and this is impossible for any positive real value of λ . Adding a factor p to the trial solution does not improve the situation.

Thus even the possibility of noncovariant solutions of the integral equation has to be excluded.

IV. DISCUSSION

The foregoing conclusions might be interpreted as casting doubt on the ability of the S-B equation to predict bound states. It might appear that the solutions of this equation obtained by various authors are merely a feature of the noncovariant approximations which they used. The present author, however, would prefer to take the view that the extreme value of the binding energy assumed by Goldstein is responsible for his failure to obtain a valid discrete value of the coupling constant. If one gave the binding energy of the ground

state its maximum value (infinity) in the nonrelativistic approximation, one would not get a solution there either. One may thus maintain that to give a binding energy equal to the total rest-energy of the two nucleons, the coupling constant would have to be infinite, and that the possibility of a discrete finite value for any other binding energy is not excluded.

Goldstein stated that an expansion of the solution in powers of the total energy appeared to be singular, and if that is so it rather supports such a conclusion. But what is really needed is independent evidence of the nature of the solutions of the S-B equation for general values of the binding energy. Such evidence should not be founded on a noncovariant approximation, as covariance is clearly the crux of the matter. The author hopes to present a completely covariant treatment of the S-B equation in the near future.

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Coulomb Functions for Large Charges and Small Velocities*

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Expansions in powers of $\eta^{-\frac{1}{2}}$, where η is defined in the introduction below, for the Coulomb wave functions $F_L(\rho)$ and $G_L(\rho)$ and their derivatives are given for special values of $\rho = 2\eta$ and $\rho = \rho_L = \eta + [\eta^2 + L(L+1)]^{\frac{1}{2}}$, the classical turning points for L=0 and any L, respectively. Expansions applicable in the vicinity of the turning point are given as a series involving Bessel functions of order $\pm n/3$ with the expansion parameter $\rho_L^{-\frac{1}{2}}$. Approximations valid for large values of η are given and discussed.

I. INTRODUCTION

UCLEAR reactions involving "heavy" charged particles^{1,2} and the inelastic scattering of charged particles by nuclei^{3,4} have recently been the object of several investigations, both theoretical and experimental. In both cases, the Coulomb interaction can be expected to play a dominant role, and the Coulomb wave functions are necessary for discussions of nuclear interactions of this type. It is evident, that for the parameter

$\eta = ZZ'e^2/\hbar v,$

which, together with $\rho = kr$ and L, characterize the Coulomb function,⁵ the values of interest will be fairly large; η , for example, lies in the range 5–15. Tabulations in this particular range of parameters are either unavailable or incomplete⁶ and the present work was undertaken to fill this need as far as feasible, with particular emphasis on large values of the parameter η . It extends and supplements the earlier work of Breit and his associates,7 and of Abramowitz and Morse,8 and in part runs parallel to or overlaps work of Newton,9

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⁵ Yost, Wheeler, and Breit, Phys. Rev. **49**, 174 (1936). ⁶ The recent appearance of tables with $1 \le \eta \le 10$ [U. S. National Bureau of Standards Report No. 3033 (unpublished)] by C. E. Froberg and P. Rabinowitz is a welcome addition in this range

⁷ Yost, Wheeler, and Breit, reference 5; G. Breit and M. H. Hull, Jr., Phys. Rev. 80, 392 (1950) and Phys. Rev. 80, 561 (1950); Bloch, Hull, Broyles, Bouricius, Freeman, and Breit, Phys. Rev. 80, 553 (1950).

⁸ M. Abramowitz, Tables of Coulomb Functions, Vol. I, U. S. National Bureau of Standards Applied Mathematics Series, No. 17 (1952). Several expansions due to Mr. Abramowitz are discussed in the introduction, pp. xv-xxvii, and one due to P. M. Morse.

⁹ T. D. Newton, Atomic Energy of Canada, Limited, Report CRT-526, 1952 (unpublished).

Tyson,¹⁰ Feshbach, Shapiro, and Weisskopf,¹¹ and more recent work of Abramowitz.¹² Two different needs have been kept in mind in this work: The desirability of having formulas for calculating the functions at given points to high accuracy for starting numerical integrations, and of being able to obtain fairly good values of the functions for any value of ρ , η , L for estimates, checks, etc. The first expressed need is met here in series which converge rapidly for large η and for $L < \eta$, $L > \eta$, $L > \eta$ at two special values of $\rho: \rho = 2\eta$ and $\rho = \rho_L \equiv \eta + [\eta^2 + L(L+1)]^{\frac{1}{2}}$. These will be recognized, respectively, as the classical turning point for L=0 and for any L. The methods of obtaining the expansions start from the integral representations of the functions (given, in the form used here, by Bloch, Hull, Broyles, Bouricius, Freeman, and Breit¹³). Use of the special points indicated leads to simplifications in the work. Expansions for arbitrary values of ρ in the vicinity of the turning points are also obtained. A noteworthy lack of dependence on L is found, and for general values of $\rho < \rho_L$ extending down to fairly small fractions of ρ_L , it has been found possible to group the functions rather close to a "universal" curve from which values for any n, L can be read.

The second need is met by an approximation by means of Bessel functions of order one-third which is an extension of the procedure given by Morse and Feshbach.¹⁴ Again the integral representation, or expressions obtained from it, is used to evaluate constants in the approximation. For the present case, it is found that the difference between the potential appearing in the equation actually solved by the usual Morse-Feshbach approximation and the true Coulomb potential is nearly proportional to ρ^{-2} . An improved approximation is easily obtained, therefore, by defining an effective value of L in the Morse-Feshbach potential. This approach is pursued, and comparisons of accuracy are made for several special values of ρ . The approximation suffers, of course, because its accuracy is not definitely assignable for arbitrary ρ , but its virtue is that it yields values of the function for any ρ with an error not expected to exceed one or two percent.

II. EXPANSIONS AT THE TURNING POINTS

Expansions at the turning points for $F_L(\rho)$ and $G_L(\rho)$ and their derivatives, valid for large values of η and moderate values of $L < \eta$, have been obtained from the integral representations for these functions given in the paper of Bloch, Hull, Broyles, Bouricius, Freeman, and Breit¹³—their equation (9). In what follows we shall use the notation of this paper. It is convenient to introduce a notation for the classical turning point, ρ_{L_1} which has the value:

$$\rho_L = \eta + [\eta^2 + L(L+1)]^{\frac{1}{2}}$$

Letting $Y_L(\rho) = F_L(\rho) + iG_L(\rho)$, one finds from reference 13, Eq. (9), that:

$$Y_{L}(\rho) = ie^{-i\rho} [(2L+1)! C_{L}\rho^{L}]^{-1} \\ \times \int_{0}^{\infty} t^{-i\eta+L} (t+2i\rho)^{i\eta+L} e^{-i} dt, \\ C_{L} \equiv [2^{L}/(2L+1)!] \{ [L^{2}+\eta^{2}] [(L-1)^{2}+\eta^{2}] \cdots \\ \times [1+\eta^{2}] \}^{\frac{1}{2}} [2\pi\eta/(e^{2\pi\eta}-1)]^{\frac{1}{2}}.$$
(1)

Consider first the expansion for $\rho = \rho_0 = 2\eta$. With $\rho = 2\eta$ and the new variable z introduced by $t = i\rho_0(z-1)$, Eq. (1) becomes

$$Y_{L}(\rho_{0}) = -\frac{e^{-\pi\eta}(2\eta)^{L+1}}{\left[C_{L}(2L+1)!\right]} \int_{1}^{1-i\infty} (1-z^{2})^{L} \\ \times \exp\left\{i\eta\left[\ln\left(\frac{1+z}{1-z}\right) - 2z\right]\right\} dz. \quad (2)$$

Introducing another change of variable defined by

$$2w^{3}/3 = \ln[(1+z)/(1-z)] - 2z,$$
 (3)

one can put Eq. (2) in the form

$$Y_{L}(\rho_{0}) = \frac{e^{-\pi\eta}(2\eta)^{L+1}}{\left[(2L+1)!C_{L}\right]} \int_{\Gamma} \left[1-z^{2}(w)\right]^{L} \\ \times \exp\left[\frac{2}{3}i\eta w^{3}\right] \frac{dz(w)}{dw} dw, \quad (4)$$

where the contour Γ is taken from $-i\infty$ to 0 and from 0 to ∞ . The desired expansion now results when $[1-z^2(w)]^L dz(w) dw$ is expanded in a power series in w. and term-by-term integration is carried out. Upon taking the real and imaginary parts separately, the desired expansions for F_L and G_L are obtained. This procedure is quite straightforward and will not be discussed in detail. The series for G_L differs from that for F_L only in that some of the terms differ in sign and there is an over-all difference in size by the factor $\sqrt{3}$. Utilizing this fact, one can express the final results in the compact form

$$\begin{cases} F_{L}(\rho_{0}) \\ G_{L}(\rho_{0})/\sqrt{3} \end{cases} = \frac{1}{2}\Gamma(\frac{1}{3})\pi^{-\frac{1}{2}}(\frac{2}{3}\eta)^{1/6}(1-e^{-2\pi\eta})^{\frac{1}{2}} \\ \times \{1\mp [3/35+L(L+1)/2]a\eta^{-4/3}-[2/225 \\ +L(L+1)/20]\eta^{-2}\mp [724/170\ 625 \\ +L(L+1)/6300-L^{2}(L+1)^{2}/8]a\eta^{-10/3}+\cdots\}, \quad (5) \end{cases}$$

¹⁰ J. K. Tyson, thesis, Massachusetts Institute of Technology (1948) (unpublished).

 ¹¹Feshbach, Shapiro, and Weisskopf, Atomic Energy Commission Reports NYO 3077, NDA 15B-5, 1953 (unpublished).
 ¹² M. Abramowitz and H. A. Antosiewicz, U. S. National Bureau of Standards Report No. 3225, 1954 (unpublished); M. Abramowitz and P. Rabinowitz (to be published).

¹³ Bloch, Hull, Broyles, Bouricius, Freeman, and Breit, 4th reference of footnote

¹⁴ P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, Chap. 9.

where

$$a \equiv \left(\frac{3}{2}\right)^{\frac{1}{3}} \Gamma\left(\frac{2}{3}\right) / \Gamma\left(\frac{1}{3}\right),$$

and where the upper sign before an expression on the right is to be taken with the upper function on the left, and similarly with the lower. This convention is utilized throughout the paper.

It should be mentioned that in obtaining Eq. (5) an expansion of the coefficient C_L [given in Eq. (1)] has been made. In addition, it might be of interest to note that the coefficients for the $\eta^{-2\nu/3}$ terms in the brackets with $\nu = 6n+1$ and $\nu = 6n+4$ always vanish.

Similar series for the derivatives, at $\rho = \rho_0$, can be obtained in two ways, either from the integral representation, Eq. (1), after differentiating, or from the recurrence relation, Eq. (11.5) of reference 13. The results are identical, of course, and have the form

$$\begin{cases} F_{L'}(\rho_{0}) \\ G_{L'}(\rho_{0})/\sqrt{3} \end{cases} = \frac{1}{2}\Gamma(\frac{2}{3})\pi^{-\frac{1}{2}}(2\eta/3)^{-1/6}(1-e^{-2\pi\eta})^{-\frac{1}{2}} \\ \times \{\pm 1+(1/10a)\eta^{-\frac{3}{2}}\pm(1/3150)\eta^{-2} \\ +([359/173\ 250-L^{2}(L+1)^{2}/16]/a)\eta^{-8/3}+\cdots\}.$$
(6)

The coefficients for the $\eta^{-2\nu/3}$ terms in brackets with $\nu = 6n+2$ and $\nu = 6n+5$ always vanish, so that the first omitted term in Eq. (6) is of order η^{-4} compared to unity.

Instead of evaluating all the functions at the same point, say ρ_0 as above, it is useful to evaluate the functions for a given L at their own turning point, ρ_L . It develops that the results one then obtains are sensibly independent of the value of L.

To accomplish this one first of all changes the variable in Eq. (1) by the substitution $t \equiv i\rho(z-1)$. Then $Y_L(\rho)$ becomes

$$Y_{L}(\rho) = \left[e^{-\pi \eta} \rho^{L+1} / C_{L}(2L+1) ! \right] \int_{1-i\infty}^{1} e^{\varphi(z)} dz,$$

$$\varphi(z) \equiv L \ln(1-z^{2}) + i\eta \ln[(1+z)/(1-z)] - i\rho z.$$
(7)



FIG. 1. $F_L(\rho_0)$ plotted as a function of L^2 for $\eta = 5$, 10, 15, 20 on a semi-log scale. Equation (5) was used in the calculations for $L \leq \eta$, and Eq. (A3) when $L \geq \eta$. The smooth variation of the curves allows easy interpolation in L for a given value of η .

If φ is differentiated with respect to z, one finds

$$d\varphi/dz = (1-z^2)^{-1} [i\rho(z+iL/\rho)^2 + i(2\eta - \rho + L^2/\rho)].$$
(8)

This suggests, first, that the variable be changed yet again from z to $s \equiv z + iL/\rho$ and, second, that one choose ρ to be that value for which $2\eta - \rho + L^2/\rho = 0$. This is not the usual "classical" turning point value for ρ [in the sense that $L(L+1) \rightarrow L^2$ it is an even more "classical" value!] but the difference is rather slight. Designating this value of ρ by $\bar{\rho}_L$, one has $\bar{\rho}_L = \eta + [\eta^2 + L^2]^{\frac{1}{2}}$. Although the work is considerably simpler for $\bar{\rho}_L$ than for ρ_L , the resulting formulas for F_L , G_L , and their derivatives assume the more compact form for $\rho = \rho_L$. The shift from $\bar{\rho}_L$ to ρ_L is easily accomplished by a Taylor's series. This apparently roundabout procedure outlined above is easier algebraically than the direct expansion at ρ_L .

Proceeding in this way, one finds that for $\rho = \bar{\rho}_L$

where

$$\varphi = \varphi_0 + \left[(i\bar{\rho}_L s^3/3 (1 + L^2/\bar{\rho}_L^2)] + \cdots, \right] \qquad (9)$$

$$\varphi_0 = L \ln(1 + L^2/\bar{\rho}_L^2) - L + 2\eta \tan^{-1}(L/\bar{\rho}_L).$$

In exact analogy to the methods used for the case where $\rho = 2\eta$, one now makes still another change of variable defined by

$$\varphi \equiv \varphi_0 + i\bar{\rho}_L w^3 / [3(1 + L^2 / \bar{\rho}_L^2)].$$

The final result is

$$Y_{L}(\bar{\rho}_{L}) = \frac{e^{(\varphi \phi - \pi \eta)} \bar{\rho}_{L}^{L+1}}{(2L+1)! C_{L}}$$
$$\times \int_{\Gamma} \exp\left(\frac{i\rho w^{3}}{3(1+L^{2}/\bar{\rho}_{L}^{2})}\right) \left(\frac{dz}{dw}\right) dw. \quad (10)$$

The contour Γ is the same as for Eq. (4), and the details of the work are exactly as earlier. The results are

$$\begin{cases} F_{L}(\bar{\rho}_{L}) \\ G_{L}(\bar{\rho}_{L})/\sqrt{3} \end{cases} = \frac{1}{2} \Gamma(\frac{1}{3}) \pi^{-\frac{1}{2}} (\bar{\rho}_{L}/3)^{1/6} (1 + L^{2}/\bar{\rho}_{L}^{2})^{-1/6} \\ \times \left\{ 1 \mp \bar{\rho}_{L}^{-\frac{1}{2}} b (1 + L^{2}/\bar{\rho}_{L}^{2})^{-\frac{3}{2}} (L/\bar{\rho}_{L}) \\ + \frac{\bar{\rho}_{L}^{-1} (L/\bar{\rho}_{L}) (2L^{2}/\bar{\rho}_{L}^{2} - 1)}{10 (1 + L^{2}/\bar{\rho}_{L}^{2})^{2}} \\ \mp \bar{\rho}_{L}^{-4/3} b (b/35 - 11L^{2}/35\bar{\rho}_{L}^{2} \\ + L^{4}/140\bar{\rho}_{L}^{4}) + \cdots \right\}, \quad (11)$$

$$\begin{cases} G_{L'(\bar{\rho}_{L})/\sqrt{3}} &= \frac{1}{2}\Gamma(\frac{2}{3})\pi^{-\frac{1}{2}}(\bar{\rho}_{L}/3)^{-1/6}(1+L^{2}/\rho_{L}^{2})^{1/6} \\ &\times \left\{ \pm 1 + \frac{\bar{\rho}_{L}^{-\frac{2}{3}}(2-L^{2}/\bar{\rho}_{L}^{2})}{10b(1+L^{2}/\bar{\rho}_{L}^{2})^{4/3}} + \cdots \right\}, \quad (12)$$

544



FIG. 2. $G_L(\rho_0)$ plotted as a function of L^2 for $\eta = 5$, 10, 15, 20 on a semilog scale. Equation (5) was used in the calculations for $L \leq \eta$, and Eq. (A4) when $L \geq \eta$. The smooth variation allows easy interpolation in L for a given value of η .

where $b=3^{\frac{1}{2}}\Gamma(\frac{2}{3})/\Gamma(\frac{1}{3})$. The next expected term in Eq. (11) and the next two in Eq. (12) contain zero factors.

It is now quite simple to obtain the desired expansions at the turning points by using a Taylor series for the shift from $\bar{\rho}_L$ to ρ_L . The results are¹⁵

$$\begin{cases} F_{L}(\rho_{L}) \\ G_{L}(\rho_{L})/\sqrt{3} \end{cases} = \frac{1}{2}\Gamma(\frac{1}{3})\pi^{-\frac{1}{2}}(\rho_{L}/3)^{1/6} [1+L(L+1)/\rho_{L}^{2}]^{-1/6} \\ \times \{1 \mp \rho_{L}^{-4/3}(6b/35)[1+L(L+1)/\rho_{L}^{2}]^{-8/3} \\ \times [1+4L(L+1)/\rho_{L}^{2}+3L^{2}(L+1)^{2}/2\rho_{L}^{4}] + \cdots \}, \quad (13) \\ \begin{cases} F_{L}'(\rho_{L}) \\ G_{L}'(\rho_{L})/\sqrt{3} \end{cases} = \frac{1}{2}\Gamma(\frac{2}{3})\pi^{-\frac{1}{2}}(\rho_{L}/3)^{-1/6} [1+L(L+1)/\rho_{L}^{2}]^{1/6} \\ \times \{+1+\frac{\rho_{L}^{-\frac{3}{2}}[1+2L(L+1)/\rho_{L}^{2}]}{2} + \cdots \}, \quad (14) \end{cases}$$

The dependence of the above results on
$$L$$
 can be
put in evidence by expanding the various factors con-
taining L in powers of L/n , which will be presumed

 $5b[1+L(L+1)/\rho_L^2]^{4/3}$

$$\{ \rho_L / [1 + L(L+1)] \rho_L^2] \}^{\pm 1/6}$$

= $(2\eta)^{\pm 1/6} [1 \pm L^2 (L+1)^2 / 96\eta^4 + \cdots].$

small. Thus,

Introducing this into Eqs. (13) and (14), one finds that $F_L(\rho_L)$ and $G_L(\rho_L)$ are independent of L to about 1 percent even when $L=\eta$, for η large.

Unlike Eqs. (5) and (6), which required $L < \eta$, Eqs. (13) and (14) [and Eqs. (11) and (12), as well] are valid for arbitrary values of L, and, in fact, can be used to obtain the asymptotic forms for $L \rightarrow \infty$. In this limit

one finds

$$\begin{cases} F_L(\rho_L) \\ G_L(\rho_L)/\sqrt{3} \\ \end{cases} \xrightarrow{\frac{1}{2}} \Gamma(\frac{1}{3}) \pi^{-\frac{1}{2}} (L/6)^{1/6}, \\ \begin{cases} F_L'(\rho_L) \\ G_L'(\rho_L)/\sqrt{3} \\ \end{cases} \xrightarrow{\frac{1}{2}} \Gamma(\frac{2}{3}) \pi^{-\frac{1}{2}} (L/6)^{-1/6}, \end{cases}$$

with $L \rightarrow \infty$.

When L and η are of the same order, and large compared to unity, ρ_L is about 25 percent larger than ρ_0 and the difference between ρ_L and ρ_0 increases as L becomes greater than η . As a consequence the regular and irregular properties of F_L and G_L , respectively, begin to appear markedly at ρ_0 , so that they are no longer of the same order numerically. This is, of course, the basis for the requirement that L be moderately small compared to η for Eqs. (5) and (6) to be valid. If one desires expansions at ρ_0 for cases when this restriction does not obtain, it is clear that a very much different approach is required. It is convenient in this case then to study F_L and G_L from the standpoint of their own integral representations. This case, where $L \ge \eta$, will not be discussed here; for reference, however, some results appropriate to this region are collected in the Appendix.

Since the calculations of Barfield and Broyles,¹⁶ for $F_0(\rho_0)$, $F_0'(\rho_0)$, and $G_L(\rho_0)$, led initially to the work described above, one of the first applications was to verify their results. It was found that for $\eta \ge 10$ the first two nonvanishing terms of Eqs. (5), (6) for L=0 gives the Barfield-Broyles values to the accuracy written by them, and for $\eta > 30$ the first term is sufficient. This result agrees with Newton,⁹ who made the same comparison.

Calculations have also been performed for $\eta \ge 5$ and arbitrary *L*. The convergence of Eqs. (5) and (6) rapidly becomes poorer as *L* increases, and for high *L* the alternative results given in the Appendix were necessary.



FIG. 3. $F_L'(\rho_0)$ plotted as a function of L^2 for $\eta = 5$, 10, 20 on a semilog scale. Equation (6) was used in the calculations for $L \leq \eta$, and Eq. (A5) when $L \geq \eta$. The smooth variation of the curves allows easy interpolation in L for a given value of η .

¹⁶ W. D. Barfield and A. A. Broyles, Phys. Rev. 88, 892 (1954).

¹⁵ M. Abramowitz and P. Rabinowitz, second reference of footnote 12, have obtained, in a preprint recently received by us, an expansion at ρ_0 for L=0 to which our Eqs. (13) and (14) reduce in that special case.



FIG. 4. $-G_{L'}(\rho_0)$ plotted as a function of L^2 for $\eta = 5$, 10, 20 on a semilog scale. Equation (6) was used in the calculations for $L \leq \eta$, and Eq. (A5) when $L \geq \eta$. The smooth variation of the curves allows easy interpolation in L for a given value of η .

The results of this numerical work are displayed in Figs. 1-4.

Further calculations have been performed for $F_L(\rho_L)$, $G_L(\rho_L)$ and their derivatives by using Eqs. (13) and (14). The range of validity of these equations is considerable, since they hold for arbitrary values of L/η provided only that η is large. In the parameter range $\eta \sim 10$, the first term alone in Eq. (13) is sufficient to give $F_L(\rho_L)$ or $G_L(\rho_L)$ to 2 percent, with accuracy improving as L increases. The results of the calculations are plotted in Figs. 5 and 6. It will be noted that these figures demonstrate the lack of sensitivity to the value of L remarked on earlier.

III. EXPANSIONS VALID IN THE VICINITY OF THE TURNING POINT

In the vicinity of the turning point, ρ_L , an expansion can be obtained by successive approximation with the aid of the Green's function for the operator d^2/dx^2+x . The equation satisfied by F_L and G_L is

$$d^{2}Y_{L}/d\rho^{2} + [1 - 2\eta/\rho - L(L+1)/\rho^{2}]Y_{L} = 0.$$
(15)

It is convenient to change the variable from ρ to $x = (\rho - \rho_L) [1/\rho_L + L(L+1)/\rho_L^3]^{\frac{1}{2}}$. Then the coefficient of Y_L in Eq. (15) can be expanded as a power series in x, so that Eq. (15) becomes

$$d^{2}Y_{L}/dx^{2} + x(1+\lambda_{1}\rho_{L}-x^{3}x+\lambda_{2}\rho_{L}-4/3}x^{2}+\cdots)Y_{L}=0,$$
(15.1)
$$\lambda_{n}=(-1)^{n}[1+L(L+1)/\rho_{L}^{2}]^{-(n+2)/3}$$

$$\times [1+nL(L+1)/\rho_{L}^{2}].$$

Two independent solutions of Eq. (15.1) will be constructed having the following behavior at x=0: f(x)shall have zero value and unit slope at x=0, g(x) shall have unit value and zero slope at x=0 (slope here means derivative with respect to x). Expand f(x) as

$$f(x) = f_0(x) + \rho_L^{-\frac{2}{3}} f_1(x) + \cdots,$$

[and g(x) similarly]. Then Eq. (15.1) leads to

$$f_{0}''(x) + xf_{0}(x) = 0,$$

$$f_{1}''(x) + xf_{1}(x) = -\lambda_{1}x^{2}f_{0}\rho_{L}^{-\frac{3}{4}},$$

$$f_{2}''(x) + xf_{2}(x) = -\lambda_{1}x^{2}f_{1}\rho_{L}^{-\frac{3}{4}} - \lambda_{2}x^{3}f_{0}\rho_{L}^{-\frac{4}{3}}.$$

(16)

The Green's function for the operator (d^2/dx^2+x) is therefore required. It is found to be

$$G(x,x') = (2\pi/3^{\frac{3}{2}})x_{<\frac{1}{2}}J_{\frac{1}{2}}(2x_{<\frac{3}{2}}/3)x_{>\frac{1}{2}}J_{-\frac{1}{2}}(2x_{>\frac{3}{2}}/3), \quad (17)$$

where x_{\leq} is the smaller of x and x', $x_{>}$ is the larger of x and x'. The solution proceeds as follows:

$$f_{0}(x) = x^{\frac{1}{2}} J_{\frac{1}{2}}(\frac{2}{3}x^{\frac{3}{2}}),$$

$$f_{1}(x) = -\lambda_{1} \int f_{0}(x')x'^{2}G(x,x')dx',$$

$$f_{2}(x) = -\lambda_{1} \int f_{1}(x')x'^{2}G(x,x')dx'$$

$$-\lambda_{2} \int f_{0}(x')x'^{3}G(x,x')dx',$$
(18)

which leads to integrals of the forms

$$\int t^{(2n+5)/3} J_{\pm \frac{1}{3}}(t) J_{\pm \frac{1}{3}}(t) dt.$$

These indefinite integrals are special cases of the Lommel integrals in Sec. 5.12 of Watson's *Bessel Functions*, or may be evaluated with their help after application of a reduction formula due to Schafheitlin (Sec. 5.14 of Watson) and extensions obtained in a manner analogous to that of Schafheitlin. The resulting expressions are sums of products of 3 Bessel functions, but have a common factor which arranges itself into a Wronskian relation, leaving sums of single Bessel functions. Suitable portions of zero order solutions had to be added to ensure the proper behavior of the high order solutions at x=0, since this procedure was found to be easier than adjusting the limits in Eq. (18) properly.

In the case of f(x), for example, $f_0(x)$ has the desired behavior at x=0, and $f_1(x)$, $f_2(x)$ were adjusted so as not to interfere with this.

The results of these calculations are:

$$\begin{split} f_{0}(x) &= x^{\frac{1}{2}}J_{\frac{1}{2}}(\frac{2}{3}x^{\frac{1}{2}}), \\ f_{1}(x) &= -(\lambda_{1}/5)x^{3}J_{4/3}(\frac{2}{3}x^{\frac{1}{2}}), \\ f_{2}(x) &= (\lambda_{1}^{2}/350) [(30x^{4}-90x)J_{-\frac{3}{2}}(\frac{2}{3}x^{\frac{1}{2}}) \\ &+ (7x^{11/2}-45x^{5/2})J_{\frac{1}{2}}(\frac{2}{3}x^{\frac{1}{2}})+90bx^{\frac{1}{2}}J_{-\frac{1}{2}}(\frac{2}{3}x^{\frac{1}{2}})] \\ &+ (\lambda_{2}/14) [(2x^{4}-6x)J_{-\frac{3}{2}}(\frac{2}{3}x^{\frac{1}{2}}) \\ &- 3x^{5/2}J_{\frac{1}{2}}(\frac{2}{3}x^{\frac{1}{2}})]+6bx^{\frac{1}{2}}J_{-\frac{1}{2}}(\frac{2}{3}x^{\frac{1}{2}})], \quad (19) \\ \end{split}$$
 where $b = 3^{\frac{1}{2}}\Gamma(\frac{2}{3})/\Gamma(\frac{1}{3}), \end{split}$

and

$$g_{0}(x) = x^{\frac{1}{2}}J_{-\frac{1}{2}}(\frac{2}{3}x^{\frac{3}{2}}),$$

$$g_{1}(x) = (\lambda_{1}/5)[x^{3}J_{-4/3}(\frac{2}{3}x^{\frac{3}{2}}) + (1/b)x^{\frac{1}{2}}J_{\frac{1}{2}}(\frac{2}{3}x^{\frac{3}{2}})],$$

$$g_{2}(x) = (\lambda_{1}^{2}/350)[(30x^{4} - 90x)J_{\frac{3}{2}}(\frac{2}{3}x^{\frac{3}{2}}) - (7x^{11/2} - 45x^{5/2})J_{-\frac{1}{2}}(\frac{2}{3}x^{\frac{3}{2}})] - (\lambda_{1}^{2}/25b)x^{3}J_{4/3}(\frac{2}{3}x^{\frac{3}{2}}) - (\lambda_{2}/14) \times [(2x^{4} - 6x)J_{\frac{3}{2}}(2x^{\frac{3}{2}}) - (\lambda_{2}/14) .$$
(20)

The expressions in Eqs. (19) and (20) are convenient for positive values of x, i.e., for $\rho > \rho_L$.

Equivalent expressions for $\rho < \rho_L$ may be written in terms of the modified Bessel functions of the first kind and order: $\pm \frac{1}{3}, \pm \frac{2}{3}, \pm$ etc. These expressions are:

$$f_0 = -y^{\frac{1}{2}} I_{\frac{1}{3}}(\frac{2}{3}y^{\frac{3}{2}}),$$

$$f_1 = (\lambda_1/5) y^3 I_{4/3}(\frac{2}{3} y^{\frac{3}{2}}),$$

$$\begin{split} f_{2} &= (\lambda_{1}^{2}/350) \big[(30y^{4} + 90y) I_{-\frac{1}{8}} (\frac{2}{3}y^{\frac{3}{2}}) \\ &- (7y^{11/2} + 45y^{5/2}) I_{\frac{1}{8}} (\frac{2}{3}y^{\frac{3}{2}}) - 90by^{\frac{1}{2}} I_{-\frac{1}{8}} (\frac{2}{3}y^{\frac{3}{2}}) \big] \\ &+ (\lambda_{2}/14) \big[- (2y^{4} + 6y) I_{-\frac{3}{8}} (\frac{2}{3}y^{\frac{3}{2}}) \\ &+ 3y^{5/2} I_{\frac{1}{8}} (\frac{2}{3}y^{\frac{3}{2}}) + 6by^{\frac{1}{2}} I_{-\frac{1}{8}} (\frac{2}{3}y^{\frac{3}{2}}) \big], \quad (21) \end{split}$$

 $y = (\rho_L - \rho) [1/\rho_L + L(L+1)/\rho_L^3]^{\frac{1}{3}},$

and

 $g_0 = y^{\frac{1}{2}} I_{-\frac{1}{3}} \left(\frac{2}{3} y^{\frac{3}{2}} \right),$

$$g_{1} = -(\lambda_{1}/5) \left[y^{3}I_{-4/3}(\frac{2}{3}y^{\frac{3}{2}}) + (1/b)y^{\frac{1}{2}}I_{\frac{1}{2}}(\frac{2}{3}y^{\frac{3}{2}}) \right],$$

$$g_{2} = (\lambda_{1}^{2}/350) \left[-(30y^{4}+90y)I_{\frac{2}{3}}(\frac{2}{3}y^{\frac{3}{2}}) + (7y^{11/2}+45y^{5/2})I_{-\frac{1}{2}}(\frac{2}{3}y^{\frac{3}{2}}) \right] + (\lambda_{2}/25b)y^{3}I_{4/3}$$

$$\times (\frac{2}{3}y^{\frac{3}{2}}) + (b/14) \left[(2y^{4}+6y)I_{\frac{3}{2}}(\frac{2}{3}y^{\frac{3}{2}}) - 3y^{5/2}I_{-\frac{1}{2}}(\frac{2}{3}y^{\frac{3}{2}}) \right]. \quad (22)$$



FIG. 5. $F_L(\rho_L)$ and $G_L(\rho_L)$ plotted as a function of L for $\eta = 5$, 10, 15, 20. Equation (13) was used in the calculations for all values of L. The slow variation of the functions with L is illustrated.



FIG. 6. $F_L'(\rho_L)$ and $-G_L'(\rho_L)$ plotted as a function of L for $\eta = 5$, 10, 15, 20. Equation (14) was used in the calculations for all values of L. The slow variation of the functions with L is illustrated.

The desired formulas for F_L and G_L are then

$$F_{L}(\rho) = F_{L}(\rho_{L})g(x) + F_{L}'(\rho_{L})[1/\rho_{L} + L(L+1)/\rho_{L}^{3}]^{\frac{1}{2}}f(x),$$

$$G_{L}(\rho) = G_{L}(\rho_{L})g(x) + G_{L}'(\rho_{L})[1/\rho_{L} + L(L+1)/\rho_{L}^{3}]^{\frac{1}{2}}f(x).$$
(23)

The forms of $F_L(\rho_L)$, $G_L(\rho_L)$, etc. of Eqs. (13) and (14) may be used with Eqs. (23) to write explicit expansions of $F_L(\rho)$, $G_L(\rho)$. These are

$$\begin{bmatrix}
F_{L}(\rho) \\
G_{L}(\rho)/\sqrt{3}
\end{bmatrix} = \frac{\pi^{\frac{1}{3}}}{3} \left(\frac{\rho_{L}}{1+L(L+1)/\rho_{L}^{2}}\right)^{1/6} \\
\times \left\{x^{\frac{1}{2}} \left[J_{-\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) \pm J_{\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)\right] \\
-\rho_{L}^{-\frac{3}{4}} \left(\frac{1+2L(L+1)/\rho_{L}^{2}}{5\left[1+L(L+1)/\rho_{L}^{2}\right]^{4/3}}\right)x^{3} \\
\times \left[J_{-4/3}\left(\frac{2}{3}x^{\frac{3}{2}}\right) \mp J_{4/3}\left(\frac{2}{3}x^{\frac{3}{2}}\right)\right] \\
+\rho_{L}^{-4/3}\left[\frac{1+2L(L+1)/\rho_{L}^{2}}{1+L(L+1)/\rho_{L}^{2}}\right]^{5/3}\left[\left(\frac{3x^{4}-9x}{35}\right)\right] \\
\times \left[J_{\frac{3}{4}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) \mp J_{-\frac{3}{4}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)\right] \\
+\rho_{L}^{-4/3}\left(\frac{1+3L(L+1)/\rho_{L}^{2}}{1+L(L+1)/\rho_{L}^{2}}\right)\left[-\left(\frac{x^{4}-3x}{7}\right)\right] \\
\times \left[J_{\frac{3}{4}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) \mp J_{-\frac{3}{4}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)\right] \\
-\left(\frac{3x^{5/2}}{14}\right)\left[J_{-\frac{1}{4}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) \pm J_{\frac{1}{4}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)\right] \\
+\cdots\right\}, (24)$$

for $\rho - \rho_L > 0$, and

$$\begin{cases} F_{L}(\rho) \\ G_{L}(\rho)/\sqrt{3} \end{cases} = \frac{\pi^{\frac{1}{2}}}{3} \left(\frac{\rho_{L}}{1 + L(L+1)/\rho_{L}^{2}} \right)^{1/6} \\ \times \left\{ y^{\frac{1}{2}} \left[I_{-\frac{1}{2}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \mp I_{\frac{1}{2}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \right] \\ + \rho_{L}^{-\frac{3}{4}} \left(\frac{1 + 2L(L+1)/\rho_{L}^{2}}{5\left[1 + L(L+1)/\rho_{L}^{2} \right]^{2/3}} \right) y^{3} \\ \times \left[I_{-4/3} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \mp I_{4/3} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \right] \\ + \rho_{L}^{-4/3} \left(\frac{\left[1 + 2L(L+1)/\rho_{L}^{2} \right]^{2}}{\left[1 + L(L+1)/\rho_{L}^{2} \right]^{2/3}} \right) \left[- \left(\frac{3y^{4} - 9y}{35} \right) \right] \\ \times \left[I_{\frac{3}{2}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \mp I_{-\frac{3}{4}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \right] \\ + \left(\frac{y^{11/2}}{50} + \frac{9y^{5/2}}{70} \right) \left[I_{-\frac{1}{2}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \mp I_{\frac{1}{2}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \right] \\ + \rho_{L}^{-4/3} \left(\frac{1 + 3L(L+1)/\rho_{L}^{2}}{\left[1 + L(L+1)/\rho_{L}^{2} \right]^{5/3}} \right) \left[\left(\frac{y^{4} + 3y}{7} \right) \\ \times \left[I_{\frac{3}{4}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \mp I_{-\frac{3}{4}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \right] \\ - \left(\frac{3y^{5/2}}{14} \right) \left[I_{-\frac{1}{4}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \mp I_{\frac{1}{4}} \left(\frac{2}{3} y^{\frac{3}{2}} \right) \right] + \cdots \right\}, \quad (25)$$

for $\rho - \rho_L < 0$.

The results given in Eqs. (24) and (25) may also be obtained directly from the integral representation of Eq. (1), by suitably expanding the integrand. The leading term, for example, yields an integral that can be put in the form of Airy's integral and leads to the Bessel functions of order one-third.¹⁷ It may be noted in Eq. (25) that the functions with positive and negative orders occur in the expression for $F_L(\rho)$ in the proper combination to make $K_{\nu}(\frac{2}{3}x^3)$.

It has already been brought out, in connection with Eqs. (13) and (14), that the dependence on L of the functions $F_L(\rho_L)$ and $G_L(\rho_L)$ is in the fourth power of L/η , in particular, the dependence is $(1+L^2(L+1)^2/96\eta^4)$ for large η . Since

$$y = (\rho_L - \rho) [1/\rho_L + L(L+1)/\rho_L^3]^{\frac{1}{3}}$$

$$\cong [(\rho_L - \rho)/(2\eta)^{\frac{1}{3}}] [1 - L^2(L+1)^2/48\eta^4],$$

Eq. (25) leads one to expect that for a fair range of parameters, $F_L(\rho)$ and $G_L(\rho)$ could be represented by "universal" curves fitted respectively to $F_L(\rho)/\eta^{1/6}$ plotted against $(\rho_L - \rho)/\eta^{\frac{1}{2}}$ and to $G_L(\rho)/\eta^{1/6}$ plotted against the same variable. Figure 7 shows such a set of curves, and illustrates indeed that the functions bunch fairly closely when plotted as suggested by the limiting forms of Eq. (25). The functions for L=10, $\eta=5$

¹⁷ M. Abramowitz and H. A. Antosiewicz, first reference of footnote 12, have obtained an expansion of $F_0(\rho)$ and $G_0(\rho)$ in terms of the Airy integrals for $|\rho - \rho_0| < \rho_0$.

deviate most, as is expected since L/η is then 2. The bunching is expected to become yet more pronounced as η exceeds L by larger and larger factors. At y=0, the values of $F_L(\rho_L)/\eta^{1/6}$ and $G_L(\rho_L)/\eta^{1/6}$ exhibit the even more pronounced (L,η) independence indicated in the discussion of Eq. (13).

Expansions similar to Eqs. (24) and (25), but valid in the vicinity of ρ_0 rather than ρ_L , have been given by Newton.⁹ His expansion converges for small values of L. For $L \sim \eta$ or larger, expansions useful near ρ_0 may be obtained by other means indicated in the Appendix.

IV. APPROXIMATE WAVE FUNCTIONS

The discussion of the previous sections has had as its object the enumeration of convenient methods for determining the Coulomb wave functions for large η to an arbitrarily given accuracy in any one of several regions of interest. There exists, however, a quite different objective, namely the need for simple functional forms for the Coulomb wave functions valid to reasonable accuracy, say ~ 1 percent, over extended regions for ρ . Although somewhat too crude for our purposes, the JWKB approximation is typical to this approach. An improved approximation along these lines has been given by Morse and Feshbach in terms of the Bessel functions of order one-third. It is characteristic of both these points of view that one seeks to relate the solution of the problem at hand to the known solutions of a differential equation that is approximately the same, the physical basis of the approximation being in all cases the small change in the potential over distances of the order of a wavelength. In order to obtain an approximate solution to

$$d^2y/dx^2 + g(x)y = 0,$$
 (26)

it is convenient to make a transformation,

$$y = CuY\left(\int^{x} u^{-2}dx\right),\tag{27}$$

where C is an arbitrary constant. One has then

$$\frac{d^2y}{dx^2} = \left(\frac{1}{u}\frac{d^2u}{dx^2} + \frac{1}{u^4}\frac{Y''}{Y}\right)y.$$
 (27.1)

So far Y(z) is an arbitrary function of argument

$$z = \int^x u^{-2} dx. \tag{28}$$

Once chosen, Y determines a function χ through

$$Y''(z) + \chi(z)Y(z) = 0,$$
 (29)

and in terms of χ substitution of (29) in (27.1) and identification with (26) gives

$$g(x) = \frac{1}{u^4} \chi \left(\int^x \frac{dx}{u^2} \right) - \frac{1}{u} \frac{d^2 u}{dx^2}.$$
 (30)

Conversely, if $\chi(z)$ is an assigned functional form, then a suitably chosen u inserted in (30) gives a solution of Eq. (26) provided one solves (29) so as to be able to insert Y in (27). Even if g(x) cannot be represented exactly by means of Eq. (30) there are available adjustments in both u and χ for its approximate representation. In terms of z

$$g(x) = (dz/dx)^{2}\chi(z(x)) + \Delta,$$

$$\Delta = -(dz/dx)^{\frac{1}{2}} \frac{d^{2}[(dz/dx)^{-\frac{1}{2}}]}{dx^{2}},$$
(30.1)

and

 $y = (dz/dx)^{-\frac{1}{2}}Y(z(x)).$ (30.2)

In the latter form z is seen to be a generalization of the phase of the JWKB approximation.

By specializing to $\chi = a = \text{const}$, Eq. (30) becomes

$$g = \frac{a}{u^4} - \frac{1}{u} \frac{d^2 u}{dx^2}.$$
 (31)

An approximate solution is then $u \cong (a/g)^{\frac{1}{2}}$ which gives

$$y \cong C(a/g)^{\frac{1}{2}} Y\left(\int^{x} (g/a)^{\frac{1}{2}} dx\right)$$
$$= C'g^{-\frac{1}{2}} \sin\left(\int^{x} g^{\frac{1}{2}} dx + C''\right), \quad (31.1)$$

where C', C'' are arbitrary constants. If Eq. (31) is solved for u more accurately, correction terms to the one term JWKB formula are obtained.

The JWKB approximation is an immediate generalization of a representation of g(x) by constant steps. An improvement in convergence of successive terms is obtained¹⁸ if g(x) is approximated by a set of straight line segments. Such an approximation is found from the transformation under discussion by setting

X

$$(z) = z \tag{31.2}$$

so that according to (30.1)

$$g(x) = z(dz/dx)^2 + \Delta. \qquad (31.3)$$

Again if Δ is not too important,

$$z^{\ddagger} = \frac{3}{2} \int^{x} g^{\ddagger} dx, \qquad (31.4)$$

$$Y(z) = z^{\frac{1}{2}} \left[A J_{\frac{1}{2}}(\frac{2}{3}z^{\frac{3}{2}}) + B J_{-\frac{1}{2}}(\frac{2}{3}z^{\frac{3}{2}}) \right], \qquad (31.5)$$

so that according to (30.2),

$$y = (\varphi/g^{\frac{1}{2}})^{\frac{1}{2}} [A'J_{\frac{1}{2}}(\varphi) + B'J_{-\frac{1}{2}}(\varphi)], \qquad (31.6)$$

where

and

$$\varphi = \int^x g^{\frac{1}{2}} dx. \tag{31.7}$$

¹⁸ R. E. Langer, Phys. Rev. 51, 669 (1937).



FIG. 7. $F_L(\rho)/\eta^{1/6}$ and $G_L(\rho)/\eta^{1/6}$ plotted as a function of $(\rho_L - \rho)/\eta^{1/3}$. These curves illustrate the possibility of representing the functions by "universal" curves, as suggested by Eq. (25). This tendency to group is lost as L exceeds η more and more and is emphasized as η exceeds L. The calculations were done by numerical integrations started at $\rho = \rho_L$ using Eqs. (13) and (14).

It should be noted that whenever the approximation is made by setting $\Delta = 0$, then according to (30.1)

$$\varphi = \int^{x} g^{\frac{1}{2}} dx \cong \int \chi^{\frac{1}{2}} dz, \qquad (32)$$

so that the geometrical optics approximation of the solutions to (26) and (29) contain the same phase. The approximation of Eq. (31.6) has been first obtained by Morse and Feshbach¹⁴ who have also worked out the differential equation satisfied by the right side of (31.6). They have found in this special case a relation equivalent to Eq. (30.1) above.

Other approximations applicable in special situations are obtainable by the same method. If, for example, g(x) can be approximately represented by a power of x then it is useful to take $\chi(z) = z^{p}$. In this case

$$y \cong (\varphi/g^{\frac{1}{2}})^{\frac{1}{2}} [AJ_{p}(\varphi) + BJ_{-p}(\varphi)],$$

$$p = 1/(\nu + 2).$$
(32.1)

For the Coulomb wave functions, the turning point has a zero of first order in g and consequently the Morse-Feshbach approximation is indicated. When the constants are adjusted to fit the boundary conditions and the values at the turning point, one finds:

For
$$\rho \ge \eta + [\eta^2 + L(L+1)]^{\frac{1}{2}}$$
,
 $g^{\frac{1}{2}} = [1 - 2\eta/\rho - L(L+1)/\rho^2]^{\frac{1}{2}}$,
 $\varphi = \rho g^{\frac{1}{2}} - \eta \ln \left(\frac{(\rho - \eta + \rho g^{\frac{1}{2}})}{[\eta^2 + L(L+1)]^{\frac{1}{2}}} \right)$
 $- [L(L+1)]^{\frac{1}{2}} \sin^{-1} \left(\frac{[L(L+1)g]^{\frac{1}{2}}}{[\eta^2 + L(L+1)]^{\frac{1}{2}}} \right)$,
 $\begin{cases} F_L(\rho) \\ G_L(\rho)/\sqrt{3} \end{cases} \cong (\pi \varphi/6g^{\frac{1}{2}})^{\frac{1}{2}} [J_{-\frac{1}{2}}(\varphi) \pm J_{\frac{1}{2}}(\varphi)]$. (33)

For $\rho \leq \eta + \lceil \eta^2 + L(L+1) \rceil^{\frac{1}{2}}$,

$$g^{\frac{1}{2}} = [L(L+1)/\rho^{2} + 2\eta/\rho - 1]^{\frac{1}{2}},$$

$$\varphi = i \left\{ \rho g^{\frac{1}{2}} - \eta \tan^{-1} \left(\frac{\rho g^{\frac{1}{2}}}{(\rho - \eta)} \right) - [L(L+1)]^{\frac{1}{2}} \sinh^{-1} \left(\frac{[L(L+1)g]^{\frac{1}{2}}}{[\eta^{2} + L(L+1)]^{\frac{1}{2}}} \right) \right\} \quad (33.1)$$
for $\rho \ge n$ and

rρ>η, a

$$=i\left\{\rho g^{\frac{1}{2}}-\pi\eta-\eta \tan^{-1}\left(\frac{\rho g^{\frac{1}{2}}}{\rho-\eta}\right)-\left[L(L+1)\right]^{\frac{1}{2}}\sinh^{-1}\left(\frac{\left[L(L+1)g\right]^{\frac{1}{2}}}{\left[\eta^{2}+L(L+1)\right]^{\frac{1}{2}}}\right)\right\}$$

for $\rho < \eta$,

$$\begin{cases} F_L(\rho) \\ G_L(\rho)/\sqrt{3} \end{cases} = |\pi\varphi/6g^{\frac{1}{2}}|^{\frac{1}{2}} [-I_{-\frac{1}{2}}(|\varphi|) \pm I_{\frac{1}{2}}(|\varphi|)]$$

One may use the definition of Whittaker and Watson, namely that $I_{-\frac{1}{2}} - I_{\frac{1}{2}} = (2\sqrt{3}/\pi)K_{\frac{1}{2}}$, to write the result for F_L in an alternative form.

The Bessel functions of order one-third are not single valued in the vicinity of x=0, whereas the functions $x^{\frac{1}{2}}J_{\pm \frac{1}{2}}(2x^{\frac{3}{2}}/3)$ are indeed single-valued in this vicinity. In consequence it is convenient to utilize the latter functions, especially since they have been tabulated for complex values of their arguments.¹⁹ Changing the



FIG. 8. The error, Δ , in the potential, given in Eq. (30.1), for the JWKB approximation, the Morse-Feshbach (MF) approxi-mation and the modified Morse-Feshbach (m) approximation plotted as a function of ρ . The variation, constant $\times \rho^{-2}$, of $\Delta_{\rm MF}$, used in making the modification, is illustrated.

¹⁹ Tables of the Modified Hankel Functions of Order One-Third and of Their Derivatives (Harvard University Press, Cambridge, 1945).

notation to facilitate the use of these tables one has

$$\begin{cases} F_L(\rho) \\ G_L(\rho)/\sqrt{3} \end{cases} = \pm (3\pi/8)^{\frac{1}{2}} |\varphi|^{1/6} |g|^{-\frac{1}{4}} \\ \times \left[\begin{cases} 1 \\ \frac{1}{3} \end{cases} \operatorname{Re} h_1(z) \mp (\frac{1}{3})^{\frac{1}{2}} \operatorname{Im} h_1(z) \end{bmatrix}, \quad (34) \end{cases}$$

where φ was defined earlier in Eqs. (33) and (33.1),

$$z = \left(\frac{3}{2}\right)^{\frac{2}{3}} \left| \varphi \right|^{\frac{3}{3}}, \qquad \rho \geqslant \rho_L,$$
$$= -\left(\frac{3}{2}\right)^{\frac{2}{3}} \left| \varphi \right|^{\frac{3}{3}}, \qquad \rho \ll \rho_L.$$

For some applications, it is useful to have similar approximations for the derivatives $dF_L/d\rho$ and $dG_L/d\rho$ which are denoted, as customary, by $F_{L'}$ and $G_{L'}$. While these derivatives follow immediately from the preceding formulae, the presence of absolute value signs (which were introduced as a convenience only) complicates the situation, and the explicit results are therefore given below,

$$\begin{cases} F_{L}'(\rho) \\ G_{L}'(\rho)/\sqrt{3} \end{cases} = \left[g^{\frac{1}{2}}/6 \right] \varphi \left| -\frac{1}{2}d \ln(g^{\frac{1}{2}})/d\rho \right] \begin{cases} F_{L}(\rho) \\ G_{L}(\rho)/\sqrt{3} \end{cases}$$

$$+ \left(\frac{2}{3} \right)^{\frac{1}{2}} (3\pi/8)^{\frac{1}{2}} \right] \varphi \left|^{-1/6} g^{\frac{1}{4}} \right]$$

$$\times \left[\left\{ \frac{1}{\frac{1}{3}} \right\} \operatorname{Re} h_{1}'(z) \pm \left(\frac{1}{3} \right)^{\frac{1}{2}} \operatorname{Im} h_{1}'(z) \right], \quad (35)$$

where z is the same as in Eq. (34). It should be mentioned that $h_1'(z)$ is tabulated along with $h_1(z)$.

It is of interest to check the Wronskian of these approximations to F_L , G_L and F_L' , G_L' . Employing the properties of $h_1(z)$ and $h'_1(z)$, one finds indeed that $F_L G_L - G_L F_L = 1$ for the functions of Eqs. (34) and (35).

The Morse-Feshbach approximation to the Coulomb wave functions is not, in general, sufficiently accurate. To get some estimate of the accuracy of the fit one can examine the values assumed by the approximate solutions at $\rho = \rho_L$ and as $\rho \rightarrow \infty$, as well as $\rho \rightarrow 0$. At $\rho = \rho_L$ one finds

$$F_L(\rho_L) \to [\Gamma(\frac{1}{3})/2\pi^{\frac{1}{2}}] \left(\frac{\rho_L}{3[1+L(L+1)/\rho_L^2]}\right)^{1/6}.$$

This differs from the exact value [see Eq. (13)] in order $\rho_L^{-4/3}$ compared to unity. In order to improve the accuracy one may proceed in several ways:

(a) The difference between the exact potential and the potential in the differential equation satisfied by the approximate solution is

$$g(x) - z(dz/dx)^{2} = -\frac{(d^{2}/dx^{2})[(dz/dx)^{-\frac{1}{2}}]}{(dz/dx)^{\frac{1}{2}}} \equiv \Delta(x).$$

Thus one can write

$$\left[d^2/dx^2 + g(x) - \Delta(x)\right]\psi = -\Delta(x)\psi = \Theta\psi,$$

and invert this equation approximately to obtain

$$\psi \cong \psi_{\mathbf{M}-\mathbf{F}} + \mathcal{O}^{-1}[\Delta(x)\psi_{\mathbf{M}-\mathbf{F}}].$$

This procedure is closely allied to that used earlier to obtain Eqs. (24) and (25), but suffers from the complicated form of $\Delta(x)$, which all but precludes anything but numerical work.

(b) One may take a more complicated function for $\chi(z)$. In practice, this amounts to a quadratic fitting of the potential at every point (just as the Morse-Feshbach approximation was a linear fitting). While of value as a general technique, it is of little interest for the problem at hand since the resulting approximate solutions involve the parabolic cylinder functions, which are certainly less thoroughly tabulated than the Coulomb functions themselves.

(c) One may introduce in place of g(x) an approximate function containing one or more arbitrary parameters and adjust the Morse-Feshbach approximation for this latter potential so as to minimize the error for the particular case at hand.

It turns out that procedure (c) is quite well suited to approximating the Coulomb functions, owing to the fortunate circumstance that the error in the potential, i.e., $\Delta(x)$, is, to a fair approximation, constant $\times \rho^{-2}$ in the region zero to infinity. Figure 8 illustrates this.

The application of this fact is immediate, since it involves no additional complication in the Morse-Feshbach approximation, requiring only a shift in the value of L. This is reminiscent somewhat of the shift $L\rightarrow L+\frac{1}{2}$ given by Kramers, and others,^{5,18} for the JWKB approximation. The value of the shift is, however, not unique; one can choose it, for example, so as to make $\Delta(\rho)$ vanish for any specified value of ρ . [$\Delta(\rho)$ is, of course dependent on the altered value of L.] A reasonable place to make $\Delta(\rho)$ vanish is at the (new) turning point. For this, one finds that if

$$g^{\frac{1}{2}} = \left[1 - 2\eta/\rho - \alpha/\rho^{2}\right]^{\frac{1}{2}},$$
$$\Delta(\rho_{a}) = -\left(\frac{3}{140\eta^{2}}\right) \left(\frac{10 + 13\alpha/\eta^{2} - 2(1 + \alpha/\rho^{2})^{\frac{1}{2}}}{(1 + \alpha/\eta^{2})\rho_{a}^{2}}\right),$$

where $\rho_a = \eta + (\eta^2 + \alpha)^{\frac{1}{2}}$. Hence to cancel the error in the potential at ρ_a one must use

$$\alpha = L(L+1) + (3/140) \left(\frac{10 + 13\alpha/\eta^2 - 2(1 + \alpha/\eta^2)^{\frac{1}{2}}}{(1 + \alpha/\eta^2)} \right)$$
$$= L(L+1) + 6/35 + (3/35\eta^2)[L(L+1) + 6/35] + \cdots$$

The approximation $\alpha = L(L+1) + 6/35$ is sufficient for η large.

To examine the usefulness of this artifice consider first L=0 in detail. The proposed approximation is, for $\rho \ge \eta + (\eta^2 + 6/35)^{\frac{1}{2}}$, given by

$$g^{\dagger} = [1 - 2\eta/\rho - 6/35\rho^{2}]^{\dagger},$$

$$\varphi = \rho g^{\frac{1}{2}} - \eta \ln[(\rho - \eta + \rho g^{\frac{1}{2}})/(\eta^{2} + 6/35)^{\frac{1}{2}}] - (6/35)^{\frac{1}{2}} \sin^{-1}[(6g/35)^{\frac{1}{2}}/(\eta^{2} + 6/35)^{\frac{1}{2}}], \quad (36)$$

$$\left\{ \frac{F_{0}(\rho)}{G_{0}(\rho)/\sqrt{3}} \right\} = (\pi \varphi/6g^{\frac{1}{2}})^{\frac{1}{2}} [J_{-\frac{1}{2}}(\varphi) \pm J_{\frac{1}{2}}(\varphi)].$$

Consider the error near the new turning point, *i.e.*, at the point where $\rho = \eta + (\eta^2 + 6/35)^{\frac{1}{2}} \equiv \rho_a$. Using the results given by Eqs. (5) and (6) in a Taylor series, one readily finds that

$$F_0(\rho_a)_{\rm approx}/F_0(\rho_a)_{\rm exact} = 1 + 1/3150\eta^2 + O(\eta^{-10/3})$$

The error is surprisingly small, particularly in view of the fact that for the unmodified value of L=0, one found earlier that

$$F_{0}(2\eta)_{\rm approx}/F_{0}(2\eta)_{\rm exact} = 1 + \eta^{-4/3} (\frac{3}{2})^{\frac{1}{2}} 3\Gamma(\frac{2}{2})/35\Gamma(\frac{1}{2}).$$

Thus the error is pushed to order η^{-2} instead of order $\eta^{-4/3}$ and moreover the coefficient is remarkably small: $\approx 1/3000$ instead of $\approx 1/20$.

It is of interest to examine in more detail the origins of this accuracy, especially for general L. First of all the series for F_L and G_L had no terms of order $\eta^{-\frac{3}{4}}$, and F_L and G_L differed in the sign of the $\eta^{-\frac{4}{3}}$ term. Since the values for F_L and $G_L/\sqrt{3}$ given by the Morse-Feshbach approximation are the same at the turning point, the error in this approximation is therefore of order $\eta^{-\frac{4}{3}}$, already one higher order than might be expected. Now the use of the modified value of L shifts the value of the turning point to

$$\begin{split} \rho_a = \rho_0 + \eta^{-1} [3/35 + L(L+1)/2] \\ + \eta^{-3} [9/2450 - L^2(L+1)^2/8] + \mathcal{O}(\eta^{-5}). \end{split}$$

[This uses the modified value for L(L+1) to be $L(L+1)+6/35+(3/35\eta^2)(L(L+1)+6/35)+\cdots$.] To obtain the value of $F_L(\rho_a)$ and $G_L(\rho_a)$ one uses a Taylor series

$$F_L(\rho_a) = F_L(\rho_0) + (1/2\eta)(6/35 + L(L+1))F_L'(\rho_0) + \cdots$$

Upon referring to Eqs. (5) and (6), it is clear that the shift from ρ_L to ρ_a is precisely that required to cancel terms of order $\eta^{-4/3}$, for both F_L and G_L . In fact, the requirement that the shift minimize the error in the wave functions seems equally as good a criterion as the equivalent requirement that the error in the potential cancel at ρ_a . The terms of order η^{-2} do not cancel and,

for general L, one has

$$\begin{cases} F_{L}(\rho_{a}) \\ G_{L}(\rho_{a})/\sqrt{3} \end{cases} = \left(\frac{\Gamma\left(\frac{1}{3}\right)}{2\pi^{\frac{1}{3}}}\right) (\frac{2}{3}\eta)^{1/6} \\ \times \left[1 - \left(\frac{1}{3150}\right)\eta^{-2} \mp \left(\frac{216a}{398\ 125}\right)\eta^{-10/3} + \cdots\right], \quad (37)$$

where $a = (\frac{3}{2})^{\frac{1}{3}} \Gamma(\frac{2}{3}) / \Gamma(\frac{1}{3})$.

This result requires η to be large and L/η to be small. Note the remarkable independence of L shown in this result.

Now the value assumed by the modified Morse-Feshbach approximation at ρ_a is the same for both F_L and G_L and turns out to be

$$\begin{cases} F_L(\rho_a) \\ G_L(\rho_a)/\sqrt{3} \end{cases} \cong \left(\frac{\Gamma(\frac{1}{3})}{2\pi^{\frac{1}{3}}}\right) (\frac{2}{3}\eta)^{\frac{1}{3}} [1 + \mathcal{O}(\eta^{-4})]. \quad (37.1)$$

Hence one obtains the result that, for general L, the modified Morse-Feshbach approximation yields

$$\begin{cases}
F_{L}(\rho_{a})_{\text{approx}}/F_{L}(\rho_{a})_{\text{exact}} \\
G_{L}(\rho_{a})_{\text{approx}}/G_{L}(\rho_{a})_{\text{exact}}
\end{cases} = 1 + \left(\frac{1}{3150}\right)\eta^{-2} \\
\pm \left(\frac{216a}{398\ 125}\right)\eta^{-10/3} + \mathcal{O}(\eta^{-4}), \quad (38)$$

which, to repeat, is both gratifyingly accurate and moreover independent of L for L/η small.

For $\rho \rightarrow \infty$ the results are also very good. As is typical of the Morse-Feshbach approximation, the approximate result differs asymptotically from the exact result only in the asymptotic phase. That is,

$$F_L(\rho) \sim \sin(\rho - L\pi/2 - \eta \ln 2\rho + \sigma_L),$$

and the approximate result differs from this exact result only by a different value for σ_L , namely, for L=0,

$$(\sigma_0)_{\text{approx}} = \pi/4 - \eta + \eta \ln\eta + (\eta/2) \ln(1 + 6/35\eta^2) - (6/35)^{\frac{1}{2}} \sin^{-1} [1/(1 + 35\eta^2/6)^{\frac{1}{2}}]. \quad (39)$$

Expanding in inverse powers of η with the help of Sterling's series for the exact phase yields the result

$$(\sigma_0)_{\text{approx}} = (\sigma_0)_{\text{exact}} - 1/420\eta + \mathcal{O}(\eta^{-3}).$$

The unmodified Morse-Feshbach result is

$$(\sigma_0)_{\text{approx}} = (\sigma_0)_{\text{exact}} + 1/12\eta + \mathcal{O}(\eta^{-3})$$

Hence the modification results in a significant improvement.

For general L, the value for σ_L which results from the

modification is

$$(\sigma_L)_{approx} = (\eta/2) \ln[\eta^2 + L(L+1) + 6/35] - \eta + (L+\frac{1}{2})(\pi/2) - [L(L+1) + 6/35]^{\frac{1}{2}} \times \sin^{-1} \left[1 / \left(1 + \frac{\eta^2}{[L(L+1) + 6/35]} \right)^{\frac{1}{2}} \right], \quad (39.1)$$

[where L(L+1) has been replaced by L(L+1)+6/35]. For large η , with L/η small, this becomes

$$(\sigma_L)_{\text{approx}} = (\sigma_L)_{\text{exact}} - 1/420\eta + \mathcal{O}(\eta^{-3}),$$

which is, once again, independent of L to the order given.

Finally these approximate wave functions can be examined for $\rho \rightarrow 0$. Using the asymptotic form for $h_1(z)$ for $z \rightarrow -\infty$ one finds

$$\begin{cases} 2F_L(\rho) \\ G_L(\rho) \end{cases} \xrightarrow[approx]{} \rightarrow |g|^{-\frac{1}{2}} e^{\mp |\varphi|} [1 \mp 5/72 |\varphi| + \cdots], \quad (40)$$
$$|\varphi| \rightarrow [L(L+1) + 6/35]^{\frac{1}{2}} [\ln \rho + \mathcal{O}(\rho^0)],$$

as $\rho \rightarrow 0$. Thus

$$\begin{cases} 2F_L(\rho) \\ G_L(\rho) \end{cases} \rightarrow \rho^{f(L)},$$
 (40.1)

where $f(L) = (\frac{1}{2}) \pm [L(L+1) + 6/35]^{\frac{1}{2}} \ln \rho + O(\rho^{0}).$

The exponents for ρ , for the exact F_L and G_L , should be, of course, L+1 and -L. The approximation yields however, $f(L)\sim \frac{1}{2}+\lfloor L(L+1)+6/35 \rfloor^{\frac{1}{2}}$ with the upper sign, and $f(L)\sim \frac{1}{2}-\lfloor L(L+1)+6/35 \rfloor^{\frac{1}{2}}$ with the lower. For moderately large L the square root can be expanded and one finds

$$f(L) \sim \frac{1}{2} \pm (L + \frac{1}{2} + \frac{1}{2} (6/35 - \frac{1}{4}) [1/(L + \frac{1}{2}) + \cdots]$$

= $\frac{1}{2} \pm (L + \frac{1}{2}) \mp 11/140(2L + 1) + \cdots$ (39.1)

The error in the exponents decreases reasonably well as L increases.

For L=0 one has as exponents $\frac{1}{2}+(6/35)^{\frac{1}{2}}\cong 32/35$ and $\frac{1}{2}-(6/35)^{\frac{1}{2}}\cong 3/35$, which are to be compared to 1 and 0 respectively. The approximation to F_0 is satisfactory, but for G_0 the approximation is very poor for extremely small ρ . Nevertheless, the 6/35 modification did result in marked improvement.

The consideration of the special values of ρ above, namely $\rho = 0$, $\rho_a = \infty$, indicate clearly that the proposed modification of the Morse-Feshbach approximation yields a very satisfactory approximation to the Coulomb wave functions over the entire positive real axis. This is, of course, largely due to the simplicity of g for the Coulomb case, since only one turning point occurs for $\rho \ge 0$. The results obtained for the approximate wave functions using these special values of ρ are summarized in Table I for convenience.

 $\begin{cases} (F_L)_{approx}/(F_L)_{exact} \\ (G_L)_{approx}/(G_L)_{exact} \end{cases} \text{ at turning point} \end{cases}$ Exponents as $\rho \rightarrow 0$ Error in σ_L at $\rho = \infty$ $\begin{array}{l} \text{MF: } \frac{1}{2}, \frac{1}{2} \\ \text{MF mod: } \frac{1}{2} + \left[\frac{6}{35} + L(L+1) \right]^{\frac{1}{2}}, \\ - \frac{1}{2} - \left[\frac{6}{35} + L(L+1) \right]^{\frac{1}{2}} \end{array}$ $1 \pm (3/35)(\frac{3}{2})^{1/3} \eta^{-4/3} \Gamma(\frac{2}{3}) / \Gamma(\frac{1}{3}) + \cdots$ $1/12\eta$ $1+1/3150\eta^2+\cdots$ $-1/420\eta$

TABLE I. Approximate wave functions for special values of ρ .

In order to illustrate the accuracy of these approximations for other than the special values of ρ used above sample calculations have been performed for F_0 and G_0 which are tabulated in Table II. It should be noted that even for $\eta = 1$, which is a severe test of the approximations, the agreement is good. The error decreases rapidly as η increases. The few comparisons made reflect primarily the lack of tables for large η .

In the discussion above for F_L and G_L at the turning point, the expansions have been made under explicit assumption that $\eta \gg 1$ and L/η is small. It is of some interest to note that the approximate wave functions are equally valid for L/η not small. At the modified turning point, ρ_a , it has already been found that

$$\begin{cases} F_L(\rho_a) \\ G_L(\rho_a)/\sqrt{3} \end{cases} \cong [\Gamma(\frac{1}{3})/2\pi^{\frac{1}{2}}] 6^{-1/6} \rho_a^{\frac{1}{2}} (\rho_a - \eta)^{-1/6}.$$

The definition of ρ_a is, in general,

Exact: L+1, -L

$$\rho_a = \eta + (\eta^2 + \alpha)^{\frac{1}{2}},$$

where α is the modified value of L(L+1) as given earlier. For $L/\eta \gg 1$ one has therefore

$$\alpha = L(L+1) + 39/140 + O(1/L).$$

As a result, one finds that

$$\rho_a = \rho_L + 39/280 \rho_L + \mathcal{O}(\rho_L^{-2}).$$

Hence the Morse-Feshbach (modified) approximation to F_L and G_L at ρ_a assumes the form

$$\begin{cases} F_L \\ G_L/\sqrt{3} \end{cases} \cong [\Gamma(\frac{1}{3})/2\pi^{\frac{1}{3}}] 6^{-1/6} \rho_L^{1/6} \\ \times [1+\eta/6\rho_L + O(1/\rho_L^2)]. \quad (41)$$

To obtain the exact value for F_L and G_L at ρ_a , one again resorts to a Taylor series. Noting that $F_L''(\rho_L)$

and $G_L''(\rho_L)$ vanish, it is found that

$$\begin{cases} F_{L}(\rho_{a}) \\ G_{L}(\rho_{a}) \end{cases} = \begin{cases} F_{L}(\rho_{L}) \\ G_{L}(\rho_{L}) \end{cases} + (39/280\rho_{L}) \begin{cases} F_{L}'(\rho_{L}) \\ G_{L}'(\rho_{L}) \end{cases} + \mathfrak{O}(\rho_{L}^{-4}) \begin{cases} F_{L} \\ G_{L} \end{cases}.$$

Under the assumptions that $L \gg \eta \gg 1$, Eqs. (13) and (14) assume the forms,

$$\begin{cases} F_L(\rho_L) \\ G_L(\rho_L)/\sqrt{3} \end{cases} \rightarrow (\Gamma(\frac{1}{3})/2\pi^{\frac{1}{3}})\rho_L^{1/6}6^{-1/6}(1-\eta/\rho_L)^{-1/6} \\ \times (1\mp 39b2^{\frac{1}{3}}\rho_L^{-4/3}/280+\cdots), \end{cases}$$

$$\begin{cases} F_{L'}(\rho_L) \\ G_{L'}(\rho_L)/\sqrt{3} \\ \end{bmatrix} \rightarrow [\Gamma(\frac{1}{3})/2\pi^{\frac{1}{2}}]\rho_L^{1/6}6^{-1/6} \\ \times [\pm b\rho^{-\frac{1}{2}}2^{\frac{1}{3}} + (3(2)^{-4/3}/5b)\rho_L^{-1} + \cdots] \\ \text{Thus.} \end{cases}$$

. .

$$\begin{cases} F_L(\rho_a) \\ G_L(\rho_a)/\sqrt{3} \end{cases} = [\Gamma(\frac{1}{3})/2\pi^{\frac{1}{2}}]\rho_L^{1/6}6^{-1/6}(1-\eta/\rho_L)^{-1/6} \\ \times [1+\mathcal{O}(\rho_L^{-2})]. \quad (41.1) \end{cases}$$

This result is seen to agree with the approximate result, Eq. (41), up to order ρ_L^{-2} . It is clear therefore that the approximate wave functions give excellent results for F_L and G_L at $\rho = \rho_a$ in both limits $L \gg \eta$ and $\eta \gg L$. This leads one to feel confident that similarly good results will hold for the transition region, $L \sim \eta$, as well. It is important to note, however, that the aforementioned results all require the use of a value for the "shifted" L(L+1), that is α , which is appropriate to the region of interest. Now α can be given quite generally, but this would require solving a quartic equation, given earlier. The result is quite unwieldy, and it was therefore considered reasonable to confine attention to limiting cases as done above.

TABLE II. Sample calculations for F_0 and G_0 .

η;ρ	$F_0(a)$				Ga(a)			
	JWKB	MF	MF mod.	Exact	JWKB	MF	MF mod.	Exact
1; 0.6 1; 3 1; 6	0.1393 1.2268 -0.2742	$0.1322 \\ 1.1111 \\ -0.2465$	$0.1177 \\ 1.0877 \\ -0.1603$	0.1071 1.0844 -0.1665	$1.644 \\ 0.4763 \\ -1.072$	$2.564 \\ 0.5591 \\ -1.074$	$2.631 \\ 0.6220 \\ -1.096$	2.792 0.6284
1.995; 1.2 3.981; 2.4	$0.04853 \\ 0.005923$	$0.04725 \\ 0.005834$	$0.04370 \\ 0.005635$	0.04343 0.005625	6.756 5.5450	7.0747 56.544	7.4526 58.162	7.5050 58.280

0

APPENDIX

For L of the same order as or larger than η , F_L and G_L are not as similar to each other at ρ_0 as they are at ρ_L , and if L is quite large compared to η , the difference may be very great. In this case it is necessary to turn to the individual integral representations of F_L and G_L as given in reference 13, Eqs. (10.3) and (10.5)

$$F_L(\rho) = \frac{e^{-\pi\eta}\rho^{L+1}}{(2L+1)!C_L} \int_0^1 (1-z^2)^L \cos(2\eta \tanh^{-1}z - \rho z) dz,$$
(A1)

$$G_L(\rho) = \frac{e^{-\pi\eta\rho^{L+1}}}{(2L+1)!C_L} \bigg\{ \int_0^1 (1-z^2)^L \sin(2\eta \tanh^{-1}z - \rho z) dz \bigg\}$$

$$+e^{\pi\eta}\int_0^\infty (1+u^2)^L \exp\left[-u\rho - 2\eta \tan^{-1}(1/u)\right] du \bigg\}.$$
 (A2)

To obtain $F_L(\rho_0)$, note that the main contribution to the integral comes from small z and expand the cosine for z small, setting $\rho = 2\eta$ wherever it occurs. Term-byterm integration, together with the use of the expansion of C_L already discussed, yields the following result for $L \ge \eta$:

$$F_{L}(\rho_{0}) \cong \left[(1/2L)^{\frac{1}{2}} \eta^{L+1} (L^{2} + \eta^{2})^{-(L/2+\frac{1}{2})} / (1+1/2L) \right]$$

$$\times \exp\{L - \eta \tan^{-1}L/\eta - 5\eta^{2}/12L^{3} - 1/8L$$

$$- L/12(L^{2} + \eta^{2})\} (1 + 11\eta^{2}/8L^{4} + 5\eta^{4}/4L^{6} + \cdots). \quad (A3)$$

The expansion for G_L at ρ_0 may be obtained in terms of the steepest descents result, given in reference 13, Eq. (9.6), for $\rho = 2\eta$. For large η , only the second integral in Eq. (A2) contributes, and corrections to their Eq. (9.6) may be obtained by expanding the integrand about $u = L/\eta$, and integrating term-by-term. The result, after treating the coefficient in the same manner as before, is

$$G_{L}(\rho_{0}) = (2/L)^{\frac{1}{2}} \eta^{-L} (L^{2} + \eta^{2})^{(L/2 + \frac{1}{4})}$$

$$\times \exp\{-L + \eta \tan^{-1}L/\eta + 5\eta^{2}/12L^{3} - 1/8L$$

$$+ L/12(L^{2} + \eta^{2})\}(1 + \eta^{2}/8L^{4} + 5\eta^{4}/4L^{6}). \quad (A4)$$

With the help of the recurrence relation given by Powell,²⁰ the derivatives of $F_L(\rho_0)$ and $G_L(\rho_0)$ were

²⁰ J. L. Powell, Phys. Rev. 72, 626 (1947).

found to be

$$F_{L}'(\rho_{0}) = F_{L}(\rho_{0}) \{ [(L+1)/2\eta] [1+\eta^{2}/L^{3} - 7\eta^{2}/2L^{4} - 5\eta^{4}/2L^{6}] \},$$

$$G_{L}'(\rho_{0}) = G_{L}(\rho_{0}) \{ -[L/2\eta] [1-\eta^{2}/L^{3} - \eta^{2}/2L^{4} - 5\eta^{4}/2L^{6}] \}.$$
(A5)

In order to obtain an expansion of $F_L(\rho)$ for arbitrary ρ in the vicinity of ρ_0 , one must return to the integral representation of Eq. (A1) and, as before, expand for z small. In the present case, an extra term $(\rho_0 - \rho)z$ appears as part of the argument of the cosine in the integrand, and necessitates use of the expression for the cosine of the sum of two angles. Noting that

$$\int_{0}^{1} (1-z^{2})^{L} z^{2m} \cos(\Delta \rho z) dz = L \, [\pi^{\frac{1}{2}} 2^{L-\frac{1}{2}} (-1)^{m} \\ \times D^{2m} [(\Delta \rho)^{-(L+\frac{1}{2})} J_{L+\frac{1}{2}} (\Delta \rho)] \equiv b_{2m}$$

where $D \equiv d/d\rho$, and

.

$$\int_{0}^{1} (1-z^{2})^{L} z^{2m+1} \sin(\Delta \rho z) dz = L ! \pi^{\frac{1}{2}} 2^{L-\frac{1}{2}} (-1)^{m} \\ \times D^{2m+1} [(\Delta \rho)^{-(L+\frac{1}{2})} J_{L+\frac{1}{2}} (\Delta \rho)] \equiv b_{2m+1},$$

where $\Delta \rho = \rho_0 - \rho$, one may write the resulting expression for $F_L(\rho)$, when $L \ge \eta$ and $(\rho_0 - \rho)$ small, as

$$F_{L}(\rho) = \left[e^{-\pi \eta \rho L + 1} / (2L + 1) ! C_{L} \right] \\ \times \left\{ b_{0} - 2\eta (b_{3}/3 + b_{5}/5 + b_{7}/7 + \cdots) - 2\eta^{2} (b_{6}/9 + 2b_{8}/15 + \cdots) + \eta^{3} b_{9}/81 + \cdots \right\}.$$
(A6)

The corresponding expression for $G_L(\rho)$ is again obtained by finding corrections to the steepest descents approximation. The result is

$$G_{L}(\rho) = [G_{L}(\rho)]_{SD} \{1 + 1/24L + [(L^{2} + \eta^{2})\rho^{2}/24L] \\ \times [5L/(X - L)^{3}(LX + \rho\eta) \\ - X^{2}/(X - L)^{2}(LX + \rho\eta)^{2}] + \cdots, \quad (A7)$$

where, according to Eq. (9.6) of reference 13,

$$[G_{L}(\rho)]_{SD} = 2^{L} (2\pi)^{\frac{1}{2}} (LX + \rho\eta)^{L + \frac{1}{2}} \\ \times \exp\{-X - 2\eta \tan^{-1}(\rho/X)\} / \\ (2L + 1) ! C_{L} \rho^{L} (X - L)^{\frac{1}{2}}, \quad (A8)$$

and $X = L + (L^2 + 2\rho\eta - \rho^2)^{\frac{1}{2}}$.