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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 defin-

ing $\epsilon = -E$ 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

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

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:

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

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

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

which gives

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

Typeset by REVTEX

which is

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

or

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

Doing it again (differentiating), we obtain

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

which leads to

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

which finally becomes

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

Generalizing, we have

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

III. PART 2

Consider Equation II

$$\[\frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho} R(\rho) - \frac{\ell(\ell+1)}{\rho^2} \] R(\rho) + \frac{2\mu Z e^2}{\hbar^2 \rho \alpha} R(\rho) - \frac{R(\rho)}{4} = 0$$

$$(3.1)$$

if we re-write it as

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

(for comparison with the following):

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

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

$$\frac{2\mu Z e^2}{\hbar^2 \alpha} \rightleftharpoons n - \frac{k-1}{2} \tag{3.4}$$

 $\rho \rightleftharpoons \frac{x}{4} \tag{3.5}$

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

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

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

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

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

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

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

$$-\frac{x}{4} y = -\frac{x^{(k+1)/2}}{4} w$$

$$-\frac{k^2 - 1}{4x} y = -\frac{k^2 - 1}{4} x^{(k-3)/2} w$$

$$= 0$$
(3.8)

or IV.

Now we let

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

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

(as noted before) to obtain

Substituting into Equation 3.8 we have:

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

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

$$xw'' = e^{-x/2} \left(\frac{x}{4}v - xv' + xv'' \right)$$

$$(k+1)w' = e^{-x/2} \left(-\frac{k+1}{2}v + (k+1)v' \right)$$

$$\left(n - \frac{k-1}{2} - \frac{x}{4} \right) w = e^{-x/2} \left(n - \frac{k-1}{2} - \frac{x}{4} \right) v = 0$$

$$(4.1)$$

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

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

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

i.e.,

or

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

which is Equation 2.5, i.e.,

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

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

so, substituting into Equation 3.8 we have

$$xw'' = e^{-x/2} \left(\frac{x}{4} v - xv' + xv'' \right)$$

$$(k+1)w' = e^{-x/2} \left(-\frac{k+1}{2} v + (k+1)v' \right)$$

$$\left(n - \frac{k-1}{2} - \frac{x}{4} \right) w = e^{-x/2} \left(n - \frac{k-1}{2} - \frac{x}{4} \right) v = 0$$

$$(4.2)$$

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

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

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

i.e.,

or

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

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

which is Equation 2.5, i.e.,

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

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

which yields

$$a_{1} = -\gamma a_{0}$$

$$a_{2} = \frac{1 - \gamma}{4} a_{1}$$

$$a_{3} = \frac{2 - \gamma}{9} a_{2}$$

$$a_{4} = \frac{3 - \gamma}{16} a_{3}$$
(5.2)

or, in general,

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

which means

$$a_{1} = -\frac{\gamma}{1}a_{0}$$

$$a_{2} = -\frac{(1-\gamma)\gamma}{(4)(1)}a_{0}$$

$$a_{3} = -\frac{(2-\gamma)(1-\gamma)\gamma}{(9)(4)(1)}a_{0}$$

$$a_{4} = -\frac{(3-\gamma)(2-\gamma)(1-\gamma)\gamma}{(16)(9)(4)(1)}a_{0}$$

$$\cdots (5.3)$$

which finally is

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

and

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

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