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MATRIX ELEMENTS BETWEEN STATES IN THE COULOMB FIELD

BY

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CONTENTS

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It is shown that the matrix elements between radial eigensolutions in a Coulomb field of functions of the type $r^p exp(-qr)$ can be expressed explicitly by means of hypergeometric functions of two variables. The calculation is made separately for the non-relativistic and relativistic case. Recursion formulae connecting the matrix elements are discussed and specializations to discrete-discrete, discrete-continuous, and continuous-continuous transitions are given.

I. Introduction.

In quantum mechanical perturbation treatments one often has to evaluate matrix elements between the eigenstates of the Coulomb field. In point of fact, this problem arose as one of the first in wave mechanics in connection with the calculation of the intensity of the hydrogen lines[1].

Other cases where one encounters Coulomb matrix elements are, e. g., the theory of bremsstrahlung, photoeffect, internal conversion, Auger effect, and Coulomb excitation, when one includes the Coulomb interaction in the unperturbed Hamiltonian.

In all these cases the integration over angles can be readily performed, giving the selection rules for the angular momenta. The remaining radial integral is generally of the type

$$\int_0^\infty R_i \, e^{-qr} \, r^p \, R_f^* \, r^2 \, dr \,,$$

where R is the radial eigenfunction in the Coulomb field belonging to either the discrete or the continuous spectrum. For $p = \pm 1$, Gordon[2] has given general formulae for discrete-discrete, discrete-continuous, and continuous-continuous transitions. For a positive integer, p, the matrix elements may be obtained by means of recursion formulae. For $p = -2$ and $q = 0$, one may use the equation of motion in the Coulomb field and reduce it to the case $p = 1$. For negative integers, $p < -2$, the matrix elements are more difficult and have until now been calculated only in some special cases of discrete-continuous transitions.

It will be shown here that a quite general explicit expression for Coulomb matrix elements of the above mentioned types can be given.

Section II of this paper is concerned with the derivation of this explicit expression for non-relativistic matrix elements. In the next section, methods will be given by which it is possible to derive recursion formulae connecting different matrix elements of the aforementioned type. Section IV deals with the specializations of the general formulae for the cases of discrete-discrete, discrete-continuous, and continuous-continuous transitions. These expressions embrace the earlier calculations of Gordon and others, corresponding to special choices of the parameters. In the last section, we shall give the exact expression also for the matrix elements with relativistic Coulomb wave functions.

The application of the method introduced here to the theory of Coulomb excitation will be given in a following paper[3].

II. Non-Relativistic Matrix Elements.

The non-relativistic eigenfunctions of a particle of charge $Z_1 e$ in a Coulomb potential $\frac{Z_2 e}{r}$ are in spherical coordinates r, θ, φ

$$\Psi_{l,m}(\lambda, r) = N_{\lambda,l}\, Y_{l,m}(\theta, \varphi)\, R_l(r/\lambda). \tag{1}$$

$N_{\lambda,l}$ is the normalization factor to be specified later; $Y_{l,m}(\theta, \varphi)$ are the normalized spherical harmonics. The radial wave function $R_l(r/\lambda)$ is a solution of the differential equation

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} - \left(\lambda^{-2} + \frac{2}{ar} + \frac{l(l+1)}{r^2}\right) R_l = 0. \tag{2}$$

l and m are the angular momentum quantum numbers. λ^{-2} is connected with the energy E and the mass m of the particle through

$$\lambda^{-2} = -\frac{2\,m}{\hbar^2}\,E. \tag{3}$$

The K orbit radius a is given by

$$a = \hbar^2/Z_1\,Z_2\,me^2, \tag{4}$$

where Z_1 and Z_2 have the signs of the charges.

The general solution of the radial equation (2) can be expressed by the confluent hypergeometric function ${}_1F_1$ or by the Whittaker function M through*

$$\left.\begin{aligned} R_l(r/\lambda) &= (2\,r/\lambda)^l\,e^{-r/\lambda}\,{}_1F_1(l+1+\lambda/a,\,2\,l+2,\,2\,r/\lambda) \\ &= (2\,r/\lambda)^{-1}\,M_{-\lambda/a,\,l+1/2}(2\,r/\lambda) \\ &= (-1)^l(-2\,r/\lambda)^{-1}\,M_{\lambda/a,\,l+1/2}(-2\,r/\lambda). \end{aligned}\right\} \tag{5}$$

A *discrete spectrum* $E < 0$ occurs only when a is negative, and one finds

$$\lambda = -\,na. \tag{6}$$

n is the principal quantum number which can take on the values $l+1,\ l+2,\ \ldots.,$ while the radial quantum number $n' = n-l-1$ takes on the values $0,\ 1,\ 2, \ldots.$ In the confluent hypergeometric function of formula (5) the first parameter is a negative integer, namely $-n'$, and the radial wave function may be expressed by a Laguerre polynomial**

$$R_l(r/\lambda) = \frac{(n-l-1)!\,(2\,l+1)!}{(l+n)!}\left(\frac{2\,r}{n\,|\,a\,|}\right)^l e^{-\frac{r}{n\,|a|}}\,L_{n-l-1}^{2\,l+1}\left(\frac{2\,r}{n\,|\,a\,|}\right).$$

* For the definition of these functions, see ERDÉLYI et al.: Higher Transcendental Functions, McGraw Hill 1953, vol. I, chap. VI. This reference will hereafter be quoted as HTF.

** HTF, vol. II, chapter X.

The normalization is given by the condition $\int |\psi|^2 d^3r = 1$, i. e.

$$N_{l,\lambda} = \frac{2}{(2l+1)!\,n^2}\sqrt{\frac{(n+l)!}{(n-l-1)!}}\,|a|^{-3/2}. \tag{7}$$

For the *continuous spectrum*, $E > 0$, one has

$$\lambda = i\eta a = \frac{i}{k}. \tag{8}$$

The "Sommerfeld number" η is defined as $\eta = \frac{Z_1 Z_2 e^2}{\hbar v}$.
In all scattering phenomena this is a very important number, since it measures the strength of the interaction. For $\eta \ll 1$ the interaction is weak and in the limit the Born approximation applies. For $\eta \gg 1$ one may similarly in the limit use classical concepts[5, 6].

The quantities $k = mv/\hbar$ and v are the wave number and the velocity, respectively, at infinity.

The normalization is here

$$N_{l,\lambda} = e^{-\frac{\pi}{2}\eta}\,\frac{|\Gamma(l+1+i\eta)|}{(2l+1)!}\,i^l, \tag{9}$$

which makes the so-called Coulomb wave function

$$F_l = N_{l,\lambda}\,kr\,R_l(-ikr)$$

real with the following asymptotic behaviour

$$F_l \cong \sin\left(kr - l\frac{\pi}{2} + \sigma_l - \eta \log 2kr\right). \tag{10}$$

The Coulomb phase σ_l is defined as

$$\sigma_l = \arg \Gamma(l+1+i\eta).$$

We shall now consider the radial matrix element of the following type

$$J_{l_i,\, l_f}^{p,\, q} = \int_0^\infty R_{l_i}(r/\lambda_{l_i})\, r^p\, e^{-qr} R_{l_f}^*(r/\lambda_f)\, r^2\, dr. \tag{11}$$

For its evaluation, we use an integral representation of the confluent hypergeometric function*

$$R_l = \left(\frac{2\,r}{\lambda}\right)^l e^{-r/\lambda} \frac{(2\,l+1)!}{\Gamma\left(l+1-\frac{\lambda}{a}\right)\Gamma\left(l+1+\frac{\lambda}{a}\right)} \int_0^1 e^{2ru/\lambda}\, u^{l+\frac{\lambda}{a}} (1-u)^{l-\frac{\lambda}{a}}\, du. \tag{12}$$

Hereby one obtains, carrying out the integration over r,

$$\left.\begin{aligned} & J_{l_i,\, l_f}^{p,\, q} = \\ & \frac{(2\,l_i+1)!\,(2\,l_f+1)!\,(2/\lambda_i)^{l_i}(2/\lambda_f^*)^{l_f}(l_i+l_f+p+2)!\left(\frac{1}{\lambda_i}+\frac{1}{\lambda_f^*}+q\right)^{-(l_i+l_f+p+3)}}{\Gamma\left(l_i+1-\frac{\lambda_i}{a}\right)\Gamma\left(l_i+1+\frac{\lambda_i}{a}\right)\Gamma\left(l_f+1-\frac{\lambda_f^*}{a}\right)\Gamma\left(l_f+1+\frac{\lambda_f^*}{a}\right)} \\ & \int_0^1\int_0^1 du\, dv\, u^{l_i+\frac{\lambda_i}{a}}(1-u)^{l_i-\frac{\lambda_i}{a}}\, v^{l_f+\frac{\lambda_f^*}{a}}(1-v)^{l_f-\frac{\lambda_f^*}{a}}(1-ux-vy)^{-(l_i+l_f+p+3)} \\ & \qquad x = \frac{2/\lambda_i}{1/\lambda_i+1/\lambda_f^*+q} \qquad y = \frac{2/\lambda_f^*}{1/\lambda_i+1/\lambda_f^*+q}. \end{aligned}\right\} \tag{13}$$

The remaining double integral is just one of the integral representations of the Appell function F_2.**

$$\left.\begin{aligned} & J_{l_i,\, l_f}^{p,\, q} = (l_i+l_f+p+2)!\, x^{l_i} y^{l_f}\left(\frac{1}{\lambda_i}+\frac{1}{\lambda_f^*}+q\right)^{-(p+3)} \\ & F_2\left(l_i+l_f+p+3,\ l_i+1+\frac{\lambda_i}{a},\ l_f+1+\frac{\lambda_f^*}{a},\ 2\,l_i+2,\ 2\,l_f+2,\ x,\ y\right). \end{aligned}\right\} \tag{14}$$

By means of the functional equation for the F_2 function (Appendix A 5) one may give alternative formulae, e. g.,***

* HTF, vol. I, chapter VI.

** HTF, vol. I, chapter V.

*** In the derivation, one has to put limits to the parameters so that the integral representation (12) has a meaning. Once, however, we have got the closed formula (14) this must be true for any values of the parameters.

The formula (14) is a special case of a general formula for the integral of products of Whittaker functions given by A. Erdélyi[7].

$$\left.\begin{aligned} J_{l_i\, l_f}^{q,\, q} &= (-1)^{l_i+p+3}\,(l_i+l_f+p+2)!\left(\frac{1}{\lambda_i}-\frac{1}{\lambda_f^*}-q\right)^{-(p+3)} u^{l_i}\, v^{l_f} \\ &F_2\left(l_i+l_f+p+3,\ l_i+1-\frac{\lambda_i}{a},\ l_f+1+\frac{\lambda_f^*}{a},\ 2\,l_i+2,\ 2\,l_f+2,\ u,\ v\right) \\ &\text{with} \\ &u=\frac{2/\lambda_i}{1/\lambda_i-1/\lambda_f^*-q} \qquad v=\frac{-2/\lambda_f^*}{1/\lambda_i-1/\lambda_f^*-q}. \end{aligned}\right\} \tag{14 a}$$

The generalized hypergeometric functions of two variables have been studied by several authors, the standard work on the subject being the monograph by APPELL and KAMPÉ DE FÉRIET[8]. Some of the properties of these functions are given in the Appendix.

The radial matrix element is given by J through

$$M_{l_i\, l_f}^{p,\, q} = N_{l_i,\,\lambda_i}\, N_{l_f,\,\lambda_f}^{*}\, J_{l_i\, l_f}^{p,\, q}. \tag{15}$$

III. Recursion Formulae.

One can derive a large number of recursion formulae which connect matrix elements with different values of l_i, l_f, and p. The general form of these recursion formulae can be determined from a theorem† which states that any five F_2 functions of the form

$$F_2\,(\alpha+n_1,\ \beta+n_2,\ \beta'+n_3,\ \gamma+n_4,\ \gamma'+n_5,\ x,\ y)$$

(where n_r are positive or negative integers) are connected by a linear relationship. The coefficients are polynomials in x and y. Since the matrix elements are proportional to an F_2 function, also five matrix elements of the form

$$M_{l_i+n',\ l_f+n''}^{p+n,\ q}$$

are linearly connected.

If the F_2 function is reduced to an F_1 function, e. g., in the case $l_i = l_f \pm (p+1)$, already four matrix elements are con-

† APPELL and KAMPÉ de FÉRIET (ref. 8, chapter I) state that this theorem holds already for four F_2 functions, but this does not seem to be true.

nected in this way. In the case where the F_2 function is reduced to an ordinary hypergeometric function, three will suffice. Since the above mentioned theorem holds for three ordinary confluent hypergeometric functions ${}_1F_1$, three radial Coulomb wave functions of the type R_{l+n} are connected by a linear relation. Some of the recursion formulae for the matrix elements can be derived from these recursion formulae. One has, e. g.,*

$$\left.\begin{aligned}&\left(\frac{l}{r}+\frac{1}{la}+\frac{d}{dr}\right) rR_l \equiv {}^+H^l rR_l = 2\,(2\,l+1)\,r/\lambda\, R_{l-1}\\&\left(\frac{l+1}{r}+\frac{1}{(l+1)\,a}-\frac{d}{dr}\right) rR_l \equiv {}^-H^{l+1} rR_l = -\frac{1}{l+1}\cdot\frac{(l+1)^2-(\lambda/a)^2}{(2\,l+2)(2\,l+3)}\frac{r}{\lambda} R_{l+1}.\end{aligned}\right\}\tag{16}$$

Recursion formulae for Coulomb matrix elements can now be obtained by considering the following expression:

$$\int_0^\infty rR_{l_i} r^p e^{-qr}\left[x_1{}^+H^{l_i+1}+x_2{}^+H^{l_f}+x_3{}^-H^{l_f+1}+x_4{}^-H^{l_i}\right] rR^*_{l_f}\,dr.$$

For the moment we leave the constant coefficients x_1 to x_4 undetermined. By partial integration in the first and fourth term and application of the recursion formulae (16) one obtains, by identifying the result with the direct evaluation

$$\left.\begin{aligned}&-x_1\frac{1}{\lambda_i(l_i+1)}\frac{(l_i+1)^2-(\lambda_i/a)^2}{(2\,l_i+2)(2\,l_i+3)} J^{p,\,q}_{l_i+1,\,l_f}+x_2\frac{2}{\lambda_f^*}(2\,l_f+1)\,J^{p,\,q}_{l_i,\,l_f-1}\\&-x_3\frac{1}{\lambda_f^*(l_f+1)}\frac{(l_f+1)^2-(\lambda_f/a)^2}{(2\,l_f+2)(2\,l_f+3)} J^{p,\,q}_{l_i,\,l_f+1}+x_4\frac{2}{\lambda_i}(2\,l_i+1)\,J^{p,\,q}_{l_i-1,\,l_f}\\&=\left[x_1(l_i+1+p)+x_2\,l_f+x_3(l_f+1)+x_4(l_i-p)\right] J^{p-1,\,q}_{l_i,\,l_f}\\&-\frac{1}{a}\left[x_1\left(\frac{1}{l_i+1}+qa\right)+x_2\frac{1}{l_f}+x_3\frac{1}{l_f+1}+x_4\left(\frac{1}{l_i}-qa\right)\right] J^{p,\,q}_{l_i,\,l_f}\\&+(x_1+x_2-x_3-x_4)\int_0^\infty rR_{l_i} r^p e^{-qr}\frac{d}{dr}(rR^*_{l_f})\,dr.\end{aligned}\right\}\tag{17}$$

* These formulae can be derived directly from the properties of the ${}_1F_1$ functions (HTF, vol. I, chapter VI) or by the factorization method[9].

To get recursion formulae between Coulomb matrix elements we choose the $x_n's$ so that the last term vanishes, i. e.,

$$x_1 + x_2 - x_3 - x_4 = 0 . \tag{18}$$

In accordance with the parity selection rule one will often employ the further condition

$$x_1\left(\frac{1}{l_i+1} + qa\right) + x_2\frac{1}{l_f} + x_3\frac{1}{l_f+1} + x_4\left(\frac{1}{l_i} - qa\right) = 0 . \tag{19}$$

In the resulting recursion relation we still have freedom in the choice of the x_n's. In particular, one can get a recursion formula with p fixed by the extra condition

$$x_1\,(l_i + p + 1) + x_2\,l_f + x_3\,(l_f + 1) + x_4\,(l_i - p) = 0 . \tag{20}$$

For $q = 0$, the relations containing $p - 1$ as well as p become singular for $p = -2$, which illustrates the more complicated character of matrix elements of the quadrupole type, as compared with that of dipole matrix elements.

Other recursion formulae may be obtained directly from the properties of the generalized hypergeometric functions. An example will be given in connection with the theory of Coulomb excitation (II).

IV. Specializations.

In this section, we give a few examples of the reduction of the general formula (14) for the case $q = 0$, which is of special interest.

a) *Discrete-discrete transitions.*

In this case, the second and third parameters in the F_2 function become negative integers, namely $l_i + 1 - n_i = - n_i'$ and $l_f + 1 - n_f = - n_f'$. The F_2 function is then reduced to a polynomial in x and y.[10]

$$\left.\begin{aligned}
M^{p}_{l_i,\, l_f} &= (l_i + l_f + p + 2)!\; a^{p} \left(\frac{1}{n_i} + \frac{1}{n_f}\right)^{-p-3} \frac{4\, x^{l_i}\, y^{l_f}}{n_i^2 n_f^2 (2\, l_i + 1)!\, (2\, l_f + 1)!} \\
&\sqrt{\frac{(n_i + l_i)!\, (n_f + l_f)!}{(n_i - l_i - 1)!\, (n_f - l_f - 1)!}} \sum_{r=0}^{n_i - l_i - 1} \sum_{s=0}^{n_f - l_f - 1} \frac{(l_i + l_f + p + 3)_{r+s} (l_i + 1 - n_i)_r (l_f + 1 - n_f)_s}{(2\, l_i + 2)_r\, (2\, l_f + 2)_s\; r!\; s!}\, x^r\, y^s \\
&\text{with} \\
&\qquad x = \frac{2\, n_f}{n_i + n_f} \qquad y = \frac{2\, n_i}{n_i + n_f}.
\end{aligned}\right\} \quad (21)$$

This formula contains, e. g., the matrix elements needed for the calculation of the intensity of hydrogen lines.

b) *Discrete-continuous transitions.*

Here, the parameter $\beta = l_i + 1 - n_i = -n_i'$ will become a negative integer. The F_2 function can, in this case, be reduced to a finite sum of ordinary hypergeometric functions (A 3).

$$\left.\begin{aligned}
M^{p}_{l_i\, l_f} &= (l_i + l_f + p + 2)!\; a^{p + 3/2} \left(\frac{1}{n_i} + \frac{i}{\eta_f}\right)^{-p-3} \frac{2\, x^{l_i}\, y^{l_f}}{n_i^2 (2\, l_i + 1)!} \sqrt{\frac{(n_i + l_i)!}{(n_i - l_i - 1)!}} \\
&\times \frac{\left| \Gamma(l_f + 1 + i\eta_f) \right|}{(2\, l_f + 1)!}\, i^{-l_f}\, e^{-\frac{\pi}{2}\eta_f} \\
&\times \sum_{r=0}^{n_i - l_i - 1} \frac{(l_i + l_p + p + 3)_r (l_i + 1 - n_i)_r}{(2\, l_i + 2)_r\;\; r!}\, x^r\, {}_2F_1(l_i + l_f + p + 3 + r,\, l_f + 1 + i\eta_f,\, 2 l_f + 2,\, y) \\
&\text{with} \\
&\qquad x = \frac{2\, i\eta_f}{n_i - i\eta_f} \qquad y = \frac{2\, n_i'}{n_i - i\eta_f}.
\end{aligned}\right\} \quad (22)$$

This formula applies, e. g., for the matrix elements occurring in the theory of electron emission by radioactive α — disintegration[11].

c) *Continuous-continuous transitions.*

In the general case, the F_2 function cannot easily be reduced to more elementary functions. The matrix element is

$$\left.\begin{aligned} M^p_{l_i\, l_f} &= (l_i + l_f + p + 2)!\; a^{p+3} \left(\frac{1}{\eta_i} - \frac{1}{\eta_f}\right)^{-p-3} \frac{x^{l_i}\, y^{l_f}\, i^{l_i - l_f + p + 3}}{(2\, l_i + 1)!\,(2\, l_f + 1)} \\ & \left| \Gamma(l_i + 1 + i\eta_i) \right| \cdot \left| \Gamma(l_f + 1 + i\eta_f) \right| e^{-\frac{\pi}{2}(\eta_i + \eta_f)} \\ & F_2\,(l_i + l_f + p + 3,\; l_i + 1 - i\eta_i,\; l_f + 1 + i\eta_f,\; 2\, l_i + 2,\; 2\, l_f + 2,\; x, y), \\ & \text{where } x = \frac{2\,\eta_f}{\eta_f - \eta_i} \quad \text{and} \quad y = \frac{-2\,\eta_i}{\eta_f - \eta_i}. \end{aligned}\right\} \quad (23)$$

Since $x + y > 1$, it is essential for the application of this formula to investigate the analytic continuation of the F_2 function beyond the domain of convergence of the series expansion (A1). This problem will be treated in detail in (II) in connection with the theory of Coulomb excitation. In the case $p = -1$ and $l_i = l_f$, the F_2 function is reduced directly to the usual hypergeometric function (A6) and one obtains an expression which is identical with the formula of Gordon (loc. cit.).

V. Relativistic Matrix Elements.

The relativistic eigensolution for an electron in a Coulomb field $-Ze/r$ is, in the notation of Rose and Osborn[12],

$$\psi_{\varkappa,\, m} = \begin{pmatrix} -i f_\varkappa\, \chi^m_{-\varkappa} \\ g_\varkappa\, \chi^m_\varkappa \end{pmatrix}, \qquad (24)$$

where

$$\chi^m_\varkappa = \sum_\tau < l_\varkappa,\, m - \tau;\; {}^1\!/_2,\, \tau \,|\, j,\, m > \chi_{{}^1\!/_2,\, \tau}\, Y_{l_\varkappa,\, m-\tau}$$

with

$$l_\varkappa = |\varkappa| + {}^1\!/_2\,(\text{sign}\,\varkappa - 1)$$

$$j = |\varkappa| - {}^1\!/_2$$

and

$$\chi_{1/2,\,1/2} = \begin{pmatrix}1\\0\end{pmatrix} \qquad \chi_{1/2,\,-1/2} = \begin{pmatrix}0\\1\end{pmatrix}.$$

The radial wave functions are solutions of the differential equations

$$\frac{d}{dr}\begin{pmatrix}f\\g\end{pmatrix} = \begin{pmatrix}\frac{\varkappa-1}{r}, & -\frac{1}{\hbar c}\left(W-mc^2-\frac{Ze^2}{r}\right)\\ \frac{1}{\hbar c}\left(W+mc^2+\frac{Ze^2}{r}\right), & -\frac{\varkappa+1}{r}\end{pmatrix}\begin{pmatrix}f\\g\end{pmatrix}, \tag{25}$$

where W is the total energy (including the rest energy). The solution may be written in the following form:

$$\begin{pmatrix}f\\g\end{pmatrix} = N_{\lambda,\varkappa}\begin{pmatrix}F\\G\end{pmatrix}, \tag{26}$$

where $N_{\lambda,\varkappa}$ is a normalization factor and

$$\begin{pmatrix}F\\G\end{pmatrix} = \sqrt{\frac{mc^2}{W}\mp 1}\left(\frac{\lambda}{r}\right)^{3/2}\left[(N-\varkappa)\,M_{\gamma+n'+1/2,\,\gamma}\left(\frac{2\,r}{\lambda}\right)\pm n' M_{\gamma+n'-1/2,\,\gamma}\left(\frac{2\,r}{\lambda}\right)\right].$$

We have used the following abbreviations:

$$\left.\begin{aligned}
\lambda &= \lambda_0\frac{mc^2}{\sqrt{m^2c^4-W^2}} & \lambda_0 &= \frac{\hbar}{mc},\\
N &= \frac{\hbar c}{a\sqrt{m^2c^4-W^2}} & a &= \frac{\hbar^2}{Zme^2},\\
\gamma &= \sqrt{\varkappa^2-Z^2\alpha^2} & \alpha &= \frac{e^2}{\hbar c},\\
n' &= \frac{\alpha ZW}{\sqrt{m^2c^4-W^2}}-\gamma. & &
\end{aligned}\right\} \tag{27}$$

For the *discrete spectrum* $W < mc^2$, n' is the radial quantum number taking on the values $0, 1 \ldots\ldots$ The quantum number N is then

$$N = \sqrt{n^{2\prime}+\varkappa^2+2\,n'\gamma} \tag{28}$$

and the parameter λ becomes

$$\lambda = Na. \tag{19}$$

The normalization is determined by the condition

$$\int \overline{\psi} \psi d^3 r = 1,$$

giving

$$N_{\gamma, \varkappa} = -\frac{\sqrt{\Gamma(2\gamma + n' + 1)}}{\Gamma(2\gamma + 1)\sqrt{(n')!}} \frac{(Na)^{-3/2}}{\sqrt{4N(N-\varkappa)\sqrt{1+\frac{\alpha^2 Z^2}{(n'+\gamma)^2}}}}. \tag{30}$$

For the *continuous spectrum* $W > mc^2$ the parameters have the following values:

$$\left.\begin{aligned} \lambda &= \frac{i}{k}, \quad k = p/\hbar, \\ N &= \frac{i}{ka}, \\ n' &= i\eta - \gamma, \quad \eta = \frac{Ze^2}{\hbar v} = Z\alpha \frac{W}{pc}, \end{aligned}\right\} \tag{31}$$

where p is the momentum at infinity. The normalization is

$$N_{\lambda, \varkappa} = k e^{i\left(\frac{\pi}{2}\gamma - \delta\right)} \frac{e^{\frac{\pi}{2}\eta} \left|\Gamma(\gamma + i\eta)\right|}{\Gamma(2\gamma + 1)} (2i)^{-3/2}, \tag{32}$$

which makes the wave function real with the following asymptotic behaviour:

$$\begin{pmatrix} f \\ g \end{pmatrix} \sim \sqrt{1 \mp \frac{W}{mc^2}} \begin{pmatrix} -\sin \\ \cos \end{pmatrix} \left[kr + \eta \log 2kr - \sigma_l + \delta - \frac{\pi}{2}\gamma\right]. \tag{33}$$

The phases σ_l and δ are defined by

$$\left.\begin{aligned} \sigma_l &= \arg \Gamma(\gamma + i\eta), \\ \delta &= \frac{1}{2} \arg \frac{-\varkappa + \frac{i}{ka}}{\gamma + i\eta}. \end{aligned}\right\} \tag{34}$$

Since the relativistic wave functions are expressed by confluent hypergeometric functions, the matrix elements of $r^p e^{-qr}$ may be calculated in the same way as the non-relativistic matrix elements (formula 14). Here, we shall give the result only:

$$\left.\begin{aligned}
&\int_0^\infty \begin{pmatrix} f_i \\ g_i \end{pmatrix} r^p e^{-qr} (f_f, g_f) r^2 dr = \\
&N_{\varkappa_i, \lambda_i} N_{\varkappa_f, \lambda_f} 2 \lambda_i \lambda_f \lambda_i^{-\gamma_i} \lambda_f^{-\gamma_f} \left(q + \frac{1}{\lambda_i} + \frac{1}{\lambda_f}\right)^{-\gamma_i - \gamma_f - p - 1} \Gamma(\gamma_i + \gamma_f + p + 1) \\
&\sqrt{\frac{(mc^2 + \varepsilon_1 W_i)(mc^2 + \varepsilon_2 W_f)}{W_i W_f}} \\
&\{\varepsilon_3 (N_i - \varkappa_i)(N_f - \varkappa_f) F_2(\gamma_i + \gamma_f + p + 1, -n_i, -n_f, 2\gamma_i + 1, 2\gamma_f + 1, x, y) \\
&\quad \varepsilon_4\, n_i\, n_f \qquad F_2(\gamma_i + \gamma_f + p + 1, -n_i + 1, -n_f + 1, 2\gamma_i + 1, 2\gamma_f + 1, x, y) \\
&\quad \varepsilon_5 (N_i - \varkappa_i)\, n_f \qquad F_2(\gamma_i + \gamma_f + p + 1, -n_i - n_f + 1, 2\gamma_i + 1, 2\gamma_f + 1, x, y) \\
&\quad \varepsilon_6 (N_f - \varkappa_f)\, n_i \qquad F_2(\gamma_i + \gamma_f + p + 1, -n_i + 1, -n_f, 2\gamma_i + 1, 2\gamma_f + 1, x, y)\}.
\end{aligned}\right\} \quad (35)$$

The signs ε_n are given by

$$\left.\begin{aligned}
\varepsilon_1 &= \begin{pmatrix} - & - \\ + & + \end{pmatrix} & \varepsilon_2 &= \begin{pmatrix} - & + \\ - & + \end{pmatrix} & \varepsilon_3 &= \begin{pmatrix} + & + \\ + & + \end{pmatrix} \\
\varepsilon_4 &= \begin{pmatrix} + & - \\ - & + \end{pmatrix} & \varepsilon_5 &= \begin{pmatrix} + & - \\ + & - \end{pmatrix} & \varepsilon_6 &= \begin{pmatrix} + & + \\ - & - \end{pmatrix}.
\end{aligned}\right\} \quad (36)$$

Further,

$$x = \frac{2/\lambda_i}{1/\lambda_i + 1/\lambda_f + q} \qquad y = \frac{2/\lambda_f}{1/\lambda_i + 1/\lambda_f + q}. \quad (37)$$

With this formula one can, e. g., write down directly the internal conversion matrix elements.

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Appendix:
Some properties of the generalized hypergeometric function of two variables, F_2.

The F_2 function is defined by a series expansion

$$F_2(\alpha, \beta, \beta', \gamma, \gamma' x, y) = \sum_{m,n=0}^{\infty} \frac{\alpha_{m+n} \beta_m \beta'_n}{\gamma_m \gamma'_n \, m! \, n!} x^m y^n, \tag{A1}$$

where

$$a_m = \frac{\Gamma(a+m)}{\Gamma(a)} = a(a+1)\cdot\cdots(a+m-1).$$

This double series has the following domain of absolute convergence

$$|x| + |y| \leqslant 1. \tag{A2}$$

By summation over n, one gets an alternative series expansion

$$F_2(\alpha, \beta, \beta', \gamma, \gamma' x, y) = \sum_{m=0}^{\infty} \frac{\alpha_m \beta_m}{\gamma_m \, m!} x^m {}_2F_1(\alpha+m, \beta', \gamma', y). \tag{A3}$$

The analytic continuation of the function F_2 beyond the domain A2 may be given by the integral representation

$$\left.\begin{aligned} F_2(\alpha, \beta, \beta', \gamma, \gamma', x, y) &= \frac{\Gamma(\gamma)\Gamma(\gamma')}{\Gamma(\beta)\Gamma(\beta')\Gamma(\gamma-\beta)\Gamma(\gamma'-\beta')} \\ \int_0^1\int_0^1 du\, dv\, u^{\beta-1} v^{\beta'-1} (1-u)^{\gamma-\beta-1}&(1-v)^{\gamma'-\beta'-1}(1-ux-vy)^{-\alpha} \end{aligned}\right\} \tag{A4}$$

The integral representation has a meaning only when the following inequalities are fulfilled,

$$Re\,\beta > 0 \quad Re\,\beta' > 0 \quad Re(\gamma - \beta) > 0 \quad Re(\gamma' - \beta') > 0.$$

There exist three transformations corresponding to the Euler transformations of the ordinary hypergeometric functions,

$$\left.\begin{aligned} F_2(\alpha, \beta, \beta', \gamma, \gamma'\, x, y) &= (1-x)^{-\alpha} F_2\left(\alpha, \gamma-\beta, \beta', \gamma, \gamma' \frac{x}{x-1}, \frac{y}{1-x}\right) \\ &= (1-y)^{-\alpha} F_2\left(\alpha, \beta, \gamma'-\beta', \gamma, \gamma' \frac{x}{1-y}, \frac{y}{y-1}\right) \\ &= (1-x-y)^{-\alpha} F_2\left(\alpha, \gamma-\beta, \gamma'-\beta', \gamma, \gamma' \frac{x}{x+y-1}, \frac{y}{x+y-1}\right). \end{aligned}\right\} \quad (A5)$$

The F_2 function reduces, for special choices of the parameters, to a simpler function.

If the first index α is a negative integer, the series A1 breaks off and the F_2 function is thus a polynomial. The same is true when both parameters β and β' are negative integers. If only one of them is a negative integer, the series A3 reduces to a finite sum of ordinary hypergeometric functions. There exist also other special reduction formulae of which we use only

$$\left.\begin{aligned} F_2(\alpha, \beta, \beta', \alpha, \alpha, x, y) &= (1-x)^{-\beta}(1-y)^{-\beta'} \\ &\times {}_2F_1\left(\beta, \beta', \alpha, \frac{xy}{(1-x)(1-y)}\right). \end{aligned}\right\} \quad (A6)$$

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