Asymptotic Expansion of Irregular Coulomb Function for Angular Momentum Zero

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A justification is given for an expansion of the irregular Coulomb function, usually denoted by G_0, in terms of Bessel functions of the second kind with an imaginary argument. This expansion has been considered speculatively by Yost, Wheeler, and Breit and explicitly verified by Breit and Bouricius for a number of terms. A general rule of replacement of the Bessel functions of the first kind with an imaginary argument in the corresponding expansion of the regular Coulomb function is here established. The formulas developed are convenient for the calculation of coefficients of the energy.

Notation

M, M' and Ze, $Z'e$, masses and charges of the particles.
μ = reduced mass; $\mu^{-1}=M^{-1}+(M')^{-1}$.
m = mass of electron.
v = relative velocity of the particles.
$k=\mu v/\hbar$.
$L\hbar$ = angular momentum.
$a=\hbar^2/\mu ZZ'e^2$.
$\eta=1/ka=ZZ'e^2/\hbar v$.
$\rho=kr$.
$x=(8\rho\eta)^{\frac{1}{2}}=(8r/a)^{\frac{1}{2}}$.
F_0, G_0 = regular and irregular solutions of the differential equation for $r\times$radial function for $L=0$; the signs and normalization are as in YWB.
$C_0^2=2\pi\eta/(e^{2\pi\eta}-1)$.
$\Phi_0=F_0/C_0\rho$ is a power series in ρ the first term of which is 1.
$\Theta_0=C_0G_0$.
$\Gamma(x)$ = gamma-function of x.
$\gamma=0.5772\cdots$ = Euler's constant.
$q=2\eta(2\gamma-1+\text{R.P.}\Gamma'(i\eta)/\Gamma(i\eta))$ for $L=0$.
$\Psi_0=\Theta_0-\rho(2\eta\ln 2\rho+q)\Phi_0$ is a power series in ρ beginning with the term 1 and having no term in ρ.
$p=2\eta$ for $L=0$.

I. INTRODUCTION

It has been shown by Yost, Wheeler, and Breit[1] that in the limit of zero energy the quotient $G_L/(D_L\rho^{-L})=\Theta_L$ approaches a finite limit,

$$\lim_{\eta=\infty}\Theta_L=-(2/(2L)!)(x/2)^{2L+1}K_{2L+1}(x), \tag{1}$$

where $K_\nu(x)$ is the Bessel function of an imaginary argument of the second kind defined by Whittaker and Watson's[2] Eq. (17.71). It has been also stated in that reference[1] that the replacement of K_{2L+1} by a series obtainable from the series for the regular Coulomb function by the substitution of the K_ν for the Bessel functions of an imaginary argument I_ν leads to values which agree in some cases with results obtained by direct calculation also at finite values of the energy. At the time there was no proof that the expansion of Θ_L in the K_ν is justifiable. For $L=0$ the expansion has been used by Breit and Bouricius.[3] These authors have verified the expansion for a number of terms by a rearrangement of the standard series for Θ_0. The quantity $\Gamma'(i\eta)/\Gamma(i\eta)$ which multiplies the regular function in the expression for Θ_0 was replaced in these calculations by Stirling's series for the logarithmic derivative of the Γ function. These calculations have been preceded by some closely related ones made by the present authors. Since then a different treatment has been published by Jackson and Blatt.[4] An explanatory note concerning the procedure of Breit and Bouricius was inserted in a footnote by Breit and Hatcher[5] and the relationship to the work of Jastrow[6] was pointed out. In the present note considerations are presented which demonstater that the replacement of the I_ν by the K_ν in the series for the regular function should lead to the result of employing Stirling's approximation for $\Gamma'(i\eta)/\Gamma(i\eta)$ in the standard expression for Θ_0. The replacements are meant to be made by means of Eqs. (7.24), (7.26) of Breit and Bouricius. These give

$$\Phi_0=\varphi_0+\varphi_1/\eta^2+\varphi_2/\eta^4+\cdots,$$
$$\varphi_0=(2/x)I_1(x),\ \cdots, \tag{2}$$
$$-2\Theta_0/x^2=\theta_0+\theta_1/\eta^2+\theta_2/\eta^4\cdots \tag{3}$$

and here the φ_i can be obtained from Eqs. (7.3), (7.31) of the same reference,[3] while the θ_i follow by replacing the I_ν by the K_ν. A proof can be given as follows.

It will first be noted that the expression for Θ_0 in terms of Ψ_0, Φ_0, p, q of YWB contains a term in $\ln\eta$ when ρ is expressed in terms of $r/a=\rho\eta$. The quantity q_0 contains $\Gamma'(i\eta)/\Gamma(i\eta)$. When Stirling's series is used for the logarithmic derivative of the gamma-function the term in $\ln\eta$ is removed everywhere, the two compensating terms occurring in the single factor $p\ln 2\rho+q$ which multiplies the regular function. The series for Θ_0 can be rearranged, therefore, as in Eq. (3). The symbols θ_i are independent of η but are functions of x. The cancellation of terms in $\ln\eta$ is essential for the validity of this form. The absence of positive powers of η is readily seen from the structure of Eq. (10) of YWB. The step of the proof, just conducted, will be referred to as step A.

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[1] Yost, Wheeler, and Breit, Phys. Rev. **49**, 174 (1936), referred to as YWB.

[2] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, London, 1920), third edition, Chapter XVII.

[3] G. Breit and W. G. Bouricius, Phys. Rev. **75**, 1029 (1949), referred to as BB.

[4] J. David Jackson and John M. Blatt, Rev. Mod. Phys. **22**, 77 (1950).

[5] G. Breit and R. D. Hatcher, Phys. Rev. **78**, 110 (1950).

[6] R. Jastrow, Phys. Rev. **73**, 60 (1948).

It will next be noted that Whittaker's integral representation of Whittaker's confluent hypergeometric function gives

$$F_0+iG_0=(ie^{-i\rho}/C_0)\int_0^\infty t^{-i\eta}(t+2i\rho)^{i\eta}e^{-t}dt$$

$$=(i/C_0)\int_{i\rho}^\infty (\tau-i\rho)^{-i\eta}(\tau+i\rho)^{i\eta}e^{-\tau}d\tau, \quad (4)$$

where each of the integrals may be taken along an arbitrary path from the lower limit to the infinitely remote part of the complex plane to the right of the axis of pure imaginaries. This requirement is essential because it is necessary to require that

$$e^{-t}t^{L-i\eta+1}(t+2i\rho)^{L+i\eta-1}$$

have vanishing values at both limits of integration. In terms of the variable τ the original path of integration from $t=0$ to $t=\infty$, along the axis of reals in the t plane, corresponds to integration along the straight line $Im\tau=\rho$. This path may be deformed into a path along two straight lines, the first from $\tau=i\rho$ to $\tau=0$, the second from $\tau=0$ to $\tau=\infty$. In the process of deforming the path one must vary $\arg t=\arg(\tau-i\rho)$ as well as $\arg(\tau+i\rho)$ continuously. Accordingly $\arg(\tau-i\rho)$ on the vertical part of the path is $-\pi/2$, while $\arg(\tau+i\rho)$ on this part of the path is $+\pi/2$. There results, therefore, the factor $\exp(-\pi\eta)$ which multiplies

$$|\tau-i\rho|^{-i\eta}|\tau+i\rho|^{i\eta}$$

in the integrand. It now follows that

$$C_0(F_0+iG_0)=e^{-\pi\eta}\rho\int_0^1 (1-u)^{-i\eta}(1+u)^{i\eta}e^{-i\rho u}du$$

$$+i\int_0^\infty \exp[-\tau-2\eta\tan^{-1}(\rho/\tau)]d\tau. \quad (5)$$

Hence

$$\Theta_0=C_0G_0=\Theta_0{}^I+\Theta_0{}^{II}, \quad (6)$$

where

$$\Theta_0{}^I=\int_0^\infty \exp[-\tau-2\eta\tan^{-1}(\rho/\tau)]d\tau \quad (6')$$

and

$$\Theta_0{}^{II}=e^{-\pi\eta}\rho\int_0^1 \sin\left[-\rho u+\eta\log\frac{1+u}{1-u}\right]du. \quad (6'')$$

The real part of Eq. (5) gives

$$F_0=(\rho e^{-\pi\eta}/2C_0)\int_{-1}^{+1}(1-u)^{-i\eta}(1+u)^{i\eta}e^{-i\rho u}du$$

$$=(\rho e^{-\pi\eta}/2C_0)[|\Gamma(1+i\eta)|^2/i\rho]M_{i\eta,\frac{1}{2}}(2i\rho)$$

$$=C_0M_{i\eta,\frac{1}{2}}(2i\rho)/(2i), \quad (7)$$

in agreement with the fact that F_0 is the regular solution which can be expressed as a power series having for the first term $C_0\rho$. The quantity $\Theta_0{}^I$ is readily transformed into

$$\Theta_0{}^I=(x/2)\int_0^\infty \exp[-(x/2)(v+1/v)]$$

$$\times\exp[2\eta(\xi-\tan^{-1}\xi)]_{\xi=x/4\eta v}dv. \quad (8)$$

The establishment of Eqs. (6)–(8) will be referred to as part B of the proof.

It will be shown next that the expansion defined by part A of the proof can be obtained from the following symbolic expression for G_0

$$C_0(G_0)_{\text{symb}}=(\Theta_0)_{\text{symb}}=(x/2)\int_0^\infty e^{-(x/2)(v+1/v)}$$

$$\times\exp\{-2\eta\Sigma_1{}^\infty(-)^n\xi^{2n+1}/(2n+1)\}_{\xi=x/4\eta v}dv. \quad (9)$$

The relation of Eq. (9) to Eq. (8) is that of replacing $\xi-\tan^{-1}\xi$ by its Taylor expansion. The employment of the symbolic expression for G_0 is meant in the sense that if one expands the exponential containing ξ in a power series in $1/\eta$ and integrates over v then one obtains a representation of $G_0=\Theta_0/C_0$ which is claimed to be identical with that obtained by the Stirling series procedure described in part A of the proof. In fact according to Eq. (3)

$$-x^2\theta_s/2=(1/s!)[\partial^s\Theta_0/\partial(\eta^{-2})^s]_{\eta=\infty}. \quad (10)$$

This relation is true irrespective of questions of convergence of the right side of Eq. (3). In fact Stirling's asymptotic series for $\Gamma'(y)/\Gamma(y)$ has the property that the coefficient of $1/y^2$ can be obtained by successive differentiation of

$$\Gamma'(y)/\Gamma(y)-\ln y+1/2y \quad (11)$$

and equating both sides of the resultant equation as though Stirling's series were a convergent rather than an asymptotic one. The reason for this circumstance is the fact that the above expression is

$$-2\int_0^\infty \frac{tdt}{(t^2+y^2)(e^{2\pi t}-1)}=I \quad (12)$$

and that Stirling's series is obtainable by expanding $1/(t^2+y^2)$ in ascending powers of t^2/y^2 and integrating term by term in accordance with Eq. (12). On the other hand,

$$\{\partial^sI/\partial(y^{-2})^s\}_{y=\infty}$$

$$=-2\int_0^\infty \frac{t}{e^{2\pi t}-1}\left\{\frac{\partial^s}{\partial(y^{-2})^s}(t^2+y^2)^{-1}\right\}_{y=\infty}dt, \quad (13)$$

and

$$\left\{\frac{\partial^s}{\partial(y^{-2})^s}(t^2+y^2)^{-1}\right\}_{y=\infty}=s!(-)^{s-1}t^{2s-2}. \quad (13')$$

The differentiation under the integral sign in Eq. (13) is legitimate because the integrals converge for all derivatives.

In the present application the variable $y=i\eta$. The The term $\ln\eta$ in Eq. (11) is removed by a similar term arising from $\ln\rho$. The term in $1/y$ does not enter because $1/y$ is purely imaginary. The expression listed as Eq. (11) is, therefore, the one of interest. The differentiation of Θ_0 involves the differentiation of Φ_0, p, q and Ψ_0, ρ. An inspection of Eq. (18) of YWB shows that $p\rho=2r/a$ does not bring in η and that Ψ_0, Φ_0, and the expression listed under Eq. (11) are the only ones containing η. Since Ψ_0, Φ_0 are absolutely convergent their differentiation with respect to η^{-2} can be performed as though they were polynomials. It has just been shown that the same may be done employing Stirling's series for the expression arising from q and listed under (11). It follows, therefore, that one may use Eq. (10) in order to evaluate θ_s even though the series for Θ_0 in powers of η^{-2} is an asymptotic one.

Returning to Eq. (6) it will now be sufficient to consider separately the contributions arising from the two parts of Θ_0. The presence of $e^{-\pi\eta}$ in Θ_0^{II} causes the disappearance of its contributions to the right side of Eq. (10). The form of Θ_0^I presented as Eq. (8) and the expansion

$$\tan^{-1}\xi=\Sigma_0^\infty(-)^n\xi^{2n+1}/(2n+1)$$

show that these derivatives can be obtained by forgetting temporarily that the expansion of $\tan^{-1}\xi$ is inapplicable for $\xi>1$ because this circumstance is irrelevant in the evaluation of successive derivatives for $\xi=0$. It now follows that the θ_s can be obtained by means of a formal expansion of Eq. (9) in powers of η^{-2}, successive differentiation with respect to η^{-2} and evaluation for $\eta=\infty$ by means of Eq. (10). The procedure of performing differentiations is unnecessary, however, because the symbolic expansion furnishes the coefficients directly. Eq. (10) had to be brought into the discussion only as a means of defining coefficients of an asymptotic series. Since the power series in ξ for the second exponential in Eq. (9) is a power series in η^{-2} it has been proved by now that the formal expansion of the integrand of Eq. (9) in ascending powers of η^{-2} yields a series which is identical with that obtained through the replacement of $\Gamma'(i\eta)/\Gamma(i\eta)$ by Stirling's series. The part of the proof just concluded will be referred to as part C. It demonstrated the equivalence of the symbolic expansion to the employment of Stirling's series.

It remains to show that the θ_s are obtainable from the φ_s by replacing the $I_\nu(x)$ by the $K_\nu(x)$. A proof of this can be given by noting that the recurrence relations for the $I_\nu(x)$ and $K_\nu(x)$ are the same, that the Taylor expansion of the second exponential factor in Eq. (9) brings in powers of x which combine with the Bessel functions and that the powers are in agreement with the lowest permissible ones occurring for Φ_0. It is hard to write out this proof briefly and unambiguously because of the necessity for distinguishing between operations on the I_ν and K_ν. A more usual type of proof will be given, therefore, making use of the possibility of expressing Φ_0 in a form similar to Eq. (9).

It follows from Eq. (7) that

$$\begin{aligned}\Phi_0&=\frac{\sinh(\pi\eta)}{2\pi\eta}\int_{-1}^{+1}(1-u)^{-i\eta}(1+u)^{i\eta}e^{-i\rho u}du\\&=\frac{\sinh(\pi\eta)}{\pi\eta}\int_{-\infty}^{\infty}\left\{\exp\left[i\eta\theta-i\frac{x^2}{8\eta}\tanh\frac{\theta}{2}\right]\right\}e^\theta(e^\theta+1)^{-2}d\theta.\end{aligned} \quad (14)$$

In the second form of Φ_0, listed above, the parts $e^{\pi\eta}/2$ and $e^{-\pi\eta}/2$ of $\sinh(\pi\eta)$ will be first considered separately. For the first, the path of integration is moved to the line $Im\theta=\pi$, going around the point $\theta=\pi i$ in a small semicircle from below. For the second part the path is moved to the line $Im\theta=-\pi$, going around $\theta=-\pi i$ in a small semicircle from above. The two integrals can then be combined into one since the contributions on the rectilinear portions of the paths cancel. One finds by a short calculation

$$\Phi_0=-\frac{1}{2\pi\eta}\int_C\left\{\exp\left[i\theta\eta-i\frac{x^2}{8\eta}(e^\theta+1)\Big/(e^\theta-1)\right]\right\}\times e^\theta(e^\theta-1)^{-2}d\theta, \quad (14')$$

where C is a contour around $\theta=0$, taken counterclockwise. Expressing this result in terms of u and introducing a variable of integration

$$\zeta=ix/(4\eta u), \quad (15)$$

one obtains

$$\begin{aligned}\Phi_0&=\frac{i}{\pi x}\int_C\left(1+\frac{ix}{4\eta\zeta}\right)^{i\eta}\left(1-\frac{ix}{4\eta\zeta}\right)^{-i\eta}e^{-x\zeta/2}d\zeta\\&=\frac{i}{\pi x}\int_C e^{-(x/2)(\zeta+1/\zeta)}\\&\quad\times\exp\{-2\eta\,\Sigma_1^\infty(-)^n(x/4\eta\zeta)^{2n+1}/(2n+1)\}d\zeta.\end{aligned} \quad (16)$$

In the last formula C denotes a counterclockwise contour around the origin in the ζ plane. This form of Φ_0 is directly comparable with

$$-(2/x^2)[\Theta_0]_{\text{symb}}.$$

It is seen by means of Eq. (9) that aside from the fact that the integrals in Eqs. (9), (16) are over different variables and different paths their integrands have the same form and that the formula for Φ_0 contains an extra factor $1/(\pi i)$. The standard integral

$$K_\nu(x)=\frac{(x/2)^\nu\Gamma(\frac{1}{2})}{\Gamma(\nu+\frac{1}{2})}\cos(\pi\nu)\int_0^\infty e^{-x\cosh\theta}\sinh^{2\nu}\theta d\theta$$

may be expressed as

$$K_\nu(x)=\frac{(x/2)^\nu\Gamma(\frac{1}{2})}{2\Gamma(\nu+\frac{1}{2})}\cos(\pi\nu)\int_0^\infty e^{-(x/2)(v+1/v)}\times\left(\frac{v}{2}-\frac{1}{2v}\right)^{2\nu}\frac{dv}{v} \quad (17)$$

and one has also

$$I_\nu(x)=\frac{(x/2)^\nu\Gamma(\frac{1}{2})}{\pi\Gamma(\nu+\frac{1}{2})}\int_0^\pi \cosh(x\cos\varphi)\sin^{2\nu}\varphi d\varphi$$
$$=\frac{(x/2)^\nu\Gamma(\frac{1}{2})}{2\pi i\Gamma(\nu+\frac{1}{2})}\cos(\pi\nu)\int_C e^{-(x/2)(\zeta+1/\zeta)}\times\left(\frac{\zeta}{2}-\frac{1}{2\zeta}\right)^{2\nu}\frac{d\zeta}{\zeta}, \quad (18)$$

the last contour being in the same sense as in Eq. (16). It will be noted that the integrands in Eqs. (17), (18) differ only by a change of the letter v to ζ, that the contours differ in the same way as in the representations of $-2\Theta_0/x^2$ and Φ_0 by Eqs. (9), (16) and that the extra factor $1/(\pi i)$ occurs in the formula for I_ν, just accounting for its presence in Eq. (16). The collection of the same powers of $1/\eta^2$ in Eq. (16) must lead to the Bessel function expansion of YWB since there can be only one such expansion. The same process applied to $-2\Theta_0/x^2$ through Eq. (9) will give in accordance with Eqs. (9), (16)–(18) the same form for the θ_s as for the φ_s but with the I_ν replaced by K_ν.

It may be mentioned that the symbolic expansion of Θ_0 and the analogous form for Φ_0 are reasonably convenient for the calculation of coefficients of η^{-2s}. The absence of the I_ν in the series for Θ_0 means that all terms of the asymptotic expansion vanish exponentially with x for large x. These terms provide, therefore, a continuous passage to the solutions of negative energy for which the particles are bound to each other by a deviation from the Coulomb law at short distances.

It is clearly possible to subtract the term in $[\Gamma'(i\eta)/\Gamma(i\eta)-\log\eta]\rho\Phi_0$ from Θ_0, expressing it by means of Stirling's series and then to add it again without the use of Stirling's series. The calculations of Jackson and Blatt[4] give a formula which has this relation to the asymptotic expansion discussed here. The law of formation of the coefficients appears to be simplest, however, for the asymptotic series and it can be used as a starting point for the modification just mentioned avoiding the somewhat laborious operations which appear to be necessary in the solution of the chain of equations for the θ_s. Whether one does so or not does not matter in the calculation of Ψ_0. This quantity is the only one used by BB.

In connection with the calculations of BB, the Bessel function expansion of Ψ_0 was compared with series calculations of Breit, Thaxton, and Eisenbud[7] for proton-proton interaction in the energy range 0.2 to 2.8 Mev, and of Thaxton and Hoisington[8] in the energy range 3 to 9 or 10 Mev. It was found that the Bessel function expansion including the term in E^2 gave values of Ψ_0 0.05 percent smaller than exact calculations at 2.8 Mev for $r=0.75e^2/mc^2$ and 0.001 percent larger for $r=e^2/mc^2$. In the higher energy range, the Bessel function expansion gave a result smaller than the results of exact calculations at 10 Mev by 0.07 percent for $r=0.75e^2/mc^2$, and at 9 Mev by 2.4 percent for $r=e^2/mc^2$. A Bessel function expansion including only the linear term in E was found to give agreement within 0.4 percent below 2.8 Mev.

[7] Breit, Thaxton, and Eisenbud, Phys. Rev. **55**, 1018 (1939).
[8] H. M. Thaxton and L. E. Hoisington, Phys. Rev. **56**, 1194 (1939).