# MATEMATISK-FYSISKE MEDDELELSER

UDGIVET AF

DET KGL. DANSKE VIDENSKABERNES SELSKAB

BIND 29



KØBENHAVN 1954–55 I KOMMISSION HOS EJNAR MUNKSGAARD



### INDHOLD

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## Det Kongelige Danske Videnskabernes Selskab

Matematisk-fysiske Meddelelser, bind 29, nr. 19

Dan. Mat. Fys. Medd. 29, no. 19 (1955)

## ON THE EXACT EVALUATION OF THE COULOMB EXCITATION

BY

KURT ALDER AND AAGE WINTHER



København 1955 i kommission hos Ejnar Munksgaard

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Printed in Denmark. Bianco Lunos Bogtrykkeri A-S. It is shown that the calculation of the total cross section for Coulomb excitation can be reduced to the calculation of radial matrix elements between eigenstates in the Coulomb potential. With the method developed in the preceding paper, one is able to give closed expressions, convenient series expansions, and recursion formulae for these matrix elements. The case of vanishing energy loss and the semi-classical limit are also discussed.

#### I. Introduction.

The exact evaluation of the Coulomb excitation cross section has hitherto only been performed in the dipole case<sup>1,2</sup>. The radial matrix elements for the higher multipoles are more complicated and have previously been treated only in the WBK approxmation<sup>3</sup>. With the method developed in the preceding paper<sup>4</sup>, one is able, however, to give closed expressions and suitable series developments of these matrix elements.

The closed expression given there contains a generalized hypergeometric function of two variables. It is one of the main points of this paper to give the analytical continuation of this function into the domain where it is of physical interest and from which the numerical evaluation can be performed. Once this is derived it will be easy to discuss the different limiting cases. We shall deal here especially with the limit of no energy loss and the classical limit. Furthermore, we shall give a number of recursion formulae which will considerably facilitate a numerical evaluation.

#### II. Reduction of the Coulomb Cross Section to Radial Matrix Elements.

The electromagnetic excitation of nuclear levels by means of impinging charged particles is a phenomenon analogous to the nuclear photoeffect, since specific nuclear properties enter only through matrix elements identical with those encountered in radiation theory. If one neglects the penetration of the projectile into the nucleus, one finds easily in the non-relativistic limit the following differential cross section for excitations by means of the electric field:

$$\frac{d\sigma}{d\Omega} = \frac{4 m_1^2 Z_1^2 e^2}{\hbar^4} \frac{v_j}{v_i} \sum_{\lambda \mu} \frac{B(E\lambda)}{(2\lambda+1)^3} \left| \langle \vec{k}_i \right| r^{-\lambda-1} Y_{\lambda \mu}(\vartheta, \varphi) \left| \vec{k}_j \right|^2.$$
(1)

 $m_1, Z_1$ , and v are the mass, the charge, and the velocity of the projectile, respectively. The indices i and f refer to the initial and final states.  $B(E\lambda)$  is the square of the nuclear  $2^{\lambda}$  pole electric transition matrix element in the notation of BOHR and MOTTELson<sup>5</sup>. The states  $|\vec{k}\rangle$  are eigenstates in the Coulomb field of the nucleus which, at distances far from the nucleus, behave as "plane waves" (distorted by the Coulomb field) with definite wave numbers k. These states may be decomposed in partial waves<sup>6</sup>:  $|\vec{k}\rangle = \sum_{l=0}^{\infty} 4\pi (-1)^m i^l e^{i\sigma_l} Y_{l-m}(\vec{k}) Y_{lm}(\vartheta, \varphi) kr F_l(kr),$  (2)

where  $\sigma_l = \arg \Gamma(l+1+i\eta)$  is the Coulomb phase and  $F_l(kr)$ the regular solution of the wave equation behaving as

$$\sin\left(kr - \frac{1}{2}l\pi - \eta \ln 2 kr + \sigma_l
ight) ext{ for } kr 
ightarrow 1.$$

Introducing this into (1) one may integrate over the angles, utilizing the formula\*

$$\int Y_{l_1 m_1} Y_{l_2 m_3} Y_{l_3 m_3} d\Omega = \sqrt{\frac{(2 l_1 + 1)(2 l_2 + 1)(2 l_3 + 1)}{4 \pi} \binom{l_1 l_2 l_3}{0 \ 0 \ 0} \binom{l_1 l_2 l_3}{m_1 m_2 m_3}}.$$
 (3)

By integrating over the direction of k one obtains the total cross section

$$\sigma_{el} = \frac{64 \pi^2 Z_1^2 e^2 m_1^2}{\hbar^4} \frac{v_l}{v_i} \sum_{\lambda} \frac{B(E\lambda)}{(2\lambda+1)^2} \times \sum_{l_i l_f} (2 l_i + 1) (2 l_f + 1) {\binom{l_i l_f \lambda}{000}}^2 |M_{l_i l_f}^{-\lambda-1}|^2$$
(4)

\* Here we use the Wigner notation for the vector addition coefficients. The relation between those and the Clebsch-Gordon coefficients of Condon and Shortley (E. U. CONDON and G. H. SHORTLEY, Theory of Atomic Spectra, Oxford 1936) is

$$\binom{l_1 \quad l_2 \quad l_3}{m_1 \, m_2 \, m_3} = \frac{(-1)^{l_1 - l_3 - m_3}}{\sqrt{2 \, l_3 + 1}} < l_1 \, m_1 \, l_2 \, m_2 \mid (l_1 \, l_2) \, l_3 - m_3 >.$$

with

$$M_{l_i l_f}^{-\lambda-1} = \frac{1}{k_i k_f} \int_0^\infty F_{l_i}(k_i r) r^{-\lambda-1} F_{l_f}^*(k_f r) dr.$$
 (5)

The selection rules for the angular momenta  $l_i$  and  $l_j$  are directly seen from equation (3):

 $|l_i - l_f| \leq \lambda \leq l_i + l_f$  and  $l_i + l_f + \lambda$  even.

The evaluation of the total cross section is thus reduced to the evaluation of the radial integrals  $M^{-\lambda-1}$ . The differential cross section and the angular distribution of subsequent  $\gamma$  quanta can also be expressed by these radial matrix elements. In a forthcoming review article<sup>7</sup>, formulae will be given for these cross sections together with a more complete discussion of electromagnetic excitations.

#### III. Evaluation of the Radial Matrix Elements.

According to the formula (22) of I, the radial matrix element is given by

$$M_{l_{i}l_{f}}^{-\lambda-1} = \frac{\left|\Gamma(l_{i}+1+i\eta_{i})\right|\left|\Gamma(l_{f}+1+i\eta_{f})\right|}{(2\,l_{i}+1)!\,(2\,l_{f}+1)!} \left(l_{i}+l_{f}-\lambda+1\right)!\,i^{l_{i}+l_{f}-\lambda+2}x^{l_{i}}y^{l_{f}}e^{-\frac{\pi}{2}(\eta_{i}+\eta_{f})}(k_{i}-k_{f})^{\lambda-2} F_{2}(l_{i}+l_{f}-\lambda+2,\,l_{i}+1-i\eta_{i},\,l_{f}+1+i\eta_{f},\,2\,l_{i}+2,\,2\,l_{f}+2,\,x,-y),\right|$$
(6)

where

$$x=rac{2\,\eta_{f}}{\xi} \quad ext{and} \quad y=rac{2\,\eta_{i}}{\xi};$$

further

$$\xi = \eta_j - \eta_i$$
 and  $\eta = \frac{Z_1 Z_2 e^2}{\hbar v}$ 

Since the series expansion of the  $F_2$  function only converges for x and y in the neighbourhood of zero, one has for the numerical evaluation to find the analytic continuation of this function in the neighbourhood of infinity.

The analytic continuation is in fact given by the Barnes integral representation<sup>8</sup>, and suitable asymptotic expansions may easily be derived from this. However, we shall here use only the analytic continuation for the special case  $l_i = l_f \pm \lambda$  and derive the other matrix elements by means of recursion formulae.

In these matrix elements, where the change of l is maximum (maximal matrix elements), the  $F_2$  function reduces to an  $F_1$  according to formula A5. This may again be expressed by an  $F_3$  function (A5) for which an analytic continuation in terms of  $F_2$  functions is known (A4). One thus obtains immediately, e.g.,

$$F_{2}(2 l + 2, l + \lambda + 1 - i\eta_{i}, l + 1 + i\eta_{f}, 2 l + 2\lambda + 2, 2 l + 2, x, -y) = (-1)^{l+1-i\eta_{f}}(2 l + 2\lambda + 1)! \left[ (-x)^{-2l-2} \frac{|\Gamma(\lambda + i\xi)|^{2}}{\Gamma(2\lambda) |\Gamma(l + \lambda + 1 + i\eta_{i})|^{2}} \right] F_{2}\left(-2\lambda + 1, l + 1 - i\eta_{f}, l + 1 + i\eta_{f}, -\lambda + 1 - i\xi, -\lambda + 1 + i\xi, \frac{1}{x}, \frac{1}{x}\right) + 2 Re\left\{ (-x)^{-2l-\lambda-2-i\xi} \frac{\Gamma(-\lambda - i\xi)}{\Gamma(l + 1 - i\eta_{f}) \Gamma(l + \lambda + 1 + i\eta_{i})} \right\}$$
(7)  
$$\times F_{2}\left(-\lambda + 1 + i\xi, l + \lambda + 1 - i\eta_{i}, l + 1 + i\eta_{f}, \lambda + 1 + i\xi, -\lambda + 1 + i\xi, \frac{1}{x}, \frac{1}{x}\right) \right\}.$$

#### With this formula one gets for the radial matrix element\*

$$M_{l+\lambda,l}^{-\lambda-1} = e^{\frac{\pi}{2}\xi} \left| \frac{\Gamma(l+1+i\eta_l)}{\Gamma(l+1+i\eta_l)} \left| \left(\frac{\eta_l}{\eta_l}\right)^l (2 k_l)^{\lambda-2} \times \left\{ \frac{|\Gamma(\lambda+i\xi)|^2}{(2 \lambda-1)!} \right\} \right|$$

$$F_2 \left(-2\lambda+1, l+1-i\eta_l, l+1+i\eta_l, -\lambda+1-i\xi, -\lambda+1+i\xi, \frac{\xi}{2 \eta_l}, \frac{\xi}{2 \eta_l}\right)$$

$$+ 2 Re \left[ \left(e^{i\pi}\frac{\xi}{2 \eta_l}\right)^{\lambda+i\xi} \frac{\Gamma(l+\lambda+1-i\eta_l) \Gamma(-\lambda-i\xi)}{\Gamma(l+1-i\eta_l)} \right]$$

$$\times F_2 \left(-\lambda+1+i\xi, l+\lambda+1-i\eta_l, l+1+i\eta_l, \lambda+1+i\xi, -\lambda+1+i\xi, \frac{\xi}{2 \eta_l}, \frac{\xi}{2 \eta_l}\right) \right]$$

$$(8)$$

\* Dr. L. C. BIEDENHARN has kindly communicated to us an independent derivation of expressions equivalent to formulae (8) and (9) which were obtained directly without explicit use of the properties of the hypergeometric functions. Similarly, for the other maximal matrix element, one obtains

$$\begin{split} M_{l,l+\lambda}^{-\lambda-1} &= e^{-\frac{\pi}{2}\xi} \left| \frac{\Gamma(l+1+i\eta_{l})}{\Gamma(l+\lambda+1+i\eta_{l})} \left| \left(\frac{\eta_{l}}{\eta_{l}}\right)^{l} (2 \ k_{l})^{\lambda-2} \times \left\{ \frac{\left| \Gamma(\lambda+i\xi) \right|^{2}}{(2 \ \lambda-1)!} \right. \right. \\ \left. F_{2} \left( -2 \ \lambda+1, l+1+i\eta_{l}, l+1-i\eta_{l}, -\lambda+1-i\xi, -\lambda+1+i\xi, \frac{-\xi}{2 \eta_{l}}, \frac{-\xi}{2 \eta_{l}} \right) \right. \\ &+ 2 \ Re \left[ \left( \frac{\xi}{2 \eta_{l}} \right)^{\lambda+i\xi} \frac{\Gamma(l+\lambda+1+i\eta_{l}) \ \Gamma(-\lambda-i\xi)}{\Gamma(l+1+i\eta_{l})} \right. \\ \left. \times F_{2} \left( -\lambda+1+i\xi, \ l+\lambda+1+i\eta_{l}, \ l+1-i\eta_{l}, \ \lambda+1+i\xi, \\ \left. -\lambda+1+i\xi, \frac{-\xi}{2 \eta_{l}}, \frac{-\xi}{2 \eta_{l}} \right) \right] \right\} \\ &= e^{-\pi\xi} \ M_{l+\lambda,l}^{-\lambda-1} \left( \eta_{l} \rightleftharpoons -\eta_{l} \right). \end{split}$$
(9)

In the first  $F_2$  function of these formulae, the first parameter,  $-2\lambda + 1$ , is a negative integer. Thus the functions are reduced to polynomials which for the lowest multipole orders are given explicitly by

$$F_{2}\left(-2\lambda+1, l+1-i\eta_{f}, l+1+i\eta_{f}, -\lambda+1-i\xi, -\lambda+1+i\xi, \frac{\xi}{2\eta_{f}}, \frac{\xi}{2\eta_{f}}\right)$$

$$= \begin{cases} 0 & \text{for } \lambda = 1 \\ \frac{1}{2(1+\xi^{2})} \cdot \frac{\eta_{i}(\eta_{i}+\eta_{f})}{\eta_{f}^{2}} & \text{for } \lambda = 2 \\ \frac{1}{2(1+\xi^{2})(4+\xi^{2})} \cdot \frac{\eta_{i}(\eta_{i}+\eta_{f})}{\eta_{f}^{4}} \left[5l(\eta_{i}+\eta_{f})\xi+4(3\eta_{f}^{2}-2\eta_{i}^{2})\right] & \text{for } \lambda = 3. \end{cases}$$
(10)

The formulae (8) and (9) are well suited for a numerical evaluation, since the series expansion of  $F_2$  converges for nearly all interesting values of the parameters. However, for  $l \gg \eta$  the convergence is rather slow.

#### **IV. Recursion Formulae.**

The non-maximal radial matrix elements can be derived from the maximal ones through recursion formulae. We shall first derive a recursion relation of this type, which we shall use for quadrupole matrix elements. Recursion relations connecting different multipoles can be used, e. g., for the calculation of the octupole matrix elements from the quadrupole ones.

For the numerical evaluation of the maximal matrix elements, it may also be advantageous to use recursion formulae connecting successive maximal matrix elements.

From the general formula I (17) one gets a recursion formula of the first type by demanding the condition

$$x_1(l_i - \lambda) + x_2 l_j + x_3(l_j + 1) + x_4(l_i + \lambda + 1) = 0 \quad (11)$$

besides the two conditions I (18, 19). In the quadrupole case, this leads to two recursion formulae, where one has to set  $l_i = l_f - 1$  and  $l_i = l_f + 1$ , respectively.

$$y_1 M_{l+1, l+1}^{-3} + y_2 M_{ll}^{-3} + y_3 M_{ll+2}^{-3} + y_4 M_{l-1, l+1}^{-3} = 0, \qquad (12)$$

$$y_{1}'M_{l+2l}^{-3} + y_{2}'M_{l+1l-1}^{-3} + y_{3}'M_{l+1l+1}^{-3} + y_{4}'M_{ll}^{-3} = 0, \qquad (13)$$

where

$$\begin{array}{l} y_{1} = k_{i}(l+2)(2l+3)|l+1+i\eta_{i}| \quad y_{1}' = -3k_{i}(l+1)(2l+1)|l+2+i\eta_{i}| \\ y_{2} = -k_{f}l(2l+1)|l+1+i\eta_{f}| \quad y_{2}' = 3k_{f}(l+1)(2l+3)|l+i\eta_{f}| \\ y_{3} = 3k_{f}(l+1)(2l+1)|l+2+i\eta_{f}| \quad y_{3}' = -k_{f}(l+2)(2l+3)|l+1+i\eta_{f}| \\ y_{4} = -3k_{i}(l+1)(2l+3)|l+i\eta_{i}| \quad y_{4}' = k_{i}l(2l+1)|l+1+i\eta_{i}|. \end{array}$$

By elimination of the matrix element  $M_{l+1, l+1}^{-3}$  from (12) and (13) one obtains a recursion formula of the desired type

$$z M_{ll}^{-3} = z_1 M_{ll+2}^{-3} + z_2 M_{l-1l+1}^{-3} + z_3 M_{l+2l}^{-3} + z_4 M_{l+1l-1}^{-3}$$
(15)

with

$$=rac{l(l+1)}{3}(\eta_l^2-\eta_i^2)$$

z

$$z_{1} = -\eta_{i}^{2} \left| l+1+i\eta_{f} \right| \left| l+2+i\eta_{f} \right| \quad z_{3} = \eta_{f}^{2} \left| l+1+i\eta_{i} \right| \left| l+2+i\eta_{i} \right| \\ z_{2} = \eta_{i}\eta_{f} \frac{2l+3}{2l+1} \left| l+i\eta_{i} \right| \left| l+1+i\eta_{f} \right| \quad z_{4} = -\eta_{i}\eta_{f} \frac{2l+3}{2l+1} \left| l+i\eta_{f} \right| \left| l+1+i\eta_{i} \right| .$$

$$(15)$$

By means of (15) the non-maximal quadrupole matrix elements are determined from the maximal ones already calculated in (8) and (9).

The recursion relation connecting matrix elements of different multipoles may also be derived from I (17). One relation involving octupole matrix elements is, e.g., obtained with the subsidiary condition  $x_1 = 0$ . This leads to

$$y'' M_{l\,l+1}^{-4} = y_1'' M_{l\,l}^{-3} + y_2'' M_{l\,l+2}^{-3} + y_3'' M_{l-1\,l+1}^{-3}, \tag{17}$$

where

$$y_{1}'' = 2 k_{f} | l + 1 + i \eta_{f} |$$

$$y'' = (l+2)(2 l+3) \quad y_{2}'' = k_{f} (2 l+1) | l + 2 + i \eta_{f} |$$

$$y_{3}'' = -k_{i} (2 l+3) | l + i \eta_{i} |.$$
(18)

In order to obtain recursion relations which involve only maximal matrix elements, we shall use the general properties of the  $F_1$ functions which occur in these matrix elements. The property which we shall utilize is the following:

$$F_{1}(\alpha + n_{1}, \beta + n_{2}, \beta' + n_{3}, \gamma + n_{4}, x, y) = \left[A(x, y) + B(x, y)\frac{\partial}{\partial x} + C(x, y)\frac{\partial}{\partial y}\right]F_{1}(\alpha, \beta, \beta', \gamma, x, y), \qquad (19)$$

where  $n_r$  are arbitrary positive or negative integers and A, B, and C rational functions in x and  $y^9$ .

A method of deriving recursion formulae is then to eliminate  $\frac{\partial}{\partial x}F_1$  and  $\frac{\partial}{\partial y}F_1$  between three such equations. The  $F_1$  function which occurs in the maximal matrix elements is, for  $l_i = l_i + \lambda$ ,

$$F_{1}(l + \lambda + 1 - i\eta_{i}, l + 1 + i\eta_{j}, l + 1 - i\eta_{f}, 2l + 2\lambda + 2, x, y) = F_{1}(l)$$
with
$$x = \frac{2\eta_{i}}{\eta_{f} + \eta_{i}} \quad y = \frac{2\eta_{f}}{\eta_{f} - \eta_{i}}.$$
(20)

One easily obtains

$$F_{1}(l+1) = \frac{(2l+2\lambda+2)(2l+2\lambda+3)}{|l+\lambda+1+i\eta_{l}|^{2}|l+1+i\eta_{f}|^{2}(x-y)} \left\{ (l+1-i\eta_{l})(x-1)\frac{\partial}{\partial x} - (l+1+i\eta_{l})(y-1)\frac{\partial}{\partial y} \right\} F_{1}(l).$$
(21)

Similar expressions for  $F_1(l-1)$  and  $F_1(l+2)$  can be derived. The elimination of the derivatives gives the desired recursion formula

$$w_1 M_{l+\lambda-3, l-3}^{-\lambda-1} + w_2 M_{l+\lambda-2, l-2}^{-\lambda-1} + w_3 M_{l+\lambda-1, l-1}^{-\lambda-1} + w_4 M_{l+\lambda, l}^{-\lambda-1} = 0$$
(22)  
with

$$\begin{split} w_{1} &= 2 \eta_{i} \eta_{f} \left| l - 2 + i \eta_{f} \right\| l - 1 + i \eta_{f} \left\| l + \lambda - 2 + i \eta_{i} \right| \\ w_{2} &= - \left| l - 1 + i \eta_{f} \right| [l^{2} (2 \eta_{i}^{2} + 4 \eta_{f}^{2}) + l [4 (\lambda - 2) (\eta_{i}^{2} + \eta_{f}^{2}) + \eta_{i}^{2} - \eta_{f}^{2}] \\ &+ (\lambda - 2) [(2 \lambda - 3) \eta_{i}^{2} - 3 \eta_{f}^{2}] + 6 \eta_{i}^{2} \eta_{f}^{2}] \\ w_{3} &= \frac{\eta_{f}}{\eta_{i}} \left| l + \lambda - 1 + i \eta_{i} \right| [l^{2} (4 \eta_{i}^{2} + 2 \eta_{f}^{2}) + l [4 (\lambda - 2) \eta_{i}^{2} + \eta_{i}^{2} - \eta_{f}^{2}] \\ &- 2 (\lambda - 2) \eta_{i}^{2} + 6 \eta_{i}^{2} \eta_{f}^{2}] \\ w_{4} &= -2 \eta_{f}^{2} \left| l + \lambda - 1 + i \eta_{i} \right\| l + \lambda + i \eta_{i} \| l + i \eta_{f} |. \end{split}$$

#### V. Limiting Cases.

We shall here study two limiting cases of the general formulae for the Coulomb matrix elements. The one is the case of vanishing energy loss, i. e.  $\eta_i - \eta_i = \xi = 0$ , where one easily can obtain a simple expression for an arbitrary Sommerfeld number. The second case is the classical limit where  $\eta_i, \eta_j \gg 1$ , while  $\eta_j - \eta_i$ is finite. This must lead to expressions identical with the usual classical integrals<sup>10, 11</sup>.

a) 
$$\xi = 0$$
.

For the maximal matrix elements, the second term of equations (8) and (9) is zero<sup>\*</sup> while the first  $F_2$  function is equal to one. One gets thus immediately the result

$$M_{l,\,l+\lambda}^{-\lambda-1} = M_{l+\lambda,\,l}^{-\lambda-1} = (2\ k)^{\lambda-2} \frac{[(\lambda-1)!]^2}{(2\ \lambda-1\,!)} \left| \frac{\Gamma(l+1+i\eta)}{\Gamma(l+\lambda+1+i\eta)} \right|.$$
(24)

The other matrix elements can be obtained by means of the recursion formulae. For the quadrupole case one may use equation  $(15)^{**}$ . However, this becomes singular for  $\xi = 0$ , and the limiting process  $\xi \to 0$  has to be performed with some care.

<sup>\*</sup> This is not true for  $\lambda = 1$ , the result (24) is, however, right also in this case.

<sup>\*\*</sup> The formula (25) has been found also by L. C. BIEDENHARN and C. M. CLASS<sup>12</sup> who have given a numerical evaluation of the total cross section and one of the coefficients for the angular distribution of the subsequent  $\gamma$ 's for the case  $\xi = 0$ .

$$M_{l,l}^{-3} = -\frac{\eta^{2}}{2(2l+1)l(l+1)} \lim_{\xi \to 0} \frac{1}{\xi} \left[ \left| \frac{\Gamma(l+1+i\eta_{l})}{\Gamma(l+1+i\eta_{l})} \right| \frac{\eta_{l}}{\eta_{l}^{2}} e^{\frac{\pi}{2}\xi} - \left| \frac{\Gamma(l+1+i\eta_{l})}{\Gamma(l+1+i\eta_{l})} \right| \frac{\eta_{l}}{\eta_{l}^{2}} \left( \frac{\eta_{l}}{\eta_{l}} \right)^{2l-2} e^{-\frac{\pi}{2}\xi} \right] = \frac{1}{2l(l+1)(2l+1)} \left\{ 2l+1 - \pi\eta + i\eta \left[ \psi(l+1-i\eta) - \psi(l+1+i\eta) \right] \right\}.$$
(25)

We have here used the expansion  $\Gamma(x+\delta) \cong \Gamma(x) [1+\delta \psi(x)]$ , where  $\psi(x)$  is the logarithmic derivative of the  $\Gamma$ -function.

For the octupole case one may use equation (17), and one gets directly

$$M_{l,l+1}^{-4} = \frac{k}{3l(l+1)(l+2)(2l+1)(2l+3)[l+1+i\eta]} \{3|l+1+i\eta|^2 \\ [2l+1-\pi\eta+i\eta(\psi(l+1-i\eta)-\psi(l+1+i\eta))] - l(l+1)(2l+1)\}.$$
(26)

The limiting case  $\eta = 0$ , i.e., the case where a plane wave Born approximation applies, is immediately obtained from (24) and (25).

For  $\eta \gg 1$  one obtains the classical limit for  $\xi = 0$ . The deflection angle  $\theta$  is there determined through  $tg \theta/2 = \eta/l$  (see below) and one gets, e.g., for the quadrupole case

$$M_{l,\,l+2}^{-3} = M_{l+2,\,l}^{-3} = \frac{1}{\eta^2} \frac{1}{6} \sin^2 \theta/2$$

$$M_{l,\,l}^{-3} = \frac{1}{\eta^2} \cdot \frac{1}{2} \operatorname{tg}^2 \theta/2 \left[ 1 - \frac{\pi - \theta}{2} \operatorname{tg} \theta/2 \right].$$
(27)

These matrix elements are just  $4/\eta^2$  times the classical integrals for  $\xi = 0$  given by Ter-Martirosyan (loc. cit.). The connection between the matrix elements and the classical integrals is obtained by the WBK approximation.

#### b) The classical limit.

In the classical limit  $\eta >> 1$ , the main contribution to the matrix element  $< \vec{k}_i | r^{-\lambda-1} Y_{\lambda\mu} | \vec{k}_i >$  of equation (1) will arise from a narrow region of l values around<sup>13</sup>

$$T = \frac{mv}{\hbar}p = \eta \operatorname{cotg} \theta/2,$$
 (28)

 $2\sin\theta/2$ 

where p is the classical impact parameter and  $\theta$  the angle between  $k_i$  and  $k_j$ .

For  $\eta \gg 1$  and  $\xi$  finite, the  $F_2$  functions of (8) and (9) approach the confluent hypergeometric functions of two variables  $\Psi_2$  according to equation (A3). One obtains thus, in view of equation (28),

$$M_{l+\lambda,l}^{-\lambda-1} = \frac{k^{\lambda-2}}{4\eta^{\lambda}} I_{\lambda,-\lambda}(\theta) = \frac{k^{\lambda-2}}{4\eta^{\lambda}} 2^{\lambda} \sin^{\lambda} \theta/2 \quad e^{-\xi(\cot\theta/2 + \theta/2 - \pi/2)} \cdot \left\{ \frac{|\Gamma(\lambda + i\xi)|^2}{(2\lambda - 1)!} \Psi_2(-2\lambda + 1, -\lambda + 1 - i\xi, -\lambda + 1 + i\xi, z, z^*) + 2Re[e^{-\pi\xi}\Gamma(-\lambda - i\xi)z^{\lambda+i\xi}\Psi_2(-\lambda + 1 + i\xi, \lambda + 1 + i\xi, -\lambda + 1 + i\xi, z, z^*)] \right\}$$

$$(29)$$
with
$$z = \frac{\xi}{(\cot\theta/2 - i)} = e^{-i\theta/2} \cdot \frac{\xi}{2}$$

The classical integrals  $I_{\lambda\mu}(\theta)$  are defined in ref. 10. Similarly, one obtains

2

$$\begin{split} M_{l\,l+\lambda}^{-\lambda-1} &= \frac{k^{\lambda-2}}{4\,\eta^{\lambda}} I_{\lambda\lambda}(\theta) \\ &= \frac{k^{\lambda-2}}{4\,\eta^{\lambda}} 2^{\lambda} \sin^{\lambda} \theta/2 \ e^{\xi\,(\cot\,\theta/2+\theta/2-\pi/2)} \\ &\times \left\{ \frac{|\Gamma(\lambda+i\xi)|^2}{(2\,\lambda-1)!} \Psi_2\,(-2\,\lambda+1,-\lambda+1-i\xi,-\lambda+1+i\xi,-z^*,-z) \right. \\ &+ 2\,Re\,[\Gamma(-\lambda-i\xi)\,(z^*)^{\lambda+i\xi}(-1)^{\lambda} \\ &\Psi_2\,(-\lambda+1+i\xi,\lambda+1+i\xi,-\lambda+1+i\xi,-z^*,-z)] \right\} \\ &= (-1)^{\lambda}\,e^{-\pi\xi}\frac{k^{\lambda-2}}{4\,\eta^{\lambda}} I_{\lambda-\lambda}(-\theta). \end{split}$$
(30)

The non-maximal matrix elements may be obtained by means of the recursion formulae.

The series expansion (A3) of the  $\Psi_2$  function converges for all values of the variables, and the formulae (29) and (30) are thus directly suited for a numerical evaluation.

Since the limiting formula (A3) also holds for any value of  $\eta$  in the limit  $l \gg 1$ , the formulae (29) and (30) constitute the limits of the general formula (6) for large values of  $l_i$  and  $l_i$ .

#### VI. Conclusions.

By means of the results obtained in this paper it is possible to calculate the exact matrix elements needed for the computation of the total and differential cross sections in Coulomb excitation. The main difficulty encountered in a numerical evaluation is the rather large number of angular momenta which contribute to the process. The main contribution will in fact arise from l values of the order  $l = \eta$ , but also much higher l values must be taken into account. A direct application of the formulae for the matrix elements is made difficult by the fact that the  $F_2$  functions converge rather slowly for  $l > \eta$ . However, this difficulty is overcome by the use of recursion formulae, whereby one may compute all matrix elements from the maximal matrix element, corresponding to l = 0.1, and 2. Furthermore, in the limit l >> 1, the matrix elements approach always the classical integrals  $k^{\lambda-2}/4 \eta^{\lambda} I_{\lambda\mu}(\theta,\xi)$ , with tg  $\theta/2 = \eta/l$ . Extensive tables of these integrals have recently been compiled\*.

#### VII. Numerical Results.\*\*

A numerical evaluation along the above mentioned lines has been carried out on the high speed electronic computer BESK in Stockholm. The first three maximal matrix elements were calculated with an accuracy of  $10^{-11}$ . A comparison between the directly evaluated matrix elements and those obtained by the recursion formulae proved that this accuracy was sufficient for the application of successive recursion from these three first matrix elements.

\* This tabulation, which was made by the authors, is not published, but parts of it are available on request.

\*\* This chapter has been added to the original manuscript on May 10th 1955. We are greatly indebted to Prof. G. BREIT for drawing our attention to an error of sign in the numerical calculation of ref. 11.





An extract of the results is shown in Figs. 1–3. The total cross section function  $f_{E2}(\eta, \xi)$  is connected with the total cross section for electric quadrupole excitation through

$$\sigma_{E2} = rac{m_1^2 v_f^2}{Z_2^2 e^2 \hbar^2} \, B(E2) \, f_{E2} \, (\eta_i, \xi).$$

With this definition one expects from the WBK approximation that the quantum mechanical corrections on f are small. Thus

$$f_{E2}(\eta_i, \xi) = rac{64 \ \pi^2}{25} \ \eta_i \eta_f \ b_i$$

$$b_{0} = \sum_{l} \left\{ \frac{3 l (l-1)}{2 (2 l-1)} \left( M_{l-2, l}^{-3} \right)^{2} + \frac{l (l+1) (2 l+1)}{(2 l-1) (2 l+3)} \left( M_{ll}^{-3} \right)^{2} + \frac{3 (l+1) (l+2)}{2 (2 l+3)} \left( M_{l+2, l}^{-3} \right)^{2} \right\}.$$

The classical limit of this function is

$$f_{E2}(\infty,\xi) = \int_0^{\pi} \sin\theta \ d\theta \ \frac{8 \pi^3}{125} \sum_{\mu} \left| Y_{2\mu}(\frac{\pi}{2},0) \right|^2 \left| I_{2\mu}(\theta,\xi) \right|^2 \sin^{-4}\theta/2.$$

This function was tabulated earlier (ref. 11) and is reproduced in Table 1. The results for the total cross section function is plotted in Fig. 1 as the ratio  $f_{E2}(\eta, \xi)/f_{E2}(\infty, \xi)$ . Within the accuracy of drawing the curves for different values of  $\xi \leq 2$  coincide for  $\eta > 1$ .

The angular distribution coefficients are given by

$$a_2 = b_2/b_0$$
 and  $a_4 = b_4/b_0$ 

with

$$\begin{split} &= \sum_{l} \left\{ \frac{3 \, l \, (l-1) \, (l-2)}{(2 \, l-1)^2} \left( M_{l-2,l}^{-3} \right)^2 - \frac{l \, (l+1) \, (2 \, l+1) \, (2 \, l-3) \, (2 \, l+5)}{(2 \, l-1)^2 \, (2 \, l+3)^2} \left( M_{l,l}^{-3} \right)^2 \right. \\ &+ \frac{3 \, (l+1) \, (l+2) \, (l+3)}{(2 \, l+3)^2} \left( M_{l+2,l}^{-3} \right)^2 \\ &- 6 \, \frac{(l-1) \, l \, (l+1)}{(2 \, l-1)^2} \, M_{l-2,l}^{-3} \, M_{l,l}^{-3} \, \cos \left(\sigma_l - \sigma_{l-2}\right) \\ &- 6 \, \frac{l \, (l+1) \, (l+2)}{(2 \, l+3)^2} \, M_{l+2,l}^{-3} \, M_{l,l}^{-3} \, \cos \left(\sigma_l - \sigma_{l+2}\right) \right\} . \\ &= - \sum_{l} \left\{ \frac{9 \, l \, (l(-1) \, (l-2) \, (l-3)}{(2 \, l-1)^2 \, (2 \, l+1)} \left( M_{l-2,l}^{-3} \right)^2 + \frac{9 \, (l-1) \, l \, (l+1) \, (l+2) \, (2 \, l+1)}{(2 \, l-1)^2 \, (2 \, l+3)^2} \left( M_{l,l}^{-3} \right)^2 \right. \\ &+ \frac{9 \, (l+1) \, (l+2) \, (l+3) \, (l+4)}{(2 \, l+1) \, (2 \, l+3)^2} \left( M_{l-2,l}^{-3} \, M_{l+2,l}^{-3} \, \cos \left(\sigma_l - \sigma_{l-2}\right) \right. \\ &- \frac{15 \, (l-2) \, (l-1) \, l \, (l+1) \, (l+2) \, (l+3)}{(2 \, l-1) \, (2 \, l+3)^2} \, M_{l+2,l}^{-3} \, m_{l,l}^{-3} \, \cos \left(\sigma_l - \sigma_{l-2}\right) \\ &- \frac{15 \, l \, (l+1) \, (l+2) \, (l+3) \, M_{l+2,l}^{-3} \, M_{l,l}^{-3} \, \cos \left(\sigma_l - \sigma_{l-2}\right) \\ &+ \frac{105 \, (l-1) \, l \, (l+1) \, (l+2) \, (l+3) \, M_{l+2,l}^{-3} \, M_{l+2,l}^{-3} \, \cos \left(\sigma_l - \sigma_{l+2}\right) \\ &+ \frac{105 \, (l-1) \, l \, (l+1) \, (l+2) \, (l+3) \, M_{l+2,l}^{-3} \, M_{l+2,l}^{-3} \, \cos \left(\sigma_{l+2} - \sigma_{l-2}\right) \right\}. \end{split}$$

The results for  $a_2$  and  $a_4$  are plotted in Figs. 2 and 3. The classical curves  $(\eta = \infty)$  calculated earlier<sup>11</sup> contain an error of sign. The curves for  $\eta_i = 0$  are discontinuous having the values

$$a_2 (\eta_i = 0, \xi) = egin{cases} rac{1}{2} & ext{for } \xi = 0 \ 2 & ext{for } \xi \pm 0 \ 2 & ext{for } \xi \pm 0 \ \end{array}$$
 $a_4 (\eta_i = 0, \xi) = egin{cases} rac{1}{16} & ext{for } \xi = 0 \ -rac{3}{2} & ext{for } \xi \pm 0 \ \end{array}$ 

Table 1.

ž	$f_{_{FP}}(\infty,\xi)\cdot 10^{+P}$	Р
0.0	0.8954	0
0.1	0.8638	0
0.2	0.7289	0
0.3	0.5608	0
0.4	0.4046	0
0.5	0.2781	0
0.6	0.1844	0
0.7	0.1189	0
0.8	0.7511	1
0.9	0.4663	1
1.0	0.2855	1
1.2	0.1035	1
1.4	0.3628	2
1.6	0.1238	2
1.8	0.4143	3
2.0	0.1363	3

The classical total cross section function for electric quadrupole excitation for  $\xi \leq 2$ .

#### Acknowledgement.

The authors wish to thank Professor NIELS BOHR and Drs. AAGE BOHR and BEN MOTTELSON for their continued interest in this work.

Dan. Mat. Fys. Medd, 29, no.19.

#### Appendix:

## Some Properties of Generalized Hypergeometric Functions of Two Variables.

Besides the function  $F_2$  defined in I, we shall here use the following Appell functions:

$$F_{1}(\alpha, \beta, \beta' \gamma, x, y) = \sum_{m, n=0}^{\infty} \frac{\alpha_{m+n} \beta_{m} \beta'_{n}}{\gamma_{m+n} m! n!} x^{m} y^{n}$$

$$F_{3}(\alpha, \alpha', \beta, \beta', \gamma, x, y) = \sum_{m, n=0}^{\infty} \frac{\alpha_{m} \alpha'_{n} \beta_{m} \beta'_{n}}{\gamma_{m+n} m! n!} x^{m} y^{n},$$
(A1)

where

$$a_n = \frac{\Gamma(a+n)}{\Gamma(a)} = a (a+1) \dots (a+n-1).$$

These double series have the following domain of absolute convergence:

$$|x| < 1 |y| < 1.$$
 (A2)

From these hypergeometric functions one can obtain related functions by a limiting process, (the so-called confluence), e. g.,

$$\lim_{\substack{\varepsilon_{1} \to 0 \\ \varepsilon_{2} \to 0}} F_{2}\left(\alpha, \frac{1}{\varepsilon_{1}}, \frac{1}{\varepsilon_{2}}, \gamma, \gamma', \varepsilon_{1} x, \varepsilon_{2} y\right) = \Psi_{2}\left(\alpha, \gamma, \gamma', x, y\right), \quad (A3)$$

where

$$\Psi_{2}(\alpha,\gamma,\gamma',xy) = \sum_{m,n=0}^{\infty} \frac{\alpha_{m+n}}{\gamma_{m}\gamma_{n}m!n!} x^{m} y^{n}$$

is a series expansion which converges for all values of x and y. There exist a large number of functional relations connecting different hypergeometric functions. Some of these represent an analytic continuation, such as

$$\begin{split} F_{3}(\alpha, \alpha, '\beta, \beta', \gamma, x, y) &= f(\alpha, \alpha', \beta, \beta') (-x)^{-\alpha} (-y)^{-\alpha'} \\ F_{2}\left(\alpha + \alpha' + 1 - \gamma, \alpha, \alpha', \alpha + 1 - \beta, \alpha' + 1 - \beta', \frac{1}{x}, \frac{1}{y}\right) \\ &+ f(\alpha, \beta', \beta, \alpha') (-x)^{-\alpha} (-y)^{-\beta'} \\ F_{2}\left(\alpha + \beta' + 1 - \gamma, \alpha, \beta', \alpha + 1 - \beta, \beta' + 1 - \alpha', \frac{1}{x}, \frac{1}{y}\right) \\ &+ f(\beta, \alpha', \alpha, \beta') (-x)^{-\beta} (-y)^{-\alpha'} \\ F_{2}\left(\beta + \alpha' + 1 - \gamma, \beta, \alpha', \beta + 1 - \alpha, \alpha' + 1 - \beta', \frac{1}{x}, \frac{1}{y}\right) \\ &+ f(\beta, \beta', \alpha, \alpha') (-x)^{-\beta} (-y)^{-\beta'} \\ F_{2}\left(\beta + \beta' + 1 - \gamma, \beta, \beta', \beta + 1 - \alpha, \beta' + 1 - \alpha', \frac{1}{x}, \frac{1}{y}\right) \\ &\text{where} \end{split}$$

$$(A4)$$

$$f(\lambda, \mu, \varrho, \sigma) = \frac{\Gamma(\gamma) \Gamma(\varrho - \lambda) \Gamma(\sigma - \mu)}{\Gamma(\varrho) \Gamma(\sigma) \Gamma(\gamma - \lambda - \mu)}.$$

Others represent the reductions which occur for special choices of the parameters. We shall here use the following reduction formulae:

$$F_{2}(\alpha, \beta, \beta', \gamma, \alpha, x, y) = (1 - y)^{-\beta'} F_{1}\left(\beta, \alpha - \beta', \beta', \gamma, x, \frac{x}{1 - y}\right)$$

$$F_{2}(\alpha, \beta, \beta', \alpha, \gamma', x, y) = (1 - x)^{-\beta} F_{1}\left(\beta', \beta, \alpha - \beta, \gamma', \frac{y}{1 - x}, y\right)$$

$$F_{3}(\alpha, \alpha', \beta, \gamma - \beta, \gamma, x, y) = (1 - y)^{-\alpha'} F_{1}\left(\beta, \alpha, \alpha', \gamma, x, \frac{y}{y - 1}\right).$$
(A5)

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indleveret til selskabet den 18. marts 1955. Færdig fra trykkeriet den 7. oktober 1955.