6.3: The Laguerre Equation

So far we used the power series method to solve equations that can be solved using simpler methods. Let's now turn our attention to differential equations that cannot be solved otherwise. One such example is the *Laguerre equation*. This differential equation is important in quantum mechanics because it is one of several equations that appear in the quantum mechanical description of the hydrogen atom. The solutions of the Laguerre equation are called the *Laguerre polynomials*, and together with the solutions of other differential equations, form the functions that describe the orbitals of the hydrogen atom.

The Laguerre equation is

$$xy'' + (1-x)y' + ny = 0$$

where $n = 0, 1, 2....$

Solving the n=0 Laguerre Equation

Here, for simplicity, we will solve the equation for a given value of n. That is, instead of solving the equation for a generic value of n, we will solve it first for $n = 0$, then for $n = 1$, and so on.

Let's start with $n = 0$. The differential equation then becomes:

$$xy'' + y' - xy' = 0. \tag{6.3.1}$$

We start by assuming that the solution can be written as:

$$y(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + \dots$$

and therefore the first and second derivatives are:

$$\begin{aligned} y'(x) &= a_1 + 2a_2x + 3a_3x^2 + 4a_4x^3 + 5a_5x^4 \dots \\ y''(x) &= 2a_2 + 2\times 3a_3x + 3\times 4a_4x^2 + 4\times 5a_5x^3 + 5\times 6a_6x^4 + \dots. \end{aligned}$$

We then plug these expressions in the differential equation (Equation 6.3.1):

$$\begin{aligned} xy'' + y' - xy' &= 0 \\ x(2a_2 + 2\times 3a_3x + 3\times 4a_4x^2 + 4\times 5a_5x^3 + 5\times 6a_6x^4 + \dots) + (a_1 + 2a_2x + 3a_3x^2 + 4a_4x^3 + 5a_5x^4 \dots) \\ - x(a_1 + 2a_2x + 3a_3x^2 + 4a_4x^3 + 5a_5x^4 + \dots) &= 0 \\ (2a_2x + 2\times 3a_3x^2 + 3\times 4a_4x^3 + 4\times 5a_5x^4 + 5\times 6a_6x^5 + \dots) + (a_1 + 2a_2x + 3a_3x^2 + 4a_4x^3 + 5a_5x^4 + \dots) \\ - (a_1x + 2a_2x^2 + 3a_3x^3 + 4a_4x^4 + 5a_5x^5 + \dots) &= 0 \end{aligned}$$

We then group the terms in the same power of x. However, to avoid writing a long equation, let's try putting the information in a table. The second column contains the terms that multiply each power of x. We know each of these terms needs to be zero, and that will give us the relationships between the coefficients we need.

x^0	a_1	$=0$	$\rightarrow a_1 = 0$
x^1	$2a_2 + 2a_2 - a_1$	$=0$	$\rightarrow a_2 = a_1/4$
x^2	$6a_3 + 3a_3 - 2a_2$	$=0$	$\rightarrow a_3 = a_2 \times 2/9$
x^3	$12a_4 + 4a_4 - 3a_3$	$=0$	$\rightarrow a_4 = a_3 \times 3/16$
x^4	$20a_5 + 5a_5 - 4a_4$	$=0$	$\rightarrow a_5 = a_4 \times 4/25$

The first row tells us that $a_1 = 0$, and from the other rows, we conclude that all other coefficients with $n > 1$ are also zero. Recall that $y(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 \dots$, so the solution is simply $y(x) = a_0$ (i.e. the solution is a constant). This solution may be disappointing to you because it is not a function of x. Don't worry, we'll get something more interesting in the next example.

Solving the n=1 Laguerre Equation

Let's see what happens when $n=1$. The differential equation becomes

$$xy''+y'-xy'+y=0. \tag{6.3.2}$$

As always, we start by assuming that the solution can be written as:

$$y(x)=a_0+a_1x+a_2x^2+a_3x^3+a_4x^4+\dots$$

and therefore the first and second derivatives are:

$$y'(x) = a_1+2a_2x+3a_3x^2+4a_4x^3+5a_5x^4+\dots \tag{6.3.3}$$

$$y''(x) = 2a_2+2\times 3a_3x+3\times 4a_4x^2+4\times 5a_5x^3+5\times 6a_6x^4+\dots \tag{6.3.4}$$

and then plug these expressions in the differential equation (Equation 6.3.2):

$$\begin{aligned} xy''+y'-xy'+y &=0 \\ x(2a_2+2\times 3a_3x+3\times 4a_4x^2+4\times 5a_5x^3+5\times 6a_6x^4\dots)+(a_1+2a_2x+3a_3x^2+4a_4x^3+5a_5x^4\dots) &=0 \\ -x(a_1+2a_2x+3a_3x^2+4a_4x^3+5a_5x^4\dots)+(a_0+a_1x+a_2x^2+a_3x^3+a_4x^4\dots) & \\ (2a_2x+2\times 3a_3x^2+3\times 4a_4x^3+4\times 5a_5x^4+5\times 6a_6x^5\dots)+(a_1+2a_2x+3a_3x^2+4a_4x^3+5a_5x^4\dots) &=0 \\ -(a_1x+2a_2x^2+3a_3x^3+4a_4x^4+5a_5x^5\dots)+(a_0+a_1x+a_2x^2+a_3x^3+a_4x^4\dots) & \end{aligned}$$

The next step is to group the terms in the same power of x. Let's make a table as we did before:

x^0	a_1+a_0	$=0$	$\rightarrow a_1=-a_0$
x^1	$2a_2+2a_2-a_1+a_1$	$=0$	$\rightarrow 4a_2=0$
x^2	$6a_3+3a_3-2a_2+a_2$	$=0$	$\rightarrow a_3=a_2\times 1/9$
x^3	$12a_4+4a_4-3a_3+a_3$	$=0$	$\rightarrow a_4=a_3\times 2/16$
x^4	$20a_5+5a_5-4a_4+a_4$	$=0$	$\rightarrow a_5=a_4\times 3/25$

We see that in this case $a_1=-a_0$, and $a_{n>1}=0$. Recall that

$$y(x)=a_0+a_1x+a_2x^2+a_3x^3+a_4x^4\dots$$

so the solution is $y(x)=a_0(1-x)$.

In physical chemistry, we define the Laguerre polynomials ($L_n(x)$) as the solution of the Laguerre equation with $a_0=n!$. This is arbitrary and somewhat field-dependent. You may find other definitions, but we'll stick with $n!$ because it is the one that is more widely used in physical chemistry.

With the last two examples we proved that $L_0(x)=1$ and $L_1(x)=1-x$. You'll obtain $L_2(x)$ and $L_3(x)$ in your homework.