2 Hermite Polynomials $H_n(x)$

The next class of orthogonal polynomials to be considered are **Hermite polynomials**, which can be defined via the generating function **A&W Sec. 13.1**

$$g(x,\, t) \;=\; \exp\{-t^2 + 2tx\} \;=\; \sum_{n=0}^{\infty} H_n(x)\, \frac{t^n}{n!} \quad . \tag{16}$$

This can be employed in the now familiar differentiation protocol to yield the recurrence relations

$$\begin{aligned} H_{n+1}(x) \;&=\; 2xH_n(x) - 2nH_{n-1}(x) \quad , \\ H_n'(x) \;&=\; 2nH_{n-1}(x) \quad . \end{aligned} \tag{17}$$

The substitutions $t \to -t$ and $x \to -x$ in the generating function simply yield the parity relation $H_n(-x) = (-1)^n H_n(x)$. These recurrence relations quickly lead to the second order Hermite ODE

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) \;=\; 0 \quad , \tag{18}$$

which is clearly not self-adjoint.

• The Rodrigues' formula can be obtained by interpreting the generating function $g(x,\, -t)$ as a Taylor series about $t = 0$, so that

$$H_n(x) \;=\; (-1)^n \frac{d^n}{dt^n} \Big[\exp\Big\{ x^2 - (t+x)^2 \Big\} \Big]_{t=0} \;=\; (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}) \quad . \tag{19}$$

This can then be used to establish the orthogonality integral

$$\int_{-\infty}^{\infty} e^{-x^2}\, H_m(x)\, H_n(x)\, dx \;=\; 0 \quad , \quad m \,\neq\, 0 \quad . \tag{20}$$

This implies that the Hermite polynomials are not self-adjoint, but the functions $\phi_n(x) = e^{-x^2/2} H_n(x)$ are, and they satisfy

$$\phi_n''(x) + [2n + 1 - x^2]\, \phi_n(x) \;=\; 0 \quad . \tag{21}$$

This is the equation of motion for a quantum mechanical simple harmonic oscillator (SHO), an important application of Hermite polynomials.

• The orthonormality condition for the Hermite polynomials needs to be determined. We proceed by squaring the generating function and multiplying by $\exp(-x^2)$:

$$e^{-x^2} e^{-s^2+2sx} e^{-t^2+2tx} \;=\; \sum_{m,n=0}^{\infty} e^{-x^2} H_m(x)\, H_n(x)\, \frac{s^m t^n}{m!\, n!} \quad . \tag{22}$$

This is now in a form to integrate over $(-\infty, \infty)$ and employ the orthogonality condition to collapse the double sum into a single one with $m = n$:

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{(st)^n}{(n!)^2} \int_{-\infty}^{\infty} e^{-x^2} \left\{H_n(x)\right\}^2 \, dx \;&=\; \int_{-\infty}^{\infty} e^{-x^2-s^2+2sx-t^2+2tx}\, dx \\ =\; e^{2st} \int_{-\infty}^{\infty} e^{-(x-s-t)^2}\, dx \;&=\; \sqrt{\pi}\, e^{2st} \;=\; \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n (st)^n}{n!} \quad . \end{aligned} \tag{23}$$

Equating the coefficients term by term yields the normalization constraint

$$\int_{-\infty}^{\infty} e^{-x^2} \left\{H_n(x)\right\}^2 \, dx \;=\; 2^n \sqrt{\pi}\, n! \quad . \tag{24}$$

• The quantum mechanical SHO with a potential energy $V = m\omega^2 z^2/2$ is described by the Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(z) + \frac{m\omega^2 z^2}{2}\, \Psi(z) \;=\; E\Psi(z) \quad . \tag{25}$$

Here ω is the angular frequency of the corresponding classical oscillator. Rescaling the spatial coordinate by $x = \alpha z$ with $\alpha = \sqrt{m\omega/\hbar}$, the ODE can be written in the form (for $\lambda = 2E/\hbar\omega$)

$$\frac{d^2\psi(x)}{dx^2} + (\lambda - x^2)\, \psi(x) \;=\; 0 \quad , \quad \psi(x) \;\equiv\; \Psi(z/\alpha) \quad . \tag{26}$$

The Frobenius series technique then yields bounded polynomial solutions for $e^{x^2/2}\psi(x)$ only of $\lambda = 2n + 1$ for integer n, thereby demarcating the quantum numbers. These solutions are the Hermite polynomials, and the energy is quantized via $E = (n+1/2)\hbar\omega$. <u>The ground state $n = 0$ therefore has finite energy $\hbar\omega/2$</u>.

3 Laguerre Functions

Laguerre functions $L_n(x)$ are also pertinent to cylindrical geometries, and are solutions of Laguerre's ordinary differential equation: **A&W Sec. 13.2**

$$x \frac{d^2y}{dx^2} + (1-x)\frac{dy}{dx} + n\,y \;=\; 0 \quad . \tag{27}$$

These are polynomials when n is an integer, and the Frobenius series is truncated at the x^n term. A new representation, which can also be obtained for other special functions, is the **Schläfli integral** representation

$$L_n(x) \;=\; \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)\,z^{n+1}}\,dz \quad . \tag{28}$$

The contour lies <u>inside the unit circle and encircles the origin</u>, i.e., $|z| < 1$. One can then form the left hand side of Eq. (27), and the result is

$$\frac{1}{2\pi i}\oint \left[\frac{x}{(1-z)^3\,z^{n-1}} - \frac{1-x}{(1-z)^2\,z^n} + \frac{n}{(1-z)\,z^{n+1}}\right] e^{-xz/(1-z)}\,dz \quad . \tag{29}$$

Grouping terms appropriately, this is equal to

$$\frac{1}{2\pi i}\oint \frac{d}{dz}\left[\frac{e^{-xz/(1-z)}}{(1-z)\,z^n}\right] dz \quad . \tag{30}$$

Obviously, since there is no simple pole within the contour, since the Laurent series of the integrand does not possess a $1/z$ term. The resulting integral is zero, and the Schläfli integral satisfies Laguerre's ODE. The generating function series identity is quickly found using the Schläfli integral form and a geometric series manipulation:

$$\begin{aligned} \sum_{n=0}^{\infty} L_n(x)\,z^n \;&=\; \sum_{n=0}^{\infty} \frac{z^n}{2\pi i}\oint \frac{e^{-xu/(1-u)}}{(1-u)\,u^n}\,\frac{du}{u} \\ &=\; \frac{1}{2\pi i}\oint \frac{e^{-xu/(1-u)}\,du}{(1-u)\,(u-z)} \end{aligned} \tag{31}$$

so that applying the Residue theorem leads to the result

$$g(x,\,z) \;=\; \frac{e^{-xz/(1-z)}}{(1-z)} \;=\; \sum_{n=0}^{\infty} L_n(x)\,z^n \quad , \quad |z| \;<\; 1 \quad . \tag{32}$$

Introducing the transformation $z = 1 - x/t$, then since the new contour in the t-plane surrounds $t = x$,

$$L_n(x) \;=\; \frac{e^x}{2\pi i}\oint \frac{t^n e^{-t}}{(t-x)^{n+1}}\,dt \quad\Rightarrow\quad L_n(x) \;=\; \frac{e^x}{n!}\,\frac{d^n}{dx^n}(x^n e^{-x}) \tag{33}$$

using Cauchy's integral formula for derivatives. We then also have the finite series form of the Laguerre polynomials:

$$L_n(x) \;=\; \sum_{s=0}^{n} \frac{(-1)^s n!\,x^s}{(n-s)!\,\{s!\}^2} \quad . \tag{34}$$

• From this it becomes obvious that the Laguerre polynomials do not possess a parity property. Nor should they, since they are basis states for the $[0,\infty)$ interval that is not symmetric about the origin.

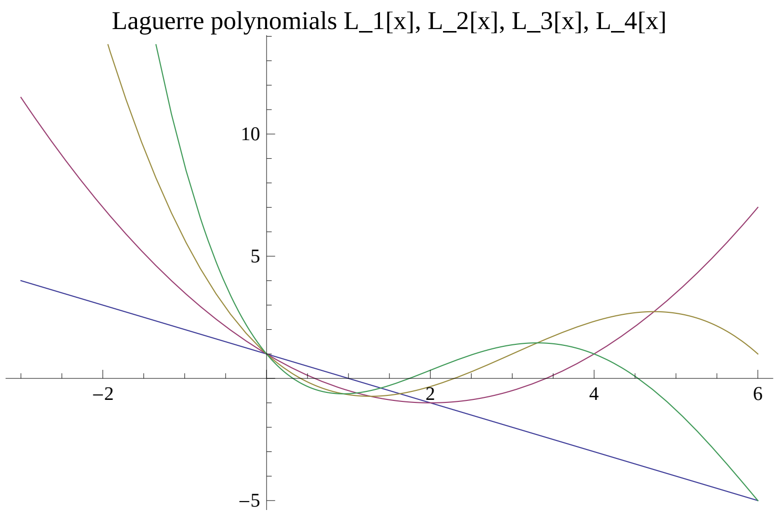

Figure 3: The Laguerre polynomials $L_1(x)$, $L_2(x)$, $L_3(x)$ and $L_4(x)$, evaluated on the real axis, highlighting the lack of parity about the origin.

Now we regurgitate a handful of standard results for the Laguerre polynomials. The first are the recurrence relations:

$$\begin{aligned}(n+1)L_{n+1}(x) &= (2n+1-x)L_n(x) - nL_{n-1}(x) \quad , \\ x\,L_n'(x) &= nL_n(x) - nL_{n-1}(x) \quad .\end{aligned} \tag{35}$$

Then we have the orthogonality relation

$$\int_0^\infty e^{-x} L_m(x)\, L_n(x)\, dx \;=\; \delta_{m,n} \quad . \tag{36}$$

This follows routinely from **Sturm-Louiville theory**, to be studied in due course, and defines the basis for computing quadrature integrations for the case of quasi-exponential integrands.

3.1 Associated Laguerre Polynomials

• As with other classes of orthogonal polynomials, we can extend to **associated Laguerre polynomials**, defined via

$$L_n^k(x) \;=\; (-1)^k \frac{d^k}{dx^k} L_{n+k}(x) \;=\; \sum_{s=0}^{n} \frac{(-1)^s (n+k)!\, x^s}{(n-s)!\,(s+k)!\,s!} \quad . \tag{37}$$

The generating function is

$$g(x,\, z) \;=\; \frac{e^{-xz/(1-z)}}{(1-z)^{k+1}} \;=\; \sum_{n=0}^{\infty} L_n^k(x)\, z^n \quad , \quad |z| \;<\; 1 \quad , \tag{38}$$

the Rodrigues' representation is

$$L_n^k(x) \;=\; \frac{e^x x^{-k}}{n!} \frac{d^n}{dx^n} \bigl(x^{n+k} e^{-x} \bigr) \quad , \tag{39}$$

and the associated Laguerre polynomials obey the ODE

$$x \frac{d^2 y}{dx^2} + (k+1-x) \frac{dy}{dx} + n\, y \;=\; 0 \quad . \tag{40}$$

Their orthogonality relation is

$$\int_0^\infty e^{-x} x^k\, L_m^k(x)\, L_n^k(x)\, dx \;=\; \frac{(n+k)!}{n!}\, \delta_{m,n} \quad . \tag{41}$$

• One of the most important applications of associated Laguerre functions is in the solution of the Schrödinger equation for the hydrogen atom, capturing the radial portion after separation of variables extracts the spherical harmonic component.

4 Hypergeometric Functions

The classes of special functions we have discussed so far can mostly be categorized as special cases of the broader class of functions known as **hypergeometric functions**, which satisfy Gauss' hypergeometric ODE

A&W Sec. 13.4

$$x(1-x)\,\frac{d^2y}{dx^2} + [c-(a+b+1)x]\,\frac{dy}{dx} - ab\,y \;=\; 0 \quad . \tag{42}$$

The solution that is bounded as $z \to 0$ is

$${}^2F^1(a,\,b,\,c;\,x) \;=\; 1 + \frac{ab}{c}\,\frac{x}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\,\frac{x^2}{2!} + \dots \tag{43}$$

for c not equal to zero or a negative integer.

- Functions that are related to hypergeometric functions are Legendre, Chebyshev, Gegenbauer and incomplete Beta functions.

There are also the **confluent hypergeometric functions**, which satisfy

A&W Sec. 13.5

$$x\,\frac{d^2y}{dx^2} + [c-x]\,\frac{dy}{dx} - a\,y \;=\; 0 \quad . \tag{44}$$

This ODE can be obtained from the hypergeometric one by merging two of its singularities.

- Functions that are related to confluent hypergeometric functions are Bessel, error, incomplete Gamma, Laguerre and Hermite functions.

12. PARTIAL DIFFERENTIAL EQUATIONS

Matthew Baring — Lecture Notes for PHYS 516, Fall 2022

1 Characterization of PDEs

• Since many problems in physics encapsulate linear, second order partial differential equations (PDEs), these will form our focus in this chapter. Examples abound in mechanics, fluid flow, diffusion, electrodynamics and quantum mechanics. Non-linear equations such as encountered in the theory of solitons, shock waves and general relativity, will not be explored. **A&W Sec. 9.1**

• The general form of the 2nd order, linear PDE is

$$\mathcal{A}\,\frac{\partial^2\psi}{\partial x^2} + 2\mathcal{B}\,\frac{\partial^2\psi}{\partial x\,\partial y} + \mathcal{C}\,\frac{\partial^2\psi}{\partial y^2} \;=\; f\left(x,\, y,\, \frac{\partial\psi}{\partial x},\, \frac{\partial\psi}{\partial x}\right) \quad . \tag{1}$$

Familiar examples include:

$$\begin{aligned}
\text{Laplace's equation}: &\quad \nabla^2\psi \;=\; 0 \quad , \\
\text{Wave equation}: &\quad \nabla^2\psi - \frac{1}{c^2}\,\frac{\partial^2\psi}{\partial t^2} \;=\; 0 \quad , \\
\text{Diffusion equation}: &\quad \nabla^2\psi - \frac{1}{\kappa}\,\frac{\partial\psi}{\partial t} \;=\; 0 \quad , \\
\text{Helmholtz equation}: &\quad \nabla^2\psi + k^2\,\psi \;=\; 0 \quad , \\
\text{Schrödinger equation}: &\quad -\frac{\hbar^2}{2m}\,\nabla^2\psi + V(\vec{x})\,\psi - i\hbar\,\frac{\partial\psi}{\partial t} \;=\; 0 \quad .
\end{aligned} \tag{2}$$

Observe that these are all **homogeneous** because $f = 0$: if ψ is a solution, then so is any multiple of ψ.

• An **inhomogenous** form for the PDE results if a **force** or **source term** is added to the RHS of these equations.

∗ e.g. The inhomogenous form of Laplace's equation is known as **Poisson's equation**.

• Observe that if $\psi \sim e^{\pm i\omega t}$, then the wave equation reduces to the Helmholtz equation with $k = \omega/c$, and if $\psi \sim e^{-\gamma t}$, then the diffusion equation reduces to the Helmholtz equation with $k^2 = \gamma/\kappa$.

• Even a homogeneous PDE can be complicated by the **boundary conditions** that enable its integration. The combined information is known as a **boundary value problem** (BVP). A homogeneous BVP requires not only a homogeneous PDE, but also homogeneous boundary conditions.

A unique solution requires sufficient boundary information but not too much, on a *boundary curve or surface*. The right level is determined by the type of equation. There are three standard types of boundary/initial conditions:

- **Dirichlet**: ψ is specified on the boundary;
- **Neumann**: $(\nabla\psi)_n$ is specified on the boundary;
- **Cauchy**: both ψ and $(\nabla\psi)_n$ are specified on the boundary.

Note that the subscript n denotes the direction *normal* to the boundary; this is required so as to propagate information into the region of interest.