Calculation of Coulomb Wave Functions for High Energies

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For high energies and moderate radii Coulomb functions are conveniently calculated by evaluating certain integrals numerically.

The power-series method[1] of calculating Coulomb wave functions is cumbersome if the radius and energy are large on account of slow convergence of the series. A way of eliminating some of the labor has been given by Wheeler,[2] who developed the phase-amplitude method using a transformation recommended for numerical work by Milne.[3] The phase-amplitude method is especially suitable for the treatment of scattering of alpha-particles by helium. Another simple method suitable for the treatment of the scattering of protons by protons is described in this note. The Coulomb functions are expressed in terms of definite integrals which can be conveniently evaluated by numerical integration. The arrangement of the calculation is such as to have $\sin\rho$, $\cos\rho$ as the first order approximations for $L=0$. Here ρ is $2\pi r/\Lambda$, Λ is the wave-length at a large distance, $L\hbar$ is the angular momentum. The regular and irregular solutions are linear combinations of $\sin\rho$ and $\cos\rho$ multiplied by slowly varying factors expressible by means of definite integrals. For high energies one of the factors is small while the other is nearly unity. The difference between the actual function and the first approximation can be estimated sufficiently accurately by using a relatively rough numerical evaluation of the integrals.

The differential equation to be solved is

$$\frac{d^2Y_L}{d\rho^2}+\left(1-\frac{2\eta}{\rho}-\frac{L(L+1)}{\rho^2}\right)Y_L=0.$$

Here η is the collision parameter $ZZ'e^2/\hbar v$ where Z, Z' are the atomic numbers of the colliding nuclei and v is the relative velocity. The equation is solved by[4]

$$Y_L=F_L+iG_L=\frac{ie^{-i\rho}}{(2L+1)!C_L\rho^L}\int_0^\infty t^{-i\eta+L}\times(t+2i\rho)^{i\eta+L}e^{-t}dt. \quad (1)$$

Here F_L, G_L are respectively the regular and irregular functions having asymptotic forms for large ρ given in reference 1. In order that (1) be a solution of the differential equation it is essential that

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

be zero for $t=0$. This is true for all real η. Negative energies correspond to imaginary η. For these Y_L is not a solution. Negative energies of relative motion are not needed, however, in the discussion of collision problems. The number C_L occurring in Eq. (1) is independent of ρ and is given by

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

For $L=0$ one obtains from Eq. (1)

$$F_0=(I_0\sin\rho+H_0\cos\rho)/C_0,$$
$$G_0=(I_0\cos\rho-H_0\sin\rho)/C_0, \quad (2)$$

where

$$I_0=\int_0^\infty e^{-t-\alpha}\cos\beta\,dt;\quad H_0=-\int_0^\infty e^{-t-\alpha}\sin\beta\,dt, \quad (3)$$

$$\alpha=\eta\tan^{-1}\frac{2\rho}{t},\quad \beta=\eta\ln\left(1+\frac{4\rho^2}{t^2}\right)^{\frac{1}{2}}. \quad (3.1)$$

[1] F. L. Yost, J. A. Wheeler and G. Breit, Phys. Rev. **49**, 174 (1935); the notation of this reference is used in present note; J. Terr. Mag. At. Elec. **40**, 443 (1935). E. R. Wicher, J. Terr. Mag. At. Elec. **41**, 389 (1936).
[2] J. A. Wheeler, Phys. Rev. **52**, 1123 (1937).
[3] W. E. Milne, Phys. Rev. **35**, 864 (1930).
[4] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Third Edition, Cambridge University Press, 1920), p. 340.

TABLE I. *Comparison of calculations by series with calculations by Eqs. (2) and (4).**

Proton Energy	Radius	No. of Integration Intervals Used		F_0	G_0	A	F_0'
2.6 Mev ($\eta=0.09805$)	$r=0.5e^2/mc^2$ ($\rho=0.24915$)	18 Intervals $t=0.0001$ to $t=6$	By integral	0.2135	1.070	1.096	0.865
			By series	0.2152	1.073	1.094	0.866
			Difference	0.8%	0.3%	0.2%	0.1%
2.6 Mev ($\eta=0.09805$)	$r=3e^2/mc^2$ ($\rho=1.4919$)	18 Intervals $t=0.0001$ to $t=6$	By integral	0.999	0.2505	1.062	0.2196
			By series	1.000	0.2502	1.0623	0.2195
			Difference	0.1%	0.1%	0.0%	0.0%
10.0 Mev ($\eta=0.0500$)	$r=e^2/mc^2$ ($\rho=0.9772$)	12 Intervals $t=0.0001$ to $t=5$	By integral	0.804	0.628	1.022	0.590
			By series	0.805	0.628	1.021	0.590
			Difference	0.1%	0.0%	0.1%	0.0%

* The first column gives the energy of protons impinging on hydrogen atoms at rest. The second column gives the distance r between the protons for which the Coulomb wave function has been computed. The third column describes the intervals used in the evaluation of the definite integrals. The series computations are the more accurate in this case. The accuracy obtained by the integral method using relatively little arithmetical labor is seen to be sufficient for most practical purposes.

The calculation of I is often carried out more conveniently by means of

$$I_0=1+\int_0^\infty e^{-t}(e^{-\alpha}\cos\beta-1)dt. \qquad (3.2)$$

For large energies η is small and, therefore, $I_0\sim 1$, $H_0\sim 0$. It is convenient to evaluate H_0 and I_0-1 numerically. The same sets of quantities occur in both integrals. Similarly the derivatives $F_0'=dF_0/d\rho$, $G_0'=dG_0/d\rho$ are computed by formulas of the same type

$$\begin{aligned}F_0'&=G_0+(1/C_0)(I_0'\sin\rho+H_0'\cos\rho),\\ G_0'&=-F_0+(1/C_0)(I_0'\cos\rho-H_0'\sin\rho)\end{aligned} \qquad (4)$$

with

$$I_0'=-\int_0^\infty 2\xi\eta(t\cos\beta+2\rho\sin\beta)e^{-t-\alpha}dt, \qquad (4.1)$$

$$H_0'=\int_0^\infty 2\xi\eta(t\sin\beta-2\rho\cos\beta)e^{-t-\alpha}dt, \qquad (4.2)$$

where $$\xi=(t^2+4\rho^2)^{-1}. \qquad (4.3)$$

For comparison with Wheeler's phase-amplitude method one has

$$C_0^2AdA/d\rho=C_0^2(F_0F_0'+G_0G_0')=I_0I_0'+H_0H_0', \qquad (5)$$

$$1=F_0'G_0-F_0G_0'=A^2+(I_0H_0'-I_0'H_0)/C_0^2, \qquad (5.1)$$

$$A^2=F_0^2+G_0^2. \qquad (5.2)$$

These formulas are also useful for checking the calculations.

The calculation of G_0, G_0' by the definite integral method is no harder than that of F_0, F_0' in contrast to the series method. The phase-amplitude method has the same advantage.

In Table I calculations by series are compared with those by means of Eqs. (2) and (4). The definite integrals were evaluated relatively crudely. The range of integration was divided into intervals. The integral in an interval $t_1<t<t_2$ was evaluated by calculating all the factors for $t=t_1$ and for $t=t_2$, then multiplying $e^{-t_1}-e^{-t_2}$ by the average value of the other factors.