Physics 464/511 Lecture K Fall, 2016

1 Some particular important functions

The Γ function

We have already seen that the Γ function

$$\Gamma(z) = \int_0^\infty e^{-u} u^{z-1} du \qquad \text{Re } x > 0$$

is an extension of $(z-1)!$ to the complex rhp (right half plane).

We have seen $\Gamma(z+1) = z\Gamma(z)$, which allows continuation to the whole plane except for simple poles at the negative integers and zero. We have also claimed

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z},$$

using the beta function $B(z, 1-z)$, which we will show is indeed $\Gamma(z)\Gamma(1-z)$, shortly.

Special values: $\Gamma(n+1) = n!$ for nonnegative integers n, $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. Here are two proofs of the last:

$$1) \qquad \int_0^\infty e^{-u} u^{-1/2} du \underset{v=\sqrt{u}}{=} 2\int_0^\infty e^{-v^2} dv = \int_{-\infty}^\infty e^{-v^2} dv = \sqrt{\pi}$$

$$2) \qquad \Gamma(\frac{1}{2})\Gamma(\frac{1}{2}) = \frac{\pi}{\sin \pi/2} = \pi.$$

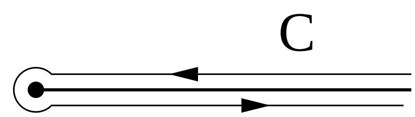
I once assigned for homework proving the infinite product formula

$$\frac{1}{\Gamma(z)} = z e^{\gamma z} \prod_{n=1}^\infty \left(1 + \frac{z}{n}\right) e^{-z/n},$$

where $\gamma = \lim_{n\to\infty} \left(-\ln n + \sum_1^n \frac{1}{k}\right)$ is the EulerMascheroni constant. This would be straightforward if you apply the technique we used for $\sin(z)$, based on the Mittag-Leffler expansion, except that the assumption that $f(z)$ doesn't blow up at infinity is not clear. Nonetheless the expression is correct, and in fact was the original definition, due to Euler, of the Gamma function.

1.1 Extension of the integral formula for $\Gamma(z)$ to all z

An expression for the Γ function in terms of a contour integral can be obtained by noting that $(-u)^\nu$ has a cut from zero to infinity.
Above the cut,



$$(-u)^\nu = \left(|u|e^{-i\pi}\right)^\nu = u^\nu e^{-i\pi\nu},$$

while below the cut $(-u)^\nu = u^\nu e^{i\pi\nu}$. Thus

$$\int_C e^{-u}(-u)^\nu\, du = -\int_0^\infty e^{-u}u^\nu e^{-i\pi\nu}\, du + \int_0^\infty e^{-u}u^\nu e^{i\pi\nu}\, du = 2i\sin\pi\nu\Gamma(\nu+1),$$

which, for $z \notin \mathbb{Z}$, gives the formula

$$\Gamma(z) = \frac{i}{2\sin\pi z}\int_C e^{-u}(-u)^{z-1}\, du.$$

Now the integral doesn't need to go near $u = 0$, so the restriction to $\mathrm{Re}\, z > 0$ is no longer necessary. The poles have been explicitly removed.

Define

$$\psi(z) = \frac{d}{dz}\ln\Gamma(z) = \frac{1}{\Gamma(z)}\frac{d\,\Gamma(z)}{dz}.$$

ψ is called the *digamma function*. From the product formula

$$\ln\Gamma(z) = -\ln z - \gamma z - \sum_{n=1}^\infty \left[\frac{-z}{n} + \ln\left(1+\frac{z}{n}\right)\right],$$

so

$$\psi(z) = -\frac{1}{z} - \gamma + \sum_{n=1}^\infty \left(\frac{1}{n} - \frac{1}{n+z}\right).$$

Thus $\psi(z)$ is also an analytic function with simple poles at zero and the negative integers.

The derivatives of ψ are called polygamma functions,

$$\psi^{(n)}(z) := \frac{d}{dz}\psi^{(n-1)}(z) = \sum_{r=0}^\infty \frac{(-1)^{n+1}n!}{(r+z)^{n+1}} \qquad n \geq 1,\ \psi^{(0)} := \psi.$$

A Maclaurin expansion for $\ln\Gamma(1+x)$ gives

$$\ln\Gamma(1+x) = \sum_{n=0}^\infty \frac{x^n}{n!}\left(\frac{d}{du}\right)^n \ln\Gamma(u)\bigg|_{u=1} = \sum_{r=0}^\infty \frac{x^{r+1}}{(r+1)!}\psi^{(r)}(1).$$

But $\psi^{(r)}(1) = (-1)^{r+1} r! \sum_{p=1}^{\infty} \frac{1}{p^{r+1}} = (-1)^{r+1} r! \zeta(r+1)$ for $r > 0$, while $\psi(1) = -\gamma$. We see the Riemann zeta function once again. So

$$\ln \Gamma(1+x) = -\gamma x + \sum_{r=2}^{\infty} \frac{(-x)^r}{r} \zeta(r).$$

This expansion converges for $|x| < 1$, which is obvious from either side, noting that $\zeta(r) \underset{r\to\infty}{\longrightarrow} 1$.

The Beta Function

We defined the beta function $B(u,v) = \int_0^1 t^{u-1}(1-t)^{v-1} dt$ previously, and claimed it was $\Gamma(u)\Gamma(v)/\Gamma(u+v)$. Let's prove this

Let $t = \cos^2\theta$

$$\begin{aligned} B(u,v) &= \int_0^{\pi/2} \cos^{2(u-1)}\theta \ \cdot \ \sin^{2(v-1)}\theta \cdot 2\cos\theta \sin\theta \, d\theta \\ &= 2\int_0^{\pi/2} \cos^{2u-1}\theta \sin^{2v-1}\theta \, d\theta. \end{aligned}$$

Then

$$\begin{aligned} B(u,v)\Gamma(u+v) &= 2\int_0^{\pi/2} \cos^{2u-1}\theta \sin^{2v-1}\theta \, d\theta \quad \underbrace{\int_0^{\infty} t^{u+v-1} e^{-t} \, dt}_{2\int_0^{\infty} r^{2u+2t-2} e^{-r^2} r \, dr} \\ &= 4\int_0^{\pi/2} d\theta \int_0^{\infty} (r\cos\theta)^{2u-1} (r\sin\theta)^{2v-1} e^{-r^2} r \, dr \\ &= 4\int_0^{\infty} x^{2u-1} e^{-x^2} dx \int_0^{\infty} y^{2v-1} e^{-y^2} dx \\ &= \int_0^{\infty} p^{u-1} e^{-p} dp \int_0^{\infty} q^{v-1} e^{-q} dq \\ &= \Gamma(u)\Gamma(v). \end{aligned}$$

In the first line we changed variables $t \to r^2$ and in the penultimate line the reverse, $x \to \sqrt{p}, y \to \sqrt{q}$. Thus we have proven

$$B(u,v) = \frac{\Gamma(u)\Gamma(v)}{\Gamma(u+v)}.$$

The beta function enjoyed great popularity in the late '60's as the Veneziano model for the scattering of elementary particles, which led to the creation of string theory.

Consider

$$\begin{aligned} B(z,z) &= 2\int_0^{\pi/2} (\cos\theta)^{2z-1}(\sin\theta)^{2z-1} d\theta \\ &= 2\int_0^{\pi/2} \left(\frac{\sin 2\theta}{2}\right)^{2z-1} d\theta \\ &= 2^{1-2z}\int_0^{\pi} \sin^{2z-1}\phi\, d\phi \\ &= 2^{1-2z}\, 2\int_0^{\pi/2} \sin^{2z-1}\phi\, \cos^{1-1}\phi\, d\phi \\ &= 2^{1-2z}\, B(z,\frac{1}{2}), \end{aligned}$$

$$\text{so} \qquad \frac{\Gamma(z)\Gamma(z)}{\Gamma(2z)} = 2^{1-2z}\frac{\Gamma(z)\Gamma(\frac{1}{2})}{\Gamma(z+\frac{1}{2})},$$

and

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma(z+\frac{1}{2}).$$

This is known as the *duplication* formula.

Now we are ready to derive the Stirling series for $\ln\Gamma(z)$, expanding the expression we found from steepest descents. Recall the Euler-Maclauren integration formula

$$\int_0^n f(x)\,dx = \frac{1}{2}f(0) + \sum_{r=1}^{n-1} f(r) + \frac{1}{2}f(n) - \sum_{p=1}^{\infty}\frac{B_{2p}}{(2p)!}\left[f^{2p-1}(n) - f^{2p-1}(0)\right]$$

Applying this to $f(x) = \dfrac{1}{(z+x)^2}$ as $n\to\infty$, using $f^{(r)}(0) = \dfrac{(-1)^r(r+1)!}{z^{r+2}}$, $f^{(r)}(\infty) = 0$, and evaluating explicitly $\displaystyle\int_0^\infty \frac{1}{(x+z)^2}dx = -\left.\frac{1}{x+z}\right|_0^\infty = \frac{1}{z}$, we have

$$\frac{1}{z} = \frac{1}{2z^2} + \sum_{r=1}^{\infty}\frac{1}{(z+r)^2} - \sum_{p=1}^{\infty}\frac{(2p)!}{(2p)!}B_{2p}z^{-2p-1}.$$

But $\psi'(z) = \sum_{r=0}^{\infty} \frac{1}{(z+r)^2}$, so $\psi'(z+1) = \sum_{r=1}^{\infty} \frac{1}{(z+r)^2}$ and

$$\psi'(z+1) = \frac{1}{z} - \frac{1}{2z^2} + \sum_{p=1}^{\infty} B_{2p} z^{-2p-1}.$$

This is an asymptotic expansion, and does not really converge. Ignoring this fine point,

$$\psi(z+1) = \int^z \psi'(u+1)\,du = C_1 + \ln z + \frac{1}{2z} - \sum_{p=1}^{\infty} \frac{B_{2p}}{2p} z^{-2p},$$

so $$\ln\Gamma(z+1) = \int^z \psi(u+1)\,du = C_3 + C_1 z - z + \left(z + \frac{1}{2}\right)\ln z + \sum_{p=1}^{\infty} \frac{B_{2p} z^{1-2p}}{2p(2p-1)},$$

which is again an asymptotic expansion. To determine C_1,

$$0 = \ln\Gamma(z+1) - \ln z - \ln\Gamma(z) \Longrightarrow C_1 - 1 + \left(z - \frac{1}{2}\right)\ln\frac{z}{z-1} + \ln z - \ln z + \mathcal{O}(1/z)$$

which tells us $C_1 = 0$. Now the log of the duplication formula tells us
$\ln\Gamma(2z) - \ln\Gamma(z) - \ln\Gamma(z+\frac{1}{2}) - (2z-1)\ln 2 + \frac{1}{2}\ln\pi \equiv 0,$

$$\begin{aligned}\rightarrow\quad & -\frac{1}{2} - C_3 + (2z - \frac{1}{2})\ln(2z-1) - (z - \frac{1}{2})\ln(z-1) - z\,\ln(z - \frac{1}{2}) \\ & -(2z-1)\ln 2 + \frac{1}{2}\ln\pi + \mathcal{O}(1/z) \;=\; -C_3 + \frac{1}{2}\ln(2\pi) = 0.\end{aligned}$$

Thus $C_3 = \frac{1}{2}\ln(2\pi)$ and

$$\begin{aligned}\ln\Gamma(z+1) \;&=\; \left(z + \frac{1}{2}\right)\ln z - z + \frac{1}{2}\ln(2\pi) \\ &\quad + \sum_{p=1}^{\infty} \frac{B_{2p}}{2p(2p-1)} z^{1-2p}.\end{aligned}$$

z	best $2p$	error in $\Gamma(z+1)$
1	6	3×10^{-4}
1.5	10	1×10^{-5}
2	14	8×10^{-7}
3	20	4×10^{-9}
4	26	2×10^{-11}
5	34	3×10^{-14}

Without the $\sum_1^\infty$ this is the Stirling approximation we found with the method of steepest descents. With the sum, this is an asymptotic expansion which does not converge for any finite z. I did some calculations for small z, and found the best p to stop at.

We have already met the incomplete gamma function

$$\Gamma(a,x) = \int_x^\infty e^{-t} t^{a-1}\,dt$$

and derived an asymptotic expansion for it,

$$\Gamma(a,x) = x^{a-1}e^{-x}\sum_{r=0}^\infty \frac{\Gamma(a)}{\Gamma(a-r)}x^{-r} = x^{a-1}e^{-x}\sum_{r=0}^\infty (-1)^r\frac{\Gamma(r-a+1)}{\Gamma(-a+1)}x^{-r}.$$

For positive integer a, the first form shows the series terminates. When it doesn't terminate the second form is more useful.

There is also the other half of the incomplete Γ,

$$\gamma(a,x) = \int_0^x e^{-t}t^{a-1}\,dt = \Gamma(a) - \Gamma(a,x).$$

We have also met $E_1(x) = \Gamma(0,x) =: -\mathrm{Ei}(-x)$. Some other functions sometimes met use the "sine integral"

$$\begin{aligned} si(x) &:= -\int_x^\infty \frac{\sin t}{t}\,dt \\ Ci(x) &:= -\int_x^\infty \frac{\cos t}{t}\,dt \\ li(x) &:= \int_0^x \frac{du}{\ln u} = \mathrm{Ei}(\ln x) = -E_1(-x) \end{aligned}$$

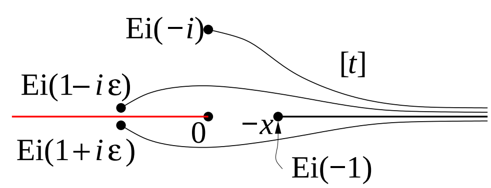
the last being called the logarithmic integral, defined for $0 < x < 1$, or as the principal part of the integral for $x > 1$.

These definitions, while suggesting real variables and integration along the real axis, can be analytically continued simply by moving the endpoint, as long as no singularity is crossed.

Thus

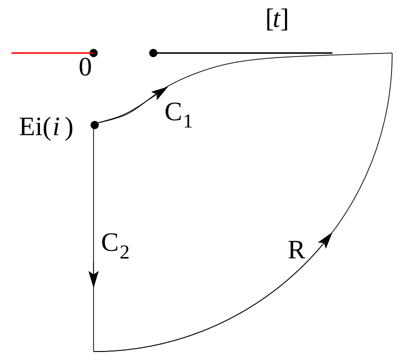
$$\mathrm{Ei}(x) = -\int_{-x}^\infty \frac{e^{-t}}{t}\,dt$$

has a real integrand for $-x$ real and positive. Analytically continuing means just moving the endpoint,



but we must specify which way to go around the pole. Thus Ei is given a cut along the positive real axis.

$$\begin{aligned}\mathrm{Ei}(ix) &= -\int_{C_1} \frac{e^{-t}}{t}\,dt \\ &= -\int_{C_2} - \underbrace{\int_R}_{\to 0} \qquad (\text{with } t = 0 - iv) \\ &= -\int_x^\infty \frac{e^{iv}}{v}\,dv = Ci(x) + i\ si(x)\end{aligned}$$



As $\mathrm{Ei}(-x)$ is real for real $x > 0$, the Schwarz reflection principle insures

$$\mathrm{Ei}(-ix) = \mathrm{Ei}^*(ix) = Ci(x) - i\ si(x),$$

so

$$\begin{aligned}Ci(x) &= \frac{1}{2}\left[Ei(ix) + Ei(-ix)\right] \\ si(x) &= \frac{1}{2i}\left[Ei(ix) - Ei(-ix)\right]\end{aligned}$$

just as for the normal exponential, cosine and sine functions.

1.2 The Error Function

The error function is defined as

$$\mathrm{erfc}(z) := \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt.$$

Changing variables to $u = t^2$,

$$\mathrm{erfc}(z) := \frac{1}{\sqrt{\pi}} \int_{z^2}^\infty u^{-1/2} e^{-u} du = \frac{1}{\sqrt{\pi}}\, \Gamma(\frac{1}{2}, z^2).$$

The erfc is an incomplete gaussian integral, useful to estimate how often a gaussian random variable (*e.g.* experimental data) can be expected to lie outside $\sqrt{2}\,z$ standard deviations from the mean. The inside function

$$\mathrm{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt = 1 - \mathrm{erfc}(z)$$

gives the probability to be within $\sqrt{2}\,z$ standard deviations.

1.3 Bessel Functions

Consider the generating function

$$G(z,t) = e^{z(t-t^{-1})/2} = \sum_{n=-\infty}^{\infty} J_n(z) t^n.$$

The functions $J_n(z)$ thus generated are called *Bessel functions of the first kind* of order n.

Expanding in powers of z,

$$\begin{aligned} G(z,t) &= e^{zt/2} e^{-zt^{-1}/2} = \sum_{r=0}^{\infty}\sum_{s=0}^{\infty} \frac{(-1)^s}{r!\, s!}\left(\frac{z}{2}\right)^{r+s} t^{r-s} \\ &= \sum_{n=-\infty}^{\infty} t^n \sum_s \frac{(-1)^s}{s!\,(n+s)!}\left(\frac{z}{2}\right)^{n+2s}, \\ \text{so} \qquad J_n(z) &= \sum_s \frac{(-1)^s}{s!\,(n+s)!}\left(\frac{z}{2}\right)^{n+2s}, \end{aligned}$$

where the sums on s are over all s without the factorial of a negative integer in the denominator.

For $n \geq 0$, the sum on s runs from 0 to ∞. This agrees with the expression we found earlier from Frobenius.

For negative n, the sum on s runs from $-n$ to ∞. Let $r = s + n = s - |n|$,

$$J_{-|n|}(z) = \sum_r \frac{(-1)^{r+|n|}}{(r+|n|)!r!}\left(\frac{z}{2}\right)^{|n|+2r} = (-1)^n J_{|n|}(z).$$

Thus J_{-n} and J_n are actually the same function, up to sign. Each has a power series expansion beginning with z^n.

Given a generating function, one can often find a recursion relation. Here

$$\frac{\partial}{\partial t} G(z,t) = \left(1 + \frac{1}{t^2}\right)\frac{z}{2}\, G(z,t) = \sum n\, t^{n-1} J_n(z) = \frac{z}{2}\sum \left(t^n + t^{n-2}\right) J_n(z).$$

Matching powers of t^{n-1},

$$nJ_n(z) = \frac{z}{2}\left(J_{n+1} + J_{n-1}\right) \qquad \text{for } n \geq 1.$$

Such relations are common for orthogonal polynomials. A formula for the derivative

$$\frac{\partial}{\partial x}G(x,t) = \left(\frac{t}{2} - \frac{1}{2t}\right)G(x,t) \Longrightarrow J_n'(x) = \frac{1}{2}J_{n-1} - \frac{1}{2}J_{n+1} = \frac{n}{x}J_n - J_{n+1}.$$

Consider any set of functions $Z_\nu(x)$ which satisfy these two equations

$$\begin{array}{lrcll} & \text{(a)} \quad 2Z_\nu'(x) & = & Z_{\nu-1}(x) - Z_{\nu+1}(x) & \quad \text{for any } \nu \\ \text{and} & \text{(b)} \quad 2\nu Z_\nu(x) & = & xZ_{\nu+1}(x) + xZ_{\nu-1}(x). & \end{array}$$

$$\begin{array}{lrcll} \text{Then} & xZ_\nu' & = & \frac{x}{2}Z_{\nu-1} - \frac{1}{2}\left(2\nu Z_\nu - xZ_{\nu-1}\right) & (1) \\ & & = & xZ_{\nu-1} - \nu Z_\nu & (2) \\ \text{Similarly} & xZ_\nu' & = & -xZ_{\nu+1} + \nu Z_\nu. & (3) \end{array}$$

Differentiate (2), write (3) with $\nu \to v{-}1$, and write (2) times ν/x:

$$\begin{array}{lcccccl} xZ_\nu'' & +(\nu{+}1)Z_\nu' & -xZ_{\nu-1}' & & -Z_{\nu-1} & = 0 \\ & & xZ_{\nu-1}' & +xZ_\nu & +(1{-}\nu)Z_{\nu-1} & = 0 \\ & -\nu Z_\nu' & & -\dfrac{\nu^2}{x}Z_\nu & +\nu Z_{\nu-1} & = 0 \\ \hline \text{Adding:}\quad xZ_\nu'' & +Z_\nu' & & +\dfrac{x^2-\nu^2}{x}Z_\nu & & = 0 \end{array}$$

or

$$x^2 Z_\nu'' + xZ_\nu' + \left(x^2 - \nu^2\right) Z_\nu = 0,$$

which is the *Bessel equation*.

Thus $J_\nu(x)$ is a solution of Bessel's equation when ν is an integer.

If we want to extract $J_n(x)$ from $G(x,t)$, the standard method is

$$\oint \frac{dt}{2\pi i t^{n+1}} G(x,t) = J_n(x),$$

where the contour circles the origin. Choosing $t = e^{i\theta}$,

$$\begin{aligned} J_n(x) &= \frac{1}{2\pi}\int_0^{2\pi} e^{-in\theta} e^{ix\sin\theta}\, d\theta \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(\underbrace{\cos(n\theta - x\sin\theta)}_{\text{sym}} - i\,\underbrace{\sin(n\theta - x\sin\theta)}_{\text{antisym}} \right) d\theta \\ &= \frac{1}{\pi}\int_0^{\pi} \cos(n\theta - x\sin\theta)\, d\theta \end{aligned}$$

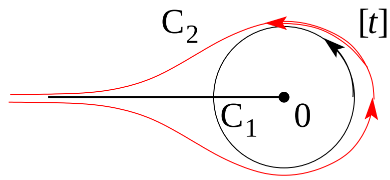
where the integral of the term antisymmetric under $\theta \to -\theta$ vanishes.

Bessel functions occur in problems with Laplace's equation in cylindrical coordinates, Fraunhofer diffraction through a circular aperature, bag models, *etc.*.

Return to the expression

$$J_n(x) = \oint \frac{dt}{2\pi i t^{n+1}} e^{\frac{x}{2}\left(t-t^{-1}\right)}.$$

The integrand is analytic everywhere in t except at $t = 0$, and vanishes rapidly as $t \to -\infty$ for $x > 0$, so the contour can be deformed



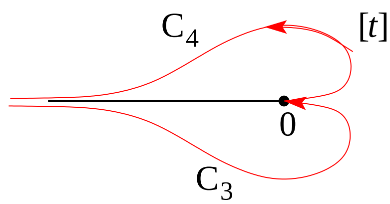
In this form, there is no particular reason to restrict n to integers, so define

$$J_\nu(x) = \int_{C_2} \frac{dt}{2\pi i t^{\nu+1}} e^{\frac{x}{2}\left(t-t^{-1}\right)} \qquad \mathrm{Re}\; x > 0.$$

As we approach $t = 0$ along positive values, the exponential again vanishes for $\mathrm{Re}\; x > 0$, so we can write

$$J_\nu(x) = \int_{C_3} + \int_{C_4}.$$

But this we recognize as



$$\frac{1}{2} H_\nu^{(1)}(x) + \frac{1}{2} H_\nu^{(2)}(x),$$

where $H_\nu^{(1)}(x)$ was met in our discussion of steepest descents, where we found

$$\begin{aligned} H_\nu^{(1)}(x) &\approx \sqrt{\frac{2}{\pi x}} e^{i(x - \nu\pi/2 - \pi/4)} \qquad x \to \infty \\ H_\nu^{(2)}(x) &= H^{(1)\,*}(x^*) \end{aligned}$$

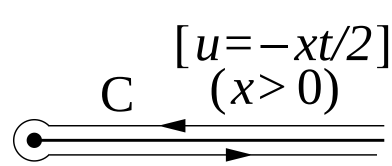
so

$$J_\nu(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - \nu\frac{\pi}{2} - \frac{\pi}{4}\right) \qquad \text{for large } x$$

Consider again $J_\nu(x)$:

$$J_\nu(x) = \int_C \frac{dt}{2\pi i\, t^{\nu+1}} e^{x\left(t-t^{-1}\right)/2}.$$

Let $u = -xt/2$, so



$$\begin{aligned}
J_\nu(x) &= -\left(\frac{x}{2}\right)^\nu \int_C \frac{du}{2\pi i(-u)^{\nu+1}} e^{-u+\frac{x^2}{4}u^{-1}} \\
&= -\left(\frac{x}{2}\right)^\nu \int_0^\infty \frac{du}{2\pi i u^{\nu+1}} \left(-e^{-i\pi\nu} + e^{i\pi\nu}\right) e^{-u} \sum_{s=0}^\infty \left(\frac{x}{2}\right)^{2s} \frac{u^{-s}}{s!} \\
&= \sum_{s=0}^\infty \left(\frac{x}{2}\right)^{\nu+2s} \underbrace{\frac{-2i\sin\pi\nu}{2\pi i}}_{(-1)^s\frac{\sin\pi(-s-\nu)}{\pi}} \frac{\Gamma(-s-\nu)}{n!}
\end{aligned}$$

But $\Gamma(x)\dfrac{\sin(\pi x)}{\pi} = \dfrac{1}{\Gamma(1-x)}$, so

$$J_\nu(x) = \sum_{s=0}^\infty (-1)^s \left(\frac{x}{2}\right)^{\nu+2s} \frac{1}{s!\,\Gamma(1+s+\nu)}. \tag{4}$$

This is exactly the form we had before for integral $\nu > 0$, but extended to all ν other than negative integers.

The definition of $J_\nu(z)$ for nonintegral ν cannot be given directly by the generating function, but is given by extending the series definition as we have derived in Eq. (4). You will show for homework that the crucial recursion relations for Z_ν are satisfied, so J_ν is a solution of Bessel's equation. For noninteger ν the sum starts at $s = 0$, so $J_{-\nu}$ starts at $x^{-|\nu|}$ and is not proportional to J_ν. Thus

$$N_\nu(x) := \frac{J_\nu(x)\cos\pi\nu - J_{-\nu}(x)}{\sin\pi\nu}$$

is nonzero, and, as a superposition of two solutions, is a solution of the Bessel equation.

When ν is an integer, this expression needs to be evaluated by l'Hôpital's rule,

$$N_n(x) = \frac{(-1)^n \left.\dfrac{\partial J_\nu(x)}{\partial\nu}\right|_{\nu=n} - \pi J_\nu \sin(\pi n) + \left.\dfrac{\partial J_{+\nu}}{\partial\nu}\right|_{\nu=-n}}{\pi\cos\pi n}.$$

The dominant term as $x \to 0$ in the $\left.\dfrac{\partial J_{+\nu}}{\partial \nu}\right|_{\nu=-n}$ term is the $s = 0$ piece, which contributes

$$\begin{aligned}&\frac{(-1)^n}{\pi}\frac{\partial}{\partial\nu}\left[\left(\frac{x}{2}\right)^\nu \frac{1}{\Gamma(\nu+1)}\right]_{\nu=-n}\\ &\quad= \frac{1}{\pi}\left(\frac{-x}{2}\right)^{-n}\frac{-\psi(-n+1)}{\Gamma(-n+1)} + \frac{1}{\pi}\ln\left(\frac{x}{2}\right)\cdot\left(\frac{-x}{2}\right)^{-n}\frac{1}{\Gamma(1-n)}.\end{aligned}$$

$\psi(z)/\Gamma(z)$ is entire and does not vanish for nonpositive integers. So for $n = 0$, for small x, $N_n(x) \sim \dfrac{1}{\pi}\ln\dfrac{x}{2}$, while for $n > 0$, it is $\propto x^{-n}$. So $N_n(x)$ is the solution of Bessel's equation which is **not regular** at the origin. It is called the *Neumann Function.*

From the asymptotic expression for J_ν,

$$J_\nu(x) \sim \sqrt{\frac{2}{\pi x}}\cos\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right),$$

we see

$$\begin{aligned}N_\nu(x) &\sim \sqrt{\frac{2}{\pi x}}\left[\frac{\cos\pi\nu\cos\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right) - \cos\left(x + \frac{\nu\pi}{2} - \frac{\pi}{4}\right)}{\sin\pi\nu}\right]\\ &\sim \sqrt{\frac{2}{\pi x}}\sin\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right).\end{aligned}$$

[the numerator inside the [ ] is of the form $\cos A\cos B - \cos(A+B)$ with $B = x - \pi\nu/2 - \pi/4$.] So N_ν is 90° out of phase with J_ν at large x. We also see that

$$J_\nu(x) + iN_\nu(x) \sim \sqrt{\frac{2}{\pi x}}\, e^{i\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right)},$$

which is just the asymptotic form of $H^{(1)}_\nu(x)$. In fact,

$$H^{(1)}_\nu(x) = J_\nu(x) + iN_\nu(x).$$

Bessel's equation $z^2 Z''_\nu + zZ'_\nu + (z^2 - \nu^2)\,Z_\nu = 0$ is satisfied by $J_\nu(z)$ and $N_\nu(z)$, for complex z. Sometimes we meet the related equation

$$x^2y'' + xy' - (x^2 + \nu^2)y = 0 \qquad \text{Modified Bessel Equation}$$

If we set $z = ix$, $y(x) = Z(ix)$, $y'(x) = iZ'(ix)$, and $y''(x) = -Z''(ix)$, so we see that $y(x)$ satifies the modified Bessel equation if Z satisfies the Bessel equation. So does any constant times y, so

$$I_\nu(x) := i^{-\nu} J_\nu(ix)$$

is a solution (regular for $\nu \in \mathbb{N}$) of the modified Bessel equation. From the power series expansion for J,

$$J_\nu(ix) = \sum_{s=0} \frac{(-1)^s}{s!\,\Gamma(s+\nu+1)} \left(\frac{ix}{2}\right)^{\nu+2s}$$

we see

$$I_\nu(x) = \sum_{s=0} \frac{1}{s!\,\Gamma(s+\nu+1)} \left(\frac{x}{2}\right)^{\nu+2s},$$

and I is a real function for real ν, *i.e.*

$$I_\nu^*(z^*) = I_\nu(z).$$

Just as for J, I_ν and $I_{-\nu}$ are independant solutions for ν not an integer, but when ν is an integer one needs another solution. The modification appled to the Hankel function

$$K_\nu(x) = \frac{\pi}{2} i^{\nu+1} H_\nu^{(1)}(ix)$$

provides such a solution.

Another equation we have met, in separating the Helmholtz equation in spherical coordinates, is

$$r^2 R'' + 2rR' + [k^2 r^2 - \ell(\ell+1)]R = 0, \tag{5}$$

which differs from Bessel's equation by the 2 on the R' term. The substitution

$$Z(x) = \sqrt{kr}\,R(kr)$$

gives $x^2 Z'' + xZ' + [x^2 - (\ell + \frac{1}{2})^2]Z = 0$, which is Bessel's equation with $\nu = \ell + \frac{1}{2}$.

The functions R, renormalized, are called *spherical Bessel functions.* In particular

$$\begin{aligned} j_\ell(x) &= \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x) \\ n_\ell(x) &= \sqrt{\frac{\pi}{2x}} N_{\ell+1/2}(x) \\ h^{(i)}_\ell(x) &= \sqrt{\frac{\pi}{2x}} H^{(i)}_{\ell+1/2}(x) \qquad i = 1, 2. \end{aligned}$$

In fact the spherical Bessel functions of integer index are really elementary functions. For example,

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}.$$

Example: A quantum mechanical particle in a spherical, infinitely deep well:

$$\begin{aligned} -\frac{\hbar^2}{2m}\nabla^2\psi = E\psi, &\qquad r < a \\ \psi = 0 &\qquad r \geq a \end{aligned}$$

This is a problem with spherical symmetry, and within $r < a$ is Helmholtz equation. We have seen that separation of variables $\psi = R(r)\,\Theta(\theta)\,\Phi(\phi)$ gives for R our equation (5), where ℓ is an integer describing the solution of the Θ equation and giving the angular momentum of the state, and $k^2 = \dfrac{2mE}{\hbar^2}$.

So the solution for R is $R(r) \propto j_\ell(kr)$. The second solution is excluded because it is singular at $r = 0$. The boundary condition $\psi = 0$ for $r = a$ requires $R(a) = 0 \Longrightarrow j_\ell(ka) = 0 \Longrightarrow J_{\ell+1/2}(ka) = 0$. We see that the zeros of the Bessel function *determine* the possible energies and angular momenta. The lowest energy state has the smallest E, smallest k. Looking at a table of zeros of $j_\ell(x)$, *e.g.* Abramowitz and Stegun p. 467, we see that the smallest one is $\ell = 0$, $x = \pi$, and the lowest energy solution is

$$E_0 = \frac{\hbar^2\pi^2}{2ma^2}.$$

Note that even though there is no potential within the sphere, the particle has a nonzero minimal energy, due roughly to Heisenberg's uncertainty in its momentum.

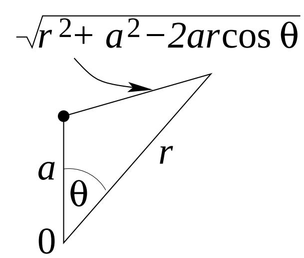
1.4 Solutions to Laplace's equation

For Laplace's equation, $k = 0$ in (5). The radial equation becomes

$$\frac{d}{dr} r^2 \frac{dR}{dr} = \ell(\ell+1)R$$

with solutions $R \propto r^\ell$ and $R \propto r^{-\ell-1}$. Outside a region of static charge, the electrostatic potential satisfies Laplace's equation and gives a potential which falls off at $r = \infty$. One can expand the potential in powers of $1/r$.

We will begin with a point charge on the z axis. Consider a charge at $z = a$ and the potential at an arbitrary point (r, θ, ϕ) in spherical polar coordinates. Then



$$\begin{aligned} \Phi &= \frac{q}{4\pi\epsilon_0} \frac{1}{(r^2 + a^2 - 2ar\cos\theta)^{1/2}} \\ &= \frac{q}{4\pi\epsilon_0} \sum_\ell \frac{a^\ell}{r^{\ell+1}} P_\ell(\cos\theta) \qquad \text{for } r > a. \end{aligned}$$

Thus the generating function for the $P_\ell(x)$ is

$$\begin{aligned} G(t,z) &= \left(1 + t^2 - 2tz\right)^{-1/2} \\ &= \sum_\ell P_\ell(z) t^\ell. \end{aligned}$$

P_ℓ are the **Legendre Polynomials**.

Conside a pair of charges, $+q$ at $z = a$ and $-q$ at $z = -a$. At (r, θ, ϕ)

$$\Phi = \frac{q}{4\pi\epsilon_0} \sum_\ell \frac{a^\ell}{r^{\ell+1}} \left[P_\ell(\cos\theta) - P_\ell(-\cos\theta)\right].$$

We note from the generating function $G(t,z) = G(-t,-z)$ so $\sum_\ell P_\ell(z)t^\ell = \sum_\ell P_\ell(-z)(-1)^\ell t^\ell$, or

$$P_\ell(-z) = (-1)^\ell P_\ell(z).$$

Thus for our two charges, the even ℓ's cancel, and

$$\Phi = \frac{2q}{4\pi\epsilon_0} \sum_{\ell \text{ odd}} \frac{a^\ell}{r^{\ell+1}} P_\ell(\cos\theta).$$

Now consider the limit where the charges get closer together but individually stronger, with $p = 2qa$ held fixed. Then the first term in the sum

$$\Phi = \frac{p}{4\pi\epsilon_0 r^2} P_1(\cos\theta) \qquad \text{survives}$$

while all the higher terms are $\mathcal{O}(pa^2) \to 0$. p is called the **dipole moment**, and as $a \to 0$, the charge distribution becomes a pure dipole.

Any localized axially symmetric distribution of charges will give a potential, outside the charged region, which can be written

$$\Phi = \sum_\ell \frac{d_\ell}{4\pi\epsilon_0 r^{\ell+1}} P_\ell(\cos\theta)$$

where $d_\ell = \int \rho\, z^\ell$.

The d_ℓ are called the **multipole moments**, but with funny names, $d_\ell =$ 2^ℓ'th pole, *e.g.*

d_0 is the monopole moment (equals the total charge)
d_1 is the dipole moment
d_2 is the quadrupole moment
d_3 is the octupole moment

etc.

The generating function method is good for finding recursion relations. Consider

$$\frac{\partial G(t,x)}{\partial t} = \frac{x-t}{(1-2xt+t^2)^{3/2}} = \sum_n n P_n(x) t^{n-1}$$

so

$$(x-t)G(t,x) = (1-2xt+t^2)\sum n P_n t^{n-1} = \sum_{\ell=0} P_\ell(x)\, t^\ell\, (x-t),$$

or, collecting terms of order t^r,

$$(r+1)P_{r+1}(x) - 2x\, r\, P_r(x) + (r-1)P_{r-1} = xP_r(x) - P_{r-1}(x)$$

$$\text{or} \qquad (2r+1)xP_r(x) = (r+1)P_{r+1}(x) + rP_{r-1}(x), \qquad (6)$$

a three term recursion relation of the usual type.

Now for derivatives:

$$\frac{\partial G}{\partial x} = \frac{t}{(1-2xt+t^2)^{3/2}} = \sum P_n'(x) t^n,$$

so $t\, G = \sum P_r t^{r+1} = (1-2xt+t^2)\sum P_n' t^n$. Again equating like powers of t, t^{r+1}:

$$P_r = P_{r+1}' - 2xP_r' + P_{r-1}'. \tag{7}$$

Twice the x derivative of (6) gives

$$(2r+1)P_r + (2r+1)\underbrace{(P_r + 2xP_r')}_{P_{r+1}'+P_{r-1}'} \;=\; (2r+1)\left(P_{r+1}' + P_{r-1}'\right) + P_{r+1}' - P_{r-1}'$$

so

$$(2r+1)P_r = P_{r+1}' - P_{r-1}'. \tag{8}$$

$$\text{Half of } ((7) + (8)) \text{ gives} \qquad (r+1)P_r = P_{r+1}' - xP_r', \tag{9}$$

$$\text{Half of } ((8) - (7)) \text{ gives} \qquad rP_r = xP_r' - P_{r-1}', \tag{10}$$

Incrementing r in (10) by one gives $(r+1)P_{r+1} = xP_{r+1}' - P_r'$, and subtracting x times (9),

$$(r+1)\left(P_{r+1} - xP_r\right) = -(1-x^2)P_r' \tag{11}$$

Differentiating and using (9)

$$\underbrace{(r+1)P_{r+1}'}_{(r+1)^2P_r+(r+1)xP_r'} - (r+1)P_r - (r+1)xP_r' + \frac{d}{dx}\left[(1-x^2)P_r'\right] = 0,$$

$$\text{or} \qquad \frac{d}{dx}(1-x^2)\frac{dP_r}{dx} + r(r+1)P_r = 0, \tag{12}$$

which is, indeed, Legendre's equation[1].

It has singular points at ± 1, and a weight function of $1 = (1-x)^0(1+x)^0$, so we see that it is a special case of Jacobi with $\alpha = \beta = 0$, with $g = (1-x^2), w = 1$. Then we expect Rodrigues' formula

$$P_r(x) = \frac{1}{a_r}\frac{d^r}{dx^r}(1-x^2)^r.$$

To evaluate a_r, note first that $P_\ell(\pm 1)$ is easy to evaluate, because

$$G(t, \pm 1) = (1 + t^2 \mp 2t)^{-1/2} = (1 \mp t)^{-1} = \sum_n (\pm t)^n = \sum_n P_N(\pm 1)t^n,$$

[1]The $m = 0$ form of the associated Legendre equation we saw in Lecture I, page 2.

so

$$P_n(\pm 1) = (\pm 1)^n, \quad \text{or} \quad \left\{ \begin{array}{c} P_n(1) = 1 \text{ all } n, \\ P_n(-1) = \begin{cases} 1 \text{ even } n, \\ -1 \text{ odd } n \end{cases} . \end{array} \right.$$

Now $$\frac{d^r}{dx^r}\left\{(1-x)^r(1+x)^r\right\}\Big|_{x=1} = (1+x)^r\,\frac{d^r}{dx^r}\left\{(1-x)^r\right\}\Big|_{x=1}$$

because all other terms have surviving factors of $1-x$, which vanish. This is $(-2)^r r!$, so $a_r = (-1)^r 2^r r!$.

In our treatment of orthogonal polynomials we showed that Rodrigues' formula satisfies the Legendre equation. We also have that the polynomials are orthogonal on $[-1,1]$:

$$\begin{aligned} \int_{-1}^{1} P_\ell(x)P_n(x)dx &= (-1)^{\ell+n}\frac{2^{-\ell-n}}{\ell!\,n!}\int \frac{d^\ell}{dx^\ell}(1-x^2)^\ell\,\frac{d^n}{dx^\ell}(1-x^2)^n\,dx \\ &= \frac{(-1)^n\,2^{-\ell-n}}{\ell!\,n!}\int(1-x^2)^\ell\left(\frac{d}{dx}\right)^{n+\ell}(1-x^2)^n\,dx, \end{aligned}$$

by integration by parts. If $\ell > n$, there are too many derivatives, and we get zero. If $n=\ell$, $(d/dx)^{2\ell}(1-x^2)^\ell = (-1)^\ell(2\ell)!$, while

$$\int_{-1}^{1}\left(1-x^2\right)^\ell dx = \int_{-1}^{1}(1-x)^\ell(1+x)^\ell dx = 2^{2\ell+1}B(\ell+1,\ell+1) = 2^{2\ell+1}\frac{\ell!^2}{(2\ell+1)!},$$

so all together,

$$\int_{-1}^{1} P_\ell^2(x)dx = \frac{(-1)^\ell 2^{-2\ell}}{\ell!^2}\,(-1)^\ell(2\ell)!\frac{2^{2\ell+1}(\ell!)^2}{(2\ell+1)!} = \frac{2}{2\ell+1}.$$

Note $G(t,\cos\theta) = (1-2t\cos\theta+t^2)^{-1/2} = \left[\left(1-te^{i\theta}\right)\left(1-te^{-i\theta}\right)\right]^{-1/2}$. Recall $(1-x)^{-1/2} = \sum_r \binom{-1/2}{r}(-1)^r x^r = \sum_r \frac{\frac{-1}{2}\frac{-3}{2}\cdots\frac{-(2r-1)}{2}}{r!}(-1)^r x^r = \sum_r 2^{-r}\frac{(2r-1)!!}{r!}x^r$, so $G(t,\cos\theta) = \sum_{rs}\frac{2^{-r-s}(2r-1)!!(2s-1)!!}{r!s!}t^{r+s}e^{i(r-s)\theta}$, and

$$\begin{aligned} &P_\ell(\cos\theta) = \text{sum of positive coefficients } \times e^{i(r-s)\theta} \\ &|P_\ell(\cos\theta)| \leq \text{sum of the same coefficients} = P_\ell(1) = 1, \end{aligned}$$

so the Legendre polynomial, on $[-1,1]$ is bounded by ± 1.

We have seen that the radial solutions r^ℓ and $r^{-\ell-1}$ of Laplace's equation are coupled to the solutions $P_\ell(\cos\theta)$ for the polar angle. Thus the electrostatic potential in chargeless space (for an axially symmetric solution) is

$$V = \sum_{n=0}^{\infty} a_n r^n P_n(\cos\theta) + \sum_{n=0}^{\infty} b_n r^{-n-1} P_n(\cos\theta).$$

Consider a neutral conducting sphere of radius r_0 in an otherwise uniform field, which would have $V = -E_0 z = -E_0 r\cos\theta$. Then at large r, the potential is unaffected and $a_1 = -E_0, a_n = 0, n > 1$. On the sphere $V = a_0 + a_1 r_0 P_1(\cos\theta) + \sum_{n=0}^{\infty} b_n r_0^{-n-1} P_n(\cos\theta) = \text{const}$, independent of θ. But the P_n's are linearly independent functions of θ, so $b_1 r_0^{-2} = -a_1 r_0$, and $b_n = 0$ for $n > 1$. $P_1(\cos\theta) = \cos\theta$, Thus

$$V = a_0 + \frac{b_0}{r} - E_0\left(r - \frac{r_0^3}{r^2}\right)\cos\theta.$$

The $1/r$ potential corresponds to a charge. Indeed, using a large sphere and Gauss' law, we can show $b_0 = Q/4\pi\epsilon_0$, where Q is the total charge on (and inside) the sphere. a_0 is an arbitrary constant but matches the conditions we've imposed ($V \to -E_0 z + 0$) if we choose $a_0 = 0$.

That problem could have been done without Legendre polynomials. Now consider a conducting thin ring of radius r_0, with a total charge q on it, lying in the x, y plane.

For $r > r_0$, the space is chargeless and, assuming no background field, and choosing $\Phi \to 0$ as $r \to \infty$, and using axial symmetry,

$$\Phi = \sum b_n r^{-n-1} P_n(\cos\theta)$$

It is easy to evaluate Φ on the z axis, because then all the charge is equally far away, at $\sqrt{z^2 + r_0^2}$, so

$$\begin{aligned}
\Phi(r, \theta = 0) &= \frac{q}{4\pi\epsilon_0}\left(r^2 + r_0^2\right)^{-1/2} \\
&= \frac{q}{4\pi\epsilon_0 r}\left(1 + \frac{r_0^2}{r^2}\right)^{-1/2} \\
&= \frac{q}{4\pi\epsilon_0}\sum_{n=0}^{\infty}\frac{r_0^{2n}}{r^{2n+1}}\binom{-1/2}{n} = \sum b_n r^{-n-1}.
\end{aligned}$$

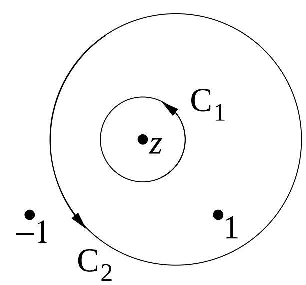
This shows $b_n = 0$ for n odd, $b_{2n} = \dfrac{q}{4\pi\epsilon_0} r_0^{2n} \dbinom{-1/2}{n} = \dfrac{q r_0^{2n}}{4\pi\epsilon_0} \dfrac{(-1)^n (2n-1)!!}{2^n\, n!}$, so in general

$$\Phi(r,\theta) = \sum_{n=0}^{\infty} \frac{q r_0^{2n}}{4\pi\epsilon_0\, r^{2n+1}} (-1)^n \frac{(2n-1)!!}{2^n\, n!} P_{2n}(\cos\theta).$$

1.5 Extension to P_ν

The Rodrigues formula

$$P_n(z) = \frac{1}{2^n\, n!} \left(\frac{d}{dz}\right)^n \left(z^2 - 1\right)^n$$

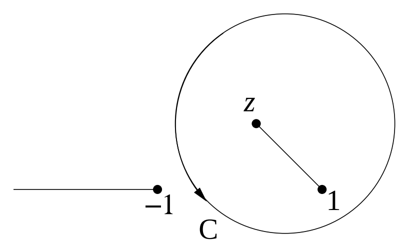


can be written

$$P_n(z) = \frac{2^{-n}}{2\pi i} \oint \frac{(t^2-1)^n}{(t-z)^{n+1}} dt$$

where the integral circles z.

We define the Legendre functions by extending this form from integer n to ν, not necessarily integral. But if n is not an integer, there are cuts starting at z, 1, and -1. We want our contour to come back to where it started, without crossing a cut. So we define the integrand with cuts from z to 1 and from -1 to ∞ along the negative real axis and define the Legendre function as



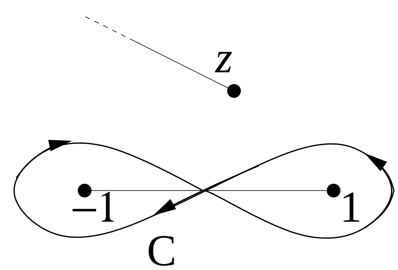
$$P_\nu(z) = \frac{2^{-\nu}}{2\pi i} \oint_C \frac{(t^2-1)^\nu}{(t-z)^{\nu+1}} dt.$$

$P_\nu(z)$ is a solution of Legendre's equation, as

$$\begin{aligned}
&\left(1-z^2\right) P_\nu''(z) - 2z P_\nu'(z) + \nu(\nu+1) P_\nu(z) \\
&\quad = \frac{2^{-\nu}}{2\pi i} \oint_C \frac{(t^2-1)^\nu}{(t-z)^{\nu+3}} dt \\
&\qquad \cdot \left[\left(1-z^2\right)(\nu+1)(\nu+2) - 2z(\nu+1)(t-z) + \nu(\nu+1)(t-z)^2\right] \\
&\quad = \frac{2^{-\nu}(\nu+1)}{2\pi i} \oint_C \frac{(t^2-1)^\nu}{(t-z)^{\nu+3}} dt \left[\nu t^2 - 2tz(v+1) + \nu + 2\right] \\
&\quad = \frac{2^{-\nu}(\nu+1)}{2\pi i} \oint_C \frac{d}{dt} \left[\frac{(t^2-1)^{\nu+1}}{(t-z)^{\nu+2}}\right] dt,
\end{aligned}$$

which, as long as we make sure our [] comes back to what we started with, must give zero.

There is another solution to the differential equation. You might expect it to be $P_{-\nu-1}$, which satisfies the same equation, but this is, in fact, just P_ν. The second function is called Q_ν, and is the integral over the figure eight contour as shown, where the cuts are to be considered running from -1 to 1 and from z to ∞. The contour goes onto the second sheet as it goes below the axis towards $z = -1$, but comes back onto the first sheet returning towards $z = 1$. Thus it never need include a discontinuity.



We will not consider these further. Whittaker and Watson "A Course in Modern Analysis" is a good reference for more.

1.6 Associated Legendre Polynomials

We have so far been restricted to axially symmetric problems. The separation of variables gave us the azimuthal dependence $\Phi(\phi) = e^{im\phi}$ with m an integer, and then for θ,

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d\Theta}{d\theta} + \left(\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right)\Theta = 0.$$

With $x = \cos\theta$, $V(x) = \Theta(\theta)$ this gives

$$(1-x^2)\frac{d^2V}{dx^2} - 2x\frac{dV}{dx} + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)V = 0.$$

Only for $m = 0$ is this the Legendre equation itself.

We can get solutions to the associated equation by differentiating Legendre's equation m times. This is essentially applying an angular momentum raising operator, if you know what that means. As you probably don't, let's just follow blindly:

$$\left(\frac{d}{dx}\right)^m \left[\left(1-x^2\right)P_\ell'' - 2xP_\ell' + \ell(\ell+1)P_\ell\right] = 0$$
$$= \left[\left(1-x^2\right)\frac{d^2}{dx^2} - 2mx\frac{d}{dx} - m(m-1) - 2x\frac{d}{dx} - 2m + \ell(\ell+1)\right]\underbrace{\left(\frac{d}{dx}\right)^m P_\ell}_{u}$$

$$\text{so}\quad \left[\left(1-x^2\right)\frac{d^2}{dx^2} - 2x(m+1)\frac{d}{dx} + \ell(\ell+1) - m(m+1)\right]u \qquad (13)$$

Now let $V = (1-x^2)^{m/2}\, u$ (which is $u \sin^m\theta$)

$$\begin{aligned} u' &= \left(1-x^2\right)^{-m/2} V' + mx\left(1-x^2\right)^{-m/2-1} V \\ \left(1-x^2\right)u'' &= \left(1-x^2\right)^{1-m/2} V'' + m\left(1-x^2\right)^{-m/2} V \\ &\qquad + m(m+2)x^2\left(1-x^2\right)^{-m/2-1} V + 2mx\left(1-x^2\right)^{-m/2} V' \end{aligned}$$

so Eq. (13) is

$$(1-x^2)^{-m/2}\left\{ \left(1-x^2\right)V'' + 2mxV' + mV + \frac{m(m+2)x^2}{1-x^2}V \right.$$
$$\left. -2x(m+1)V' - 2m(m+1)\frac{x^2}{1-x^2}V + (\ell(\ell+1) - m(m+1))V \right\} = 0$$

or $\left(1-x^2\right)V'' - 2xV' + \left[\ell(\ell+1) - \dfrac{m^2}{1-x^2}\right]V = 0$, and V satisfies the Associated Legendre Equation. We call V

$$P_\ell^m(x) := \left(1-x^2\right)^{m/2}\left(\frac{d}{dx}\right)^m P_\ell(x) \quad \text{for } m > 0.$$

From Rodrigues, $P_\ell(x) = \dfrac{(-1)^\ell}{2^\ell\,\ell!}\left(\dfrac{d}{dx}\right)^\ell \left(1-x^2\right)^\ell$, we have

$$P_\ell^m(x) := \frac{(-1)^\ell}{2^\ell\,\ell!}\left(1-x^2\right)^{m/2}\left(\frac{d}{dx}\right)^{\ell+m}\left(1-x^2\right)^\ell$$

which applies to negative m's as well, as long as $m \geq -\ell$.

1.7 Orthogonality

Consider a fixed m, but let ℓ vary. Then we would expect orthogonality with the weight funtion $w = 1$. Indeed,

$$\int_{-1}^{1} P_\ell^m(x) P_n^m(x) = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}\delta_{\ell n}.$$

This is shown in gory detail in Arfken. With $\ell = n$ but m varying, there is orthogonality with weight $w = 1/(1-x^2)$, but this is not useful. In physical problems, orthogonality in the m's comes from the ϕ equation, $\Phi(\phi) = e^{im\phi}$. It is really the combination

$$Y_\ell^m(\theta,\phi) := (-1)^m \left(\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right)^{1/2} P_\ell^m(\cos\theta) e^{im\phi}$$

which has physical significance. These are called the **spherical harmonics**. The angular integral

$$\begin{aligned}
&\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, Y_{\ell_1}^{m_1\,*}(\theta,\phi)\, Y_{\ell_2}^{m_2}(\theta,\phi) \\
&\quad = \int_{-1}^{1} dx\, P_{\ell_1}^{m_1}(x) P_{\ell_2}^{m_2}(x) \int_0^{2\pi} e^{i(m_2-m_1)\phi} d\phi \\
&\qquad\qquad (-1)^{m_1+m_2}\left\{\frac{(2\ell_1+1)(2\ell_2+1)}{(4\pi)^2}\frac{(\ell_1-m_1)!}{(\ell_1+m_1)!}\frac{(\ell_2-m_2)!}{(\ell_2+m_2)!}\right\}^{1/2}
\end{aligned}$$

The ϕ integral gives $2\pi\delta_{m_1,m_2}$, and then, as the m's are now equal, the x integral gives $\dfrac{2}{2\ell_1+1}\dfrac{(\ell_1+m_1)!}{(\ell_1-m_1)!}\,\delta_{\ell_1,\ell_2}$, so

$$\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, Y_{\ell_1}^{m_1\,*}(\theta,\phi) Y_{\ell_2}^{m_2}(\theta,\phi) = \delta_{\ell_1,\ell_2}\delta_{m_1,m_2}.$$

The Y_ℓ^m's are a set of complete functions on the **2-sphere**.

In quantum mechanics, the wave functions in a spherically symmetric problem are proportional to spherical harmonics, with angular momentum $\hbar\ell$ and z-component $m\hbar$. The angular momentum operator itself is $\vec{L} = -i\hbar\vec{r}\times\vec{\nabla}$, and the spherical harmonics are eigenfunctions of L^2 and L_z:

$$\begin{aligned}
L^2\, Y_\ell^m &= \hbar^2 \ell(\ell+1)\, Y_\ell^m \\
L_z\, Y_\ell^m &= \hbar m\, Y_\ell^m
\end{aligned}$$

1.8 Other Orthogonal Polynomials

We have extensively considered the Legendre polynomials, one special case of the Jacobi orthogonal polynomials associated with the interval $[-1, 1]$. We will not consider the others except to mention that Chebyshev polynomials are in this class, and are useful in some contexts, especially computation.

We now consider the other two classes. First, the Hermite polynomials, associated with $(-\infty, \infty)$ with a weight function $w = e^{-x^2}$ and $g = 1$. Rodrigues' formula gives

$$H_n(x) = (-1)^n e^{x^2} \left(\frac{d}{dx}\right)^n e^{-x^2},$$

where I have chosen $a_n = (-1)^n$ by convention.

From this expression it is clear that $H_n(-x) = (-1)^n H_n(x)$. Rewriting it as $D^n\,1$, where D is the differential *operator* $-e^{x^2}\frac{d}{dx}e^{-x^2} = 2x - \frac{d}{dx}$, it is clear that H_n is a polynomial of degree n.

We can write the $\left(\frac{d}{dx}\right)^n e^{-x^2}$ as a Cauchy integral

$$H_n(x) = (-1)^n e^{x^2} \frac{n!}{2\pi i} \oint \frac{e^{-z^2}\,dz}{(z-x)^{n+1}}.$$

First, get rid of the $(-1)^n$ by changing the sign of x

$$\begin{aligned} H_n(x) &= (-1)^n H_n(-x) = e^{x^2} \frac{n!}{2\pi i} \oint \frac{e^{-z^2}\,dz}{(z+x)^{n+1}} \\ &= \frac{n!}{2\pi i} \oint \frac{e^{-t^2+2xt}}{t^{n+1}} dt \end{aligned}$$

where the contour in t circles the origin. This is clearly $n!$ times the coefficient of t^n in $e^{-t^2+2xt} = G(x, t)$, so

$$G(x, t) = \sum_{n=0}^{\infty} \frac{1}{n!} t^n H_n(x).$$

[Note G generates $H_n(x)/n!$ using our usual definition]

Clearly

$$\begin{aligned} \frac{\partial}{\partial t} G(x, t) = \sum_n \frac{t^n}{n!} H_{n+1}(x) &= -2(t - x)G(x, t) \\ &= -2 \sum \frac{t^n}{(n-1)!} H_{n-1} + 2x \sum \frac{t^n}{n!} H_n \end{aligned}$$

$$\text{so} \qquad H_{n+1} = -2nH_{n-1} + 2xH_n. \tag{14}$$

$$\frac{\partial G(x,t)}{\partial x} = \sum_n \frac{t^n}{n!} H_n'(x) = 2tG(x,t) = 2 \sum \frac{t^n}{(n-1)!} H_{n-1}$$

so

$$H_n'(x) = 2nH_{n-1}(x) \tag{15}$$

Plug (15) into (14): $H_{n+1} = -H_n' + 2xH_n$ and differentiate

$$H_{n+1}' = -H_n'' + 2H_n + 2xH_n' = 2(n+1)H_n,$$

so $H_n'' - 2xH_n' + 2nH_n = 0$.

To get the equation in self-adjoint form with $p = w = e^{-x^2}$ as expected, multiply by e^{-x^2} to get

$$\frac{d}{dx}\, e^{-x^2} \frac{dH_n}{dx} + 2ne^{-x^2} H_n = 0$$

so $\lambda = 2n$.

These are orthogonal polynomials, so

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) = h_n \delta_{mn}.$$

h_n can be evaluated, and the orthogonality verified, by using the generating function

$$\sum_{m,n} \frac{s^m t^n}{m!\,n!} \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) = \int_{-\infty}^{\infty} e^{-x^2} e^{-t^2+2tx-s^2+2sx}\, dx$$

$$= \int_{-\infty}^{\infty} e^{-(x-t-s)^2} dx\; e^{2ts} = e^{2ts} \int_{-\infty}^{\infty} e^{-u^2} du = \sqrt{\pi} \sum_n \frac{2^n s^n t^n}{n!}$$

$$\text{so} \qquad \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) = \sqrt{\pi}\, 2^n\; n!\; \delta_{mn}.$$

The wave functions for the quantum mechanical harmonic oscillator are

$$\psi_n(x) = \underbrace{2^{-n/2}\pi^{-1/4}(n!)^{-1/2}}_{\text{normalization constant}}\; e^{-x^2/2} H_n(x),$$

which are orthogonal and satisfy

$$\left(-\frac{d^2}{dx^2} + x^2\right)\psi = (2n+1)\psi.$$

If appropriately scaled, this becomes the Schrödinger equation for a potential $V = \frac{1}{2}kx^2$.

The last equation to consider in detail from the orthogonal polynomial discussion is the **Generalized Laguerre**, with singular points at 0 and ∞,

$$\left(\frac{d}{dx}x^{\alpha+1}e^{-x}\frac{d}{dx} + \lambda x^\alpha e^{-x}\right) y = 0.$$

For $\alpha = 0$, this is the **Laguerre** equation, with regular solutions $L_n(x)$ for $\lambda = n$ an integer, with $g(x) = x$ and $w(x) = e^{-x}$.

Rodrigues gives

$$L_n(x) = \frac{e^x}{n!}\left(\frac{d}{dx}\right)^n \left(x^n e^{-x}\right) = \frac{e^x}{2\pi i}\oint \frac{z^n\, e^{-z}}{(z-x)^{n+1}}dz,$$

so

$$\begin{aligned} G(x,t) &= \sum L_n t^n = \frac{e^x}{2\pi i}\oint \sum_{n=0}\left(\frac{zt}{(z-x)}\right)^n \frac{e^{-z}}{z-x}dz \\ &= \frac{e^x}{2\pi i}\oint \frac{1}{1-\frac{zt}{z-x}}\frac{e^{-z}}{z-x}dz \\ &= \frac{e^x}{2\pi i}\oint \frac{e^{-z}}{z-zt-x}\,dz = \frac{e^x e^{-\frac{x}{1-t}}}{1-t} = \frac{e^{-xt/(1-t)}}{1-t}. \end{aligned}$$

For $\alpha = k, \lambda = n$ we can rewrite the *generalized Laguerre* equation, with $g(x) = x$, $w(x) = x^k\, e^{-x}$, and $\lambda = n$ as

$$\left(x\frac{d^2}{dx^2} + (k+1-x)\frac{d}{dx} + n\right) L_n^k(x) = 0.$$

Rodrigues gives $L_n^k = \dfrac{x^{-k}}{n!}e^x\dfrac{d^n}{dx^n}x^{n+k}e^{-x}$, (well, with the normalization I chose).

The wave function for a hydrogenic atom (a single electron of charge $-e$ rotating nonrelativistically around a nucleus of charge Ze) is

$$\psi_{n\ell m}(r,\theta,\phi) \propto e^{-\alpha r/2}(\alpha r)^\ell L_{n-\ell-1}^{2\ell+1}(\alpha r) Y_\ell^m(\theta,\phi)$$

where $\alpha = 2\dfrac{Ze^2 m}{\hbar^2 n}$, where $n = 1, 2, 3, \ldots$ is called the **shell**, and ℓ and m are the angular momentum and its z component, respectively, in units of $\hbar$.

The hydrogen atom and the harmonic oscillator are basically the only radial problems in quantum mechanics which are exactly solvable. Thus the other functions in this chapter do not have direct physical applications, although they are interesting in mathematical contexts. I just mention that

- Chebyshev polynomials are used in numerical methods for polynomial approximations on a bounded interval.
- The hypergeometric functions ${}_2F_1(a, b, c, x)$ is a broad class coming from a second order differential equation with three regular singular points, including infinity. Many other functions are special cases of this function. The confluent hypergeometric function ${}_1F_1(a, c, x)$ is a singular limit
$$ {}_1F_1(a, c, x) = \lim_{\lambda \to \infty} {}_2F_1(a, \lambda, c, x/\lambda) $$
which has a regular singularity at 0 and an irregular one at ∞. The erf, J_ν, I_ν, L_n, and L_n^k are special cases.