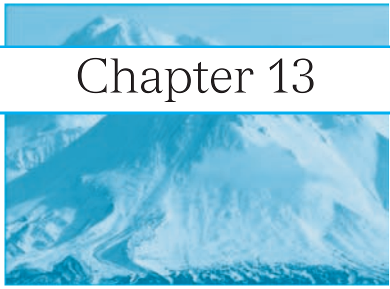


Chapter 13

Hermite and Laguerre Polynomials

In this chapter we study two sets of orthogonal polynomials, Hermite and Laguerre polynomials. These sets are less common in mathematical physics than the Legendre and Bessel functions of Chapters 11 and 12, but Hermite polynomials occur in solutions of the simple harmonic oscillator of quantum mechanics and Laguerre polynomials in wave functions of the hydrogen atom.

Because the general mathematical techniques are similar to those of the preceding two chapters, the development of these functions is only outlined. Some detailed proofs, along the lines of Chapters 11 and 12, are left to the reader. We start with Hermite polynomials.

13.1 Hermite Polynomials

Quantum Mechanical Simple Harmonic Oscillator

For the physicist, Hermite polynomials are synonymous with the one-dimensional (i.e., simple) harmonic oscillator of quantum mechanics. For a potential energy

$$V = \frac{1}{2}Kz^2 = \frac{1}{2}m\omega^2 z^2, \qquad \text{force} \quad F_z = -\partial V/\partial z = -Kz,$$

the Schrödinger equation of the quantum mechanical system is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\Psi(z) + \frac{1}{2}Kz^2\Psi(z) = E\Psi(z). \tag{13.1}$$

Our oscillating particle has mass m and total energy E. From quantum mechanics, we recall that for bound states the boundary conditions

$$\lim_{z\to\pm\infty}\Psi(z) = 0 \tag{13.2}$$

restrict the energy eigenvalue E to a discrete set $E_n = \lambda_n \hbar\omega$, where ω is the angular frequency of the corresponding classical oscillator. It is introduced by rescaling the coordinate z in favor of the dimensionless variable x and transforming the parameters as follows:

$$x = \alpha z \quad \text{with} \quad \alpha^4 \equiv \frac{mK}{\hbar^2} \equiv \frac{m^2\omega^2}{\hbar^2},$$
$$2\lambda_n \equiv \frac{2E_n}{\hbar}\left(\frac{m}{K}\right)^{1/2} = \frac{2E_n}{\hbar\omega}. \tag{13.3}$$

Eq.(13.1) becomes [with $\Psi(z) = \Psi(x/\alpha) = \psi(x)$] the ordinary differential equation (ODE)

$$\frac{d^2\psi_n(x)}{dx^2} + (2\lambda_n - x^2)\psi_n(x) = 0. \tag{13.4}$$

If we substitute $\psi_n(x) = e^{-x^2/2}H_n(x)$ into Eq. (13.4), we obtain the ODE

$$H_n'' - 2xH_n' + (2\lambda_n - 1)H_n = 0 \tag{13.5}$$

of Exercise 8.5.6. A power series solution of Eq. (13.5) shows that $H_n(x)$ will behave as e^{x^2} for large x, unless $\lambda_n = n + 1/2,\ n = 0, 1, 2, \ldots$. Thus, $\psi_n(x)$ and $\Psi_n(z)$ will blow up at infinity, and it will be impossible for the wave function $\Psi(z)$ to satisfy the boundary conditions [Eq. (13.2)] unless

$$E_n = \lambda_n\hbar\omega = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2 \ldots \tag{13.6}$$

This is the key property of the harmonic oscillator spectrum. We see that the energy is quantized and that there is a minimum or zero point energy

$$E_{\min} = E_0 = \frac{1}{2}\hbar\omega.$$

This zero point energy is an aspect of the uncertainty principle, a genuine quantum phenomenon. Also, with $2\lambda_n - 1 = 2n$, Eq. (13.5) becomes Hermite's ODE and $H_n(x)$ are the Hermite polynomials. The solutions ψ_n (Fig. 13.1) of Eq. (13.4) are proportional to the Hermite polynomials[1] $H_n(x)$.

This is the differential equations approach, a standard quantum mechanical treatment. However, we shall prove these statements next employing the method of ladder operators.

Raising and Lowering Operators

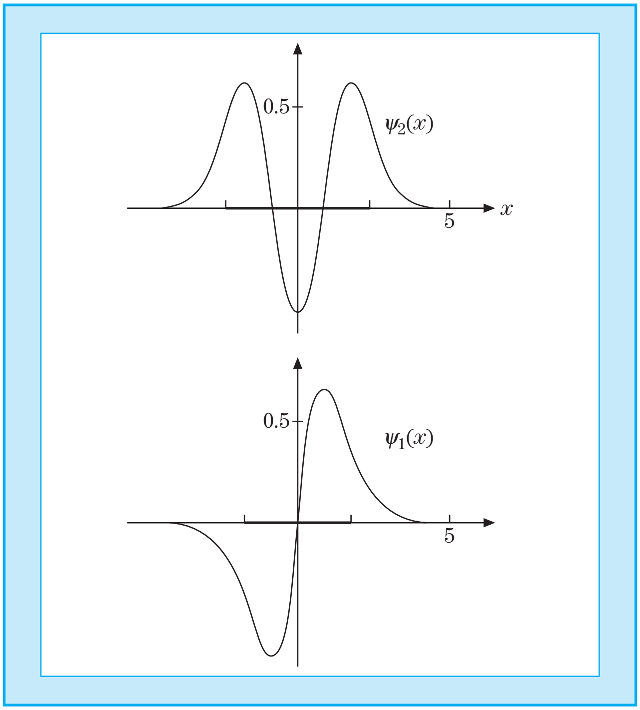
The following development is analogous to the use of the raising and lowering operators for angular momentum operators presented in Section 4.3. The key aspect of Eq. (13.4) is that its Hamiltonian

$$-2\mathcal{H} \equiv \frac{d^2}{dx^2} - x^2 = \left(\frac{d}{dx} - x\right)\left(\frac{d}{dx} + x\right) + \left[x, \frac{d}{dx}\right] \tag{13.7}$$

[1]Note the absence of a superscript, which distinguishes Hermite polynomials from the unrelated Hankel functions in Chapter 12.

Figure 13.1

Quantum Mechanical Oscillator Wave Functions. The Heavy Bar on the *x*-Axis Indicates the Allowed Range of the Classical Oscillator with the Same Total Energy



almost factorizes. Using naively $a^2 - b^2 = (a-b)(a+b)$, the basic commutator $[p_x, x] = \hbar/i$ of quantum mechanics [with momentum $p_x = (\hbar/i)d/dx$] enters as a correction in Eq. (13.7). [Because p_x is Hermitian, d/dx is anti-Hermitian, $(d/dx)^\dagger = -d/dx$.] This commutator can be evaluated as follows. Imagine the differential operator d/dx acts on a wave function $\psi(x)$ to the right, as in Eq. (13.4), so that

$$\frac{d}{dx}(x\psi) = x\frac{d}{dx}\psi + \psi \tag{13.8}$$

by the product rule. Dropping the wave function ψ from Eq. (13.8), we rewrite Eq. (13.8) as

$$\frac{d}{dx}x - x\frac{d}{dx} \equiv \left[\frac{d}{dx}, x\right] = 1, \tag{13.9}$$

a constant, and then verify Eq. (13.7) directly by expanding the product. The product form of Eq. (13.7), up to the constant commutator, suggests introducing the non-Hermitian operators

$$\hat{a}^\dagger \equiv \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right), \qquad \hat{a} \equiv \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right), \tag{13.10}$$

with $(\hat{a})^\dagger = \hat{a}^\dagger$. They obey the commutation relations

$$[\hat{a}, \hat{a}^\dagger] = \left[\frac{d}{dx}, x\right] = 1, \qquad [\hat{a}, \hat{a}] = 0 = [\hat{a}^\dagger, \hat{a}^\dagger], \tag{13.11}$$

which are characteristic of these operators and straightforward to derive from Eq. (13.9) and

$$[d/dx, d/dx] = 0 = [x, x] \quad \text{and} \quad [x, d/dx] = -[d/dx, x].$$

Returning to Eq. (13.7) and using Eq. (13.10), we rewrite the Hamiltonian as

$$\mathcal{H} = \hat{a}^\dagger \hat{a} + \frac{1}{2} = \hat{a}^\dagger \hat{a} + \frac{1}{2}[\hat{a}, \hat{a}^\dagger] = \frac{1}{2}(\hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger) \tag{13.12}$$

and introduce the Hermitian **number operator** $N = \hat{a}^\dagger \hat{a}$ so that $\mathcal{H} = N + 1/2$. We also use the simpler notation $\psi_n = |n\rangle$ so that Eq. (13.4) becomes

$$\mathcal{H}|n\rangle = \lambda_n |n\rangle.$$

Now we prove the key property that N has nonnegative integer eigenvalues

$$N|n\rangle = \left(\lambda_n - \frac{1}{2}\right)|n\rangle = n|n\rangle, \quad n = 0, 1, 2, \ldots, \tag{13.13}$$

that is, $\lambda_n = n + 1/2$. From

$$|\hat{a}|n\rangle|^2 = \langle n|\hat{a}^\dagger \hat{a}|n\rangle = \left(\lambda_n - \frac{1}{2}\right) \geq 0, \tag{13.14}$$

we see that N has nonnegative eigenvalues.

We now show that the commutation relations

$$[N, \hat{a}^\dagger] = \hat{a}^\dagger, \qquad [N, \hat{a}] = -\hat{a}, \tag{13.15}$$

which follow from Eq. (13.11), characterize N as the number operator that counts the oscillator quanta in the eigenstate $|n\rangle$. To this end, we determine the eigenvalue of N for the states $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$. Using $\hat{a}\hat{a}^\dagger = N + 1$, we see that

$$N(\hat{a}^\dagger|n\rangle) = \hat{a}^\dagger(N+1)|n\rangle = \left(\lambda_n + \frac{1}{2}\right)\hat{a}^\dagger|n\rangle = (n+1)\hat{a}^\dagger|n\rangle, \tag{13.16}$$

$$N(\hat{a}|n\rangle) = (\hat{a}\hat{a}^\dagger - 1)\hat{a}|n\rangle = \hat{a}(N-1)|n\rangle = \left(\lambda_n - \frac{1}{2}\right)\hat{a}|n\rangle$$
$$= (n-1)\hat{a}|n\rangle.$$

In other words, N acting on $\hat{a}^\dagger|n\rangle$ shows that $\hat{a}^\dagger$ has raised the eigenvalue n of $|n\rangle$ by one unit; hence its name **raising or creation operator**. Applying $\hat{a}^\dagger$ repeatedly, we can reach all higher excitations. There is no upper limit to the sequence of eigenvalues. Similarly, $\hat{a}$ lowers the eigenvalue n by one unit; hence, it is a **lowering or annihilation operator**. Therefore,

$$\hat{a}^\dagger|n\rangle \sim |n+1\rangle, \qquad \hat{a}|n\rangle \sim |n-1\rangle. \tag{13.17}$$

Applying $\hat{a}$ repeatedly, we can reach the lowest or ground state $|0\rangle$ with eigenvalue λ_0. We cannot step lower because $\lambda_0 \geq 1/2$. Therefore, $\hat{a}|0\rangle \equiv 0$, suggesting we construct $\psi_0 = |0\rangle$ from the (factored) **first-order** ODE

$$\sqrt{2}\hat{a}\psi_0 = \left(\frac{d}{dx} + x\right)\psi_0 = 0. \tag{13.18}$$

Integrating

$$\frac{\psi_0'}{\psi_0} = -x, \tag{13.19}$$

we obtain

$$\ln \psi_0 = -\frac{1}{2}x^2 + \ln c_0, \tag{13.20}$$

where c_0 is an integration constant. The solution

$$\psi_0(x) = c_0 e^{-x^2/2} \tag{13.21}$$

can be normalized, with $c_0 = \pi^{-1/4}$ using the error integral. Substituting ψ_0 into Eq. (13.4) we find

$$\mathcal{H}|0\rangle = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|0\rangle = \frac{1}{2}|0\rangle \tag{13.22}$$

so that its energy eigenvalue is $\lambda_0 = 1/2$ and its number eigenvalue is $n = 0$, confirming the notation $|0\rangle$. Applying $\hat{a}^\dagger$ repeatedly to $\psi_0 = |0\rangle$, all other eigenvalues are confirmed to be $\lambda_n = n + 1/2$, proving Eq. (13.13). The normalizations in Eq. (13.17) follow from Eqs. (13.14), (13.16), and

$$|\hat{a}^\dagger|n\rangle|^2 = \langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|\hat{a}^\dagger\hat{a} + 1|n\rangle = n + 1, \tag{13.23}$$

showing

$$\sqrt{n+1}|n+1\rangle = \hat{a}^\dagger|n\rangle, \qquad \sqrt{n}|n-1\rangle = \hat{a}|n\rangle. \tag{13.24}$$

Thus, the excited-state wave functions, ψ_1, ψ_2, and so on, are generated by the raising operator

$$|1\rangle = \hat{a}^\dagger|0\rangle = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)\psi_0(x) = \frac{x\sqrt{2}}{\pi^{1/4}}e^{-x^2/2}, \tag{13.25}$$

yielding [and leading to Eq. (13.5)]

$$\psi_n(x) = N_n H_n(x) e^{-x^2/2}, \qquad N_n = \pi^{-1/4}(2^n n!)^{-1/2}, \tag{13.26}$$

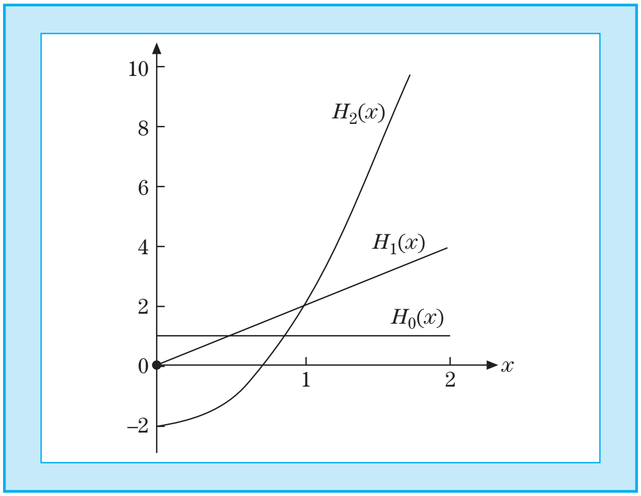
where H_n are the Hermite polynomials (Fig. 13.2).

Biographical Data

Hermite, Charles. Hermite, a French mathematician, was born in Dieuze in 1822 and died in Paris in 1902. His most famous result is the first proof that e is a transcendental number; that is, e is not the root of any polynomial with integer coefficients. He also contributed to elliptic and modular functions. Having been recognized slowly, he became a professor at the Sorbonne in 1870.

Figure 13.2

Hermite Polynomials



Recurrence Relations and Generating Function

Now we can establish the recurrence relations

$$2xH_n(x) - H_n'(x) = H_{n+1}(x), \qquad H_n'(x) = 2nH_{n-1}(x), \tag{13.27}$$

from which

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{13.28}$$

follows by adding them. To prove Eq. (13.27), we apply

$$x - \frac{d}{dx} = -e^{x^2/2}\frac{d}{dx}e^{-x^2/2} \tag{13.29}$$

to $\psi_n(x)$ of Eq. (13.26) and recall Eq. (13.24) to find

$$N_{n+1}H_{n+1}e^{-x^2/2} = -\frac{N_n}{\sqrt{2(n+1)}}e^{-x^2/2}(-2xH_n + H_n'), \tag{13.30}$$

that is, the first part of Eq. (13.27). Using $x + d/dx$ instead, we get the second half of Eq. (13.27).

EXAMPLE 13.1.1

The First Few Hermite Polynomials We expect the first Hermite polynomial to be a constant, $H_0(x) = 1$, being normalized. Then $n = 0$ in the recursion relation [Eq. (13.28)] yields $H_1 = 2xH_0 = 2x$; $n = 1$ implies $H_2 = 2xH_1 - 2H_0 = 4x^2 - 2$, and $n = 2$ implies

$$H_3(x) = 2xH_2(x) - 4H_1(x) = 2x(4x^2 - 2) - 8x = 8x^3 - 12x.$$

Comparing with Eq. (13.27) for $n = 0, 1, 2$, we verify that our results are consistent: $2xH_0 - H_0' = H_1 = 2x \cdot 1 - 0$, etc. For convenient reference, the first several Hermite polynomials are listed in Table 13.1. ■

Table 13.1

Hermite Polynomials

$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_3(x) = 8x^3 - 12x$
$H_4(x) = 16x^4 - 48x^2 + 12$
$H_5(x) = 32x^5 - 160x^3 + 120x$
$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120$

The Hermite polynomials $H_n(x)$ may be summed to yield the **generating function**

$$g(x, t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}, \tag{13.31}$$

which we derive next from the recursion relation [Eq. (13.28)]:

$$0 \equiv \sum_{n=1}^{\infty} \frac{t^n}{n!}(H_{n+1} - 2xH_n + 2nH_{n-1}) = \frac{\partial g}{\partial t} - 2xg + 2tg. \tag{13.32}$$

Integrating this ODE in t by separating the variables t and g, we get

$$\frac{1}{g}\frac{\partial g}{\partial t} = 2(x - t), \tag{13.33}$$

which yields

$$\ln g = 2xt - t^2 + \ln c, \qquad g(x, t) = e^{-t^2+2xt}c(x), \tag{13.34}$$

where c is an integration constant that may depend on the parameter x. Direct expansion of the exponential in Eq. (13.34) gives $H_0(x) = 1$ and $H_1(x) = 2x$ along with $c(x) \equiv 1$.

EXAMPLE 13.1.2

Special Values Special values of the Hermite polynomials follow from the generating function for $x = 0$; that is,

$$g(x = 0, t) = e^{-t^2} = \sum_{n=0}^{\infty} H_n(0)\frac{t^n}{n!} = \sum_{n=0}^{\infty}(-1)^n\frac{t^{2n}}{n!}.$$

A comparison of coefficients of these power series yields

$$H_{2n}(0) = (-1)^n\frac{(2n)!}{n!}, \qquad H_{2n+1}(0) = 0. \tag{13.35}$$

■

EXAMPLE 13.1.3

Parity Similarly, we obtain from the generating function identity

$$g(-x, t) = e^{-t^2-2tx} = g(x, -t) \tag{13.36}$$

the power series identity

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

which implies the important **parity relation**

$$H_n(x) = (-1)^n H_n(-x). \tag{13.37}$$

In quantum mechanical problems, particularly in molecular spectrosopy, a number of integrals of the form

$$\int_{-\infty}^{\infty} x^r e^{-x^2} H_n(x) H_m(x) dx$$

are needed. Examples for $r = 1$ and $r = 2$ (with $n = m$) are included in the exercises at the end of this section. Many other examples are contained in Wilson *et al.*[2] The oscillator potential has also been employed extensively in calculations of nuclear structure (nuclear shell model) and quark models of hadrons.

There is a second independent solution to Eq. (13.4). This Hermite function is an infinite series (Sections 8.5 and 8.6) and of no physical interest yet.

Alternate Representations

Differentiation of the generating function[3] n times with respect to t and then setting t equal to zero yields

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{13.38}$$

This gives us a Rodrigues representation of $H_n(x)$. A second representation may be obtained by using the calculus of residues (Chapter 7). If we multiply Eq. (13.31) by t^{-m-1} and integrate around the origin, only the term with $H_m(x)$ will survive:

$$H_m(x) = \frac{m!}{2\pi i} \oint t^{-m-1} e^{-t^2+2tx} dt. \tag{13.39}$$

Also, from Eq. (13.31) we may write our Hermite polynomial $H_n(x)$ in series form:

$$\begin{aligned} H_n(x) &= (2x)^n - \frac{2n!}{(n-2)!2!}(2x)^{n-2} + \frac{4n!}{(n-4)!4!}(2x)^{n-4} 1 \cdot 3 \cdots \\ &= \sum_{s=0}^{[n/2]} (-2)^s (2x)^{n-2s} \binom{n}{2s} 1 \cdot 3 \cdot 5 \cdots (2s-1) \\ &= \sum_{s=0}^{[n/2]} (-1)^s (2x)^{n-2s} \frac{n!}{(n-2s)!s!}. \end{aligned} \tag{13.40}$$

This series terminates for integral n and yields our Hermite polynomial.

[2]Wilson, E. B., Jr., Decius, J. C., and Cross, P. C. (1955). *Molecular Vibrations*. McGraw-Hill, New York. Reprinted, Dover, New York (1980).

[3]Rewrite the generating function as $g(x, t) = e^{x^2} e^{-(t-x)^2}$. Note that

$$\frac{\partial}{\partial t} e^{-(t-x)^2} = -\frac{\partial}{\partial x} e^{-(t-x)^2}.$$

EXAMPLE 13.1.4

The Lowest Hermite Polynomials For $n = 0$, we find from the series, Eq. (13.40), $H_0(x) = (-1)^0(2x)^0 \frac{0!}{0!0!} = 1$; for $n = 1$, $H_1(x) = (-1)^0(2x)^1 \frac{1!}{1!0!} = 2x$; and for $n = 2$, the $s = 0$ and $s = 1$ terms in Eq. (13.40) give

$$H_2(x) = (-1)^0(2x)^2 \frac{2!}{2!0!} - (2x)^0 \frac{2!}{0!1!} = 4x^2 - 2,$$

etc. ■

Orthogonality

The recurrence relations [Eqs. (13.27) and (13.28)] lead to the second-order ODE

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0, \tag{13.41}$$

which is clearly **not** self-adjoint.

To put Eq. (13.41) in self-adjoint form, we multiply by $\exp(-x^2)$ (Exercise 9.1.2). This leads to the orthogonality integral

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}dx = 0, \quad m \neq n, \tag{13.42}$$

with the weighting function $\exp(-x^2)$ a consequence of putting the differential equation into self-adjoint form. The interval $(-\infty, \infty)$ is dictated by the boundary conditions of the harmonic oscillator, which are consistent with the Hermitian operator boundary conditions (Section 9.1). It is sometimes convenient to absorb the weighting function into the Hermite polynomials. We may define

$$\varphi_n(x) = e^{-x^2/2}H_n(x), \tag{13.43}$$

with $\varphi_n(x)$ no longer a polynomial.

Substituting $H_n = e^{x^2/2}\varphi_n$ into Eq. (13.41) yields the quantum mechanical harmonic oscillator ODE [Eq. (13.4)] for $\varphi_n(x)$:

$$\varphi_n''(x) + (2n + 1 - x^2)\varphi_n(x) = 0, \tag{13.44}$$

which is self-adjoint. Thus, its solutions $\varphi_n(x)$ are orthogonal for the interval $(-\infty < x < \infty)$ with a unit weighting function. The problem of normalizing these functions remains. Proceeding as in Section 11.3, we multiply Eq. (13.31) by itself and then by e^{-x^2}. This yields

$$e^{-x^2}e^{-s^2+2sx}e^{-t^2+2tx} = \sum_{m,n=0}^{\infty} e^{-x^2}H_m(x)H_n(x)\frac{s^m t^n}{m!n!}. \tag{13.45}$$

When we integrate over x from $-\infty$ to $+\infty$ the cross terms of the double sum drop out because of the orthogonality property[4]

$$\sum_{n=0}^{\infty}\frac{(st)^n}{n!n!}\int_{-\infty}^{\infty}e^{-x^2}[H_n(x)]^2dx = \int_{-\infty}^{\infty}e^{-x^2-s^2+2sx-t^2+2tx}\,dx$$

$$= \int_{-\infty}^{\infty}e^{-(x-s-t)^2}e^{2st}\,dx = \pi^{1/2}e^{2st} = \pi^{1/2}\sum_{n=0}^{\infty}\frac{2^n(st)^n}{n!}. \qquad (13.46)$$

By equating coefficients of like powers of st, we obtain

$$\int_{-\infty}^{\infty}e^{-x^2}[H_n(x)]^2\,dx = 2^n\pi^{1/2}n! \qquad (13.47)$$

which yields the normalization N_n in Eq. (13.26).

SUMMARY

Hermite polynomials are solutions of the simple harmonic oscillator of quantum mechanics. Their properties directly follow from writing their ODE as a product of creation and annihilation operators and the Sturm–Liouville theory of their ODE.

EXERCISES

13.1.1 In developing the properties of the Hermite polynomials, start at a number of different points, such as
(1) Hermite's ODE, Eqs. (13.5) and (13.44);
(2) Rodrigues's formula, Eq. (13.38);
(3) Integral representation, Eq. (13.39);
(4) Generating function, Eq. (13.31); and
(5) Gram–Schmidt construction of a complete set of orthogonal polynomials over $(-\infty, \infty)$ with a weighting factor of $\exp(-x^2)$, Section 9.3.

Outline how you can go from any one of these starting points to all the other points.

13.1.2 From the generating function, show that

$$H_n(x) = \sum_{s=0}^{[n/2]}(-1)^s\frac{n!}{(n-2s)!s!}(2x)^{n-2s}.$$

13.1.3 From the generating function, derive the recurrence relations

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x),$$

$$H_n'(x) = 2nH_{n-1}(x).$$

[4] The cross terms ($m \neq n$) may be left in, if desired. Then, when the coefficients of $s^{\alpha}t^{\beta}$ are equated, the orthogonality will be apparent.

13.1.4 Prove that

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

Hint. Check out the first couple of examples and then use mathematical induction.

13.1.5 Prove that

$$|H_n(x)| \le |H_n(ix)|.$$

13.1.6 Rewrite the series form of $H_n(x)$ [Eq. (13.40)] as an **ascending** power series.

ANS.
$$H_{2n}(x) = (-1)^n \sum_{s=0}^{n} (-1)^{2s} (2x)^{2s} \frac{(2n)!}{(2s)!(n-s)!},$$
$$H_{2n+1}(x) = (-1)^n \sum_{s=0}^{n} (-1)^{s} (2x)^{2s+1} \frac{(2n+1)!}{(2s+1)!(n-s)!}.$$

13.1.7 (a) Expand x^{2r} in a series of even-order Hermite polynomials.
(b) Expand x^{2r+1} in a series of odd-order Hermite polynomials.

ANS. (a) $$x^{2r} = \frac{(2r)!}{2^{2r}} \sum_{n=0}^{r} \frac{H_{2n}(x)}{(2n)!(r-n)!},$$
(b) $$x^{2r+1} = \frac{(2r+1)!}{2^{2r+1}} \sum_{n=0}^{r} \frac{H_{2n+1}(x)}{(2n+1)!(r-n)!}, \qquad r = 0, 1, 2, \dots .$$

Hint. Use a Rodrigues representation of $H_{2n}(x)$ and integrate by parts.

13.1.8 Show that

(a) $$\int_{-\infty}^{\infty} H_n(x) \exp[-x^2/2]dx \begin{cases} 2\pi n!/(n/2)!, & n \text{ even} \\ 0, & n \text{ odd.} \end{cases}$$

(b) $$\int_{-\infty}^{\infty} x H_n(x) \exp[-x^2/2]dx \begin{cases} 0, & n \text{ even} \\ 2\pi \dfrac{(n+1)!}{((n+1)/2)!}, & n \text{ odd.} \end{cases}$$

13.1.9 Show that

$$\int_{-\infty}^{\infty} x^m e^{-x^2} H_n(x)\, dx = 0 \quad \text{for } m \text{ an integer,} \quad 0 \le m \le n-1.$$

13.1.10 The transition probability between two oscillator states, m and n, depends on

$$\int_{-\infty}^{\infty} x e^{-x^2} H_n(x) H_m(x) dx.$$

Show that this integral equals $\pi^{1/2}2^{n-1}n!\delta_{m,n-1} + \pi^{1/2}2^n(n+1)!\delta_{m,n+1}$. This result shows that such transitions can occur only between states of adjacent energy levels, $m = n \pm 1$.
Hint. Multiply the generating function [Eq. (13.31)] by itself using two different sets of variables (x, s) and (x, t). Alternatively, the factor x may be eliminated by a recurrence relation in Eq. (13.27).

13.1.11 Show that

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x)H_n(x)dx = \pi^{1/2}2^n n!\left(n + \frac{1}{2}\right).$$

This integral occurs in the calculation of the mean square displacement of our quantum oscillator.
Hint. Use a recurrence relation Eq. (13.27) and the orthogonality integral.

13.1.12 Evaluate

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x)H_m(x)dx$$

in terms of n and m and appropriate Kronecker delta functions.

ANS. $2^{n-1}\pi^{1/2}(2n+1)n!\delta_{n,m} + 2^n\pi^{1/2}(n+2)!\delta_{n+2,m} + 2^{n-2}\pi^{1/2}n!\delta_{n-2,m}$.

13.1.13 Show that

$$\int_{-\infty}^{\infty} x^r e^{-x^2} H_n(x)H_{n+p}(x)dx = \begin{cases} 0, & p > r \\ 2^n\pi^{1/2}(n+r)!, & p = r. \end{cases}$$

n, p, and r are nonnegative integers.
Hint. Use a recurrence relation, Eq. (13.27), p times.

13.1.14 (a) Using the Cauchy integral formula, develop an integral representation of $H_n(x)$ based on Eq. (13.31) with the contour enclosing the point $z = -x$.

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

(b) Show by direct substitution that this result satisfies the Hermite equation.

13.1.15 (a) Verify the operator identity

$$x - \frac{d}{dx} = -\exp[x^2/2]\frac{d}{dx}\exp[-x^2/2].$$

(b) The normalized simple harmonic oscillator wave function is

$$\psi_n(x) = (\pi^{1/2}2^n n!)^{-1/2}\exp[-x^2/2]H_n(x).$$

Show that this may be written as

$$\psi_n(x) = (\pi^{1/2}2^n n!)^{-1/2}\left(x - \frac{d}{dx}\right)^n \exp[-x^2/2].$$

Note. This corresponds to an n-fold application of the raising operator.

13.1.16 Write a program that will generate the coefficients a_s in the polynomial form of the Hermite polynomial, $H_n(x) = \sum_{s=0}^{n} a_s x^s$.

13.1.17 A function $f(x)$ is expanded in a Hermite series:

$$f(x) = \sum_{n=0}^{\infty} a_n H_n(x).$$

From the orthogonality and normalization of the Hermite polynomials the coefficient a_n is given by

$$a_n = \frac{1}{2^n \pi^{1/2} n!}\int_{-\infty}^{\infty} f(x)H_n(x)e^{-x^2}\, dx.$$

For $f(x) = x^8$, determine the Hermite coefficients a_n by the Gauss–Hermite quadrature. Check your coefficients against AMS-55, Table 22.12.

13.1.18 Calculate and tabulate the normalized linear oscillator wave functions

$$\psi_n(x) = 2^{-n/2}\pi^{-1/4}(n!)^{-1/2}H_n(x)\exp(-x^2/2) \quad \text{for } x = 0.0 \text{ to } 5.0$$

in steps of 0.1 and $n = 0, 1, \ldots, 5$. Plot your results.

13.1.19 Consider two harmonic oscillators that are interacting through a potential $V = cx_1x_2$, $|c| < m\omega^2$, where x_1 and x_2 are the oscillator variables, m is the common mass, and ω's the common oscillator frequency. Find the exact energy levels. If $c > m\omega^2$, sketch the potential surface $V(x_1, x_2)$ and explain why there is no ground state in this case.

13.2 Laguerre Functions

Differential Equation—Laguerre Polynomials

If we start with the appropriate generating function, it is possible to develop the Laguerre polynomials in analogy with the Hermite polynomials. Alternatively, a series solution may be developed by the methods of Section 8.5. Instead, to illustrate a different technique, let us start with Laguerre's ODE and obtain a solution in the form of a contour integral. From this integral representation a generating function will be derived. We want to use Laguerre's ODE

$$xy''(x) + (1 - x)y'(x) + ny(x) = 0 \tag{13.48}$$

over the interval $0 < x < \infty$ and for integer $n \geq 0$, which is motivated by the radial ODE of Schrödinger's partial differential equation for the hydrogen atom.

We shall attempt to represent y, or rather y_n since y will depend on n, by the contour integral

$$y_n(x) = \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)z^{n+1}}dz, \qquad (13.49)$$

and demonstrate that it satisfies Laguerre's ODE. The contour includes the origin but does not enclose the point $z = 1$. By differentiating the exponential in Eq. (13.49), we obtain

$$y_n'(x) = -\frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)^2 z^{n}}dz, \qquad (13.50)$$

$$y_n''(x) = \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)^3 z^{n-1}}dz. \qquad (13.51)$$

Substituting into the left-hand side of Eq (13.48), we obtain

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

which is equal to

$$-\frac{1}{2\pi i}\oint \frac{d}{dz}\left[\frac{e^{-xz/(1-z)}}{(1-z)z^n}\right]dz. \qquad (13.52)$$

If we integrate our perfect differential around a contour chosen so that the final value equals the initial value (Fig. 13.3), the integral will vanish, thus verifying that $y_n(x)$ [Eq. (13.49)] is a solution of Laguerre's equation. We also see how the coefficients of Laguerre's ODE [Eq. (13.48)] determine the exponent of the

Figure 13.3

Laguerre Function Contour

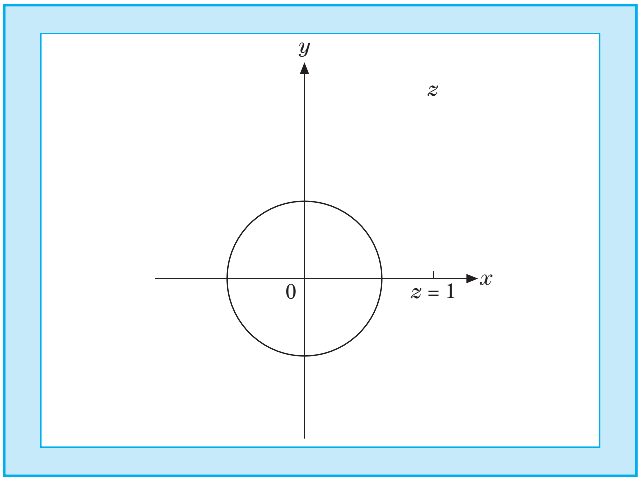
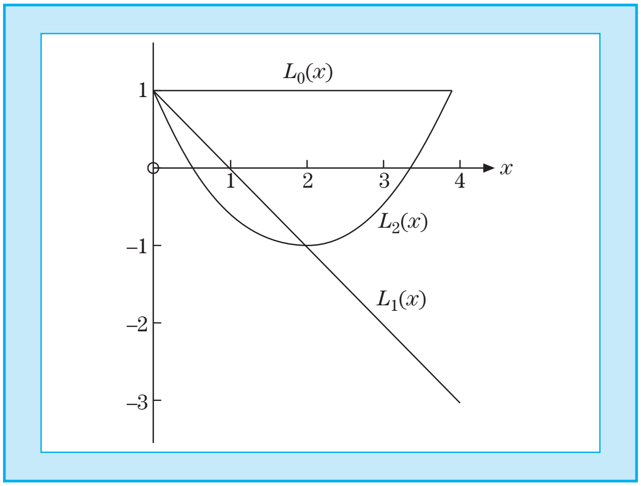


Figure 13.4

Laguerre Polynomials



generating function by comparing with Eq. (13.52), thus making Eq. (13.49) perhaps a bit less of a lucky guess.

It has become customary to define $L_n(x)$, the Laguerre polynomial (Fig. 13.4), by[5]

$$L_n(x) = \frac{1}{2\pi i}\oint \frac{e^{-xz/(1-z)}}{(1-z)z^{n+1}}\,dz. \tag{13.53}$$

This is exactly what we would obtain from the series

$$g(x, z) = \frac{e^{-xz/(1-z)}}{1-z} = \sum_{n=0}^{\infty} L_n(x) z^n, \quad |z| < 1 \tag{13.54}$$

if we multiplied it by z^{-n-1} and integrated around the origin. Applying the residue theorem (Section 7.2), only the z^{-1} term in the series survives. On this basis we identify $g(x, z)$ as the **generating function** for the Laguerre polynomials.

With the transformation

$$\frac{xz}{1-z} = s - x \quad \text{or} \quad z = \frac{s-x}{s}, \tag{13.55}$$

$$L_n(x) = \frac{e^x}{2\pi i}\oint \frac{s^n e^{-s}}{(s-x)^{n+1}}\,ds, \tag{13.56}$$

the new contour enclosing the point $s = x$ in the s-plane. By Cauchy's integral formula (for derivatives)

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x}) \quad (\text{integral } n), \tag{13.57}$$

[5]Other notations of $L_n(x)$ are in use. Here, the definitions of the Laguerre polynomial $L_n(x)$ and the associated Laguerre polynomial $L_n^k(x)$ agree with AMS-55 (Chapter 22).

giving Rodrigues's formula for Laguerre polynomials. From these representations of $L_n(x)$ we find the series form (for integral n),

$$L_n(x) = \frac{(-1)^n}{n!}\left[x^n - \frac{n^2}{1!}x^{n-1} + \frac{n^2(n-1)^2}{2!}x^{n-2} - \cdots + (-1)^n n!\right]$$
$$= \sum_{m=0}^{n} \frac{(-1)^m n! x^m}{(n-m)!m!m!} = \sum_{s=0}^{n} \frac{(-1)^{n-s} n! x^{n-s}}{(n-s)!(n-s)!s!}. \qquad (13.58)$$

EXAMPLE 13.2.1

Lowest Laguerre Polynomials For $n = 0$, Eq. (13.57) yields $L_0 = \frac{e^x}{0!}(x^0 e^{-x}) = 1$; for $n = 1$, we get $L_1 = e^x \frac{d}{dx}(xe^{-x}) = e^x(e^{-x} - xe^{-x}) = 1 - x$; and for $n = 2$,

$$L_2 = \frac{1}{2}e^x \frac{d^2}{dx^2}(x^2 e^{-x}) = \frac{1}{2}e^x \frac{d}{dx}(2xe^{-x} - x^2 e^{-x})$$
$$= \frac{1}{2}e^x(2 - 2x - 2x + x^2)e^{-x} = 1 - 2x + \frac{1}{2}x^2,$$

etc., the specific polynomials listed in Table 13.2 (Exercise 13.2.1). ■

Table 13.2

Laguerre Polynomials

$L_0(x) = 1$
$L_1(x) = -x + 1$
$2!L_2(x) = x^2 - 4x + 2$
$3!L_3(x) = -x^3 + 9x^2 - 18x + 6$
$4!L_4(x) = x^4 - 16x^3 + 72x^2 - 96x + 24$
$5!L_5(x) = -x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120$
$6!L_6(x) = x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720$

EXAMPLE 13.2.2

Recursion Relation Carrying out the innermost differentiation in Eq. (13.57), we find

$$L_n(x) = \frac{e^x}{n!}\frac{d^{n-1}}{dx^{n-1}}(nx^{n-1} - x^n)e^{-x} = L_{n-1}(x) - \frac{e^x}{n!}\frac{d^{n-1}}{dx^{n-1}}x^n e^{-x},$$

a formula from which we can derive the recursion $L'_n = L'_{n-1} - L_{n-1}$. To generate L_n from the last term in the previous equation, we multiply it by e^{-x} and differentiate it, getting

$$\frac{d}{dx}(e^{-x}L_n(x)) = \frac{d}{dx}(e^{-x}L_{n-1}(x)) - \frac{1}{n!}\frac{d^n}{dx^n}(x^n e^{-x}),$$

which can also be written as

$$e^{-x}(-L_n + L'_n + L_{n-1} - L'_{n-1}) = -\frac{1}{n!}\frac{d^n}{dx^n}(x^n e^{-x}).$$

Multiplying this result by e^x and using the definition [Eq. (13.57)] yields

$$L'_n(x) = L'_{n-1}(x) - L_{n-1}(x). \qquad (13.59)$$

■

By differentiating the generating function in Eq. (13.54) with respect to x we can rederive this recursion relation as follows:

$$(1-z)\frac{\partial g}{\partial x} = -\frac{z}{1-z}e^{-xz/(1-z)} = -zg(x, z).$$

Expanding this result according to the definition of the generating function, Eq. (13.54), yields

$$\sum_n L_n'(z^n - z^{n+1}) = \sum_{n=0}^{\infty}(L_n' - L_{n-1}')z^n = -\sum_{n=1}^{\infty} L_{n-1}z^n,$$

which implies the recursion relation [Eq. (13.59)].

By differentiating the generating function in Eq. (13.54) with respect to x and z, we obtain other recurrence relations

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x),$$
$$xL_n'(x) = nL_n(x) - nL_{n-1}(x). \tag{13.60}$$

Equation (13.60), modified to read

$$L_{n+1}(x) = 2L_n(x) - L_{n-1}(x) - [(1+x)L_n(x) - L_{n-1}(x)]/(n+1) \tag{13.61}$$

for reasons of economy and numerical stability, is used for computation of numerical values of $L_n(x)$. The computer starts with known numerical values of $L_0(x)$ and $L_1(x)$ (Table 13.2) and works up step by step. This is the same technique discussed for computing Legendre polynomials in Section 11.2.

EXAMPLE 13.2.3

Special Values From Eq. (13.54) for $x = 0$ and arbitrary z, we find

$$g(0, z) = \frac{1}{1-z} = \sum_{n=0}^{\infty} z^n = \sum_{n=0}^{\infty} L_n(0)z^n,$$

and, therefore, the special values

$$L_n(0) = 1, \tag{13.62}$$

by comparing coefficients of both power series. ■

As is seen from the form of the generating function, the form of Laguerre's ODE, or from Table 13.2, the Laguerre polynomials have neither odd nor even symmetry (parity).

The Laguerre ODE is not self-adjoint and the Laguerre polynomials, $L_n(x)$, do not by themselves form an orthogonal set. However, following the method of Section 9.1, if we multiply Eq. (13.48) by e^{-x} (Exercise 9.1.1) we obtain

$$\int_0^{\infty} e^{-x}L_m(x)L_n(x)dx = \delta_{mn}. \tag{13.63}$$

This orthogonality is a consequence of the Sturm–Liouville theory (Section 9.1). The normalization follows from the generating function. It is sometimes convenient to define orthogonal Laguerre functions (with unit weighting function) by

$$\varphi_n(x) = e^{-x/2} L_n(x). \tag{13.64}$$

EXAMPLE 13.2.4

Special Integrals Setting $z = 1/2$ in the generating function, Eq. (13.54), gives the relation

$$g\left(x, \frac{1}{2}\right) = 2e^{-x} = \sum_{n=0}^{\infty} L_n(x) 2^{-n}.$$

Multiplying by $e^{-x} L_m(x)$, integrating, and using orthogonality yields

$$2\int_0^{\infty} e^{-2x} L_m(x) dx = 2^{-m}.$$

Setting $z = -1/2, \ \pm 1/3$, etc., we can derive numerous other special integrals. ■

Our new orthonormal function $\varphi_n(x)$ satisfies the ODE

$$x\varphi_n''(x) + \varphi_n'(x) + \left(n + \frac{1}{2} - \frac{x}{4}\right)\varphi_n(x) = 0, \tag{13.65}$$

which is seen to have the (self-adjoint) Sturm–Liouville form. Note that it is the boundary conditions in the Sturm–Liouville theory that fix our interval as $(0 \le x < \infty)$.

Biographical Data

Laguerre, Edmond Nicolas. Laguerre, a French mathematician, was born in 1834 and died in Bar-le-Duc in 1886. He contributed to continued fractions and the theory of algebraic equations, and he was one of the founders of modern axiomatic geometry.

Associated Laguerre Polynomials

In many applications, particularly the hydrogen atom wave functions in quantum theory, we also need the associated Laguerre polynomials as in Example 13.2.5 defined by[6]

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x). \tag{13.66}$$

From the series form of $L_n(x)$,

$$\begin{aligned} L_0^k(x) &= 1 \\ L_1^k(x) &= -x + k + 1 \\ L_2^k(x) &= \frac{x^2}{2} - (k+2)x + \frac{(k+2)(k+1)}{2}. \end{aligned} \tag{13.67}$$

[6] Some authors use $\mathcal{L}_{n+k}^k(x) = (d^k/dx^k)[L_{n+k}(x)]$. Hence our $L_n^k(x) = (-1)^k \mathcal{L}_{n+k}^k(x)$.

In general,

$$L_n^k(x) = \sum_{m=0}^{n} (-1)^m \frac{(n+k)!}{(n-m)!(k+m)!m!} x^m, \quad k > -1. \tag{13.68}$$

A generating function may be developed by differentiating the Laguerre generating function k times. Adjusting the index to L_{n+k}, we obtain

$$\frac{e^{-xz/(1-z)}}{(1-z)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x) z^n, \quad |z| < 1. \tag{13.69}$$

From this, for $x = 0$, the binomial expansion yields

$$L_n^k(0) = \frac{(n+k)!}{n!k!}. \tag{13.70}$$

Recurrence relations can easily be derived from the generating function or by differentiating the Laguerre polynomial recurrence relations. Among the numerous possibilities are

$$(n+1)L_{n+1}^k(x) = (2n+k+1-x)L_n^k(x) - (n+k)L_{n-1}^k(x), \tag{13.71}$$

$$x\frac{dL_n^k(x)}{dx} = nL_n^k(x) - (n+k)L_{n-1}^k(x). \tag{13.72}$$

From these or from differentiating Laguerre's ODE k times, we have the associated Laguerre ODE

$$x\frac{d^2L_n^k(x)}{dx^2} + (k+1-x)\frac{dL_n^k(x)}{dx} + nL_n^k(x) = 0. \tag{13.73}$$

When associated Laguerre polynomials appear in a physical problem, it is usually because that physical problem involves the ODE [Eq. (13.73)].

A Rodrigues representation of the associated Laguerre polynomial is

$$L_n^k(x) = \frac{e^x x^{-k}}{n!} \frac{d^n}{dx^n}(e^{-x}x^{n+k}). \tag{13.74}$$

Note that all these formulas for $g(x)$ reduce to the corresponding expressions for $L_n(x)$, when $k = 0$.

The associated Laguerre equation [Eq. (13.73)] is not self-adjoint, but it can be put in self-adjoint form by multiplying by $e^{-x}x^k$, which becomes the weighting function (Section 9.1). We obtain

$$\int_0^{\infty} e^{-x}x^k L_n^k(x)L_m^k(x)dx = \frac{(n+k)!}{n!}\delta_{mn}, \tag{13.75}$$

which shows the same orthogonality interval $[0, \infty)$ as that for the Laguerre polynomials. However, with a new weighting function, we have a new set of orthogonal polynomials, the associated Laguerre polynomials.

By letting $\psi_n^k(x) = e^{x/2} x^{k/2} L_n^k(x)$, $\psi_n^k(x)$ satisfies the self-adjoint equation

$$x\frac{d^2\psi_n^k(x)}{dx^2} + \frac{d\psi_n^k(x)}{dx} + \left(-\frac{x}{4} + \frac{2n+k+1}{2} - \frac{k^2}{4x}\right)\psi_n^k(x) = 0. \qquad (13.76)$$

The $\psi_n^k(x)$ are sometimes called **Laguerre functions**. Equation (13.65) is the special case $k = 0$.

A further useful form is given by defining[7]

$$\Phi_n^k(x) = e^{-x/2} x^{(k+1)/2} L_n^k(x). \qquad (13.77)$$

Substitution into the associated Laguerre equation yields

$$\frac{d^2\Phi_n^k(x)}{dx^2} + \left(-\frac{1}{4} + \frac{2n+k+1}{2x} - \frac{k^2-1}{4x^2}\right)\Phi_n^k(x) = 0. \qquad (13.78)$$

The corresponding normalization integral is

$$\int_0^\infty e^{-x} x^{k+1} \left[L_n^k(x)\right]^2 \, dx = \frac{(n+k)!}{n!}(2n+k+1). \qquad (13.79)$$

Notice that the $\Phi_n^k(x)$ do **not** form an orthogonal set (except with x^{-1} as a weighting function) because of the x^{-1} in the term $(2n+k+1)/2x$.

EXAMPLE 13.2.5

The Hydrogen Atom The most important application of the Laguerre polynomials is in the solution of the Schrödinger equation for the hydrogen atom. This equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{Ze^2}{4\pi\epsilon_0 r}\psi = E\psi, \qquad (13.80)$$

where $Z = 1$ for hydrogen, 2 for singly ionized helium, and so on. Separating variables, we find that the angular dependence of ψ is on the spherical harmonics $Y_L^M(\theta, \varphi)$ (see Section 11.5). The radial part, $R(r)$, satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{Ze^2}{4\pi\epsilon_0 r}R + \frac{\hbar^2}{2m}\frac{L(L+1)}{r^2}R = ER. \qquad (13.81)$$

For bound states $R \to 0$ as $r \to \infty$, and R is finite at the origin, $r = 0$. These are the boundary conditions. We ignore the continuum states with positive energy. Only when the latter are included do the hydrogen wave functions form a complete set. By use of the abbreviations (resulting from rescaling r to the dimensionless radial variable ρ)

$$\rho = \beta r \quad \text{with} \quad \beta^2 = -\frac{8mE}{\hbar^2}, \qquad E < 0, \qquad \lambda = \frac{mZe^2}{2\pi\epsilon_0\beta\hbar^2}, \qquad (13.82)$$

[7]This corresponds to modifying the function ψ in Eq. (13.76) to eliminate the first derivative (compare Exercise 8.6.3).

Eq. (13.81) becomes

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\chi(\rho)}{d\rho}\right)+\left(\frac{\lambda}{\rho}-\frac{1}{4}-\frac{L(L+1)}{\rho^2}\right)\chi(\rho)=0, \tag{13.83}$$

where $\chi(\rho) = R(\rho/\beta)$. A comparison with Eq. (13.78) for $\Phi_n^k(x)$ shows that Eq. (13.83) is satisfied by

$$\chi(\rho) = e^{-\rho/2}\rho^L L_{\lambda-L-1}^{2L+1}(\rho), \tag{13.84}$$

in which k is replaced by $2L+1$ and n by $\lambda - L - 1$.

We must restrict the parameter λ by requiring it to be an integer n, $n = 1, 2, 3, \ldots$.[8] This is necessary because the Laguerre function of nonintegral n would diverge as $\rho^n e^\rho$, which is unacceptable for our physical problem with the boundary condition

$$\lim_{r\to\infty} R(r) = 0.$$

This restriction on λ, imposed by our boundary condition, has the effect of quantizing the energy

$$E_n = -\frac{Z^2 m}{2n^2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2. \tag{13.85}$$

The negative sign indicates that we are dealing here with bound states, as $E = 0$ corresponds to an electron that is just able to escape to infinity, where the Coulomb potential goes to zero. Using this result for E_n, we have

$$\beta = \frac{me^2}{2\pi\epsilon_0\hbar^2}\cdot\frac{Z}{n} = \frac{2Z}{na_0}, \qquad \rho = \frac{2Z}{na_0}r \tag{13.86}$$

with

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}, \qquad \text{the Bohr radius.}$$

Thus, the final normalized hydrogen wave function is written as

$$\psi_{nLM}(r,\theta,\varphi) = \left[\left(\frac{2Z}{na_0}\right)^3\frac{(n-L-1)!}{2n(n+L)!}\right]^{1/2} e^{-\beta r/2}(\beta r)^L L_{n-L-1}^{2L+1}(\beta r) Y_L^M(\theta,\varphi). \tag{13.87}$$

■

SUMMARY

Laguerre polynomials arise as solutions of the Coulomb potential in quantum mechanics. Separating the Schrödinger equation in spherical polar coordinates defines their radial ODE. The Sturm–Liouville theory of this ODE implies their properties.

[8] This is the conventional notation for λ. It is not the same n as the index n in $\Phi_n^k(x)$.

EXERCISES

13.2.1 Show with the aid of the Leibniz formula that the series expansion of $L_n(x)$ [Eq. (13.58)] follows from the Rodrigues representation [Eq. (13.57)].

13.2.2 (a) Using the explicit series form [Eq. (13.58)], show that

$$L'_n(0) = -n$$
$$L''_n(0) = \frac{1}{2}n(n-1).$$

(b) Repeat without using the explicit series form of $L_n(x)$.

13.2.3 From the generating function derive the Rodrigues representation

$$L_n^k(x) = \frac{e^x x^{-k}}{n!} \frac{d^n}{dx^n}(e^{-x}x^{n+k}).$$

13.2.4 Derive the normalization relation [Eq. (13.75)] for the associated Laguerre polynomials.

13.2.5 Expand x^r in a series of associated Laguerre polynomials $L_n^k(x)$, k fixed and n ranging from 0 to r (or to ∞ if r is not an integer).
Hint. The Rodrigues form of $L_n^k(x)$ will be useful.

$$\textit{ANS.} \quad x^r = (r+k)!r! \sum_{n=0}^{r} \frac{(-1)^n L_n^k(x)}{(n+k)!(r-n)!}, \qquad 0 \le x \le \infty.$$

13.2.6 Expand e^{-ax} in a series of associated Laguerre polynomials $L_n^k(x)$, k fixed and n ranging from 0 to ∞. Plot partial sums as a function of the upper limit $N = 1, 2, \ldots, 10$ to check the convergence.
(a) Evaluate directly the coefficients in your assumed expansion.
(b) Develop the desired expansion from the generating function.

$$\textit{ANS.} \quad e^{-ax} = \frac{1}{(1+a)^{1+k}} \sum_{n=0}^{\infty} \left(\frac{a}{1+a}\right)^n L_n^k(x), \qquad 0 \le x \le \infty.$$

13.2.7 Show that

$$\int_0^\infty e^{-x} x^{k+1} L_n^k(x) L_n^k(x)\, dx = \frac{(n+k)!}{n!}(2n+k+1).$$

Hint. Note that

$$xL_n^k = (2n+k+1)L_n^k - (n+k)L_{n-1}^k - (n+1)L_{n+1}^k.$$

13.2.8 Assume that a particular problem in quantum mechanics has led to the ODE

$$\frac{d^2y}{dx^2} - \left[\frac{k^2-1}{4x^2} - \frac{2n+k+1}{2x} + \frac{1}{4}\right] y = 0.$$

Write $y(x)$ as

$$y(x) = A(x)B(x)C(x)$$

with the requirements that

(a) $A(x)$ be a **negative** exponential giving the required asymptotic behavior of $y(x)$; and

(b) $B(x)$ be a **positive** power of x giving the behavior of $y(x)$ for $0 \le x \ll 1$.

Determine $A(x)$ and $B(x)$. Find the relation between $C(x)$ and the associated Laguerre polynomial.

$$\textit{ANS.} \quad A(x) = e^{-x/2}, \qquad B(x) = x^{(k+1)/2}, \qquad C(x) = L_n^k(x).$$

13.2.9 From Eq. (13.87) the normalized radial part of the hydrogenic wave function is

$$R_{nL}(r) = \left[\beta^3 \frac{(n-L-1)!}{2n(n+L)!}\right]^{1/2} e^{-\beta r}(\beta r)^L L_{n-L-1}^{2L+1}(\beta r),$$

where $\beta = 2Z/na_0 = Zme^2/(2\pi\epsilon_0\hbar^2)$. Evaluate

(a) $\langle r \rangle = \displaystyle\int_0^\infty rR_{nL}(\beta r)R_{nL}(\beta r)r^2\,dr,$

(b) $\langle r^{-1} \rangle = \displaystyle\int_0^\infty r^{-1}R_{nL}(\beta r)R_{nL}(\beta r)r^2\,dr.$

The quantity $\langle r \rangle$ is the average displacement of the electron from the nucleus, whereas $\langle r^{-1} \rangle$ is the average of the reciprocal displacement.

$$\textit{ANS.} \quad \langle r \rangle = \frac{a_0}{2}[3n^2 - L(L+1)] \qquad \langle r^{-1} \rangle = \frac{1}{n^2 a_0}.$$

13.2.10 Derive the recurrence relation for the hydrogen wave function expectation values:

$$\frac{s+2}{n^2}\langle r^{s+1} \rangle - (2s+3)a_0\langle r^s \rangle + \frac{s+1}{4}[(2L+1)^2 - (s+1)^2]a_0^2\langle r^{s-1} \rangle = 0,$$

with $s \ge -2L-1$ and $\langle r^s \rangle$ defined as in Exercise 13.2.9(a).

Hint. Transform Eq. (13.83) into a form analogous to Eq. (13.78). Multiply by $\rho^{s+2}u' - c\rho^{s+1}u$. Here, $u = \rho\Phi$. Adjust c to cancel terms that do not yield expectation values.

13.2.11 The hydrogen wave functions, Eq. (13.87), are mutually orthogonal, as they should be since they are eigenfunctions of the self-adjoint Schrödinger equation

$$\int \psi^*_{n_1L_1M_1}\psi_{n_2L_2M_2}r^2 dr d\Omega = \delta_{n_1n_2}\delta_{L_1L_2}\delta_{M_1M_2}.$$

However, the radial integral has the (misleading) form

$$\int_0^\infty e^{-\beta r/2}(\beta r)^L L_{n_1-L-1}^{2L+1}(\beta r)e^{-\beta r/2}(\beta r)^L L_{n_2-L-1}^{2L+1}(\beta r)r^2 dr,$$

which **appears** to match Eq. (13.79) and not the associated Laguerre orthogonality relation [Eq. (13.75)]. How do you resolve this paradox?

ANS. The parameter β is dependent on n. The first three β previously shown are $2Z/n_1 a_0$. The last three are $2Z/n_2 a_0$. For $n_1 = n_2$, Eq. (13.79) applies. For $n_1 \neq n_2$, neither Eq. (13.75) nor Eq. (13.79) is applicable.

13.2.12 A quantum mechanical analysis of the Stark effect (in parabolic coordinates) leads to the ODE

$$\frac{d}{d\xi}\left(\xi\frac{du}{d\xi}\right) + \left(\frac{1}{2}E\xi + L - \frac{m^2}{4\xi} - \frac{1}{4}F\xi^2\right)u = 0,$$

where F is a measure of the perturbation energy introduced by an external electric field. Find the unperturbed wave functions ($F = 0$) in terms of associated Laguerre polynomials.

ANS. $u(\xi) = e^{-\varepsilon\xi/2}\xi^{m/2}L_p^m(\varepsilon\xi)$, with $\varepsilon = \sqrt{-2E} > 0$, $p = \alpha/\varepsilon - (m+1)/2$, a nonnegative integer.

13.2.13 The wave equation for the three-dimensional harmonic oscillator is

$$-\frac{\hbar^2}{2M}\nabla^2\psi + \frac{1}{2}M\omega^2 r^2\psi = E\psi,$$

where ω is the angular frequency of the corresponding classical oscillator. Show that the radial part of ψ (in spherical polar coordinates) may be written in terms of associated Laguerre functions of argument (βr^2), where $\beta = M\omega/\hbar$.
Hint. As in Exercise 13.2.8, split off radial factors of r^l and $e^{-\beta r^2/2}$. The associated Laguerre function will have the form $L_{(n-l-1)/2}^{l+1/2}(\beta r^2)$.

13.2.14 Write a program (in Basic or Fortran or use symbolic software) that will generate the coefficients a_s in the polynomial form of the Laguerre polynomial, $L_n(x) = \sum_{s=0}^{n} a_s x^s$.

13.2.15 Write a subroutine that will transform a finite power series $\sum_{n=0}^{N} a_n x^n$ into a Laguerre series $\sum_{n=0}^{N} b_n L_n(x)$. Use the recurrence relation Eq. (13.60).

13.2.16 Tabulate $L_{10}(x)$ for $x = 0.0$ to 30.0 in steps of 0.1. This will include the 10 roots of L_{10}. Beyond $x = 30.0$, $L_{10}(x)$ is monotonically increasing. Plot your results.

Check value. Eighth root $= 16.279$.

Additional Reading

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