However, since this correction is rather small compared with that arising from the change in ξ, it is neglected here.

Finally, we consider the effect of the finite nuclear size. This effect influences the electronic S wave functions in the neighbourhood of the nucleus. However, the effect on the matrix elements for ionization is very small since the characteristic distances in the radial integrals are of the order of the larger of the two quantities $\frac{1}{q_0}$ and d. Under the conditions here considered, the characteristic distance is many times larger than the nuclear radius, and therefore the change in the electronic wave functions caused by the finite nuclear size is small. Moreover, this change vanishes in the non-relativistic approximation.

e. Discussion and comparison with experimental cross sections

The present treatment of the ionization process has one feature in common with those of HENNEBERG(7) and of JAMNIK and ZUPANČIČ(8). In all three treatments the cross sections are obtained as series developments in the quantity α/q_0. Accordingly, the evaluated formulae can only be applied to experiments where the inequality (1.3) is fulfilled, i.e. where the energy of the incident particle is so small that α/q_0 is less than unity. The other approximations involved in the three methods are such, however, that they may be said to have somewhat different regions of application.

The relativistic effects in the electron wave functions, which are important in the heavier elements (see below), are dealt with in the work of JAMNIK and ZUPANČIČ only.

The advantage of Henneberg's calculations is that he succeeds in transforming the expressions for the cross section so as to give a rather fast convergence up to $\alpha/q_0 \simeq 1$.

The present method is evidently most favourably applied to the region of small energies, where the Coulomb deflection is of importance.

For bombarding energies so great that α is close to q_0, one thus expects Henneberg's formula to represent the best approximation, but with decreasing energy the Coulomb deflections rather soon become significant (for $\varkappa \gtrsim 12\, Z_1$). In the transition region where these effects begin to play a part and where α/q_0 is still not very small, none of the available treatments are very reliable, since as yet no estimate has been made of the deflection effects for the higher multipole transitions.

The relativistic effects have so far been considered only for straight-line orbits (8), for which it is found that correction terms of the relative order of $(Z_2\zeta)^2 \frac{q_0}{\alpha}$ arise in the monopole matrix element $\left(\zeta = \frac{e^2}{c\hbar}\right.$ is the fine-structure $\left.\text{constant}\right)$. An extension of this treatment to the case of curved orbits leads to integrals which are difficult to evaluate, but it seems reasonable to expect a similar correction. Thus, a rough approximation to the relativistic straight-line cross section may be obtained by evaluation of the expression (11) of Jamnik and Zupančič[(8)] for the monopole excitations to lowest order in α/q_0*; one finds that in this case their integral I is proportional to

$$\left.\begin{aligned} &\left(\frac{\alpha}{q_0}\right)^{2(\gamma+1)}\left(1+\delta(1-\gamma)\frac{q_0}{\alpha}\right), \\ \text{where}\quad &\gamma=\sqrt{1-(\zeta Z_2)^2} \\ &\delta=\frac{2(3+2\gamma)}{5+4\gamma}\frac{\pi}{4} \end{aligned}\right\} \tag{3.46}$$

($\gamma = 1$ corresponds to the nonrelativistic case).

By multiplying the cross section deduced from (3.46) by the appropriate curvature factors found by the non-relativistic methods (cf. (3.41)) one expects to obtain an approximate value for the cross section also in the case of heavier target elements.

In figs. 3.6, 3.7, 3.8, and 3.9 the calculated cross sections are compared with the experimental data. From (3.41) we obtain the differential cross section, from which the total cross section for K-ionization is found by graphical integration, allowance being made for the fact that there are two electrons in the K-shell. Moreover, the formula (3.41) is modified so as to take the screening into account in accordance with the prescriptions given in sec. 3, *d*.

For the lighter elements, the theoretical values agree rather well with the experiments and are seen to represent a considerable improvement on those for straight-line orbits. The agreement appears to extend to $\varkappa$-values as low as about 12, for which the α/q_0 corrections are rather large and for which the accuracy of the present theory is therefore questionable.

For the heavier elements (Mo and Ag) the experimental values appear to be significantly in excess of the theoretical estimates, but it seems likely that the deviation is to be attributed mainly to relativistic corrections, which are expected to enlarge the cross sections for these elements appreciably. A simple estimate of these corrections, obtained in the manner described

* In eqs. (14) of ref. 8, which must be used for this purpose, there is a misprint. In the equation for q_m the numerator in the coefficient of the second confluent hypergeometric function should be $4m+2$ instead of $4m$.

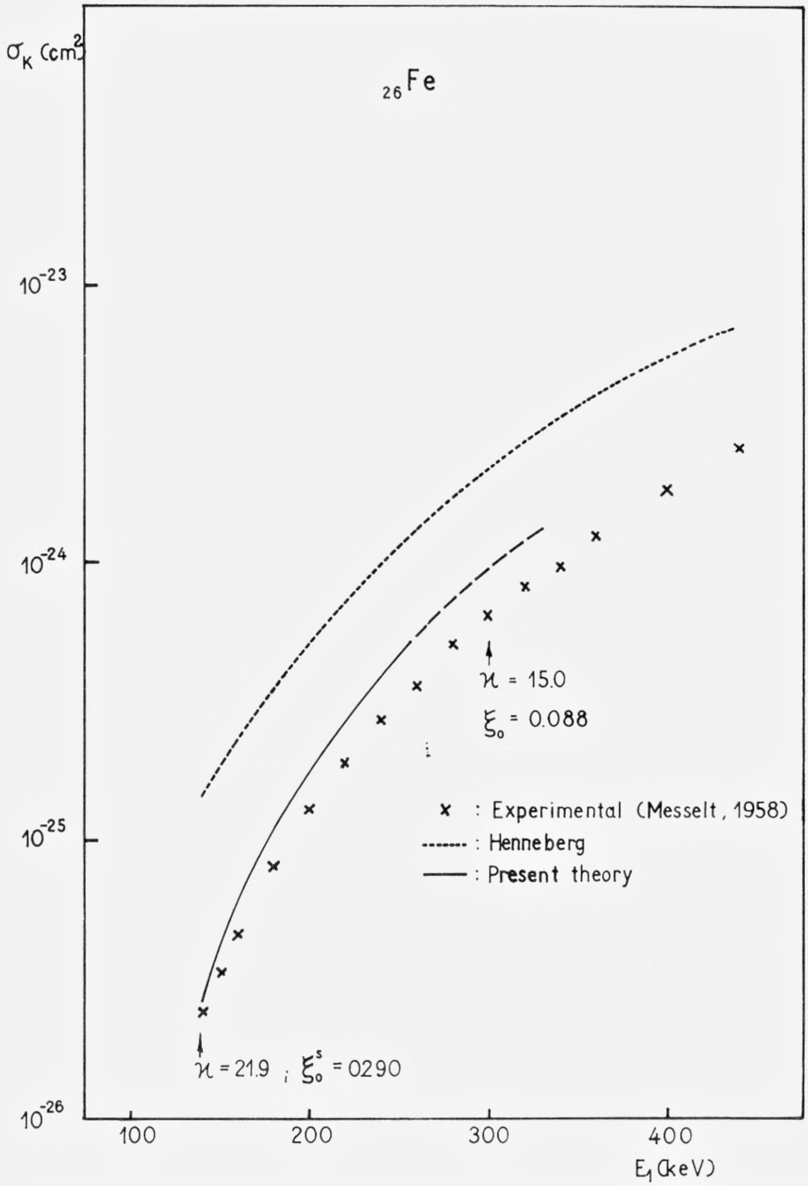

Fig. 3.6. K-ionization cross section for an iron target as a function of the proton energy. In this and the following calculations, five terms in the series development (3.39) have been taken into account. The dotting of the theoretical curve indicates the energy region in which the convergence of the series becomes slow and in which higher multipoles in the interaction may begin to contribute significantly.

For comparison, the values obtained from Henneberg's expression (as evaluated by Messelt[(4)]) are shown.

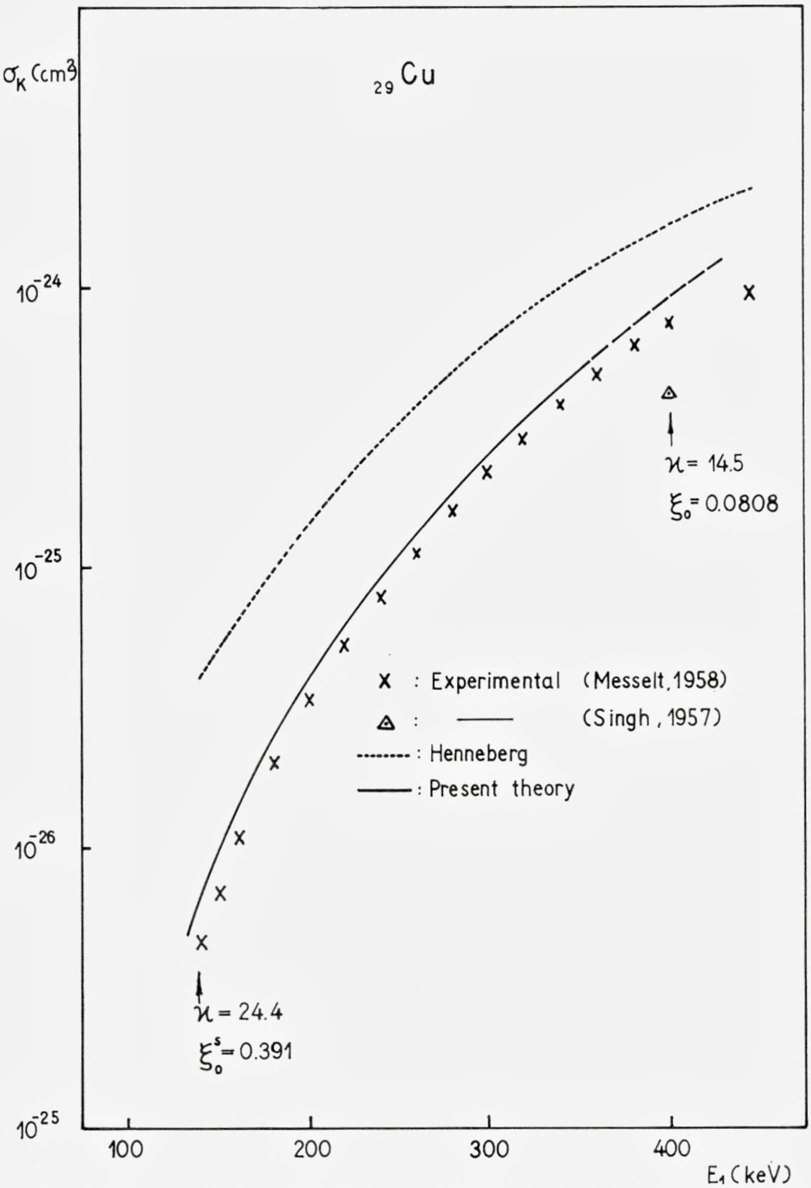

Fig. 3.7. *K*-ionization cross section for a copper target as a function of the proton energy. For further details see the text of fig. 3.6.

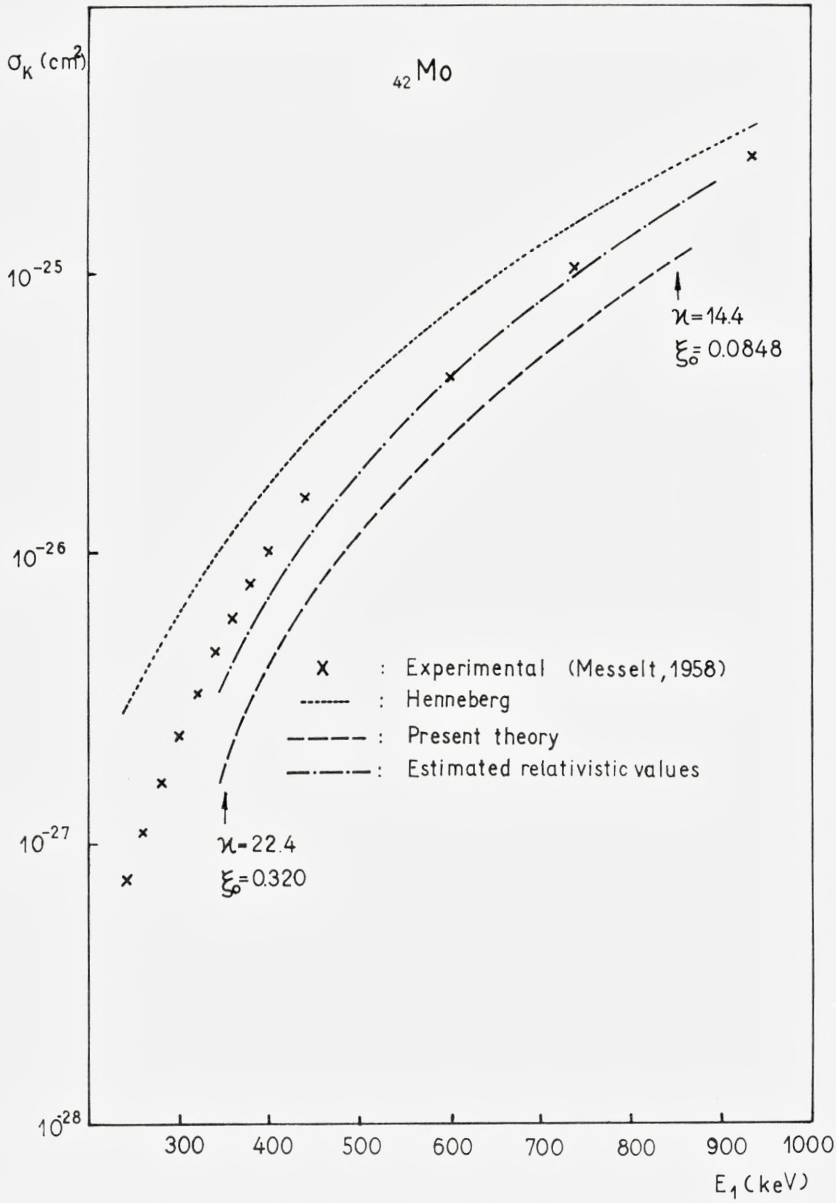

Fig. 3.8. σ_K for a molybdenum target as a function of the proton energy E_1. The non-relativistic theory is incapable of explaining the observed data. The dot-and-dash curve shows the approximate relativistic values obtained on multiplication of the dominating terms in Jamnik and Zupančič's formula(8) by the curvature factors found by the non-relativistic methods.

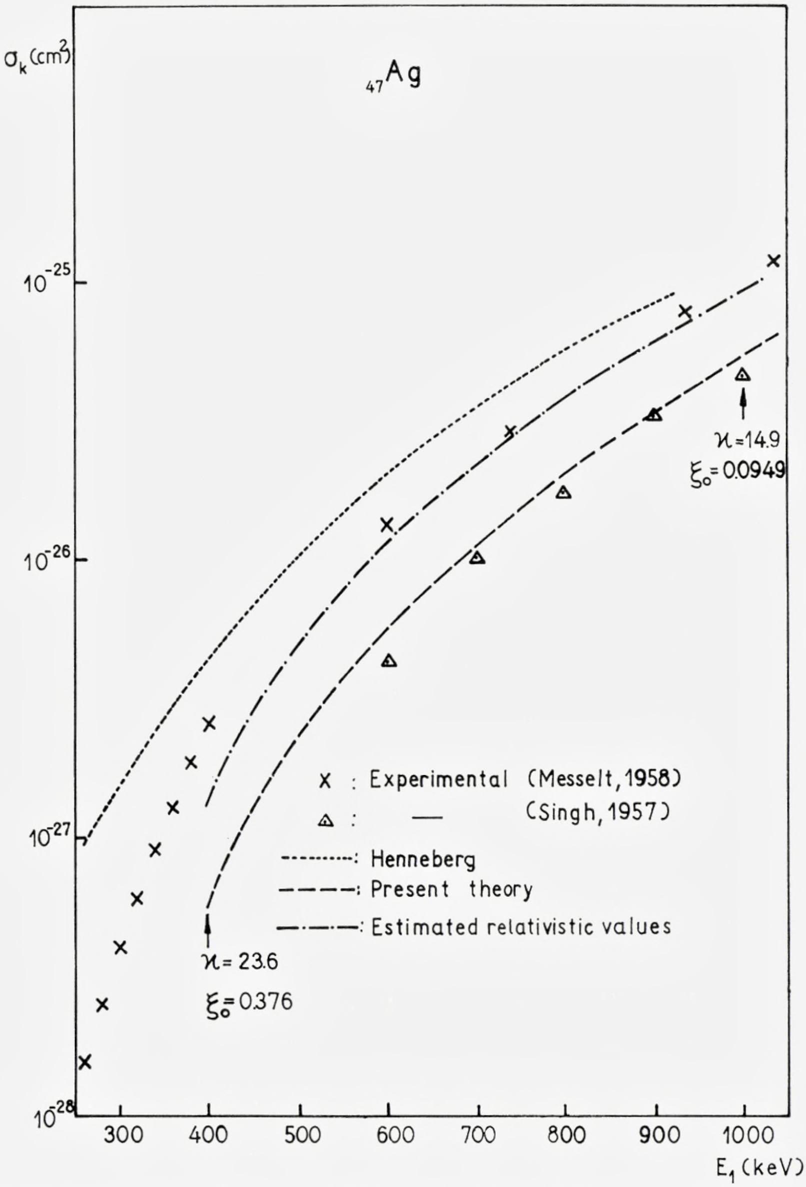

Fig. 3.9. σ_K for a silver target as a function of the proton energy. The relativistic effects are here more pronounced than for molybdenum.

above, is seen in the figures; it appears to improve the agreement with experiments considerably.

In consequence of the domination of the monopole terms, the angular distribution of the ejected electrons should be approximately isotropic.

For higher bombarding energies $\left(\frac{\alpha}{q_0} > 1\right)$ the angular distribution of the ejected electrons should in principle be evaluated by the methods of MASSEY and MOHR (cf. ref. 23)*.

4. Pair Production by Slow Protons

The cross section for pair production by protons impinging on tantalum was recently investigated by STEPHENS and STAUB[11, 12]. Their proton energy was $E_1 = 1.5$ MeV. The cross section was found to be less than $2 \cdot 10^{-32}$ cm^2 and thus smaller by a factor of a hundred or more than the value predicted by Born-approximation calculations as made by HEITLER and NORDHEIM[13].

One observes that the $\varkappa$ and ξ_0 values corresponding to this process are about 19 and 3 respectively. The use of methods analogous to the one applied to the K-ionization should therefore be justified.

In the present energy region we may carry through the calculations by taking into account only the electrostatic interactions between the particles (see ref. 13).

Considerations analogous to those in 3, b, (i) lead to the conclusion that only contributions from S-states play a part in the calculation of cross sections. This is due to the smallness of the parameter k/q_0, where k is now any of the electron momenta. One has for sufficiently small values of E_1

$$k/q_0 \leq \frac{\sqrt{4\, E_1 \dfrac{m}{M_1}(\Delta E - 2\, mc^2)}}{\Delta E} < \sqrt{\frac{4\, m}{M_1}\left(1 - \frac{2\, mc^2}{E_1}\right)} \ll 1. \qquad (4.1)$$

The cross section for pair production is then given by a formula completely analogous to eq. (3.16). Following simple hole-theory arguments,

* Note the misprints in this reference.

one inserts for the final and initial states the Coulomb wave functions for an electron and a hole in the continuum. By using integral representations of these functions[15] one gets

$$\left.\begin{aligned}\frac{d\sigma}{d(E^+E^-)} &= \frac{2\pi}{\hbar^2} d^2 e^4 \,|\, N_+ \,|^2 \,|\, N_- \,|^2 \int_1^\infty \varepsilon\, d\varepsilon \\ &\times \left| \int_{-\infty}^{+\infty} dt e^{i\omega t} \left\{ \frac{1}{\Gamma(1-i\eta_-)\,\Gamma(1+i\eta_-)\,\Gamma(1-i\eta_+)\,\Gamma(1+i\eta_+)} \right.\right. \\ &\times \left.\left. \int_0^1 du \left(\frac{u}{1-u}\right)^{i\eta_-} \int_0^1 dv \left(\frac{v}{1-v}\right)^{i\eta_+} \left[\int_0^R \frac{dr}{R} r^2 e^{-rb} + \int_R^\infty dr\, r\, e^{-rb} \right] \right\} \right|^2, \end{aligned}\right\} \quad (4.2)$$

where

$$\omega = \frac{\Delta E}{\hbar}$$

and

$$\left.\begin{aligned} b &= -ik_- + 2\,ik_- u \\ &\quad -ik_+ + 2\,ik_+ v. \end{aligned}\right\} \quad (4.3)$$

Following the procedure given in 3, b, (i), we obtain a formula identical with (3.23). This formula is valid on conditions similar to (2.9) and (2.10). As, in the cases of interest, ξ is of the order of magnitude one or larger, only small values of ε will contribute to the cross section. In the case considered here

$$\left.\begin{aligned} |\, b \,|\, d &\simeq \frac{kZ_1 Z_2 e^2}{2 E_1} = \frac{kZ_1 Z_2 e^2 \Delta E}{2 \Delta E \quad E_1} \\ &< \frac{k Z_1 Z_2 e^2 \Delta E}{2 \cdot 2\, mc^2 \; E_1} = \frac{1}{4} \zeta\, Z_1\, Z_2\, \beta_{el} \frac{\Delta E}{E_1} \ll 1 \\ &\left(\zeta \simeq \frac{1}{137},\; \beta_{el} = v/c\right). \end{aligned}\right\} \quad (4.4)$$

Because of this inequality only the first term of k_0' in the equation corresponding to (3.26, a) will be of importance. The u and v integrations are then trivial. (In the case of the general term b^{2n}, an F_2-function will enter.) The ε integration is now easily carried out, giving

$$\frac{d\sigma}{d(E_+ E_-)} = \frac{2\pi}{\hbar^2} \frac{d^2 e^4}{v_1^2} \,|\, N_+ \,|^2 \,|\, N_- \,|^2 \frac{2\, e^{-\pi\xi}}{9} \frac{d^6}{\xi^4} \,|\, K_{i\xi}'(\xi) \,|^2. \quad (4.5)$$

The expression (4.5) as a function of ξ shows that the important contributing electron energies are confined to values much smaller than the K binding energy of the target. Thus the inequality

$$|\eta_{\pm}| > 1 \tag{4.6}$$

is well fulfilled.

An approximate formula for $K'_{i\xi}(\xi)$ can be found from ref. 17, sec. 8.42. Then

$$\frac{d\sigma}{d(E^+E^-)} = C_1 \frac{Z_2^{10}}{E_1^9} S \frac{e^{-2\pi\xi}}{\xi^{16/3}} \tag{4.7}$$

Here

$$C_1 = \left(\frac{2}{3}\right)^4 \pi \left(\frac{\pi\, 6^{\frac{2}{3}}}{\Gamma\left(\frac{1}{3}\right)}\right)^2 \left(\frac{e^2}{2\,a_0}\right)^7 \frac{M_1}{m} a_0^2$$

and

$$S = \frac{1}{\left(1 - e^{-2\pi\frac{\alpha}{k_-}}\right)\left(e^{2\pi\frac{\alpha}{k_+}} - 1\right)} \tag{4.8}$$

(a_0 is the Bohr radius).

In order to obtain the total σ we must perform the integrations over E^+ and E^-. Because of the inequality (4.6) we have

$$\sigma = C_1 \frac{Z_2^{10}}{E_1^9} \int_0^{E^+_{\max}} dE^+ e^{-2\pi\frac{\alpha}{k_+}} \int_0^{E^-_{\max}} dE^- f(E^+, E^-) \tag{4.9}$$

with

$$f = \frac{e^{-2\pi\mu(2mc^2 + E^+ + E^-)}}{(\mu\,(2\,mc^2 + E^+ + E^-))^{16/3}}$$

$$\mu = \frac{Z_2 \cdot \zeta}{2\,E_1\,\beta} \tag{4.10}$$

$$\left(\beta = \frac{v_1}{c}\right).$$

Expanding the function f around $E^+ + E^- = 0$ and introducing the notation

$$\gamma_1 = 2\,\mu\, mc^2 = Z_2 \cdot \zeta \frac{mc^2}{\beta E_1}, \tag{4.11}$$

we obtain

with

$$\left.\begin{aligned} f &\simeq \frac{e^{-2\pi\gamma_1}}{\gamma_1^{16/3}}\left(1-\delta_1\left(E^+ + E^-\right)\right) \\ \delta_1 &= \frac{2\mu}{\gamma_1}\left(\pi\gamma_1+\frac{8}{3}\right). \end{aligned}\right\} \quad (4.12)$$

Consistently with (4.12) we introduce the following values for the maximum electron energies:

$$\left.\begin{aligned} E_{max}^- &= \frac{1-\delta_1 E^+}{\delta_1} \\ E_{max}^+ &= \frac{1}{\delta_1}. \end{aligned}\right\} \quad (4.13)$$

Although the expansion in $E^+ + E^-$ may not always be very accurate, the errors involved are not serious for our present purpose of obtaining an estimate of the order of magnitude of the cross section.

The double integration can now easily be carried out, leading to

$$\left.\begin{aligned} \sigma &= 4\pi^2 \frac{e^2}{2a_0} C_1 \frac{Z_2^{12}}{E_1^9} \frac{e^{-2\pi\gamma_1}}{\delta_1 \gamma_1^{16/3}} \\ &\times \left\{ I_1 - \delta_1 W I_2 + \left(\frac{\delta_1 W}{2}\right)^2 I_3 \right\} \end{aligned}\right\} \quad (4.14)$$

with

$$\left.\begin{aligned} I_{i\,(=1,2,3)} &= \int_t^\infty \frac{e^{-x}}{x^{2i+1}}\,dx;\ t = \frac{2\pi\alpha\hbar}{\sqrt{2mE_{max}^+}} \\ W &= 8\pi^2 Z_2^2 \frac{e^2}{2a_0}. \end{aligned}\right\} \quad (4.14,\ a)$$

A numerical evaluation by means of this formula gives $\sigma \simeq 10^{-48}$ cm^2 $\simeq$ $10^{-13}\,\sigma_{Born}$. This result is indeed consistent with the experimental results of Stephens and Staub. The direct curvature effects, $e^{-2\pi\xi}$, give rise to a factor of about 10^{-10} in the cross section. In addition comes the factor $e^{-2\pi\eta_+}$ resulting from the use of Coulomb wave functions for the positrons. Because of the inequality (4.6) this factor, together with the possible errors introduced through the evaluation of the integrals in (4.9), accounts well for the remaining divergence from the earlier calculations. Hence, the conclusion is that, in the low-energy region, the Coulomb repulsion very greatly reduces the cross sections for pair production by heavy, charged particles.

Acknowledgements

We want to express our deep gratitude to Professor NIELS BOHR for excellent working conditions at the Institute for Theoretical Physics in Copenhagen.

We are also very much indebted to Professor AAGE BOHR and Dr. BEN R. MOTTELSON for numerous discussions during all stages of this work. To A. WINTHER, K. ALDER and Č. ZUPANČIČ we are grateful for several valuable suggestions. Further we wish to thank various members of the Institute and NORDITA for their interest in this investigation.

We are greatly indebted to NORDITA for the research fellowships granted us by that institute. One of us (J. M. H.) further wants to thank the Royal Norwegian Council for Scientific and Industrial Research for a grant during the first part of his stay in Copenhagen.

NORDITA – Nordisk Institut for Teoretisk Atomfysik
Copenhagen, Denmark

Appendix I

The Equivalence Between First-order, Time-dependent Perturbation Theory and the Born Approximation at High Energies

1. Let the physical situation be as in fig. 3.2. It is then easily shown (cf. eqs. (3.1), (3.2) and (3.4)) that

$$\left.\begin{aligned}\int_{-\infty}^{\infty} \frac{e^{i\omega t}}{|\underline{r} - \underline{R}(t)|}\,dt &= \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{x^2 + (p-y)^2 + (v_1 t - z)^2}}\,dt \\ &= \frac{2}{v_1} e^{i\frac{\omega}{v_1}z} K_0\left(\frac{\omega}{v_1}\varrho\right)\end{aligned}\right\} \quad \text{(A I, 1)}$$

(see ref. 17, p. 172).

Introducing the energy and mass of the projectile, we find

$$\left.\begin{aligned}\frac{d\sigma}{dE_f} = 4\pi Z_1^2 \frac{M_1}{E_1}\frac{e^4}{\hbar^2} &\int d\tau\, \psi_f^*(\underline{r})\,\psi_i(\underline{r}) \int d\tau'\,\psi_f(\underline{r}')\,\psi_i^*(\underline{r}') \\ &\times e^{i\frac{\omega}{v_1}(z-z')} \int_0^{\infty} p\,dp\, K_0\left(\frac{\omega}{v_1}\varrho\right) K_0\left(\frac{\omega}{v_1}\varrho'\right).\end{aligned}\right\} \quad \text{(A I, 2)}$$

In Appendix II, a it is shown that

$$\int_0^{\infty} pdp\, K_0(q_0\varrho)\, K_0(q_0\varrho') = \frac{r_1 K_1(q_0 r_1)}{2\, q_0}, \qquad \text{(A I, 3)}$$

where

$$r_1^2 = (x-x')^2 + (y-y')^2.$$

The cross section may thus be written as

$$\frac{d\sigma}{dE_f} = 2\pi Z_1^2 \frac{M_1}{E_1}\frac{e^4}{\hbar^2}\frac{1}{q_0}\int d\tau\, \psi_f^* \psi_i \int d\tau'\, \psi_f \psi_i^*\, e^{iq_0(z-z')}\, r_1 K_1(q_0 r_1). \qquad \text{(A I, 4)}$$

2. Within the range of validity of the first Born approximation the above cross section is given by

$$\left.\begin{aligned} \frac{d\sigma}{dE_f} &= \frac{1}{4\pi^2} Z_1^2 M_1^2 \frac{e^4}{\hbar^4}\frac{k_f}{k_i}\int d\Omega \\ &\times \left| \int\!\!\int \exp\{i(k_f \underline{n}_1 - k_i \underline{n}_0)\underline{R}_c\}\, \psi_i(\underline{r})\, \psi_f^*(\underline{r})\, d\tau_c\, d\tau \frac{1}{|\underline{R}_c - \underline{r}|}\right|^2 \end{aligned}\right\} \qquad \text{(A I, 5)}$$

(see ref. 24, Chapters 11 and 12); $k_i \cdot \hbar \cdot \underline{n}_0$ and $k_f \cdot \hbar \cdot \underline{n}_1$ are the initial and final momentum vectors of the colliding particle. $\underline{R}_c$ is its position vector and $d\tau_c$ the volume element in the bombarding-particle space.

By a theorem given by Bethe[(6)] this may be written as

$$\left.\begin{aligned} \frac{d\sigma}{dE_f} &= 4 Z_1^2 M_1^2 \frac{e^4}{\hbar^4}\frac{k_f}{k_i}\int d\tau\, \psi_i \psi_f^* \int d\tau'\, \psi_i^* \psi_f \\ &\times \int d\varphi\, d\theta_e \sin\theta_e \frac{\exp\{i(k_f \underline{n}_1 - k_i \underline{n}_0)(\underline{r}' - \underline{r})\}}{|k_f \underline{n}_1 - k_i \underline{n}_0|^4}. \end{aligned}\right\} \qquad \text{(A I, 6)}$$

We choose the axis of the polar coordinate system in the direction of the incoming particle.

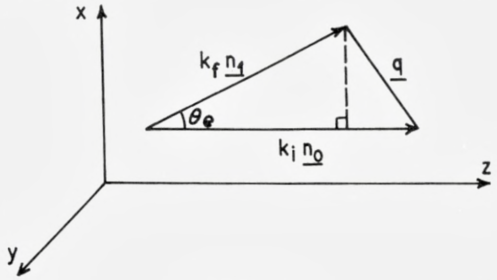

Fig. A I, 1.

Then

$$\left.\begin{aligned} |k_f n_1 - k_i \underline{n}_0|^2 &= k_f^2 + k_i^2 - 2\,k_i k_f \cos\theta_e \\ &= q_0^2 + 2\,k_i k_f (1-\cos\theta_e) \\ q_0 &= k_i - k_f. \end{aligned}\right\} \quad \text{(A I, 7)}$$

We define

$$\left.\begin{aligned} \underline{R}_1 &= \underline{r} - \underline{r}' \\ \underline{R}_1 &= (x-x',\; y-y',\; z-z'). \end{aligned}\right\} \quad \text{(A I, 8)}$$

Consequently,

$$\left.\begin{aligned} (k_f \underline{n}_1 - k_i \underline{n}_0)(-\underline{R}_1) = -(x-x')\,k_f \sin\theta_e \sin\varphi \\ -(y-y')\,k_f \sin\theta_e \cos\varphi - (z-z')\,k_f(\cos\theta_e - 1) + (z-z')\,q_0, \end{aligned}\right\} \quad \text{(A I, 9)}$$

and hence

$$\left.\begin{aligned} I &= \int d\varphi \sin\theta_e\, d\theta_e \frac{\exp\{i(k_f \underline{n}_1 - k_i \underline{n}_0)(\underline{r}' - \underline{r})\}}{|k_f \underline{n}_1 - k_i \underline{n}_0|^4} \\ &= e^{iq_0(z-z')} \int d\varphi \sin\theta_e\, d\theta_e \\ &\times \frac{\exp\{i[-k_f \sin\theta_e((x-x')\sin\varphi + (y-y')\cos\varphi) - k_f(z-z')(\cos\theta_e - 1)]\}}{(q_0^2 + 2\,k_i k_f(1-\cos\theta_e))^2}. \end{aligned}\right\} \quad \text{(A I, 10)}$$

From simple geometrical considerations this may be written as

$$\left.\begin{aligned} I &= \frac{e^{iq_0(z-z')}}{q_0^4} \int d\varphi_1 \sin\theta_e\, d\theta_e \frac{\exp\{i[-k_f r_1 \cos\varphi_1 \sin\theta_e - k_f(z-z')(\cos\theta_e - 1)]\}}{\left(1 + \frac{2\,k_i k_f}{q_0^2}(1-\cos\theta_e)\right)^2} \\ r_1^2 &= (x-x')^2 + (y-y')^2. \end{aligned}\right\} \quad \text{(A I, 11)}$$

As

$$\int_0^{2\pi} d\varphi_1 \exp\left\{-ik_f r_1 \sin\theta_e \cos\varphi_1\right\} = 2\pi J_0(k_f r_1 \sin\theta_e), \quad \text{(A I, 12)}$$

we have

$$I = 2\pi \frac{e^{iq_0(z-z')}}{q_0^4} \int_0^{\pi} \sin\theta_e\, d\theta_e \frac{J_0(k_f r_1 \sin\theta_e) \exp\{-ik_f(z-z')(\cos\theta_e - 1)\}}{\left(1 + \frac{2\,k_i k_f}{q_0^2}(1-\cos\theta_e)\right)^2}. \quad \text{(A I, 13)}$$

The incoming particle is supposed to suffer little momentum change in the collision:

$$q_0^2 \ll k_i k_f. \quad \text{(A I, 14)}$$

Putting in the denominator

$$1 - \cos\theta_e \approx \frac{\theta_e^2}{2}$$

and in the numerator

$$\cos\theta_e - 1 \approx 0,$$

we deduce the approximate relation

$$I \approx 2\pi \frac{e^{iq_0(z-z')}}{q_0^4} \int_0^{\pi} \theta_e d\theta_e \frac{J_0(k_f r_1 \theta_e)}{\left(1 + \frac{k_i k_f}{q_0^2}\theta_e^2\right)^2}. \qquad \text{(A I, 15)}$$

Using an integral formula given by Watson (ref. 17, p. 425), we find the following expression

$$I \approx \frac{2\pi e^{iq_0(z-z')}}{q_0^4} \frac{q_0^2}{k_i k_f} \int_0^{\infty} \frac{y dy J_0(q_0 r_1 y)}{(1+y^2)^2} = \frac{\pi e^{iq_0(z-z')}}{q_0 k_i k_f} r_1 K_1(q_0 r_1). \qquad \text{(A I, 16)}$$

Together with (A I, 6) this gives

$$\frac{d\sigma}{dE_f} = 4\pi Z_1^2 M_1^2 \frac{e^4}{\hbar^4} \frac{k_f}{k_i} \int d\tau\, \psi_i \psi_f^* \int d\tau' \psi_i^* \psi_f \frac{e^{iq_0(z-z')}}{q_0 k_i k_f} r_1 K_1(q_0 r_1). \qquad \text{(A I, 17)}$$

Introducing the kinetic energy of the bombarding particle, we finally get

$$\frac{d\sigma}{dE_f} = 2\pi Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \frac{1}{q_0} \int d\tau\, \psi_i \psi_f^* \int d\tau'\, \psi_i^* \psi_f e^{iq_0(z-z')} r_1 K_1(q_0 r_1), \qquad \text{(A I, 18)}$$

which is identical with the expression (A I, 4).

A proof similar to this one was given by Frame as early as 1931 (14). However, he did not calculate the probability of ionization as a function of the impact parameter.

Appendix II

Mathematical Details of the Calculations

a. An integral formula involving two modified Bessel functions of the third kind and of zeroth order

The integral in eq. (A I, 3) can be written

$$I_1 = \int_0^\infty p\,dp\, K_0(q_0\varrho)\, K_0(q_0\varrho') = \frac{1}{2\pi}\int d\underline{p}\, K_0(q_0 p)\, K_0(q_0|\underline{r}_1 - \underline{p}|). \qquad \text{(A II, 1)}$$

The last integration is performed in the (p, φ) – plane, where φ is the angle $(\underline{p}, \underline{r}_1)$.

Using the relation

$$2\pi K_0(q_0 r_1)\, I_0(q_0 p) = \int_{-\pi}^{\pi} K_0(q_0|\underline{r}_1 - \underline{p}|)\, d\varphi, \; r_1 > p \qquad \text{(A II, 2)}$$

and the corresponding one for $r_1 < p$ (see H.T.F. 2, Chapter 7), we get

$$I_1 = K_0(q_0 r_1)\int_0^{r_1} p\,dp\, I_0(q_0 p)\, K_0(q_0 p) + I_0(q_0 r_1)\int_{r_1}^{\infty} p\,dp\, K_0^2(q_0 p) = A + B. \qquad \text{(A II, 3)}$$

It is easily shown by application of well-known integral formulae that

$$\left.\begin{aligned} A &= K_0(q_0 r_1)\frac{r_1^2}{2}\left(K_0(q_0 r_1)\, I_0(q_0 r_1) + K_1(q_0 r_1)\, I_1(q_0 r_1)\right) \\ B &= I_0(q_0 r_1)\frac{r_1^2}{2}\left(K_1^2(q_0 r_1) - K_0^2(q_0 r_1)\right) \end{aligned}\right\} \qquad \text{(A II, 4)}$$

or

$$\left.\begin{aligned} A + B &= \frac{r_1^2}{2} K_1(q_0 r_1)\left(I_0 K_1 + K_0 I_1\right) \\ I_1 &= \frac{r_1}{2\, q_0} K_1(q_0 r_1). \end{aligned}\right\} \qquad \text{(A II, 5)}$$

b. Evaluation of the straight-line matrix element

(i) *General procedure*

When the non-relativistic Coulomb eigenfunctions are put into eq. (3.3), the φ-part of the integration is easily carried out:

$$\left.\begin{aligned}&\int_{-\pi}^{\pi} d\varphi\, e^{-im\varphi} K_0\left(q_0\left(r^2\sin^2\theta+p^2-2\,pr\sin\theta\cos\varphi\right)^{1/2}\right)\\&\qquad=2\pi\begin{cases}K_m(q_0\, r\sin\theta)\, I_m(q_0\, p), & r\sin\theta > p\\ K_m(q_0\, p)\, I_m(q_0\, r\sin\theta), & r\sin\theta < p\end{cases}\\&\qquad=2\pi\int_0^{\infty} dt\,\frac{t}{t^2+q_0^2}\, J_m(pt)\, J_m(rt\sin\theta)\end{aligned}\right\}\quad \text{(A II, 6)}$$

(see H.T.F. 7.14, 2, eqs. (77) and (57)).

Then

$$\left.\begin{aligned}&\mathrm{M}_p(l,m)=2\pi\, N_i\, N_f^{l,k}(-1)^m\left[\frac{2\,l+1}{4\pi}\,\frac{(l-m)!}{(l+m!)}\right]^{1/2}\frac{1}{2\sqrt{\pi}}\\&\quad\times\int_0^{\infty}dt\,\frac{t}{t^2+q_0^2}\, J_m(pt)\int r^2\, dr\sin\theta\, d\theta\, e^{-\alpha r}\, e^{iq_0 r\cos\theta}\\&\qquad\times P_l^m(\cos\theta)\, R_l\left(\frac{r}{\lambda}\right) J_m(rt\sin\theta)\end{aligned}\right\}\quad\text{(A II, 7)}$$

with

$$\lambda = i/k = i\eta a,\quad a=\frac{a_0}{Z_2}.$$

The θ-part of the integral is given by

$$I_\theta=\int_0^{\pi} d\theta\sin\theta\, e^{iq_0 r\cos\theta}\, P_l^m(\cos\theta)\, J_m(rt\sin\theta).\qquad\text{(A II, 8)}$$

Introducing the Gegenbauer polynomials, we obtain

$$\left.\begin{aligned}I_\theta&=\frac{(-1)^m(2\,m)!}{2^m\, m!}\int_0^{\pi}d\theta(\sin\theta)^{m+1}\, e^{iq_0 r\cos\theta}\, C_{l-m}^{m+\frac{1}{2}}(\cos\theta)\, J_m(rt\sin\theta)\\&=\frac{(-1)^m(2\,m)!}{2^m\, m!}\, i^{l-m}\sqrt{2\pi}\,(rs)^{-\frac{1}{2}}\left(\frac{t}{s}\right)^m C_{l-m}^{m+\frac{1}{2}}\left(\frac{q_0}{s}\right) J_{l+\frac{1}{2}}(sr)\end{aligned}\right\}\quad\text{(A II, 9)}$$

(cf. ref. 17, p. 379, eq. (1)).

Here

$$s^2=t^2+q_0^2.$$

From this we have

$$\left.\begin{aligned} \mathrm{M}_p(l,m) = \sqrt{\pi}\, N_i N_f^{l,k} \frac{(2m)!}{2^m\, m!}\left[\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}\right]^{1/2} i^{l-m} \\ \times \int_0^\infty dt\, t^{m+1} J_m(pt)\, s^{-m-\frac{5}{2}}\, C_{l-m}^{m+\frac{1}{2}}\left(\frac{q_0}{s}\right) \\ \times \int_0^\infty r^2\, dr\, r^{-\frac{1}{2}} e^{-\alpha r} J_{l+\frac{1}{2}}(sr)\, R_l(r/\lambda). \end{aligned}\right\} \text{(A II, 10)}$$

Expressing the ordinary Bessel function $J_{l+\frac{1}{2}}(s\,r)$ in terms of a Whittaker function, we obtain the following radial integral:

$$I_r = \frac{2^{-2l-\frac{5}{2}}\, i^{-l-1}\, \lambda}{\Gamma\left(l+\frac{3}{2}\right)}\, s^{-\frac{1}{2}} \int_0^\infty dr\, e^{-\alpha r} M_{0,l+\frac{1}{2}}(2\,i\,sr)\, M_{-i\eta,\,l+\frac{1}{2}}(-2\,ikr). \qquad \text{(A II, 11)}$$

This integral can be evaluated by means of a formula given by ERDÉLYI[(25)]:

$$\left.\begin{aligned} \int_0^\infty dr\, e^{-\alpha r} M_{0,\,l+\frac{1}{2}}(2\,isr)\, M_{-i\eta,\,l+\frac{1}{2}}(-2\,ikr) \\ = (2\,is)^{l+1}(-2\,ik)^{l+1}(\alpha + i(s-k))^{-(2l+3)}\, \Gamma(2l+3) \\ \times F_2\left\{2l+3,\, l+1,\, l+1+i\eta,\, 2l+2,\, 2l+2;\, \frac{2\,is}{\alpha+i(s-k)}, \frac{-2\,ik}{\alpha+i(s-k)}\right\}. \end{aligned}\right\} \text{(A II, 12)}$$

Eq. (3.5) is now easily derived.

(ii) *Simplification of some hypergeometric functions*

1. Using relations given by APPELL and KAMPÉ DE FÉRIET[(26)], we find

$$\left.\begin{aligned} \alpha_1 F_2(\alpha_1+1, \beta, \beta', \alpha_1, \alpha_1; x, y) = (\alpha_1-\beta-\beta')\, F_2(\alpha_1, \beta, \beta', \alpha_1, \alpha_1; x, y) \\ +\beta F_2(\alpha_1, \beta+1, \beta', \alpha_1, \alpha_1; x, y) + \beta' F_2(\alpha_1, \beta, \beta'+1, \alpha_1, \alpha_1; x, y) \\ = (1-x)^{-\beta}(1-y)^{-\beta'}\Big\{[(\alpha_1-\beta-\beta')-(\beta'-\beta)(1-x)^{-1}] \\ \times {}_2F_1\left(\beta, \beta', \alpha_1; \frac{xy}{(1-x)(1-y)}\right) \\ +\beta'[(1-x)^{-1}+(1-y)^{-1}]\, {}_2F_1\left(\beta, \beta'+1, \alpha_1; \frac{xy}{(1-x)(1-y)}\right)\Big\}. \end{aligned}\right\} \text{(A II, 13)}$$

Putting

$$\left.\begin{aligned} \alpha_1 &= 2\,l+2 \\ \beta &= l+1 \\ \beta' &= l+1+i\eta \\ x &= \frac{2\,is}{\alpha+i\,(s-k)} \\ y &= \frac{-2\,ik}{\alpha+i\,(s-k)}\,, \end{aligned}\right\} \qquad \text{(A II, 14)}$$

we deduce

$$\left.\begin{aligned} F_2 = \frac{1}{l+1}\left(\frac{\alpha-i\,(s+k)}{\alpha+i\,(s-k)}\right)^{-(l+1)} & \left(\frac{\alpha+i\,(s+k)}{\alpha+i\,(s-k)}\right)^{-(l+1+i\eta)} \\ \times \frac{1}{\alpha-i\,(s+k)}\Bigg\{(-i\eta)\,(\alpha-ik)\,{}_2F_1\left(l+1,l+1+i\eta,2\,l+2;\frac{4\,sk}{\alpha^2+(s+k)^2}\right) \\ +\,(l+1+i\eta)\,\alpha\,\frac{\alpha+i\,(s-k)}{\alpha+i\,(s+k)}\,{}_2F_1\left(l+1,l+2+i\eta,\,2\,l+2;\frac{4\,sk}{\alpha^2+(s+k)^2}\right)\Bigg\}. \end{aligned}\right\} \qquad \text{(A II, 15)}$$

2. According to H.T.F. 2.8, eq. (9) we have

$${}_2F_1(1,1+i\eta,2;-z) = \sum_{n=1}^{\infty}\binom{-i\eta}{n} z^n \frac{1}{z(-i\eta)} = ((1+z)^{-i\eta}-1)\frac{1}{(-z\,i\eta)}. \qquad \text{(A II, 16)}$$

Using the analogous formula for ${}_2F_1(1,2+i\eta,2;-z)$, we easily deduce eq. (3.8).

c. Some integrals leading to modified Bessel functions of the third kind and of complex order

In eq. (3.21) we treat the terms in the integral separately. In

$$I_1 = \int_{-\infty}^{\infty} dw\, e^{i\,\xi\varepsilon\,\sinh w + i\,\xi\,w} \qquad \text{(A II, 17)}$$

we make the transformation

$$w \longrightarrow -w',$$

which leads to

$$I_1 = 2\,e^{-\frac{\pi}{2}\xi}\,K_{i\,\xi}(\varepsilon\,\xi) \qquad \text{(A II, 18)}$$

(cf. ref. 17, p. 182, eq. (10)).

In

$$I_2 = \int_{-\infty}^{\infty} dw\, e^{i\xi\,(\varepsilon \sinh w + w) - bd\,\varepsilon \cosh w} \tag{A II, 19}$$

we put

$$e^w = y.$$

Then

$$I_2 = \int_0^{\infty} \frac{dy}{y^{1-i\xi}} e^{\frac{\varepsilon}{2}\left((-y\,(-i\xi + bd) - \frac{1}{y}\,(i\xi + bd)\right)}.$$

Making the substitution

$$y \frac{\varepsilon}{2} (bd - i\xi) = t,$$

we obtain

$$I_2 = \left(\frac{2}{\varepsilon}\frac{1}{bd - i\xi}\right)^{i\xi} \int_0^{\infty - i\infty} \frac{dt}{t^{1-i\xi}} e^{\left(-t - \frac{\varepsilon^2}{4t}\,(b^2 d^2 + \xi^2)\right)}.$$

Hence,

$$I_2 = \left(\frac{bd + i\xi}{bd - i\xi}\right)^{\frac{i\xi}{2}} K_{-i\xi}\left(\varepsilon\sqrt{b^2 d^2 + \xi^2}\right) \tag{A II, 20}$$

(cf. ref. 17, p. 183, eq. (15)).

The integrals

$$I_3 = \int_{-\infty}^{\infty} dw\, e^{i\xi\,(\varepsilon \sinh w + w) + w - bd\,\varepsilon \cosh w} \tag{A II, 21}$$

and

$$I_4 = \int_{-\infty}^{\infty} dw\, e^{i\xi\,(\varepsilon \sinh w + w) - w - bd\,\varepsilon \cosh w} \tag{A II, 22}$$

may be treated in exactly the same way as I_2.

Thus,

$$I_3 = 2\left(\frac{bd + i\xi}{bd - i\xi}\right)^{\frac{1 + i\xi}{2}} K_{-1-i\xi}\left(\varepsilon\sqrt{b^2 d^2 + \xi^2}\right) \tag{A II, 23}$$

$$I_4 = 2\left(\frac{bd + i\xi}{bd - i\xi}\right)^{\frac{-1 + i\xi}{2}} K_{1-i\xi}\left(\varepsilon\sqrt{b^2 d^2 + \xi^2}\right). \tag{A II, 24}$$

References

(1) H. W. Lewis, B. E. Simmons and E. Merzbacher, Phys. Rev. **91** (1953) 943.
(2) J. M. Hansteen and S. Messelt, Nucl. Phys. **2** (1956/57) 526.
(3) B. Singh, Phys. Rev. **107** (1957) 711.
(4) S. Messelt, Nucl. Phys. **5** (1958) 435.
(5) N. F. Mott, Proc. Cambr. Phil. Soc. **27** (1931) 553.
(6) H. Bethe, Annalen d. Phys. **5** (1930) 325.
(7) W. Henneberg, ZS. f. Phys. **86** (1933) 592.
(8) D. Jamnik and Č. Zupančič, Mat. Fys. Medd. Dan. Vid. Selsk. **31,** no. 2 (1957).
(9) E. Merzbacher and H. W. Lewis, Handbuch der Physik **34** (1958) 166.
(10) Niels Bohr, Mat. Fys. Medd. Dan. Vid. Selsk. **18,** no. 8 (1948).
(11) W. E. Stephens and H. H. Staub, Helv. Phys. Acta **30** (1957) 261.
(12) W. E. Stephens and H. H. Staub, Phys. Rev. **109** (1958) 1196.
(13) W. Heitler and L. Nordheim, Journ. de Phys. et le Rad. **5** (1934) 449.
(14) J. W. Frame, Proc. Cambr. Soc. **27** (1931) 511.
(15) K. Alder and A. Winther, Mat. Fys. Medd. Dan. Vid. Selsk. **29,** no. 18 (1955).
(16) A. Erdélyi et al., Higher Transcendental Functions (McGraw Hill, New York, 1953).
(17) G. N. Watson, Theory of Bessel Functions (The University Press, Cambridge, 1944).
(18) T. Huus, J. H. Bjerregaard and B. Elbek, Mat. Fys. Medd. Dan. Vid. Selsk. **30,** no. 17 (1956).
(19) K. A. Ter-Martirosyan, Žurnal eksper. i teor. fiz. **22** (1952) 284.
(20) N. W. McLachlan, Bessel Functions for Engineers, 2. ed. (The Clarendon Press, Oxford, 1955).
(21) K. Alder, A. Bohr, T. Huus, B. Mottelson, and A. Winther, Revs. Mod. Phys. **28** (1956) 432.
(22) P. Gombás, Die statistische Theorie des Atoms (Springer-Verlag Wien, 1949).
(23) H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. of London **A 140** (1930) 613.
(24) N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions, 2. ed. (Oxford University Press, 1949).
(25) A. Erdélyi, Math. ZS. **40** (1936) 693.
(26) P. Appell and J. Kampé de Fériet, Fonctions hypergéométriques et hypersphériques (Gauthiers-Villars, Paris, 1926).

Indleveret til selskabet den 6. januar 1959.
Færdig fra trykkeriet den 15. maj 1959.