Wave Functions for Large Arguments by the Amplitude-Phase Method

John A. Wheeler

University of North Carolina, Chapel Hill, North Carolina (Received August 17, 1937)

The two independent solutions of the radial wave equation required in the treatment of collision problems may be expressed in terms of a common amplitude and phases differing by $\pi/2$, following a method due to Milne. The determination of phase shifts is simplified by this procedure. Analytical expressions for the amplitude and phase and their derivatives are given in the case of zero field for L=0, 1, 2, 3, 4. In other cases these quantities may rapidly be determined for large arguments by numerical integration of Eqs. (7) and (5b). Values of the amplitude and phase of the coulomb functions needed in the treatment of the scattering of alpha-particles in helium for L=0 and L=2 were obtained in this way and are tabulated.

I N the treatment of questions of nuclear scattering and disintegration and similar problems in atomic physics,¹ the radial wave function describing the relative motion of the two particles under consideration may be divided into two parts. The first part, $F^*(r)$, defined over the region from the origin out to a certain separation r^* , depends upon the special nature of the interaction between the two particles or systems, whilst the second, extending from r^* to infinite distance, requires for its determination the solution of the Schroedinger equation for some relatively simple analytic law of force.

Characteristic of the problems mentioned is the requirement that both independent solutions of the wave equation be known for $r > r^*$ —the so-called "regular" and "irregular" functions. Difficulty in obtaining numerical values of the irregular function and its derivative often occurs as a serious obstacle in applying collision theory to actual problems. Adequate tables must give both functions and their derivatives at intervals relatively small in comparison with the wavelength, since these quantities change rapidly even in regions where they do not oscillate. However, the calculation of the two wave functions and their derivatives for a single value of r for a given impact energy is often a time-taking process, especially if r is large and the customary power series calculation is employed.

The introduction of slowly varying functions, representing essentially the amplitude and phase of the two functions, makes it possible to increase the size of the interval of tabulation by a large factor, gives a method of computing the wave function for large arguments which is often much more rapid than expansion in power series about the origin, and in addition makes a certain simplification in the calculation of phase shifts in scattering problems.

The functions under consideration may be defined as follows:

F (regular function) satisfies the wave equation; vanishes at r=0 when prolonged inward to the origin; has unit amplitude at $r = \infty$. Example: $F(r) = (kr)^{-1} \sin kr - \cos kr$ (scattering of a neutron with one unit of angular momentum).

G (irregular function) satisfies same equation; has unit amplitude and is 90° in advance of *F* at infinity. (In example, $G(r) = (kr)^{-1} \cos kr + \sin kr$). From the definitions of *F* and *G* and the properties of the Schroedinger equation it follows that

$$GdF/dr - FdG/dr = k (\equiv [2\mu E/\hbar^2]^{\frac{1}{2}}).$$
(1)

In applications, the equations of fit are applied at $r = r^*$:

$$aF + bG = F^*, \tag{2a}$$

$$adF/dr + bdG/dr = dF^*/dr$$
 (r=r*), (2b)

and the values found for a and b are used to evaluate the collision cross section (determined by the phase shift $K = \arccos a/b$) and the probability of interpenetration (proportional to $[a^2+b^2]^{-1}$) of the two particles of given angular momentum.

Milne² has shown that a simple differential

¹ Cf. Mott and Massey, *The Theory of Atomic Collisions* (Oxford, 1933).

² W. E. Milne, Phys. Rev. **35**, 864 (1930). Cf. also L. A. Young, Phys. Rev. **38**, 1612 (1931), who has given the name "local momentum" to the quantity $P(r) = A^{-2}(r)$ and shown its natural connection with the Bohr-Sommer-feld quantum conditions.

equation (essentially (5a) below) is satisfied by the amplitude function $A(r) = [F^2(r) + G^2(r)]^{\frac{1}{2}}$, and has used this equation to obtain solutions of the wave equation for certain problems in the discrete spectrum. We introduce in addition a phase function $\Phi(r)$ defined as follows:

$$F(r) = A(r) \sin \Phi(r); \quad G(r) = A(r) \cos \Phi(r); \\ \Phi(0) = 0. \quad (3)$$

If a satisfactory method is already available for obtaining F and G, Eq. (3) is needed only for purposes of interpolation; otherwise, the following differential equations may readily be deduced³ for the direct determination of A and Φ :

$$\frac{d^{2}A/dr^{2}+2\mu/\hbar^{2}[E-V(r)]A}{-(d\Phi/dr)^{2}A=0, \quad (4a)}$$

$$\frac{1/kd\Phi/dr=1/A^{2}. \quad (4b)}{kd\Phi/dr=1/A^{2}}$$

On combining and introducing $\rho = kr$ for independent variable, we have equations by which

first A and then Φ may be determined:

$$d^{2}A/d\rho^{2} + (1 - V/E - 1/A^{4})A = 0,$$

$$A(\infty) = 1, \ dA/d\rho(\infty) = 0, \quad (5a)$$

 $d\Phi/d\rho = 1/A^2$, $\Phi(0) = 0$. (5b)

These equations clearly reduce to the Jeffreys-W.K.B. approximation on neglecting

$1/Ad^2A/d ho^2$.

FUNCTIONS IN FIELD FREE SPACE

When there is no interaction between the two particles, we have $V(r) = L(L+1)\hbar^2/2\mu r^2$, representing the effect of centrifugal force alone. The analytical expressions for F and G are in this case well known,⁴ and the expressions for A and Φ can be obtained directly from the equations of definition. The asymptotic value of Φ for large ρ is $\rho - L\pi/2$; we therefore write $\Phi = \rho - L\pi/2 + \varphi$; also $z = \rho^{-1} = (kr)^{-1}$.

$$L=0, \ A=1, \ \varphi=0, \ \frac{r}{A}\frac{dA}{dr}=0, \ \frac{r}{dr}\frac{d\varphi}{dr}=0,$$

$$L=1, \ A=(1+z^2)^{\frac{1}{2}}, \ \text{tg } \varphi=z, \ \frac{r}{A}\frac{dA}{dr}=-\frac{z^2}{1+z^2}, \ \frac{r}{dr}=-\frac{z}{1+z^2},$$

$$L=2, \ A=(1+3z^2+9z^4)^{\frac{1}{2}}, \ \text{tg } \varphi=\frac{3z}{1-3z^2}, \ \frac{r}{A}\frac{dA}{dr}=-\frac{3z^2+18z^4}{1+3z^2+9z^4}, \ \frac{r}{dr}=-\frac{3z+9z^3}{1+3z^2+9z^4},$$

$$L=3, \ A=(1+6z^2+45z^4+225z^6)^{\frac{1}{2}}, \ \text{tg } \varphi=\frac{6z-15z^3}{1-15z^2}, \ \frac{r}{A}\frac{dA}{dr}=-\frac{6z^2+90z^4+675z^6}{1+6z^2+45z^4+225z^6},$$

$$L=4, \ A=(1+10z^2+135z^4+1575z^6+11025z^8)^{\frac{1}{2}}, \ \text{tg } \varphi=\frac{10z-105z^3}{1-45z^2+105z^4},$$

$$L=4, \ A=(1+10z^2+135z^4+4725z^6+44100z^8), \ \text{tg } \varphi=\frac{10z+135z^3+1575z^5+11025z^7}{1-45z^2+105z^4},$$

dr

NUMERICAL INTEGRATION

A dr

 $1+10z^{2}+135z^{4}+1575z^{6}+11025z^{8'}$

Ordinarily solutions of (5) for a given V(r) cannot be obtained in terms of polynomials or

simple analytical expressions. As we are primarily interested in the solution of the wave equation for large arguments, we solve Eq. (5a) by numerical integration from infinity inward.

 $1+10z^{2}+135z^{4}+1575z^{6}+11025z^{8}$

⁸ We make use of the fact that the real part of $G+iF = A \exp(i\Phi)$ satisfies the wave equation to get (4a) and derive (4b) from condition (1).

⁴ $F = (\pi kr/2)^{\frac{1}{2}}J_{L+\frac{1}{2}}(kr)$; $G = (\pi kr/2)^{\frac{1}{2}}J_{-L-\frac{1}{2}}(kr)$, in terms of Bessel functions.

Hartree has already pointed⁵ out that the nonlinear nature of a second-order differential equation causes no difficulties in the calculations; the essential point is to see that the equation involves no first derivatives. Hence, if we introduce $z=1/\rho$ as new independent variable suitable for integrating (5a) inward, we must also change the dependent variable to M = zA to compensate the first derivatives which would otherwise creep into the equation. We then obtain

$$M'' = M^{-3} - M(1 - V/E)z^{-4}, M(0) = 0,$$

 $M'(0) = 1$ (7)

on using dashes to represent differentiation with respect to z.

In the numerical computation, the range of zof interest is divided into equal intervals (say $z=0.00, 0.05, 0.10, \cdots$ to 0.50) and a power series expansion for M in the neighborhood of z=0 is used to start the integration. The first few steps of the calculation must be made with high accuracy, since M'' appears as the small difference between large quantities. A rapid procedure for integrating second order differential equations which are free of first derivatives, together with a discussion of stability and accuracy, is given in Hartree's paper.⁵

The most convenient check on the calculation of M may be made by means of Φ , provided one knows from other considerations the value of the constant C in the asymptotic expression for the phase:

$$\Phi \sim \int^{\rho} (1 - V/E)^{\frac{1}{2}} d\rho + C \quad (\rho \to \infty).$$

(For example, it follows⁶ from the asymptotic expansion of the contour integrals for the Coulomb functions that

$$\Phi \sim \rho - \eta \ln 2\rho - L\pi/2 + \sigma_L,$$

where $\sigma_L = \arg \Gamma(L+1+i\eta)$.) Starting with this value for Φ at $\rho = \infty$, and integrating (5*b*) inwards toward the origin, it is easy to determine how closely $\Phi(\rho)$ approaches to having the value zero at the origin; this gives a direct check on the calculation of Φ and hence (from (5b)) on the accuracy of A.

	2245	$-(\rho/A)dA/d\rho$	0.0000 .0116 .0240 .0368 .0500	.0629 .0756 .0877 .0991 .1100	
uncertain.	$\sigma_0 = -0.2245$		0.4444 .4488 .4521 .4540 .4546	.4538 .4517 .4484 .4443 .4387	
	ak = 2.25	9.	0.0000 .0047 .0089 .0124 .0153	.0175 .0190 .0199 .0202 .0199	
		Ą	1.0000 1.0114 1.0234 1.0359 1.0488	$\begin{array}{c} 1.0621 \\ 1.0755 \\ 1.0891 \\ 1.1028 \\ 1.1164 \\ 1.1164 \end{array}$	
Last digit	$\sigma_0 = -0.2440$	$-(\rho/A)dA/d\rho$	0.0000 .0131 .0273 .0421 .0575	.0727 .0877 .1022 .1158 .1158	.1396
<i>z</i> ; <i>z</i> =1/kr.		ρ—ρdΦ/dρ	0.5000 .5057 .5101 .5130 .5142	.5139 .5116 .5082 .5036 .4981	.4916
: 1/ak		9	0.0000 0.0060 0114 0161 0201	.0232 .0256 .0271 .0279 .0279	.0275
unctions for $L=0$. F, $G=A$ sin, cos Φ . $\Phi=\rho-\eta \ln 2\rho+\sigma_0+\varphi$; $\eta=1/ak$; $z=1/kr$. Last digit uncertain	ak = 2.00	A	L.0000 L.0129 L.0265 L.0409 L.0558	L0712 L0869 L1029 L1191 L1353	1.1525
	0.2657	$-(\rho/A)dA/d\rho$	0.0000 0151 .0151 .0493 .0677	.0861 .1044 .1221 .1396 .1549	.1695
	ø₀=−0.2657	p−pdΦ/dp	0.5714 .5790 .5852 .5895 .5917	.5921 .5921 .5864 .5811 .5745	.5586 .5586
	1.75	9.	0.0000 .0079 .0152 .0216 .0272	.0318 .0354 .0380 .0397 .0404	.0403
	ak = 1.75	A	1.0000 1.0148 1.0306 1.0474 1.0650	L.0834 L.1023 L.1217 L.1414 L.1613	1.1813
	σ₀=−0.2873	$-(\rho/A)dA/d\rho$	0.0000 .0178 .0377 .0593 .0824	.1057 .1289 .1516 .1734 .1937	.2126 .2299 .2456 .2726 .2726
		dp/₫bq—q	0.6667 .6772 .6862 .6931 .6970	.6986 .6989 .6929 .6866 .6785	.6688 .6580 .6463 .6339 .6311 .6081
nctio	ak = 1.50	9.	0.0000 0108 0210 0303 0385	.0455 .0512 .05555 .0587 .0605	.0613 .0610 .0598 .0576 .0547
TABLE I. Coulomb fur		Ą	$\begin{array}{c} 1.0000\\ 1.0174\\ 1.0362\\ 1.0362\\ 1.0564\\ 1.0779\end{array}$	1.1007 1.1244 1.1244 1.1490 1.1741 1.1998	1.2257 1.2518 1.2780 1.3041 1.3559 1.3559
	$\sigma_0 = -0.3044$	$-(\rho/A)dA/d\rho$	0.0000 .0217 .0266 .0746 .1044	.1362 .1685 .1995 .2291 .2569	.2824 .3056 .3253 .3301 .3301
		ρ−ρdΦ/dρ	0.8000 .8155 .8293 .8403 .8484	.8505 .8506 .8462 .8383 .8272	.8139 .7987 .7823 .7823 .7469 .7104
	ak = 1.25	9.	0.0000 .0157 .0308 .0308 .0449 .0577	.0688 .0781 .0781 .0856 .0913 .0951	.0973 .0979 .0971 .0971 .0978
		¥	$\begin{array}{c} 1.0000\\ 1.0210\\ 1.0442\\ 1.0697\\ 1.0974\end{array}$	$\begin{array}{c} 1.1270\\ 1.1587\\ 1.1920\\ 1.1920\\ 1.2265\\ 1.2621\end{array}$	1.2985 1.3354 1.3727 1.4476 1.4476
	L=0	N	0.00 .05 .15 .20		80.27.26.68. 80.27.26.68.

⁵ D. R. Hartree, Memoirs and Proc. Manchester Lit. and Phil. Soc. **77**, 91 (1932–33). ⁶ Cf., for example, reference 1, p. 39.

COULOMB FUNCTIONS⁷

In the case of the interaction $V(r) = ZZ'e^2/r$ + $L(L+1)\hbar^2/2\mu r^2$, we use the notation

 $a = \hbar^2 / \mu Z Z' e^2$

(characteristic radius), $\eta = 1/ak = \lambda/2\pi a = \lambda/a$ (reduced wave-length). Expanding the solution of

$$M'' = M^{-3} - M[1 - 2\eta z - L(L+1)z^2]/z^4 \quad (8)$$

in a power series about the point z=0,

$$M = z + a_1 z^2 + a_2 z^3 + \cdots, \tag{9}$$

.

we have for the first few coefficients

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$$a_{1} = \eta/2; \quad a_{2} = 5\eta^{2}/8 + L(L+1)/4; a_{3} = 15\eta^{3}/16 + 5\eta L(L+1)/8 - \eta/8; a_{4} = 195\eta^{4}/128 + 45\eta^{2}L(L+1)/32$$
(10)
$$-23\eta^{2}/16 + 5L^{2}(L+1)^{2}/32 - 3L(L+1)/8; a_{5} = 663\eta^{5}/256 - 91\eta^{3}/16 + 195\eta^{3}L(L+1)/64 + 45\eta L^{2}(L+1)^{2}/64 - 23\eta L(L+1)/8 + 3\eta/4.$$

The choice of interval of integration is governed by the practical rate of convergence of the series for the value of η under consideration.

⁷ Cf. F. L. Yost, John A. Wheeler, and G. Breit, Phys. Rev. **49**, 174 (1936), for analytic properties of these functions. For numerical values for $\rho < 1$, cf. same authors, J. Terr. Magn. At. El., 443, Dec. (1935), and E. R. Wicher, J. Terr. Magn. At. El., 389, Dec. (1936).

In calculating the phase, we use as dependent variable the quantity φ defined by

$$\Phi(\rho) = \rho - \eta \ln 2\rho - L\pi/2 + \arg \Gamma(L+1+i\eta) + \varphi(\rho), \quad (11)$$

and take $z=1/\rho$ for independent variable. The integration of the first-order differential equation for φ ,

$$d\varphi/dz = (1 - \eta z)/z^4 - 1/M^2,$$
 (12)

is simple (cf. Hartree, for example). Near z=0 we have

$$d\varphi/dz = [L(L+1)+\eta^2]/2+\cdots$$

Numerical values are given in Tables I and II for L=0 and L=2 for the range of values of interest in the problem of the scattering of alphaparticles in helium, and applicable also to scattering and disintegration problems involving other light nuclei. The last digit is uncertain.

EQUATIONS OF FIT

In the amplitude phase notation, the general solution of the wave equation from r^* to ∞ has the form

$$cA(r)\sin\left[\Phi(r)+K\right],\tag{13}$$

where c and K are constants determined by the equations of fit (2a and 2b) at $r=r^*$. These equations may be put as follows:

TABLE II. Coulomb functions for L=2. F, G=A sin, cos Φ . $\Phi=\rho-\eta \ln 2\rho+\sigma_2-\pi+\varphi$; $\eta=1/ak$; z=1/kr. Last digit uncertain.

L=2	$ak = 1.25$ $\sigma_2 - \pi = -2.3906$		$ak = 1.50$ $\sigma_2 - \pi = -2.5192$		$ak = 1.75$ $\sigma_2 - \pi = -2.6098$		$ak = 2.00$ $\sigma_2 - \pi = -2.6770$		$ak = 2.25$ $\sigma_2 - \pi = -2.7292$			
z	A	φ		φ	A	φ.	A	φ	Α	φ		
0.00	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000		
.05	1.0252	.1689	1.0215	.1634	1.0189	.1601	1.0169	.1579	1.0154	.1564		
.10	1.0633	.3437	1.0545	.3315	1.0485	.3240	1.0440	.3191	1.0406	.3156		
.15	1.1192	.5235	1.1030	.5034	1.0920	.4912	1.0841	.4830	1.0782	.4772		
.20	1.1991	.7050	1.1717	.6767	1.1534	.6594	1.1408	.6478	1.1312	.6396		
.25	1.3128	.8836	1.2678	.8480	1.2388	.8257	1.2186	.8109	1.2036	.8003		
.30	1.4673	1.0542	1.3967	1.0127	1.3524	.9866	1.3217	.9690	1.2993	.9562		
.35	1.6692	1.2103	1.5639	1.1658	1.4987	1.1375	1.4540	1.1182	1.4220	1.1040		
.40	1.9239	1.3481	1.7734	1.3039	1.6812	1.2754	1.6188	1.2555	1.5743	1.2410		
.45	2.2342	1.4664	2.0278	1.4252	1.9023	1.3982	1.8179	1.3792	1.7581	1.3653		
.50	2.6021	1.5657	2.3286	1.5297	2.1633	1.5058	2.0527	1.4888	1.9745	1.4762		
.55	3.0281	1.6480	2.6763	1.6186	2.4677	1.5988	2.3236	1.5846	2.2241	1.5740		
.60	3.5125	1.7156	3.0712	1.6935	2.8066	1.6786	2.6308	1.6678	2.5070	1.6595		
.70	4.6568	1.8154	4.0019	1.8085	3.6115	1.8046	3.3533	1.8013	3.1722	1.7986		
.80	6.0347	1.8807	5.1195	1.8892	4.5765	1.8959	4.2188	1.9003	3.9683	1.9034		
.90	7.6460	1.9223	6.4229	1.9452	5.7001	1.9620	5.2254	1.9739	4.8936	1.9827		
1.00	9.4910	1.9476	7.9115	1.9844	6.9813	2.0101	6.3271	2.0290	5.9468	2.0431		
1.10	11.5701		9.5850	2.0112	8.4194	2.0450	7.6579		7.1269	2.0895		
					l				l			

$$rd\Phi/dr$$
 ctg $(\Phi+K) = r/F^*dF^*/dr$

$$-r/AdA/dr;$$
 (14a)
 $cA \sin (\Phi+K) = F^*$ ($r=r^*$). (14b)

Eq. (14a) determines the phase shift, K, of the wave function in the actual field of force with respect to the wave function which would describe the motion if the "outer" potential $(r > r^*)$ extended in to the origin. In scattering problems only K is needed; in the treatment of nuclear interpenetration, K from (14a) is substituted into (14b) to find c, giving the ratio between the amplitudes of the wave function in the inner and outer regions. The derivatives appearing in (14a) are independent of scale:

$$rd\Phi/dr =
ho d\Phi/d
ho = -zd\Phi/dz$$

etc. Eqs. (6) and Tables I and II give the information needed for applying the corresponding functions to collision problems.

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The Nuclear Moment of Barium

A. N. BENSON AND R. A. SAWYER University of Michigan, Ann Arbor, Michigan (Received October 20, 1937)

New data have been obtained on the hyperfine structure of several lines of barium. These have been studied in the attempt to determine more definitely the nuclear moment of the odd isotopes of barium, reported as $2\frac{1}{2}$ by Kruger, Gibbs and Williams, and as $1\frac{1}{2}$ by Schüler and by Murakawa. Studies of the separation of the 6^2S_3 and 7^2S_4 components from the center of gravity, and of the spacing and patterns of the $5^{3}D_{3}$ and $6^{3}P_{2}$ terms all lead to the conclusion that $I=1\frac{1}{2}$ is the correct value of nuclear moment.

 $\mathbf{I}_{\text{the value of the nuclear moment of the odd}}^{\text{N}}$ spite of several researches on the subject, isotopes of barium remains in doubt. The various investigators differ both in experimental findings and in interpretation of the data. McLennan and Allen¹ first found hyperfine structure in a number of the arc and spark lines of barium, but their results have never been confirmed by other workers. Frisch² found all lines sharp. The first accurate observations were those of Ritschl and Sawyer³ who observed structure in several lines and published measurements on the resonance lines of Ba II, $6^2S_{\frac{1}{2}} - 6^2P_{\frac{1}{2}, \frac{1}{2}}$, from which Schüler and Jones⁴ deduced $1\frac{1}{2}$ as the nuclear moment of the odd isotopes. However, from their own measurements on the same lines, Kruger, Gibbs, and Williams⁵ concluded that the moment is probably $2\frac{1}{2}$, while Murakawa,⁶ from

observations on these and other lines, considered $1\frac{1}{2}$ to be correct. Recent compilations of nuclear moments⁷⁻⁹ have given $2\frac{1}{2}$ as the moment of barium but have indicated that uncertainty exists.

The difficulty in the determination of the moment from hyperfine structure observations arises from the fact that barium is a mixture of several isotopes. The recent measurements of Sampson and Bleakney¹⁰ give for the isotopes and their percentage abundance:

mass number 130 132 134 135 136 137 138 percentage 0.16 0.015 1.72 5.7 8.5 10.8 73.1

The even isotopes thus make up 83.5 percent of the atoms and all observers are agreed that these even isotopes, in common with all observed even isotopes save N14, have no hyperfine structure. In all barium h.f.s. patterns, the five even isotopes fall together in a very heavy central

¹ McLennan and Allen, Phil. Mag. **8**, 515 (1929). ² Frisch, Zeits. f. Physik **68**, 758 (1931). ³ Ritschl and Sawyer, Zeits. f. Physik **72**, 36 (1931).

⁴ Kallman and Schüler, Ergebn. d. Exakt. Naturwiss. 11. 134 (1932)

Kruger, Gibbs, and Williams, Phys. Rev. 41, 322 (1932). ⁶ Murakawa, Sci. Papers Tokyo I. P. C. R. 18, 304 (1932).

⁷ White, Introduction to Atomic Spectra (McGraw Hill, 1934), p. 372.

⁸ Darrow, Bell Tech. J. 14, 319 (1935).

⁹ Bacher and Bethe, Rev. Mod. Phys. 8, 82 (1936)

¹⁰ Sampson and Bleakney, Phys. Rev. 50, 456 (1936).