

Multipole expansion of the Newtonian potential in 3D

Legendre 1782:

$$\frac{1}{|\mathbf{r} - \mathbf{r}_1|} = \frac{1}{\sqrt{r^2 - 2rr_1 \cos \theta + r_1^2}} = \frac{1}{r} \sum_{n=0}^{\infty} P_n(\cos \theta) \left(\frac{r_1}{r}\right)^n \quad (1)$$

where $\mathbf{r} \cdot \mathbf{r}_1 = rr_1 \cos \theta$, $r = |\mathbf{r}|$, $r_1 = |\mathbf{r}_1|$. In terms of $x = \cos \theta$ and $t = r_1/r$, that is

$$\boxed{\frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n.} \quad (2)$$

The function $G(x, t) = (1 - 2xt + t^2)^{-1/2}$ is called the *generating function* for $P_n(x)$, in the sense (2) that the expansion of $G(x, t)$ in powers of t *generates* the coefficients $P_n(x)$. Many properties of the $P_n(x)$ follow from (2).

Binomial expansion

The binomial formula of elementary algebra

$$(1 + q)^n = \sum_{k=0}^n \binom{n}{k} q^k \quad (3a)$$

for integer $n \geq 0$, generalizes to the *binomial series*

$$(1 + q)^\alpha = 1 + \alpha q + \frac{\alpha(\alpha - 1)}{2} q^2 + \cdots = \sum_{k=0}^{\infty} \binom{\alpha}{k} q^k \quad (3b)$$

that is the Taylor series expansion of $f(q) = (1 + q)^\alpha$ about $q = 0$, with

$$\binom{\alpha}{k} = \frac{\alpha(\alpha - 1) \cdots (\alpha - k + 1)}{k!}.$$

For integer $\alpha = n$, the series (3b) terminates at $k = n$, recovering the binomial formula (3a).

Applying (3b) to the Legendre generating function (2) with $\alpha = -1/2$ and $q = -2xt + t^2$ yields

$$\begin{aligned} \frac{1}{\sqrt{1 - 2xt + t^2}} &= 1 - \frac{1}{2}(t^2 - 2xt) + \frac{3}{8}(t^2 - 2xt)^2 + \cdots \\ &= 1 + xt + \frac{3x^2 - 1}{2} t^2 + O(t^3) \end{aligned} \quad (4)$$

thus $P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = (3x^2 - 1)/2$, $\dots$

Pushing to all orders using the binomial formula to expand the factors $(-2xt + t^2)^k$ yields

$$\begin{aligned} (1 - 2xt + t^2)^{-1/2} &= \sum_{k=0}^{\infty} \binom{-1/2}{k} (-2xt + t^2)^k \\ &= \sum_{k=0}^{\infty} \binom{-1/2}{k} \sum_{l=0}^k \binom{k}{l} (-2x)^{k-l} t^{k+l} \\ &= \sum_{n=0}^{\infty} \left(\sum_{l=0}^{\lfloor n/2 \rfloor} \binom{-1/2}{n-l} \binom{n-l}{l} (-2x)^{n-2l} \right) t^n \end{aligned} \quad (5)$$

with a switch of summation indices $(k, l) \rightarrow (n, l)$, with $n = k + l$ and

$$0 \leq k < \infty, 0 \leq l \leq k \rightarrow 0 \leq n < \infty, 0 \leq l \leq k = n - l$$

that is $0 \leq 2l \leq n$ and thus $0 \leq l \leq \lfloor n/2 \rfloor$, where $\lfloor n/2 \rfloor = n/2$ when n is even, and $\lfloor n/2 \rfloor = (n-1)/2$ when n is odd, is the *floor* of $n/2$. The coefficient of t^n in (2) and (5) is

$$\begin{aligned} P_n(x) &= \sum_{l=0}^{\lfloor n/2 \rfloor} \binom{-1/2}{n-l} \binom{n-l}{l} (-2x)^{n-2l} \\ &= \sum_{l=0}^{\lfloor n/2 \rfloor} (-1)^l \frac{(2n-2l)!}{2^n (n-l)! l! (n-2l)!} x^{n-2l} \end{aligned} \tag{6}$$

It is nice to have an explicit formula, but the following is much more useful.

Polynomial Recurrence

Differentiating both sides of (2) with respect to t yields

$$\frac{\partial G}{\partial t} = \frac{x-t}{(1-2xt+t^2)^{3/2}} = \sum_{n=0}^{\infty} n P_n(x) t^{n-1}.$$

Substituting for $(1-2xt+t^2)^{-1/2}$ from (2) and multiplying by $(1-2xt+t^2)$ yields

$$(x-t) \sum_{n=0}^{\infty} P_n(x) t^n - (1-2xt+t^2) \sum_{n=0}^{\infty} n P_n(x) t^{n-1} = 0$$

and collecting powers of t

$$\sum_n \left(x P_n(x) - P_{n-1}(x) - (n+1) P_{n+1}(x) + 2x n P_n(x) - (n-1) P_{n-1}(x) \right) t^n = 0$$

yields the three-term recurrence formula

$$\boxed{(2n+1) x P_n(x) = (n+1) P_{n+1}(x) + n P_{n-1}(x).} \tag{7}$$

Starting from $P_0(x) = 1$, $P_1(x) = x$ yields

$$\begin{aligned} P_2(x) &= \frac{1}{2} (3x P_1(x) - P_0(x)) = \frac{1}{2} (3x^2 - 1), \\ P_3(x) &= \frac{1}{3} (5x P_2(x) - 2P_1(x)) = \frac{1}{2} (5x^3 - 3x), \end{aligned}$$

and so on.

Derivative Recurrences

Differentiating (2) with respect to x yields recurrence relations for derivatives of $P_n(x)$.

$$\frac{\partial G}{\partial x} = \frac{t}{(1-2xt+t^2)^{3/2}} = \sum_{n=0}^{\infty} \frac{dP_n}{dx} t^n.$$

Substituting for $(1 - 2xt + t^2)^{-1/2}$ from (2) and multiplying by $(1 - 2xt + t^2)$ yields

$$t \sum_{n=0}^{\infty} P_n(x) t^n - (1 - 2xt + t^2) \sum_{n=0}^{\infty} \frac{dP_n}{dx} t^n = 0$$

and collecting powers of t^{n+1}

$$\sum_n \left(P_n(x) - \frac{dP_{n+1}}{dx} + 2x \frac{dP_n}{dx} - \frac{dP_{n-1}}{dx} \right) t^{n+1} = 0$$

yields the derivative recurrence

$$\frac{dP_{n+1}}{dx} + \frac{dP_{n-1}}{dx} = 2x \frac{dP_n}{dx} + P_n(x). \quad (8)$$

Differentiating the polynomial recurrence (7) gives

$$(2n+1)P_n(x) + (2n+1)x \frac{dP_n}{dx} = (n+1) \frac{dP_{n+1}}{dx} + n \frac{dP_n}{dx}, \quad (9)$$

eliminating the $x dP_n/dx$ term between (8) and (9) yields the recurrence

$$\boxed{\frac{dP_{n+1}}{dx} - \frac{dP_{n-1}}{dx} = (2n+1)P_n(x).} \quad (10)$$

Next, adding and subtracting (8) and (10) yields

$$\frac{dP_{n+1}}{dx} = x \frac{dP_n}{dx} + (n+1)P_n, \quad (11)$$

$$\frac{dP_{n-1}}{dx} = x \frac{dP_n}{dx} - nP_n. \quad (12)$$

Writing (11) for $n-1$ in place of n , then substituting for dP_{n-1}/dx from (12) yields

$$(1-x^2) \frac{dP_n}{dx} + nxP_n = nP_{n-1}. \quad (13)$$

Differentiating (13), then substituting for dP_{n-1}/dx from (12) yields Legendre's equation

$$\boxed{\frac{d}{dx} \left((1-x^2) \frac{dP_n}{dx} \right) + n(n+1)P_n = 0.} \quad (14)$$

This is a singular Sturm-Liouville equation in $-1 \leq x \leq 1$,

$$\frac{d}{dx} \left(p(x) \frac{d\Phi}{dx} \right) + q(x)\Phi = -\lambda w(x)\Phi \quad (15)$$

with

$$p(x) = 1 - x^2 \geq 0, \quad q(x) = 0, \quad w(x) = 1, \quad \lambda = n(n+1),$$

with eigenfunctions $P_n(x)$ orthogonal in $-1 < x < 1$ with weight $w(x) = 1$

$$\int_{-1}^1 P_m(x) P_n(x) dx = \delta_{mn} \int_{-1}^1 (P_n(x))^2 dx. \quad (16)$$

But Sturm and Liouville's work dates from around 1836, more than 50 years after Legendre's work on the Legendre polynomials.

Helmholtz equation in spherical coordinates

The Helmholtz equation $\nabla^2 u + k^2 u = 0$ arises from looking for eigenfunctions of the *heat*, *wave* and *Schrödinger* equations,

$$\left. \begin{aligned} \partial_t v &= \kappa \nabla^2 v, & v &= e^{-\kappa k^2 t} u, \\ \partial_t^2 v &= c^2 \nabla^2 v, & v &= e^{\pm i c k t} u, \\ \partial_t \psi &= \frac{i\hbar}{2m} \nabla^2 \psi, & \psi &= e^{-\frac{i\hbar}{2m} k^2 t} u, \end{aligned} \right\} \Rightarrow \nabla^2 u + k^2 u = 0, \quad (17)$$

and $\lambda = k^2$ is the eigenvalue of the negative Laplacian operator $-\nabla^2$.

In spherical coordinates (r, θ, φ) with $\hat{\mathbf{z}} \cdot \mathbf{r} = r \cos \theta$ and $\hat{\mathbf{x}} \cdot \mathbf{r} = r \sin \theta \cos \varphi$, the Helmholtz equation reads

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial u}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \varphi^2} + k^2 u = 0. \quad (18)$$

Looking for separated solutions $u = e^{im\varphi} f(r)g(\theta)$ yields the equations

$$\frac{d}{dr} \left(r^2 \frac{df}{dr} \right) + (k^2 r^2 - \mu) f = 0, \quad (19)$$

$$\frac{d}{d\theta} \left(\sin \theta \frac{dg}{d\theta} \right) + \left(\mu \sin \theta - \frac{m^2}{\sin \theta} \right) g = 0, \quad (20)$$

where μ is a separation constant, and an eigenvalue for the $g(\theta)$ equation, and m is an integer for period 2π in the azimuthal coordinate φ . Both (19), (20) are singular Sturm-Liouville problems (15) in $0 \leq r \leq a$ and $0 \leq \theta \leq \pi$, respectively.

Sturm-Liouville theory, and the Rayleigh quotient, predicts a countable infinity of positive eigenvalues $\mu_n^{(m)}$ for each m

$$0 < \mu_1^{(m)} < \mu_2^{(m)} < \dots$$

as long as $g(\theta)$ is bounded at the singular point $\theta = 0, \pi$, with eigenfunctions $g_n^{(m)}(\theta)$ orthogonal with respect to the weight $w(\theta) = \sin \theta$. Likewise, there is a countable infinity of positive eigenvalues $\lambda = k^2$, for each μ ,

$$0 < \lambda_1^{(\mu)} < \lambda_2^{(\mu)} < \dots$$

with corresponding eigenfunctions $f_l^{(\mu)}(r)$ orthogonal with respect to the weight $w(r) = r^2$.

The general solution to the heat equation, for example, would read

$$u(r, \theta, \varphi, t) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{l=1}^{\infty} A_{mnl} e^{im\varphi} g_n^{(m)}(\theta) f_l^{(mn)}(r) e^{-\kappa \lambda_{mnl} t},$$

with A_{mnl} obtained from the known initial condition $u(r, \theta, \varphi, 0)$ at $t = 0$ by projection onto the orthogonal eigenfunctions. The functions $Y_n^m(\theta, \varphi) = e^{im\varphi} g_n^{(m)}(\theta)$ are called *spherical harmonics*.

The change of variable $x = \cos \theta$, transforms (20) into the *associated Legendre equation*

$$\frac{d}{dx} \left((1-x^2) \frac{dg}{dx} \right) + \left(\mu - \frac{m^2}{1-x^2} \right) g = 0, \quad (21)$$

that reduces to (14) for $m = 0$. Equation (21) has regular singular points at $x = \pm 1$. Asymptotic analysis near those points shows that $g(x) \sim (1+x)^{\pm m/2}$ near $x = -1$, and $g(x) \sim (1-x)^{\pm m/2}$ near $x = 1$.