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Laguerre Polynomials, an Introduction

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I. SYNOPSIS

The radial part of the Schrödinger Equation for the H-atom consists of functions related to Laguerre polynomials, hence this introduction

II. INTRODUCTION

The radial equation for the H-atom is [1]:

$$-\frac{\hbar^2}{2\mu}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}\right]R(r)-\frac{Ze^2}{r}R(r)=ER(r)$$

which we need to bring to dimensionless form before proceeding (text book form). Cross multiplying, and defining $\epsilon = -E$ we have

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}\right]R(r)+\frac{2\mu Ze^2}{\hbar^2 r}R(r)-\frac{2\mu\epsilon}{\hbar^2}R(r)=0$$

and where we are going to only solve for states with $\epsilon > 0$, i.e., negative energy states.

Defining a dimensionless distance, $\rho = \alpha r$ we have

$$\frac{d}{dr}=\frac{d\rho}{dr}\frac{d}{d\rho}=\alpha\frac{d}{d\rho}$$

so that the equation becomes

$$\alpha^2\left[\frac{d^2}{d\rho^2}+\frac{2}{\rho}\frac{d}{d\rho}-\frac{\ell(\ell+1)}{\rho^2}\right]R(\rho)+\frac{2\mu Ze^2\alpha}{\hbar^2\rho}R(\rho)-\frac{2\mu\epsilon}{\hbar^2}R(\rho)=0$$

which is, upon dividing through by α^2,

$$\left[\frac{d^2}{d\rho^2}+\frac{2}{\rho}\frac{d}{d\rho}-\frac{\ell(\ell+1)}{\rho^2}\right]R(\rho)+\frac{2\mu Ze^2}{\hbar^2\rho\alpha}R(\rho)-\frac{2\mu\epsilon}{\hbar^2\alpha^2}R(\rho)=0$$

Now, we *choose* α as

$$\left(\frac{\alpha}{2}\right)^2=\frac{2\mu\epsilon}{\hbar^2}$$

so To continue, we re-start our discussion with Laguerre's differential equation:

$$x\frac{d^2y^*}{dx^2}+(1-x)\frac{dy^*}{dx}+\alpha y^*=0 \tag{2.1}$$

To show that this equation is related to Equation II we differentiate Equation 2.1

$$\frac{d\left(x\frac{d^2y^*}{dx^2}+(1-x)\frac{dy^*}{dx}+\alpha y^*=0\right)}{dx} \tag{2.2}$$

which gives

$$y^{*\prime\prime}+xy^{*\prime\prime\prime}-y^{*\prime}+(1-x)y^{*\prime\prime}+\alpha y^{*\prime}=0$$

which is

$$xy^{*\prime\prime\prime}+(2-x)y^{*\prime\prime}+(\alpha-1)y^{*\prime}=0$$

or

$$\left(x\frac{d^2}{dx^2}+(2-x)\frac{d}{dx}+(\alpha-1)\right)\frac{dy^*}{dx}=0 \tag{2.3}$$

Doing it again (differentiating), we obtain

$$\frac{d\left(xy^{*\prime\prime\prime}+(2-x)y^{*\prime\prime}+(\alpha-1)y^{*\prime}=0\right)}{dx}$$

which leads to

$$y^{*\prime\prime\prime}+xy^{*\prime\prime\prime\prime}-y^{*\prime\prime}+(2-x)y^{*\prime\prime\prime}+(\alpha-1)y^{*\prime\prime}=0$$

which finally becomes

$$\left(x\frac{d^2}{dx^2}+(3-x)\frac{d}{dx}+(\alpha-2)\right)\frac{d^2y^*}{dx^2}=0 \tag{2.4}$$

Generalizing, we have

$$\left(x\frac{d^2}{dx^2} + (k+1-x)\frac{d}{dx} + (\alpha - k)\right)\frac{d^k y^*}{dx^k} = 0 \quad (2.5)$$

III. PART 2

Consider Equation II

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho}R(\rho) - \frac{\ell(\ell+1}{\rho^2}\right]R(\rho) + \frac{2\mu Ze^2}{\hbar^2\rho\alpha}R(\rho) - \frac{R(\rho)}{4} = 0 \quad (3.1)$$

if we re-write it as

$$\left[\rho\frac{d^2}{d\rho^2} + 2\frac{d}{d\rho} - \frac{\ell(\ell+1}{\rho}\right]R(\rho) + \frac{2\mu Ze^2}{\hbar^2\alpha}R(\rho) - \frac{\rho}{4}R(\rho) = 0 \quad (3.2)$$

(for comparison with the following):

$$xy'' + 2y' + \left(n - \frac{k-1}{2} - \frac{x}{4} - \frac{k^2-1}{4x}\right)y = 0 \quad (3.3)$$

Notice the similarity if $\rho \sim x$, i.e., powers of x, x^{-1} etc.,

$$\frac{2\mu Ze^2}{\hbar^2\alpha} \rightleftharpoons n - \frac{k-1}{2} \quad (3.4)$$

$$\rho \rightleftharpoons \frac{x}{4} \quad (3.5)$$

$$\frac{k^2-1}{4x} \rightleftharpoons \frac{\ell(\ell+1)}{\rho} \quad (3.6)$$

We force the asymptotic form of the solution y(x) to be exponentially decreasing, i.e.,

$$y = e^{-x/2}x^{(k-1)/2}v(x) \quad (3.7)$$

and "ask" what equation $v(x)$ solves. We do this in two steps, first assuming

$$y(x) = x^{(k-1)/2}w(x)$$

and then assuming that w(x) is

$$w(x) = e^{-x/2}v(x)$$

So, assuming the first part of Equation 3.7, we have

$$y'(x) = \frac{k-1}{2}x^{(k-3)/2}w(x) + x^{(k-1)/2}w'(x)$$

and

$$y''(x) = \frac{k-1}{2}\frac{k-3}{2}x^{(k-5)/2}w(x) + \frac{k-1}{2}x^{(k-3)/2}w'(x) + \frac{k-1}{2}x^{(k-3)/2}w'(x) + x^{(k-1)/2}w''(x) = 0$$

which we now substitute into Equation 3.3 to obtain

$$\begin{aligned} xy'' &= \frac{k-1}{2}\frac{k-3}{2}x^{(k-3)/2}w(x) + (k-1)x^{(k-1)/2}w'(x) + x^{(k+1)/2}w''(x) \\ 2y' &= 2\frac{k-1}{2}x^{(k-3)/2}w(x) + 2x^{(k-1)/2}w'(x) \\ ny &= nx^{(k-1)/2}w(x) \\ -\frac{k-1}{2}y &= -\frac{k-1}{2}x^{(k-1)/2}w \\ -\frac{x}{4}y &= -\frac{x^{(k+1)/2}}{4}w \\ -\frac{k^2-1}{4x}y &= -\frac{k^2-1}{4}x^{(k-3)/2}w \\ &= 0 \end{aligned} \quad (3.8)$$

or

$$xw'' + (k+1)w' + \left(n - \frac{k-1}{2} - \frac{x}{4}\right)w = 0 \quad (3.9)$$

IV.

Now we let

$$w = e^{-x/2}v(x)$$

(as noted before) to obtain

$$w' = -\frac{1}{2}e^{-x/2}v + e^{-x/2}v'$$

$$w'' = \frac{1}{4}e^{-x/2}v - e^{-x/2}v' + e^{-x/2}v''$$

Substituting into Equation 3.8 we have:

$$\begin{aligned} xw'' &= e^{-x/2}\left(\frac{x}{4}v - xv' + xv''\right) \\ (k+1)w' &= e^{-x/2}\left(-\frac{k+1}{2}v + (k+1)v'\right) \\ \left(n - \frac{k-1}{2} - \frac{x}{4}\right)w &= e^{-x/2}\left(n - \frac{k-1}{2} - \frac{x}{4}\right)v = 0 \end{aligned} \tag{4.1}$$

so, v solves Equation 2.5 if $\alpha = n$. Expanding the r.h.s. of Equation 4.1 we have

$$\frac{x}{4}v - \frac{x}{4} + xv'' + (k+1-x)v' + \left(n - \frac{k-1}{2} - \frac{k+1}{2}\right)v = 0$$

i.e.,

$$xv'' + (k+1-x)v' + (n-k)v = 0$$

which *is* Equation 2.5, i.e.,

$$v = \frac{d^k y}{dx^k}$$

and

$$y = e^{-x/2}x^{(k-1)/2}\frac{d^k y^*}{dx^k}$$

or

$$w'' = \frac{1}{4}e^{-x/2}v - e^{-x/2}v' + e^{-x/2}v''$$

so, substituting into Equation 3.8 we have

$$\begin{aligned} xw'' &= e^{-x/2}\left(\frac{x}{4}v - xv' + xv''\right) \\ (k+1)w' &= e^{-x/2}\left(-\frac{k+1}{2}v + (k+1)v'\right) \\ \left(n - \frac{k-1}{2} - \frac{x}{4}\right)w &= e^{-x/2}\left(n - \frac{k-1}{2} - \frac{x}{4}\right)v = 0 \end{aligned} \tag{4.2}$$

so, v solves Equation 2.5 if $\alpha = n$. Expanding the r.h.s. of Equation 4.2 we have

$$\frac{x}{4}v - \frac{x}{4} + xv'' + (k+1-x)v' + \left(n - \frac{k-1}{2} - \frac{k+1}{2}\right)v = 0$$

i.e.,

$$xv'' + (k+1-x)v' + (n-k)v = 0$$

which *is* Equation 2.5, i.e.,

$$v = \frac{d^k y^*}{dx^k}$$

and

$$y = e^{-x/2}x^{(k-1)/2}\frac{d^k y^*}{dx^k}$$

or

$$R(\rho) = e^{-\rho/2}\rho^{(k-1)/2)}L^k_{n*}(\rho)$$

where y^* and $R(\rho)$ are solutions to Laguerre's Equation of degree n. Wow.

V. PART 3

Now, all we need do is solve Laguerre's differential equation Equation 2.1 (we drop the superscript star now):

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

where γ is a constant (to be discovered). We let

$$y = \sum_{\lambda=0}^{?} a_\lambda x^\lambda$$

and proceed as normal

$$\begin{aligned} xy'' &= 2a_2x + (3)(2)a_3x^2 + (4)(3)a_4x^3 + \cdots \\ +y' &= (1)a_1 + (2)a_2x + (3)a_3x^2 + (4)a_4x^3 + \cdots \\ -xy' &= -a_1x - (2)a_2x^2 - (3)a_3x^3 - \cdots \\ +\gamma y &= \gamma a_0 + \gamma a_1 x + \gamma a_2 x^2 + \cdots = 0 \end{aligned} \tag{5.1}$$

which yields

$$\begin{aligned} a_1 &= -\gamma a_0 \\ a_2 &= \frac{1-\gamma}{4} a_1 \\ a_3 &= \frac{2-\gamma}{9} a_2 \\ a_4 &= \frac{3-\gamma}{16} a_3 \end{aligned} \tag{5.2}$$

or, in general,

$$a_{j+1} = \frac{j-\gamma}{(j+1)^2} a_j$$

which means

$$\begin{aligned} a_1 &= -\frac{\gamma}{1} a_0 \\ a_2 &= -\frac{(1-\gamma)\gamma}{(4)(1)} a_0 \\ a_3 &= -\frac{(2-\gamma)(1-\gamma)\gamma}{(9)(4)(1)} a_0 \\ a_4 &= -\frac{(3-\gamma)(2-\gamma)(1-\gamma)\gamma}{(16)(9)(4)(1)} a_0 \\ &\cdots \end{aligned} \tag{5.3}$$

which finally is

$$a_j = -\frac{\Pi_{k=0}^{j-1}(k-\gamma)}{\Pi_{k=1}^{j}(k^2)} a_0$$

and

$$a_{j+1} = -(j-\gamma)\frac{\Pi_{k=0}^{j-1}(k-\gamma)}{(j+1)^2\Pi_{k=1}^{j}(k^2)} a_0 = \frac{j-\gamma}{(j+1)^2} a_j$$

which implies that

$$\frac{a_{j+1}}{a_j} = \frac{j-\gamma}{(j+1)^2} \sim \frac{1}{j}$$

as $j \to \infty$. This is the behaviour of $y = e^x$, which would overpower the previous Ansatz, so we must have truncation through an appropriate choice of γ (i.e., $\gamma = n^*$).

VI.

If γ were an integer, then as j increased, and passed into γ we would have a zero numerator in the expression

$$a_{j+1} = \frac{(j-\gamma)}{(j+1)^2} a_j$$

and all higher a's would be zero! But

$$\left(\frac{\alpha}{2}\right)^2 = \frac{2\mu\epsilon}{\hbar^2} = -\frac{2\mu E}{\hbar^2}$$

so, from Equation 3.6 we have

$$\frac{k^2-1}{4} = \ell(\ell+1)$$

$$k^2 - 1 = 4\ell^2 + 4\ell$$

$$k = 2\ell + 1$$

so

$$\frac{k-1}{2} = \frac{2\ell+1-1}{2} = \ell \tag{6.1}$$

and therefore Equation 3.3 and its successors tells us that using Equation 6.1 we have

$$\left(n^* - \frac{k-1}{2}\right) = n^* - \ell = \frac{2\mu Z e^2}{\hbar^2 \alpha}$$

implies

$$\alpha = \frac{2\mu Z e^2}{\hbar^2 (n^* - \ell)}$$

$$\left(\frac{\alpha}{2}\right)^2 = -\frac{2\mu E}{\hbar^2} = \frac{4\mu^2 Z^2 e^4}{4\hbar^4 (n^* - \ell)^2}$$

i.e.,

$$E = -\frac{\mu Z^2 e^4}{2\hbar^2 (n^* - \ell)^2}$$

which is the famous Rydberg/Bohr formula.

[1] l2h:Laguerre.tex