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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

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

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

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

Now, we choose \( \alpha \) 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:

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

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

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

which gives

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

Typeset by REVTEX
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
\[
\left[ \frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho} R(\rho) - \frac{\ell(\ell + 1)}{\rho^2} \right] R(\rho) + \frac{2\mu Z e^2}{\hbar^2 \alpha} R(\rho) - \frac{R(\rho)}{4} = 0
\]
if we re-write it as
\[
\left[ \frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho} - \frac{\ell(\ell + 1)}{\rho^2} \right] R(\rho) + \frac{2\mu Z e^2}{\hbar^2 \alpha} R(\rho) - \frac{\rho}{4} R(\rho) = 0
\]
(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.,
\[
\frac{2\mu Z e^2}{\hbar^2 \alpha} \mapsto n - \frac{k - 1}{2}
\]
(3.4)

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

which we now substitute into Equation 3.3 to obtain
\[
x y'' = \frac{k - 1}{2} k - 3 x^{(k-3)/2} w(x) + (k - 1) x^{(k-1)/2} u'(x) + x^{(k+1)/2} w''(x)
\]
\[
2y' = \frac{k - 1}{2} x^{(k-3)/2} u'(x) + 2 x^{(k-1)/2} u''(x)
\]
\[
y n y = n x^{(k-1)/2} u(x)
\]
\[
- \frac{k - 1}{2} y = - \frac{k - 1}{2} x^{(k-1)/2} u
\]
\[
- \frac{x}{4} y = - \frac{x}{4} x^{(k+1)/2} w
\]
\[
- \frac{k^2 - 1}{4x} y = - \frac{k^2 - 1}{4} x^{(k-3)/2} w
\]
\[
= 0 \quad (3.8)
\]

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

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
\[
y'(x) = k - 1 \quad 2 x^{(k-3)/2} w(x) + x^{(k-1)/2} w'(x)
\]
and
\[
y''(x) = \frac{1}{2} x^{(k-3)/2} u(x) + x^{(k-1)/2} u'(x)
\]
(3.5)
(3.6)

### 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:

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

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

\[ \left(n - \frac{k - 1}{2} - \frac{x}{4}\right)w = e^{-x/2}\left(n - \frac{k - 1}{2} - \frac{x}{4}\right)v = 0 \]  \hspace{1cm} (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.,

\[ v = \frac{d^k y}{dx^k} \]

so, substituting into Equation 3.8 we have

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

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

\[ \left(n - \frac{k - 1}{2} - \frac{x}{4}\right)w = e^{-x/2}\left(n - \frac{k - 1}{2} - \frac{x}{4}\right)v = 0 \]  \hspace{1cm} (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.,

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

so, \( R(\rho) = e^{-\rho/2}x^{(k-1)/2}L^k_{\alpha+}(\rho) \)

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 \( \gamma \) is a constant (to be discovered). We let

\[ y = \sum_{\lambda=0}^{\gamma} a_{\lambda} x^{\lambda} \]

and proceed as normal

\[ xy'' = 2a_2 x + (3)(2)a_3 x^2 + (4)(3)a_4 x^3 + \cdots \]

\[ + y' = (1)a_1 + (2)a_2 x + (3)x a_3 x^2 + (4)a_4 x^3 + \cdots \]

\[ - xy' = -a_1 x - (2)a_2 x^2 - (3)a_3 x^3 - \cdots \]

\[ + \gamma y = \gamma a_0 + \gamma a_1 x + \gamma a_2 x^2 + \cdots = 0 \]

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

\[ a_1 = \frac{-\gamma}{2} a_0 \]

\[ a_2 = -\frac{(1 - \gamma)\gamma}{4}(1) a_0 \]

\[ a_3 = -\frac{(2 - \gamma)\gamma}{9}(1) a_0 \]

\[ a_4 = -\frac{(3 - \gamma)(2 - \gamma)\gamma}{16}(1) a_0 \]

\[ \cdots \]

(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 \( \gamma \) (i.e., \( \gamma = n^* \)).

VI.

If \( \gamma \) were an integer, then as \( j \) increased, and passed into \( \gamma \) 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

\[ \left( \frac{\alpha}{2} \right)^2 = \frac{2\mu e}{\hbar^2} = -\frac{2\mu E}{\hbar^2} \]

so, from Equation 6.1 we have

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

\[ k^2 - 1 = 4\ell^2 + 4\ell \]

\[ k = 2\ell + 1 \]

so

\[ \frac{k - 1}{2} = \frac{2\ell + 1 - 1}{2} = \ell \]

(6.1)

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

\[ \left( n^* - \frac{k - 1}{2} \right) = n^* - \ell = \frac{2\mu Ze^2}{\hbar^2 \alpha} \]

implies

\[ \alpha = \frac{2\mu Ze^2}{\hbar^2 (n^* - \ell)} \]

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

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