Methods of Calculation of Radial Wave Functions and New Tables of Coulomb Functions

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In connection with the tabulation of Coulomb wave functions special methods of obtaining numerical results having an accuracy of about one percent have been developed and are reported. Some of the methods are applicable also to other problems. Many of them are concerned with the calculation of the second solution of an ordinary differential equation of second order making use of the first solution. The present paper contains an introduction to the use of new Coulomb Functions tables which cover ranges of parameters required for the calculation of nuclear reactions of protons, deuterons and alpha-particles from hydrogen to oxygen in the energy range of a few Mev. The ranges covered are 0 to 6 for ρ, 0 to 3.98 for η. For alpha-particles the tables suffice for the treatment of reactions up to about 10 Mev for $Z=9$(F) and 5 Mev for $Z=2$(He). For protons the tables cover an energy range of roughly 4 times that for alpha-particles.

I. INTRODUCTION

THE availability of Coulomb functions is of obvious importance for the development of nuclear physics. The computation of these functions was started in 1946 under the auspices of the ONR and approximate values of the functions sufficing for the treatment of nuclear reactions of protons, deuterons, and alpha-particles bombarding elements from hydrogen up to oxygen have been obtained at the close of June 1948. The tables have been tried out in some applications during the last year and a few minor errors have been found. They are now available for distribution.[1]

During the course of the work it has been found possible to employ some short cuts and methods of approximation which should be of help in the calculation of radial wave functions not only in the Coulomb case but also for more general central fields. A summary of these methods is presented below. A characteristic feature of the problem is the fact that one needs two functions for each energy, the regular and the irregular functions. The regular solution can be started as a power series at $r=0$ and its calculation is easier than that of the irregular function. Means of making use of available relations between the two functions have been found. It also proved possible to make use of solutions for the special case of zero charge in the calculation of functions for the case of a non-vanishing charge and the method employed in this connection has considerable generality.

The introduction of high speed computational machines decreases the importance of approximation methods. Nevertheless, there is still a large need for being able to obtain approximate answers without the aid of such machines or of large computational projects. This is especially true for problems in which a systematic tabulation covering large ranges of parameters is not needed. The tables referred to above may be considered to be an extension of those published by Yost, Wheeler and Breit;[2,3] Breit, Condon, and Present;[4] Breit, Thaxton, and Eisenbud;[5] Thaxton and Hoisington;[6] Wicher;[7] Wheeler;[8] and Pavinsky.[9] It is understood that new and much more complete tables will be published soon by the National Bureau of Standards.

Notation

(a) Physical quantities

$L\hbar$ = angular momentum.
v = relative velocity of colliding particles.
e = electronic charge.
Λ = wave-length of relative motion.
μ = reduced mass.
$a = \hbar^2/\mu e^2$.
Z, Z' = atomic numbers of colliding particles.
$k/2\pi = 1/\Lambda$ = wave number.
$\eta = ZZ'e^2/\hbar v$.
r = distance between particles.
$\rho = kr$.
Q = energy evolved in a reaction.

(b) Functional symbols and mathematical abbreviations

$\Gamma(x)$ = gamma-function of argument x.
$\sigma_L = \arg\Gamma(L+1+i\eta)$.
$' = d/d\rho$.
F_L = regular Coulomb function otherwise defined by being a solution of $d^2F_L/d\rho^2 + [1-2\eta/\rho - L(L+1)/\rho^2]F_L = 0$ and having its asymptotic form $F_L \sim \sin(\rho - L\pi/2 - \eta \ln 2\rho + \sigma_L)$ at $\rho = \infty$.

² Yost, Wheeler, and Breit, Phys. Rev. 49, 174 (1936), referred to hereafter as YWB.
³ Yost, Wheeler, and Breit, J. Terr. Mag. At. El. 40, 443 (1935).
⁴ Breit, Condon, and Present, Phys. Rev. 50, 825 (1936).
⁵ Breit, Thaxton, and Eisenbud, Phys. Rev. 55, 1018 (1939), hereafter referred to as BTE.
⁶ H. M. Thaxton and L. E. Hoisington, Phys. Rev. 56, 1194 (1939).
⁷ E. R. Wicher, J. Terr. Mag. At. El. 41, 389 (1936).
⁸ J. A. Wheeler, Phys. Rev. 52, 1123 (1937).
⁹ P. P. Pavinsky, J. Exper. Theor. Phys. 9, 411 (1939) (in Russian).

$G_L=$ irregular Coulomb function satisfying the same differential equation as F_L, otherwise defined by its asymptotic form $G_L \sim \cos(\rho - L\pi/2 - \eta \ln 2\rho + \sigma_L)$.

$C_L = \{[1+\eta^2/L^2][1+\eta^2/(L-1)^2]\cdots[1+\eta^2/1^2]\}^{\frac{1}{2}} \times [2\pi\eta/(e^{2\pi\eta}-1)]^{\frac{1}{2}}/[1\cdot3\cdot5\cdots(2L+1)]$.

$D_L = 1/[(2L+1)C_L]$.

$y_L = dF_L/F_L d\rho$, $y = dF/Fd\rho$.

$p_L = (2L+1)(e^{2\pi\eta}-1)C_L^2/\pi$.

$$q_L = p_L\left[\Sigma_1^L\frac{s}{s^2+\eta^2}-\Sigma_1^{2L+1}\frac{1}{s}+2\gamma+\text{R.P.}\frac{\Gamma'(i\eta)}{\Gamma(i\eta)}\right]$$
$$+(-)^{L+1}\frac{2^L}{(2L)!}\text{I.P.}\left\{\frac{2^{-L}}{2L+1}+\frac{2^{1-L}(i\eta-L)}{1!(2L)}+\cdots\right.$$
$$+\frac{2^{s+1-L}(i\eta-L)(i\eta-L+1)\cdots(i\eta-L+s)}{(s+1)!(2L-s)}+\cdots$$
$$\left.+\frac{2(i\eta-L)(i\eta-L+1)\cdots(i\eta+L-1)}{(2L)!}\right\}.^{10}$$

$\gamma = $ Euler's constant $= 0.5772\cdots$.

Φ_L, $\Theta_L = $ quantities defined by $F_L = C_L\rho^{L+1}\Phi_L$, $G_L = D_L\rho^{-L}\Theta_L$.

Φ_L^*, $\Theta_L^* = $ quantities defined by $F_L' = C_L\rho^L\Phi_L^*$, $G_L' = D_L\rho^{-L-1}\Theta_L^*$.

$\mathfrak{g}_L = 1 - 2\eta/\rho - L(L+1)/\rho^2$.

$$H(\rho) = -F(\rho)\int_{\rho_1}^{\rho} F^{-2}(\rho')d\rho'.$$

$A_L = |F_L^2 + G_L^2|^{\frac{1}{2}}$.

$\varphi_L = $ phase of the phase amplitude method, defined by $F_L = A_L\sin\varphi_L$, $G_L = A_L\cos\varphi_L$ with the additional requirement $\varphi_L = 0$ when $\rho = 0$.

General convention: subscript L will be dropped when no confusion will arise by doing so.

II. RICCATI EQUATION METHOD

The differential equation

$$F'' + \mathfrak{g}F = 0, \qquad (1)$$

is equivalent to

$$y' + y^2 + \mathfrak{g} = 0, \qquad (2)$$

where

$$y = dF/Fd\rho, \qquad (2.1)$$

is the logarithmic derivative of F. A way of expanding y in terms of one or more parameters has been described by Breit, Thaxton, and Eisenbud.[2] By means of their Eqs. (9), (9.1) one can compute successive derivatives of y with respect to parameters κ, λ, μ, ν, $\cdots$ entering linearly in

$$\mathfrak{g} = \kappa + \lambda\mathfrak{g}^{(\lambda)} + \mu\mathfrak{g}^{(\mu)} + \cdots. \qquad (2.2)$$

If the boundary conditions are such that F^2y_κ, F^2y_λ, $\cdots$, $F^2y_{\kappa\lambda\mu\nu}\ldots$ vanish at $\rho = 0$ then there result formulas[11]

$$y_\kappa = -F^{-2}\int_0^\rho F^2 d\rho, \quad y_\lambda = -F^{-2}\int_0^\rho F^2\mathfrak{g}^{(\lambda)}d\rho, \quad \cdots$$

$$y_{\lambda\lambda} = -2F^{-2}\int_0^\rho F^2 y_\lambda^2 d\rho,$$

$$y_{\kappa\lambda} = -2F^{-2}\int_0^\rho y_\kappa y_\lambda F^2 d\rho, \quad \cdots \qquad (2.3)$$

$$y_{\lambda\lambda\lambda} = -6F^{-2}\int_0^\rho y_\lambda y_{\lambda\lambda}F^2 d\rho,$$

$$y_{\lambda\lambda\mu} = -F^{-2}\int_0^\rho (4y_\lambda y_{\lambda\mu} + 2y_\mu y_{\lambda\lambda})F^2 d\rho, \quad \cdots.$$

A few additional formulas are available in Eq. (9.1) of Breit, Thaxton, and Eisenbud for the calculation of derivatives with respect to four parameters.

By means of these expansions it is possible to calculate y for the regular Coulomb function from y for the corresponding field free function, with the same L. The values tabulated by Yost, Wheeler, and Breit[3] served as a convenient starting point. In a few cases their accuracy had to be improved in order to secure sufficient reliability of the final values.

The application of the BTE expansion is convenient if it is desired to obtain the values of y and F for a number of values of η and if the expansion for y converges sufficiently rapidly. If this is not the case the following procedure works satisfactorily. The equation corresponding to Eq. (1) for which a solution is available is

$$F^{(0)''} + \mathfrak{g}^{(0)}F^{(0)} = 0, \qquad (3)$$

and the relations corresponding to Eqs. (2), (2.1) are

$$y^{(0)'} + y^{(0)2} + \mathfrak{g}^{(0)} = 0, \qquad (3.1)$$

$$y^{(0)} = dF^{(0)}/F^{(0)}d\rho. \qquad (3.2)$$

Denoting the difference between the two logarithmic derivatives by

$$\delta y = y - y^{(0)}, \qquad (3.3)$$

there results

$$\frac{d}{d\rho}[F^{(0)2}\delta y] + [(\delta y)^2 + (\delta\mathfrak{g})]F^{(0)2} = 0, \qquad (3.4)$$

where

$$\delta\mathfrak{g} = \mathfrak{g} - \mathfrak{g}^{(0)}. \qquad (3.5)$$

If one neglects the term in $(\delta y)^2$ in Eq. (3.4) there results an approximation for δy identical with that obtainable

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[10] A misprint in Eq. (16) of YWB, the omission of 2γ in the formula for λ_L, is here corrected.

[11] The formula for $y_{\lambda\lambda\mu}$ in Eq. (9.1) of Breit, Thaxton, and Eisenbud contains a misprint $2y_\lambda^2 y_\mu$ for $2y_\mu y_{\lambda\lambda}$ under the integral sign.

from Eqs. (2.3) by neglecting contributions to δy which arise from derivatives of higher order than the first. It has been found possible to employ Eq. (3.4) for a step by step construction of δy by the following procedure. The range of needed values of ρ is divided into suitably chosen relatively small intervals and the value of δy at one end of an interval is found from the value at the beginning of the same interval. This is accomplished by integrating Eq. (3.4) through the interval. Quantities corresponding to the smaller value of ρ in the interval will be here designated by the subscript 1, those for the larger by 2. For an interval that is not too large one has with sufficient accuracy

$$(\delta y)_2 = [F^{(0)2}(\rho_1)/F^{(0)2}(\rho_2)](\delta y)_1$$
$$- (\rho_2-\rho_1)[F^{(0)}(\rho_2)]^{-2}\tfrac{1}{2}\{[F^{(0)}(\rho_2)]^2$$
$$+ [F^{(0)}(\rho_1)]^2\{\tfrac{1}{2}[\delta g(2)+\delta g(1)]$$
$$+ \tfrac{1}{2}[(\delta y)_1{}^2+(\delta y)_2{}^2]\}. \quad (3.6)$$

On the right side, in this equation, there is only one unknown quantity $(\delta y)_2{}^2$. By employing the value of δy_2 which results from an extrapolation from lower ρ for $(\delta y)_2{}^2$ on the right side of the equation one obtains a first approximation to $(\delta y)_2$ which can be improved by inserting the first approximation for $(\delta y)_2{}^2$, and repeating the procedure if necessary. This iteration procedure is simply a convenient way of solving a quadratic equation for δy_2.

In the application to Coulomb functions the initial values are

$$(\delta y)_{\rho=0} = \eta/(L+1), \quad (3.7)$$
and
$$\delta g = -2\eta/\rho. \quad (3.8)$$

III. CALCULATION OF THE IRREGULAR FUNCTION FROM THE REGULAR FUNCTION BY QUADRATURE

Omitting the subscript L, one has

$$G(\rho_2)/F(\rho_2)-G(\rho_1)/F(\rho_1)+\int_{\rho_1}^{\rho_2} F^{-2}(\rho)d\rho = 0. \quad (4)$$

This formula is closely related to the Wronskian relation

$$F'G-G'F = 1, \quad (4.1)$$

and in fact the latter is the differential form of the former. By means of Eq. (4) one can obtain $G(\rho_2)$ if one knows $F(\rho_1)$, $G(\rho_1)$, $F(\rho_2)$ and if there is enough information about $F(\rho)$ between ρ_1 and ρ_2 to enable a numerical quadrature to be made for the integral occurring in Eq. (4). The computation of the regular function F is usually easier than that of the irregular function G and Eq. (4) is, therefore, more frequently applicable than the similar relation

$$F(\rho_2)/G(\rho_2)-F(\rho_1)/G(\rho_1)-\int_{\rho_1}^{\rho_2} G^{-2}(\rho)d\rho = 0. \quad (4.2)$$

In applying Eq. (4) special methods recommend themselves whenever the integrand varies rapidly and in such a manner that the accuracy of the numerical quadrature becomes questionable. In particular this is the case whenever a node of F falls in the interval $\rho_1<\rho<\rho_2$. At the node then one of the two terms G/F becomes infinite and so does the integrand. However, the quantity needed is G rather than G/F and in the equation,

$$G(\rho)=[G(\rho_1)/F(\rho_1)]F(\rho)-F(\rho)\int_{\rho_1}^{\rho} F^{-2}(\rho')d\rho', \quad (4.3)$$

the two terms representing $G(\rho)$ remain finite as one goes through a node. The only practical question is, therefore, that of carrying the second term across a small interval surrounding the node. Two general procedures which have been found useful for doing so will now be described. In this discussion the node of F will be referred to as ρ_0, the point to which the quadrature has carried the solution as $\rho_<$ and the point at which the quadrature is resumed as $\rho_>$.

(a) The value of the second term on the right side of Eq. (4.3) is obtained on one side of the node from that on the other by noting that this term, $H(\rho)$, satisfies the original differential equation and that the values of the term and of its first derivative,

$$H'(\rho_<)=\left[-F^{-1}(\rho)-F'(\rho)\int_{\rho_1}^{\rho} F^{-2}(\rho')d\rho'\right]_{\rho=\rho_<}, \quad (4.3')$$

are available from the quadratures. The values of any desired number of successive derivatives are, therefore, also available at $\rho=\rho_<$ from the result of differentiating the original differential equation. Thus H'' can be determined as $-gH$, H''' is obtainable from

$$H'''+g'H+gH' = 0, \quad (4.4)$$

and so on. The value of $H(\rho_>)$ is thus obtainable from $H(\rho_<)$ by a Taylor Series expansion around $\rho=\rho_<$. The series is

$$H = \{h-h^3g(\rho_<)/6-h^4g'(\rho_<)$$
$$+h^5[g^2(\rho_<)-3g''(\rho_<)]+\cdots\}/F(\rho_<), \quad (4.5)$$
where
$$h = \rho-\rho_<. \quad (4.6)$$

This series applies on either side of the node. If it is desired to obtain the integral in Eq. (4) for $\rho_1=\rho_<$, $\rho_2=\rho$, the same series may be used on division by $F(\rho)$. The right side of Eq. (4.5) varies smoothly on going through the node. The integral varies rapidly and behaves to a first approximation as $h/F(\rho_<)F(\rho)$.

(b) The Taylor Series expansion just described is used with a small number of terms in the series to calculate the values of $H(\rho)$ at $\rho=\rho_<+h$, $\rho_<+2h$, $\rho_<+3h$. These values of $H(\rho)$ are then used as starting values of a numerical integration of the Hartree type[12] for the

[12] D. R. Hartree, Memoirs and Proc. Man. Lit. Phil. Soc. 77, 91 (1932-33).

differential equation $H'' + gH = 0$. This procedure is superior to (a) if it is desired to have a higher accuracy. A larger interval $\rho_> - \rho_<$ can be handled by this means and the numerical integration of H can be used to check on the accuracy of the numerical quadrature for $\int F^{-2}d\rho$ by arranging for an overlap of the two procedures. The main inaccuracies in the numerical quadrature arise for values of ρ close to $\rho_<$ and $\rho_>$ and an occasional check of the type just described has been found to be a useful precaution.

It is desirable to point out that usual quadrature formulas are not especially suitable for the integration of F^{-2} as one approaches the node. In this region one deals essentially with integrals of the type

$$\int_a^b dx/x^2 = (b-a)/ab. \tag{5}$$

This circumstance suggests the approximation,

$$\int_\rho^{\rho+h} F^{-2}(\rho)d\rho \cong h/[F(\rho)F(\rho+h)], \tag{5.1}$$

which is often better than Simpson's rule. A still better approximation is obtainable from Eq. (4.5) by applying it to the intervals $(\rho-h, \rho)$, $(\rho, \rho+h)$ and employing values of g, g', g'' at ρ. One obtains in this manner

$$\int_{\rho-h}^{\rho+h} F^{-2}(\rho)d\rho \cong [h/F(\rho)]$$
$$\times [1/F(\rho+h)+1/F(\rho-h)][1-h^2g(\rho)/6], \tag{5.2}$$

where all terms in an expansion in powers of h have been kept up to h^3. This equation is often more reliable than the Newton-Cotes five point quadrature formula. It will be noted that the methods just discussed are applicable not only to Coulomb functions and that the numerical procedure for obtaining a second solution of an ordinary differential equation of second order is not made impractical by the presence of a node of the first solution within the desired range of values of the independent variable.

It is desirable to caution against the employment of a value of ρ_1 close to a node of $F(\rho)$ in Eq. (4.3). In such a case $|G(\rho_1)/F(\rho_1)|$ will be greater than the absolute value of the integral in (4.3) through most of the range of values of ρ and the numerical accuracy will be poor. It is desirable to have, therefore, a starting value of $G(\rho_1)$ at a value of ρ reasonably close to a maximum of $|F(\rho)|$ or a node of $G(\rho_1)$. If ρ_1 is made to be a node of G the accuracy close to the node of F suffers because the second term in Eq. (4.3) is then the only one present and the fractional accuracy of the factor multiplying F becomes poor close to its node unless the interval $\rho_> - \rho_<$ is made large enough.

The function F has a node also at $\rho = 0$. Here there is no need of carrying G across the node of F. Some convenient approximations can be made, however. They

will be listed consecutively with methods (a), (b). The first of these approximations is:

(c) For small ρ and especially for large L the integrand of

$$I_L(\rho) = \int_\rho^\infty d\rho/F_L^2 \tag{6}$$

varies rapidly primarily on account of the factor ρ^{L+1} which is present in F_L. This circumstance suggests the introduction of

$$\chi_L = \Phi_L^{-2}, \tag{6.1}$$

and integration by parts as follows

$$C_L^2 I_L(\rho) = \int_\rho^\infty \rho^{-2L-2}\chi_L d\rho$$

$$= \Sigma_n + \frac{(2L+1-n)!}{(2L+1)!} \int_\rho^\infty \rho^{-2L-2+n}\chi_L^{(n)}d\rho, \tag{6.2}$$

where

$$\chi_L^{(n)} = d^n\chi_L/d\rho^n, \tag{6.3}$$

$$\Sigma_n = \Sigma_1^{n-1}\frac{(2L-i)!}{(2L+1)!}\chi_L^{(i)}\rho^{-(2L+1-i)}. \tag{6.4}$$

The sum Σ_n often converges very rapidly for small ρ and large L. Under these circumstances the method is very convenient because two or three terms suffice for high accuracy. Thus, for example, for $\eta = 0.1585$, $\rho = 1.4$, $L = 4$ the second term is of the order of 3 percent and the third of the order of 0.1 percent of the first. In cases of such rapid convergence the calculation of derivatives of χ_L need not be accurate for the higher i. The first term of the series gives

$$C_L^2 I_L \cong 1/[(2L+1)\rho^{2L+1}\Phi_L^2], \tag{6.5}$$

so that

$$G_L \cong \rho^{-L}/[(2L+1)C_L\Phi_L], \tag{6.6}$$

and

$$\Phi_L\Theta_L \cong 1. \tag{6.7}$$

This relation corresponds to what one expects from the JWKB approximation, in the $(L+\frac{1}{2})^2$ modification, which is applicable to these conditions and yields[13]

$$F_L G_L \cong \rho/[2(L+\frac{1}{2})], \tag{6.8}$$

in agreement with Eq. (6.7). The first derivative of Φ_L has been available in the present work through the calculation of the series Φ_L^*.

(d) A related method applicable under similar circumstances makes use of an effective value of L which will be referred to as L^* and which is defined by

$$L^* + 1 = \rho F'/F. \tag{7}$$

There are appreciable ranges of values of ρ for fixed η

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[13] Equation (38) of YWB.

for which L^* varies nearly linearly with ρ. If it is assumed that the variation of L^* between ρ_1 and ρ_2 is exactly linear then one obtains

$$[2\langle L^*\rangle+1]\int_{\rho_1}^{\rho_2}\frac{d\rho}{F^2}=\frac{\rho_1}{F^2(\rho_1)}-\frac{\rho_2}{F^2(\rho_2)}$$

$$+\frac{b/\langle L^*\rangle}{2\langle L^*\rangle+1}\left\{\frac{\rho_1{}^2}{F^2(\rho_1)}-\frac{\rho_2{}^2}{F^2(\rho_2)}\right.$$

$$\left.-\langle L^*\rangle(\rho_2-\rho_1)\left[\frac{\rho_1}{F^2(\rho_1)}-\frac{\rho_2}{F^2(\rho_2)}\right]\right\},\quad(7.1)$$

where

$$b=-[L^*(\rho_2)-L^*(\rho_1)]/(\rho_2-\rho_1),\qquad(7.2)$$

and

$$\langle L^*\rangle=[L^*(\rho_1)+L^*(\rho_2)]/2.\qquad(7.3)$$

The accuracy obtainable by this method is illustrated in Table I for intervals with $\rho_2-\rho_1=0.4$, $\eta=0$, $L=4$.

(e) A modification of the χ_L procedure for $L=0$.

The procedure described under (c) is not convenient for $L=0$. A modification is possible in this case which makes the numerical quadrature appreciably more manageable than it would be in a direct application of general quadrature formulas. The integral $I(\rho)$ is integrated partially once, yielding

$$C_0{}^2I(\rho)=-\rho^{-1}\Phi_0{}^{-2}(\rho)\bigg|_{\rho_1}^{\rho_2}+\int_{\rho_1}^{\rho_2}(1/\rho)(d\Phi_0{}^{-2}/d\rho)d\rho$$

$$=C_0{}^2\int_{\rho_1}^{\rho_2}d\rho/F_0{}^2.$$

By singling out the dominant term for small ρ under the integral sign, subtracting it from the integrand and integrating it separately there results

$$C_0{}^2I(\rho)=\left[-\frac{1}{\rho\Phi_0{}^2}-2\eta\ln\rho\right]\bigg|_{\rho_1}^{\rho_2}$$

$$+\int_{\rho_1}^{\rho_2}\left\{\frac{2\eta}{\rho}-\frac{2(\Phi_0{}^*-\Phi_0)}{\rho^2\Phi_0{}^3}\right\}d\rho.\quad(8)$$

For $\rho>1$, in the range of parameters used, this formula is only slightly better than a direct quadrature. For smaller ρ, however, the transformed form listed above as Eq. (8) gives a considerably higher accuracy than the original.

The special methods (c), (d), (e) described for small ρ have been valuable because the numerical integration of the differential equation has to be used with caution when G varies rapidly. A transformation of the independent variable to

$$\ln\rho$$

makes it feasible[7] to handle this region by the Hartree type of numerical integration. The methods (c), (d),

TABLE I. Values of error introduced by approximation of Eq. (7.1) for $\eta=0$, $L=4$, $\rho_2-\rho_1=0.4$.

$\rho_1=0.6$	3	4.6	5.0
Error (percent) 0.03	0.22	1.2	5.7

however, have the advantage of representing $G(\rho)$ very simply. In the work for the tabulations use has been made of the logarithmic transformation for occasional checks and some overlap between methods applicable to adjacent ranges of parameters was usually arranged for.

IV. NUMERICAL CALCULATION BY CONTOUR INTEGRATION

Most of the methods described in the preceding section are applicable only if the value of the irregular function $G(\rho)$ is available in some other way. An exception to the general rule is found for small ρ and large L. In this case the contributions to the integral in Eq. (4) from the region of small ρ outweight everything else and the result is very insensitive to the value of $G(\rho_1)$. In the general case, however, it is necessary to obtain $G(\rho_1)$ by some other means. An obvious way of doing so is to calculate one or a few values by the series listed by YWB. It has also been found practical to calculate the values by means of a numerical quadrature of one of the integral representations of the functions in the complex plane. The general method is similar to that of Hoisington and Breit.[14]

The same integral representation can be used[15] for the establishment of corrections to the expressions obtained by the application of the method of steepest descents. The latter are of special value for heavy elements and can be used for the theory of α-decay. Formulas by means of which one can evaluate corrections to the expressions obtained by the method of steepest descents will be also listed.

The starting point is the definite integral

$$Y_L=F_L+iG_L$$

$$=\frac{ie^{-i\rho}}{(2L+1)!C_L\rho^L}\int_0^\infty t^{-i\eta+L}(t+2i\rho)^{i\eta+L}e^{-t}dt,\quad(9)$$

where the integral may be terminated in any part of the complex plane for which $Re(t)=+\infty$. The saddle point lies at

$$t_0=\tau_0-i\rho,\quad\tau_0=L+(L^2+2\rho\eta-\rho^2)^{\frac{1}{2}},\qquad(9.1)$$

where the quantity τ_0 is supposed to be real. The path is led from $t=0$ to $t=-i\rho$ and from $t=-i\rho$ along a line parallel to the real axis to $-i\rho+\infty$. Its direction at t_0 is the same as that of the path of steepest descents. The integrand is expressed as an exponential, the integral is first approximated by neglecting all terms in the Taylor

[14] L. E. Hoisington and G. Breit, Phys. Rev. 54, 627 (1938).
[15] A. A. Broyles and J. L. Powell, Phys. Rev. 72, 155A (1947).

TABLE II. Values of $G_0/(G_0)_{SD}$.

$\rho=$	11	14	18	10	30	35
$\eta=$	16	16	16	20	20	20
$G_0/(G_0)_{SD}=$	1.012	1.013	1.016	1.010	1.027	1.099

expansion of the exponent around the saddle point and carrying out the integration from $-\infty$ to $+\infty$ for the variable $\tau=\tau_0-i\rho$. This approximation will be referred to here as the "steepest descents approximation." The difference between Y_L and its steepest descents approximation is evaluated by subtracting the integrands in the two integrals and correcting for the presence in the steepest descents approximation of an extra integral from $\tau=-\infty$ to $\tau=0$ and for the true function from $t=0$ to $t=-i\rho$. It is found in this manner that

$$G_L/(G_L)_{SD}=1+\frac{(\tau_0-L)^{\frac{1}{2}}}{(2\pi\rho\eta)^{\frac{1}{2}}(1+L\tau_0/\rho\eta)^{\frac{1}{2}}}$$

$$\times \int_0^\infty \exp[g(\tau_0)-g(\tau)]$$

$$-\exp[-(\tau-\tau_0)^2 g''(\tau_0)/2]d\tau$$

$$-\frac{1}{2}\left[1-\Phi\left(\frac{\tau_0(\tau_0-L)^{\frac{1}{2}}}{2^{\frac{1}{2}}(L\tau_0+\rho\eta)^{\frac{1}{2}}}\right)\right]$$

$$-\frac{(\tau_0-L)^{\frac{1}{2}}\rho^{2L+1}\exp[-\pi\eta+\tau_0+2\eta\,\tan^{-1}(\rho/\tau_0)]}{(2\pi)^{\frac{1}{2}}2^L(L\tau_0+\rho\eta)^{L+\frac{1}{2}}}$$

$$\times\int_0^1 (1-z^2)^L \sin\left(\rho z+\eta\,\ln\frac{1-z}{1+z}\right)dz, \quad (9.2)$$

where

$$\tau_0=L+(L^2+2\rho\eta-\rho^2)^{\frac{1}{2}}, \quad (9.3)$$

$$g(\tau)=\tau+2\eta\,\tan^{-1}(\rho/\tau)-L\ln(\rho^2+\tau^2), \quad (9.4)$$

$$g''(\tau_0)=(L^2-\rho^2+2\rho\eta)^{\frac{1}{2}}/(L\tau_0+\rho\eta), \quad (9.5)$$

and the value obtained by taking into account only the main term in the steepest descents integral is

$$(G_L)_{SD}=\frac{2^L(2\pi)^{\frac{1}{2}}(L\tau_0+\rho\eta)^{L+\frac{1}{2}}\exp[-\tau_0-2\eta\,\tan^{-1}(\rho/\tau_0)]}{(2L+1)!C_L\rho^L(\tau_0-L)^{\frac{1}{2}}}. \quad (9.6)$$

Equation (9.2) gives the correction factor which must be applied to $(G_L)_{SD}$ in order to obtain G_L. Values of $G_0/(G_0)_{SD}$ obtained by means of these formulas are reproduced in Table II. This quantity has the value 1.01 for $\eta=23$, $\rho=8$, 10, 13; $\eta=30$, $\rho=7$, 10. Variations in the correction factor occur in the latter cases in the third place after the decimal. Similarly for $\eta=20$, $\rho=10$

the correction factor has values 1.010, 1.0097, 1.0093, 1.0089 for $L=0$, 1, 2, 3 respectively; for $\eta=20$, $\rho=30$ it has the values 1.027, 1.025, 1.022, 1.018, 1.017 for $L=0$, 2, 4, 6, 7 and for $\eta=16$, $\rho=18$ the correction factor is 1.015, 1.014 for $L=0$, 1. The JWKB method yields a very similar approximation

$$(G_L)_{JWKB}=\frac{\rho^{\frac{1}{2}}(lT_0+\rho\eta)^l\exp\{\pi\eta-T_0-2\eta(\rho/T_0)+l-\eta\,\tan^{-1}(l/\eta)\}}{\rho^l\{\eta+l^2/[\eta+(l^2+\eta^2)^{\frac{1}{2}}]^l\}(T_0-l)^{\frac{1}{2}}}, \quad (10)$$

where

$$l=[L(L+1)]^{\frac{1}{2}}, \quad (10.1)$$

$$T_0=l+(l^2+2\rho\eta-\rho^2)^{\frac{1}{2}}. \quad (10.2)$$

The quantity $(G_L)_{JWKB}$ behaves similarly to $(G_L)_{SD}$. The correction factor $G_L/(G_L)_{JWKB}$ has the values 1.010, 1.0096, 1.011, 1.011 for $L=0$, 1, 2, 3 with $\eta=20$, $\rho=10$; 1.027, 1.026, 1.025, 1.023, 1.020 for $L=0$, 2, 4, 6, 7 with $\eta=20$, $\rho=30$. The values of ρ and η referred to above are in the general range needed for the calculation of the escape of alpha-particles from naturally radioactive nuclei. Thus, for example, a nuclear radius of 10^{-12} cm for atomic number $Z=80$ corresponds approximately to $\eta=22$, $\rho=10$.

The contour integral has proved to be useful for the calculation of F_L and G_L at the classical turning point; i.e., for values of ρ and η for which $\mathfrak{g}=0$. For this pur-

pose it proved practical to use

$$F_L=[D_L e^{-\pi\eta}\rho^{L+1}/(2L)!]\int_0^1 (1-z^2)^L \cos\xi dz, \quad (10.3)$$

$$G_L=[D_L e^{-\pi\eta}\rho^{L+1}/(2L)!]\int_0^1 (1-z^2)^L \sin\xi dz$$

$$+[\rho^{L+1}D_L/(2L)!]\int_0^\infty (1+u^2)^L$$

$$\times\exp[-u\rho-2\eta\,\tan^{-1}(1/u)]du, \quad (10.4)$$

where

$$\xi=2\eta\,\tanh^{-1}z-\rho z. \quad (10.5)$$

This computation has been carried out with the aid of auxiliary tables of $\tanh^{-1}z$, $\tan^{-1}(1/u)$, $(1+u^2)^L$, $(1-z^2)^L$ and for each η of $2\eta\,\tanh^{-1}z$, $\exp[-2\eta\,\tan^{-1}(1/u)]$, C_0,

$e^{-\pi\eta}$. In much of the numerical work it proved useful to replace dz in the integrals by $(dz/d\xi)d\xi$. Integration by parts when applied to $\int(\sin\xi)(dz/d\xi)d\xi$ gives outside the integral a result which would be exact if $dz/d\xi$ were constant, a second integration by parts gives a result which would be exact if $d^2z/d\xi^2$ were constant. By repeating this procedure convenient series have been obtained by means of which it has proved practical to evaluate the contributions to the integrals arising from regions within which the integrand has an oscillatory character.

V. RECURRENCE FORMULAS

A set of recurrence formulas developed by Powell[16] has proved to be very useful, especially as a means of checking values obtained by other means. A convenient set of formulas suitable for intercomparison of F_L, G_L for different L is

$$-\beta_{L-1}Y_{L-1}+\alpha_LY_L+\alpha_{L-1}Y_{L-2}=0, \qquad (11)$$

$$(\alpha_L{}^2-\beta_L\beta_{L-1})Y_L+\alpha_{L-1}\alpha_LY_{L-2} \\ +\beta_{L-1}\alpha_{L+1}Y_{L+1}=0, \quad (11.1)$$

$$(\beta_L\beta_{L-1}\beta_{L-2}-\alpha_{L-1}{}^2\beta_L-\alpha_L{}^2\beta_{L-2})Y_L \\ +(\alpha_{L-1}{}^2\alpha_{L+1}-\alpha_{L+1}\beta_{L-1}\beta_{L-2})Y_{L+1} \\ -\alpha_L\alpha_{L-1}\alpha_{L-2}Y_{L-3}=0, \quad (11.2)$$

$$\alpha_L(F_{L-1}G_L-F_LG_{L-1})=1, \qquad (11.3)$$

$$\alpha_L=[1+\eta^2/L^2]^{\frac12}, \\ \beta_L=(2L+1)\{\eta/[L(L+1)]+1/\rho\}. \qquad (11.4)$$

Equations (11.1), (11.2) are obtainable from Eq. (11). They are reproduced here so as to provide convenient ways of checking tables. An additional relation due to Powell which was also found to provide useful checks is

$$Y_L'+\alpha_{L+1}Y_{L+1}=\left[\frac{L+1}{\rho}+\frac{\eta}{L+1}\right]Y_L. \qquad (11.5)$$

A disadvantage of recurrence formulas as a means of checking is the frequent lack of indication as to which of the values is at fault if agreement is not secured.

VI. ADDITIONAL METHODS

The phase amplitude method has been found convenient as a means of checking. By means of it, values at smaller ρ can be compared with values in the region within which the Coulomb functions become essentially sinusoidal. It has also proved useful to tabulate the phase and the amplitude as a means of detecting slips in calculation. The smooth behavior of phase and amplitude as functions of ρ enable better detection of erroneous values than is readily possible with F_L, G_L. The relation

$$\varphi_L(\rho_2)-\varphi_L(\rho_1)=\int_{\rho_1}^{\rho_2}A_L{}^{-2}(\rho)d\rho$$

[16] J. L. Powell, Phys. Rev. 72, 626 (1947).

provides for an additional check. It is also possible to relate the phase amplitude method to the JWKB approximation for the larger ρ, as will be discussed presently.

The Hartree form of arranging a numerical integration of a differential equation is convenient as a means of extending tabulations to values of ρ not covered by other means. Numerical quadrature of $F''=-\mathfrak{g}F$ or $G''=-\mathfrak{g}G$ to check on F', G' and of these quantities for intercomparison with F, G is practically equivalent to a check by a numerical integration of the differential equation. Being somewhat simpler it has proved very useful in detecting slips. The JWKB method of approximation has been of occasional value in the work reported on. It suffers, however, from the disadvantage of having an accuracy which is difficult to ascertain except under special circumstances such as exist for the high repulsive barriers when alpha-particles react with heavy elements.

VII. VALUES OF PARAMETERS FOR NUCLEAR REACTIONS

In the notation,

$$M_u=\text{mass of oxygen atom}/16,$$
$$M_i=\text{mass of incident particle},$$
$$M_b=\text{mass of bombarded particle},$$

and on the assumption that the bombarded particle is at rest one has for the parameters of the first stage of the reaction

$$\eta=0.1574ZZ'E_{\text{Mev}}{}^{-\frac12}(M_i/M_u)^{\frac12}, \qquad (12)$$

where E_{Mev} is the energy of the incident particle measured in Mev.

$$\rho\eta=(ZZ'\mu/M_u)[r/(2.905\times10^{-12}\ \text{cm})], \quad (12.1)$$

where

$$\mu=M_iM_b/(M_i+M_b).$$

The set of units used is such that

$$\hbar/[(M_um)^{\frac12}c]=0.9043\times10^{-12}\ \text{cm}, \qquad (12.2)$$

and

$$\rho\eta=0.3113(\mu/M_u)ZZ'[r(M_um)^{\frac12}c/\hbar] \\ =0.0969(2)(\mu/M_u)ZZ'(rmc^2/e^2). \qquad (12.3)$$

If the reaction gives rise to two outgoing particles of masses M_1 and M_2 with an energy release Q then the value of η for the end products is

$$\eta=0.1574Z_1Z_2(E_{\text{Mev}}')^{-\frac12}(\mu'/M_u)^{\frac12}, \qquad (12.4)$$

where

$$\mu'=M_1M_2/M, \quad M=M_1+M_2, \qquad (12.5)$$

is the reduced mass for the second stage of the reaction and

$$E'=(M_b/M)E+Q, \qquad (12.6)$$

is the energy available in the rest system after disintegration.

TABLE III. Comparison of coefficients of series for A_L given by J.W.K.B. approximation and asymptotic series.

n	Coefficient of $(1/\rho)^n$ asymptotic series
0	1
1	$\dfrac{\eta}{2}.$
2	$\dfrac{5\eta^2}{8}+\dfrac{L(L+1)}{4}.$
3	$\dfrac{15\eta^3}{16}+\dfrac{5\eta L(L+1)}{8}-\dfrac{\eta}{4}.$
4	$\dfrac{195\eta^4}{128}+\dfrac{45\eta^2 L(L+1)}{32}-\dfrac{23\eta^2}{16}+\dfrac{5L^2(L+1)^2}{32}-\dfrac{3L(L+1)}{8}.$
5	$\dfrac{663\eta^5}{256}-\dfrac{91\eta^3}{16}+\dfrac{195\eta^3 L(L+1)}{64}+\dfrac{45\eta L^2(L+1)^2}{64}$ $-\dfrac{23\eta L(L+1)}{8}+\dfrac{3\eta}{4}.$
6	$\dfrac{4641\eta^6}{1024}-\dfrac{2431\eta^4}{128}+\dfrac{3315\eta^4 L(L+1)}{512}+\dfrac{585\eta^2 L^2(L+1)^2}{256}$ $-\dfrac{455\eta^2 L(L+1)}{32}+\dfrac{281\eta^2}{32}+\dfrac{15L^3(L+1)^3}{128}-\dfrac{13L^2(L+1)^2}{32}$ $+\dfrac{15L(L+1)}{8}.$

	J.W.K.B. approximation
0	1
1	$\dfrac{\eta}{2}.$
2	$\dfrac{5\eta^2}{8}+\dfrac{L(L+1)}{4}.$
3	$\dfrac{15\eta^3}{16}+\dfrac{5\eta L(L+1}{8}.$
4	$\dfrac{195\eta^4}{128}+\dfrac{45\eta^2 L(L+1)}{32}+\dfrac{5L^2(L+1)^2}{32}.$
5	$\dfrac{663\eta^5}{256}+\dfrac{195\eta^3 L(L+1)}{64}+\dfrac{45\eta L^2(L+1)^2}{64}.$
6	$\dfrac{4641\eta^6}{1024}+\dfrac{3315\eta^4 L(L+1)}{512}+\dfrac{585\eta^2 L^2(L+1)^2}{256}+\dfrac{15L^3(L+1)^3}{128}.$

VIII. QUANTITIES CONVENIENT FOR INTERPOLATION AND SOME RELATIONS USEFUL IN APPLICATIONS

For smaller ρ, especially for the higher L, the Coulomb functions F_L, G_L vary too rapidly for accurate interpolation. Here the quantities Φ_L, $\Phi_L\Theta_L$, $\Phi_L{}^*/\Phi_L$ form a convenient set. The latter two have the advantage of giving the combinations which are needed in the calculation of the amplitude of the wave function at the nuclear boundary in a "potential well" picture of the nucleus. The formula for the latter is[17]

$$\mathfrak{F}=F/(1-FG\delta-iF^2\delta),\qquad(13)$$

where

$$\delta=F'/F-\mathfrak{F}'/\mathfrak{F}.\qquad(13.1)$$

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[17] G. Breit and F. L. Yost, Phys. Rev. 48, 204 (1935).

At the nuclear boundary one knows $\mathfrak{F}'/\mathfrak{F}$ from the internal solution and one has it available for substitution into Eq. (13.1). It is convenient to deal with $FG\delta$ as

$$(FG/\rho)(\rho\delta).$$

The quantity $\rho\delta$ contains

$$\rho F'/F=\Phi^*/\Phi.\qquad(13.2)$$

The remaining quantity

$$\rho\mathfrak{F}'/\mathfrak{F}=xd\mathfrak{F}/\mathfrak{F}dx,\qquad(13.3)$$

where x is length expressed in any unit. The latter circumstance is convenient. The factor multiplying $\rho\delta$ is

$$F_L G_L/\rho=\Phi_L\Theta_L/(2L+1).\qquad(13.4)$$

The phase amplitude variables A_L, φ_L defined in the section on notation are very useful in applications and have good interpolation properties. They are connected by

$$A_L{}^2 d\varphi_L=d\rho,\qquad(13.5)$$

which make it possible to calculate differences in φ_L from values of A_L. In applying the phase amplitude variables it is natural to express results in terms of the phase shift K_L. A formula for the latter has been given by Wheeler.[8] Substituting for φ_L' its value in terms of $A_L{}^{-2}$ his formula becomes

$$xd\mathfrak{F}/\mathfrak{F}dx-\rho A'/A=(\rho/A^2)\cot(\varphi+K).\qquad(14)$$

Having K one can obtain $\mathfrak{F}$ at the nuclear boundary from

$$\mathfrak{F}=e^{iK}(F\cos K+G\sin K).\qquad(14.1)$$

Equation (14) is convenient when $\rho dA/Ad\rho$ is readily available. If this is not the case use can be made of

$$\cot(\varphi+K)-\cot\varphi=(\mathfrak{F}'/\mathfrak{F}-F'/F)A^2.\qquad(14.2)$$

A knowledge of the behavior of A_L for large ρ is helpful in determining values of the functions in regions not covered by the tables. It also can be used for starting a numerical integration of the differential equation for A_L toward smaller ρ. A list of coefficients of powers of $1/\rho$ in the asymptotic series for A_L is given in Table III. In this table the coefficients are compared with those corresponding to the usual JWKB approximation; i.e., to the approximation $A_L\cong\mathfrak{g}_L{}^{-1}$.

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