

Coulomb Functions for Nuclear Physics

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References for Coulomb Functions

- ▶ M. Abramowitz, *Coulomb Wave Functions*, in M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover Publications (New York), 1965.
- ▶ I.J. Thompson, *Coulomb Functions*, in F.W. Olver *et al.*, *NIST Handbook of Mathematical Functions*, Cambridge University Press (New York), 2010.
- ▶ I.J. Thompson, *Coulomb Functions*, in F.W. Olver *et al.*, *NIST Digital Library of Mathematical Functions*, <http://dlmf.nist.gov/>.

Speaking of NIST, here is a useful website for the fundamental physical constants:

<https://physics.nist.gov/cuu/Constants/index.html>.

The Differential Equation

- ▶ In terms of physical parameters, a Coulomb function u in coordinate space satisfies

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u}{dr^2} + \frac{Z_1 Z_2 e^2}{r} u + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} u = E u,$$

where $r \geq 0$ is the radial coordinate, E is the center-of-mass energy, μ is the reduced mass.

- ▶ We also have

$$V_c = \frac{Z_1 Z_2 e^2}{r},$$

the repulsive Coulomb potential,

- ▶ and

$$V_{\text{eff}} = \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2},$$

an effective repulsive potential corresponding to the centrifugal or angular momentum barrier.

Dimensionless Parameters

- ▶ In terms of the dimensionless parameters ρ and η , we have $u(\ell, \eta, \rho)$ and this equation becomes

$$u'' + \left[1 - \frac{2\eta}{\rho} - \frac{\ell(\ell + 1)}{\rho^2} \right] u = 0,$$

where $\rho = kr$, $k = \sqrt{2\mu E/\hbar^2}$, $\eta k = Z_1 Z_2 e^2 \mu/\hbar^2$, and $' \equiv d/d\rho$.

- ▶ Note that $\rho \propto \sqrt{E}$ and $\eta \propto 1/\sqrt{E}$.
- ▶ One can consider Coulomb functions to be functions of the two variables (E, r) or (η, ρ) .

The Functions

- ▶ $F_\ell(\eta, \rho)$: the regular Coulomb function, $F_\ell(\eta, \rho \rightarrow 0) \propto \rho^{\ell+1}$
- ▶ $G_\ell(\eta, \rho)$: the irregular Coulomb function, $G_\ell(\eta, \rho \rightarrow 0) \propto \rho^{-\ell}$
- ▶ $H_\ell^\pm(\eta, \rho) = G_\ell(\eta, \rho) \pm iF_\ell(\eta, \rho)$
- ▶ Wronskian: $F_\ell' G_\ell - F_\ell G_\ell' = 1$

Various Phases

- ▶ The Coulomb phase shift σ_ℓ is also sometimes needed:

$$e^{2i\sigma_\ell} = \frac{\Gamma(1 + \ell + i\eta)}{\Gamma(1 + \ell - i\eta)} = \frac{(\ell + i\eta) \dots (1 + i\eta)}{(\ell - i\eta) \dots (1 - i\eta)} e^{2i\sigma_0}.$$

Note that $\sigma_\ell - \sigma_0$ does not require the Γ function.

- ▶ The asymptotic phase θ_ℓ is defined to be

$$\theta_\ell = \rho - \eta \log(2\rho) - \frac{1}{2}\ell\pi + \sigma_\ell.$$

- ▶ For $\rho \rightarrow \infty$, we have

$$H_\ell^\pm \sim \exp(\pm i\theta_\ell),$$

which is useful for calculating the S matrix.

Amplitude, Phase, Penetration, and Shift

- ▶ The Amplitude A_ℓ , Phase ϕ_ℓ , Penetration P_ℓ , and Shift S_ℓ are defined according to:

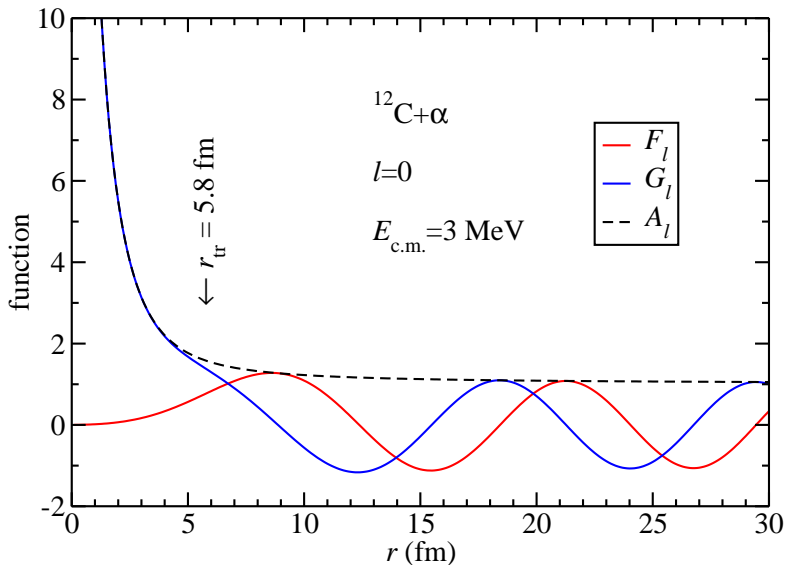
$$\begin{aligned}A_\ell &= (F_\ell^2 + G_\ell^2)^{1/2} \\ \phi_\ell &= \tan^{-1} F_\ell/G_\ell \\ H_\ell^\pm &= A_\ell \exp(\pm i\phi_\ell) \\ P_\ell &= \frac{\rho}{A_\ell^2} \\ S_\ell &= \frac{\rho A'_\ell}{A_\ell} = \frac{\rho(A_\ell^2)'}{2A_\ell^2}\end{aligned}$$

- ▶ Note that we also have $S_\ell + iP_\ell = \rho \frac{H_\ell^{+'}}{H_\ell^+}$, which can be shown using the Wronskian.
- ▶ In R -matrix calculations, one traditionally uses P_ℓ , S_ℓ , and ϕ_ℓ (you only need three).

Classical Turning Radius

- ▶ Consider the quantity $1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}$ in the differential equation.
- ▶ When it is > 0 , the Coulomb functions are oscillatory.
- ▶ When it is < 0 , the Coulomb functions are exponential.
- ▶ It $= 0$ for $\rho_{\text{tr}} = \eta + [\eta^2 + \ell(\ell + 1)]^{1/2}$.
- ▶ *Classical Turning Radius, r_{tr}* : $kr_{\text{tr}} = \rho_{\text{tr}}$.
- ▶ The location of r_{tr} relative to the nuclear surface strongly impacts the physics. In particular, if r_{tr} is well outside the nuclear surface, the reaction probability will be strongly reduced by Coulomb and/or angular momentum barriers.

An Example Plot



Interestingly, both A_ℓ and ϕ_ℓ are monotonic functions of r , for $0 \leq r < \infty$.

Limiting Forms for Small and Large ρ

quantity	$\rho \rightarrow 0$	$\rho \rightarrow \infty$
H_ℓ^+	$[\rho^\ell(2\ell+1)C_\ell(\eta)]^{-1} + \dots + i[\rho^{\ell+1}C_\ell(\eta) + \dots]$	$\exp(i\theta_\ell) \left[1 + \frac{\eta}{2\rho} + i\frac{\eta^2 + \ell(\ell+1)}{2\rho} + \dots \right]$
A_ℓ^2	$[\rho^\ell(2\ell+1)C_\ell(\eta)]^{-2} + \dots$	$1 + \frac{\eta}{\rho} + \frac{3\eta^2 + \ell(\ell+1)}{2\rho^2} + \dots$
ϕ_ℓ	$\rho^{2\ell+1}(2\ell+1)C_\ell^2(\eta) + \dots$	$\theta_\ell + \frac{\eta^2 + \ell(\ell+1)}{2\rho} + \dots$
P_ℓ	$\rho^{2\ell+1}[(2\ell+1)C_\ell(\eta)]^2 + \dots$	$\rho - \eta - \frac{\eta^2 + \ell(\ell+1)}{2\rho} + \dots$
S_ℓ	$-\ell + \dots$	$-\frac{\eta}{2\rho} - \frac{2\eta^2 + \ell(\ell+1)}{2\rho^2} + \dots$

See C.R. Brune, G.M. Hale, and M.W. Paris, *Monotonic properties of the shift and penetration factors*, Phys. Rev. C **97**, 024603 (2018), <https://doi.org/10.1103/PhysRevC.97.024603>

The Gamow factor is defined to be

$$C_\ell(\eta) = \frac{2^\ell e^{-\pi\eta/2} [\Gamma(\ell+1+i\eta)\Gamma(\ell+1-i\eta)]^{1/2}}{\Gamma(2\ell+2)},$$

which for $\ell = 0$ becomes

$$C_0 = \left[\frac{2\pi\eta}{\exp(2\pi\eta) - 1} \right]^{1/2}.$$

Low-Energy Limit

- ▶ For $E \rightarrow 0$, with radius fixed, we have

$$F_\ell \rightarrow \frac{C_0 x}{2\eta} \frac{x}{2} I_{2\ell+1}(x)$$
$$G_\ell \rightarrow \frac{x}{C_0} K_{2\ell+1}(x),$$

where $x = (8\eta\rho)^{1/2}$ is independent of energy and $\propto \sqrt{r}$, and $I_{2\ell+1}(x)$ and $K_{2\ell+1}(x)$ are the regular and irregular *Modified Bessel Functions*, respectively.

- ▶ See J. Humblet, *Bessel functions expansions of Coulomb wave functions*, J. Math. Phys. **26**, 656-659, 1985
<https://doi.org/10.1063/1.526602>.
- ▶ This implies

$$P_\ell \rightarrow \frac{\pi \exp(-2\pi\eta)}{4K_{2\ell+1}^2(x)}.$$

Negative Energies

- ▶ For negative energies, we need the exponentially-decaying Whittaker function:

$$W_{-\eta_b, \ell+1/2}(2\kappa_b r),$$

where $\kappa_b = \sqrt{-2\mu E/\hbar^2}$ and $\eta_b \kappa_b = Z_1 Z_2 e^2 \mu/\hbar^2$.

- ▶ It is proportional to the analytic continuation of H_ℓ^+ to negative energies.
- ▶ For $E < 0$, we have $P_\ell = 0$ and

$$S_\ell = \frac{r}{W} \frac{dW}{dr}.$$

- ▶ $S_\ell(E)$ is continuous across $E = 0$, with a value of

$$S_\ell(0) = -\ell - \frac{x K_{2\ell}(x)}{K_{2\ell+1}(x)}.$$

- ▶ In practice, ϕ_ℓ is not needed for $E < 0$.

The Tail a Bound State

- ▶ Using the differential equation, it can be shown that

$$\frac{\hbar^2}{2\mu} \left[\frac{W^2}{r} \frac{dS}{dE} \right]_{r=a} = \int_a^\infty W^2 dr,$$

see Eq. (A.29) in the appendix of Lane and Thomas.

- ▶ Normalization condition:

$$N + \sum_c C_c^2 \int_{a_c}^\infty W_c^2 dr_\alpha = 1$$

$$C_c = \frac{(2\mu_\alpha a_c)^{1/2}}{\hbar W_\ell(a_c)} N^{1/2} \gamma_c$$

$$N \left[1 + \sum_c \gamma_c^2 \frac{dS_c}{dE} \Big|_{E_R} \right] = 1$$

- ▶ $\frac{dS}{dE}$ can be computed by a continued fraction technique.

Computer Codes

- ▶ I.J. Thompson and A.R. Barnett, *COULCC: A continued-fraction algorithm for Coulomb functions of complex order with complex arguments*, Computer Physics Communications **36**, 363-372 (1985),
[https://doi.org/10.1016/0010-4655\(85\)90025-6](https://doi.org/10.1016/0010-4655(85)90025-6),
fortran90, code available from
<http://www.ianthompson.org/computation.htm>
- ▶ N. Michel, *Precise Coulomb wave functions for a wide range of complex ℓ , η and z* , Computer Physics Communications **176**, 232-249 (2007),
<https://doi.org/10.1016/j.cpc.2006.10.004>, c++, code available from CPC Program Library
- ▶ GNU Scientific Library (GSL),
<https://www.gnu.org/software/gsl/>, c++

Thank you for your attention.