Coulomb Functions for Nuclear Physics

Carl R. Brune

Ohio University

24 June 2024

AZURE2 R-matrix Summer School
University of Edinburgh
June 23-28, 2024

CRB supported in part by the U.S. D.O.E. through grants No. DE-FG02-88ER40387 and DE-NA0004065

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

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

  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 $\eta \propto 1/\sqrt{E}$.

- For a given pair of nuclei and ℓ, 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, $F_\ell(\eta, \rho \to 0) \propto \rho^{\ell+1}$
- $G_\ell(\eta, \rho)$: the irregular Coulomb function, $G_\ell(\eta, \rho \to 0) \propto \rho^{-\ell}$
- $H_\ell^\pm(\eta, \rho) = G_\ell(\eta, \rho) \pm iF_\ell(\eta, \rho)$
- 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 $\rho \to \infty$, 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:

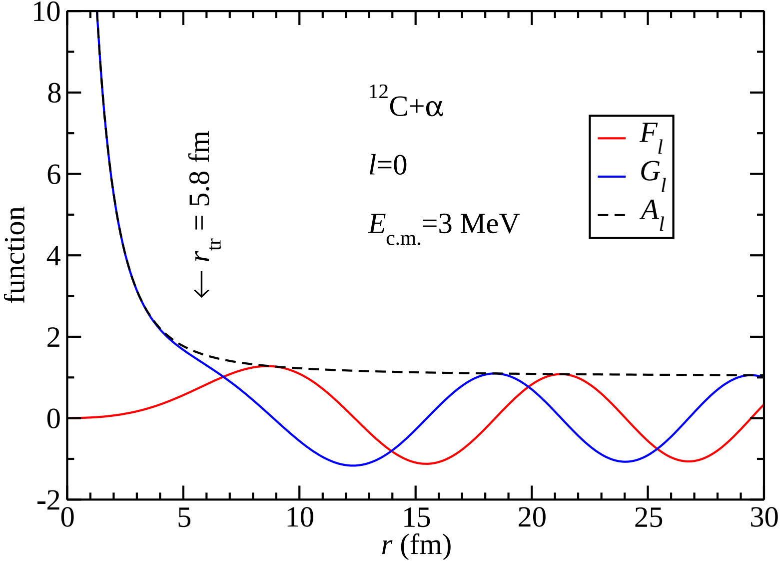
$$
\begin{aligned}
A_\ell &= (F_\ell^2 + G_\ell^2)^{1/2} \\
\phi_\ell &= \tan^{-1} F_\ell / G_\ell \\
H_\ell^\pm &= A_\ell \exp(\pm i \phi_\ell) \\
P_\ell &= \frac{\rho}{A_\ell^2} \\
S_\ell &= \frac{\rho A_\ell'}{A_\ell} = \frac{\rho (A_\ell^2)'}{2 A_\ell^2}
\end{aligned}
$$

- Note that we also have $S_\ell + i P_\ell = \rho \frac{H_\ell^{+\prime}}{H_\ell^+}$, 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 $0 \le r < \infty$.

Limiting Forms for Small and Large ρ

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

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

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

which for $\ell = 0$ becomes

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

Low-Energy Limit

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

$$
\begin{aligned}
F_\ell &\to \frac{C_0}{2\eta}\frac{x}{2} I_{2\ell+1}(x) \\
G_\ell &\to \frac{x}{C_0} K_{2\ell+1}(x),
\end{aligned}
$$

  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

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

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:

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

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

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

- $\frac{dS}{dE}$ 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`, fortran90-ish, verson 36, 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

Computer Codes, continued

- GNU Scientific Library (GSL), `https://www.gnu.org/software/gsl/`, c
- A.R. Barnett, *COULFG: Coulomb and Bessel functions and their derivatives, for real arguements, by Steed's method*, Computer Physics Communications **27**, 147-166 (1982), `https://doi.org/10.1016/0010-4655(82)90070-4`, fortran, c version is available from the LLNL github: `https://github.com/LLNL/fudge`
- I will refer to these as `coulcc`, `cwfcomp`, `gsl`, and `coulfg`, respectively.

Comparisons

- For the comparisons, I have considered ${}^{12}\mathrm{C} + \alpha$, $a = 5.5$ fm, $\ell = 2$ and varied the energy from near zero to 10 MeV.
- The radius is typical of the channel radius that one would utilize for an R-matrix analysis of this system.
- This energy range spans from far below to above the Coulomb and angular momentum barriers.

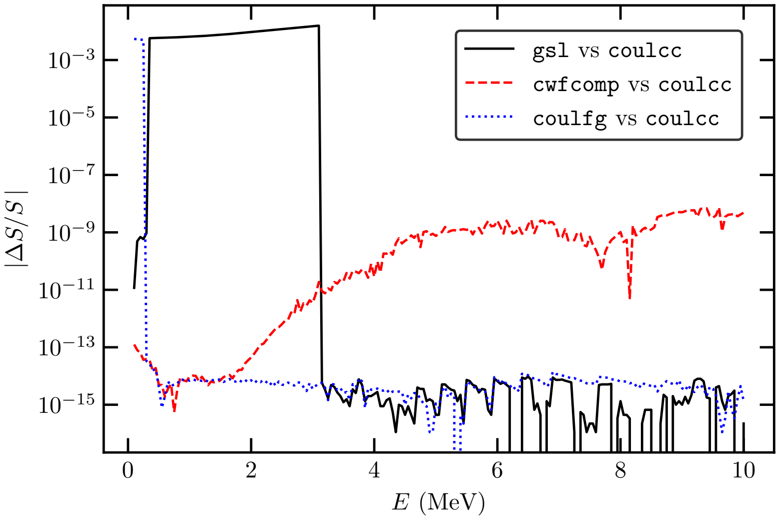
Caveats

- This study is only looking at a limited region of parameter space.
- Just because two codes agree, that does not mean they are correct.
- In the case of `cwfcomp`, I have used the default computational parameters (also the AZURE2 default):

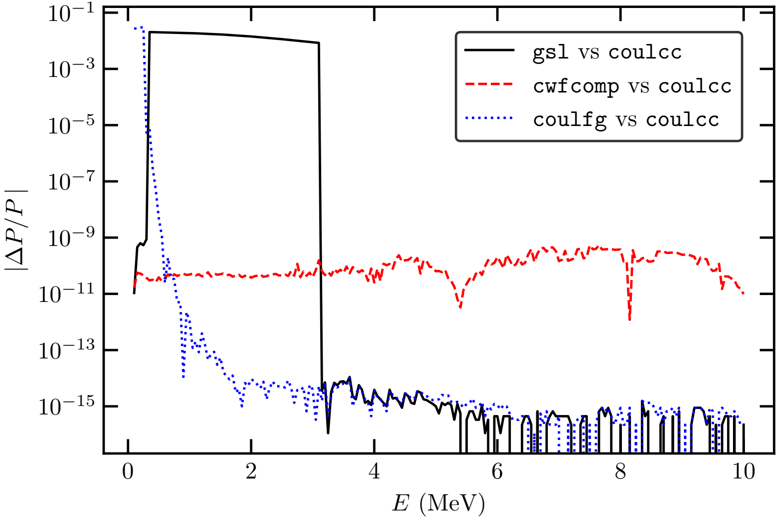
$$\begin{aligned} \texttt{precision} &= \texttt{1E}-\texttt{10} \\ \texttt{sqrt\_precision} &= \texttt{1E}-\texttt{5}. \end{aligned}$$

  Decreasing these values brings the `cwfcomp` results closer to `coulcc`, and increases the computational time.

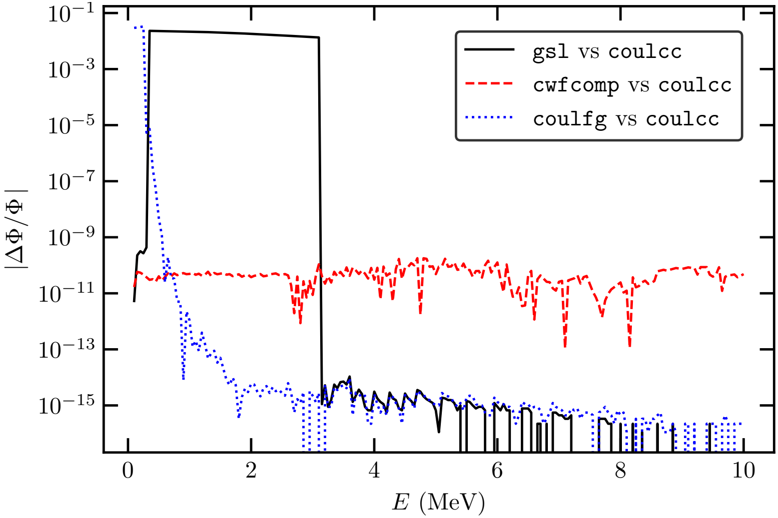
Shift Function



Penetration

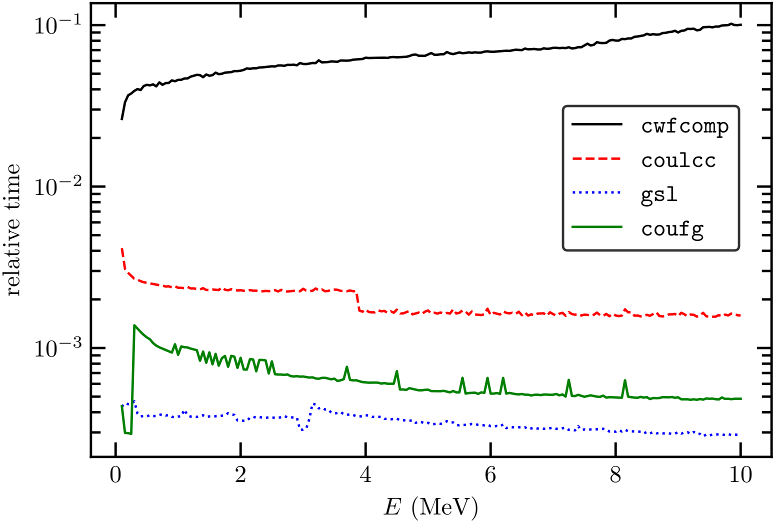


Phase



gsl vs coulcc
cwfcomp vs coulcc
coulfg vs coulcc
$|\Delta\Phi/\Phi|$
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
10^{-15}
0
2
4
6
8
10
E (MeV)

Computational Time



Findings

- `coulcc` and `cwfcomp` agree reasonably well for all energies considered.
- `gsl` agrees with the other codes for very low energies and energies above 3 MeV.
- `gsl` shows significant disagreements with the other codes for $0.3 < E < 3$ MeV.
- `coulfg` agrees will with `coulcc` and `cwfcomp`, except for very low energies.
- There are significant differences in computational speeds: `gsl` is the fastest, followed by `coulfg`, then by `coulcc`, and finally `cwfcomp`.

What is going on with `gsl`?

- It turns out that `gsl` uses a WKB approximation when $1.2 \leq \rho < 2\eta$. For $\rho < 1.2$, the power series are used. For $\rho \geq 2\eta$, continued fractions are used. Note that $\rho = 2\eta$ corresponds to the classical turning radius for $\ell = 0$.

- The range $1.2 \leq \rho < 2\eta$ corresponds to $0.3 < E < 3$ MeV for $^{12}\mathrm{C} + \alpha$ at 5.5 fm, which is a critical region of parameter space for this case. The WKB approximation is just not very accurate.

- Besides not being particularly accurate, the `gsl` Coulomb functions are not continuous functions of energy and radius. This may cause problems for parameter search algorithms in phenomenological R-matrix applications.

- User beware!

What about `coulfg`?

- It is fast and works very well, except for very low energies.
- The issue here is a loss of accuracy in the continued fraction method when $P \ll S$, which is a known issue. Other codes use different method in this regime.

Conclusions

- There are significant differences in the accuracy and computational speed of four commonly used codes for computing Coulomb functions.
- I believe there is room for a new code that optimizes speed and accuracy for ρ and η real and positive.
- However, if computational speed is a truly limiting factor, other approaches, such as interpolation from pre-computed tables, should be considered.

Thank you for your attention.