

The use of these generating functions was illustrated in example 11-26 as intermediate results in calculating spherical harmonics.

The first few Legendre polynomials are listed in table 10-1. Our interest in those is to generate associated Legendre functions. The first few associated Legendre polynomials are listed in table 10-2.

$$\begin{array}{ll} P_0(x) = 1 & P_3(x) = \frac{1}{2}(5x^3 - 3x) \\ P_1(x) = x & P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3) \\ P_2(x) = \frac{1}{2}(3x^2 - 1) & P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x) \end{array}$$

Table 10 - 1. The First Six Legendre Polynomials.

$$\begin{array}{ll} P_{0,0}(x) = 1 & P_{2,0}(x) = \frac{1}{2}(3x^2 - 1) \\ P_{1,1}(x) = -\sqrt{1-x^2} & P_{3,3}(x) = -15(\sqrt{1-x^2})^3 \\ P_{1,0}(x) = x & P_{3,2}(x) = 15x(1-x^2) \\ P_{2,2}(x) = 3(1-x^2) & P_{3,1}(x) = -\frac{3}{2}(5x^2 - 1)\sqrt{1-x^2} \\ P_{2,1}(x) = -3x\sqrt{1-x^2} & P_{3,0}(x) = \frac{1}{2}(5x^3 - 3x) \end{array}$$

Table 10 - 2. The First Few Associated Legendre Polynomials.

Two comment concerning the tables are appropriate. First, notice  $P_l = P_{l,0}$ . That makes sense. If the Legendre equation is the same as the associated Legendre equation with  $m = 0$ , the solutions to the two equations must be the same when  $m = 0$ . Also, many authors will use a positive sign for all associated Legendre polynomials. This is a different choice of phase. We addressed that following table 11-1 in comments on spherical harmonics. We choose to include a factor of  $(-1)^m$  with the associated Legendre polynomials, and the sign of all spherical harmonics will be positive as a result.

Finally, remember the change of variables  $x = \cos \theta$ . That was done to put the differential equation in a more elementary form. In fact, a dominant use of associated Legendre polynomials is in applications where the argument is  $\cos \theta$ . One example is the generating function for spherical harmonic functions,

$$Y_{l,m}(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_{l,m}(\cos \theta) e^{im\phi} \quad m \geq 0, \quad (10-10)$$

and

$$Y_{l,-m}(\theta, \phi) = Y_{l,m}^*(\theta, \phi), \quad m < 0,$$

where the  $P_{l,m}(\cos \theta)$  are associated Legendre polynomials. If we need a spherical harmonic with  $m < 0$ , we will calculate the spherical harmonic with  $m = |m|$ , and then calculate the adjoint.

To summarize the last three sections, we separated the angular equation into an azimuthal and a polar portion. The solutions to the azimuthal angle equation are exponentials including the magnetic moment quantum number in the argument. The solutions to the polar angle equation are the associated Legendre polynomials, which are different for each choice of orbital angular momentum and magnetic moment quantum number. Both quantum numbers are introduced into

the respective differential equations as separation constants. Since we assumed a product of the two functions to get solutions to the azimuthal and polar parts, the solutions to the original angular equation (10–7) are the products of the two solutions  $P_{l,m}(\cos \theta) e^{im\phi}$ . These factors are included in equation (10–10). All other factors in equation (10–12) are simply normalization constants. The products  $P_{l,m}(\cos \theta) e^{im\phi}$  are the spherical harmonic functions, the alternating sign and radical just make the orthogonal set orthonormal.

## Associated Laguerre Polynomials and Functions

The azimuthal equation was easy, the polar angle equation a little more substantial, but you will likely perceive the solution to the radial equation as plain, old heavy! There is no easy way to do this. Our approach will be to relate the radial equation to the associated Laguerre equation, for which the associated Laguerre functions are solutions. A popular option to solve the radial equation is a power series solution, for which we will refer you to Griffiths<sup>3</sup>, or Cohen–Tannoudji<sup>4</sup>.

Laguerre polynomials are solutions to the Laguerre equation

$$x L_j''(x) + (1 - x) L_j'(x) + j L_j(x) = 0.$$

The first few Laguerre polynomials are listed in table 10–3.

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

Table 10 – 3. The First Seven Laguerre Polynomials.

Laguerre polynomials of any order can be calculated using the generating function

$$L_j(x) = e^x \frac{d^j}{dx^j} e^{-x} x^j.$$

The Laguerre polynomials do not form an orthogonal set. The related set of **Laguerre functions**,

$$\phi_j(x) = e^{-x/2} L_j(x) \quad (10 - 13)$$

is orthonormal on the interval  $0 \leq x < \infty$ . The Laguerre functions are not solutions to the Laguerre equation, but are solutions to an equation which is related.

Just as the Legendre equation becomes the associated Legendre equation by adding an appropriate term containing a second index, the associated Laguerre equation is

$$x L_j^{k''}(x) + (1 - x + k) L_j^{k'}(x) + j L_j^k(x) = 0, \quad (10 - 14)$$

<sup>3</sup> Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, Englewood Cliffs, New Jersey, 1995), pp. 134–141.

<sup>4</sup> Cohen–Tannoudji, Diu, and Laloe, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), pp. 794–797.

which reduces to the Laguerre equation when  $k = 0$ . The first few associated Laguerre polynomials are

$L_0^0(x) = L_0(x)$	$L_0^2(x) = 2$
$L_1^0(x) = L_1(x)$	$L_3^0(x) = L_3(x)$
$L_1^1(x) = -2x + 4$	$L_3^1(x) = -4x^3 + 48x^2 - 144x + 96$
$L_0^1(x) = 1$	$L_2^3(x) = 60x^2 - 600x + 1200$
$L_2^0(x) = L_2(x)$	$L_3^3(x) = -120x^3 + 2160x^2 - 10800x + 14400$
$L_2^1(x) = 3x^2 - 18x + 18$	$L_2^2(x) = -20x^3 + 300x^2 - 1200x + 1200$
$L_2^2(x) = 12x^2 - 96x + 144$	$L_1^3(x) = -24x + 96$
$L_1^2(x) = -6x + 18$	$L_0^3(x) = 6$

Table 10 – 4. Some Associated Laguerre Polynomials.

Notice  $L_j^0 = L_j$ . Also notice the indices are all non-negative, and either index may assume any integral value. We will be interested only in those associated Laguerre polynomials where  $k < j$  for hydrogen atom wave functions.

Associated Laguerre polynomials can be calculated from Laguerre polynomials using the generating function

$$L_j^k(x) = (-1)^k \frac{d^k}{dx^k} L_{j+k}(x).$$

**Example 10–5:** Calculate  $L_3^1(x)$  starting with the generating function.

We first need to calculate  $L_4(x)$ , because

$$L_j^k(x) = (-1)^k \frac{d^k}{dx^k} L_{j+k}(x) \Rightarrow L_3^1(x) = (-1)^1 \frac{d^1}{dx^1} L_{3+1}(x) = -\frac{d}{dx} L_4(x).$$

Similarly, if you want to calculate  $L_3^2$ , you need to start with  $L_5$ , and to calculate  $L_4^3$ , you need to start with  $L_7$ . So using the generating function,

$$\begin{aligned} L_4(x) &= e^x \frac{d^4}{dx^4} e^{-x} x^4 \\ &= e^x \frac{d^3}{dx^3} \left( -e^{-x} x^4 + e^{-x} 4x^3 \right) \\ &= e^x \frac{d^2}{dx^2} \left( e^{-x} x^4 - e^{-x} 4x^3 - e^{-x} 4x^3 + e^{-x} 12x^2 \right) = e^x \frac{d^2}{dx^2} \left( e^{-x} x^4 - e^{-x} 8x^3 + e^{-x} 12x^2 \right) \\ &= e^x \frac{d}{dx} \left( -e^{-x} x^4 + e^{-x} 4x^3 + e^{-x} 8x^3 - e^{-x} 24x^2 - e^{-x} 12x^2 + e^{-x} 24x \right) \\ &= e^x \frac{d}{dx} \left( -e^{-x} x^4 + e^{-x} 12x^3 - e^{-x} 36x^2 + e^{-x} 24x \right) \\ &= e^x \left( e^{-x} x^4 - e^{-x} 4x^3 - e^{-x} 12x^3 + e^{-x} 36x^2 + e^{-x} 36x^2 - e^{-x} 72x - e^{-x} 24x + e^{-x} 24 \right) \\ &= e^x e^{-x} \left( x^4 - 16x^3 + 72x^2 - 96x + 24 \right) \\ &= x^4 - 16x^3 + 72x^2 - 96x + 24, \end{aligned}$$