University of Connecticut
DigitalCommons@UConn

Chemistry Education Materials | Department of Chemistry

1-1-2009

Continued Fraction Solutions to Hermite's, Legendre's and Laguerre's Differential Equation

Carl W. David
University of Connecticut, Carl.David@uconn.edu

Follow this and additional works at: http://digitalcommons.uconn.edu/chem_educ

Part of the Physical Chemistry Commons

Recommended Citation
David, Carl W., "Continued Fraction Solutions to Hermite's, Legendre's and Laguerre's Differential Equation" (2009). *Chemistry Education Materials*. Paper 77.
http://digitalcommons.uconn.edu/chem_educ/77

This Article is brought to you for free and open access by the Department of Chemistry at DigitalCommons@UConn. It has been accepted for inclusion in Chemistry Education Materials by an authorized administrator of DigitalCommons@UConn. For more information, please contact digitalcommons@uconn.edu.

Continued Fractions Solutions to Hermite's, Legendre's and Laguerre's Differential Equations

C. W. David*
Department of Chemistry
University of Connecticut
Storrs, Connecticut 06269-3060
(Dated: March 31, 2009)

I. SYNOPSIS

The continued fraction method for solving the differential equations of quantum mechanics is not well known, but since the method is used to deal with tunneling problems and the Mathieu Equation, it makes sense to familiarize ourselves with the method, in a non-rigorous manner.

II. HERMITE'S DIFFERENTIAL EQUATION

Hermite polynomials are usually generated using the differential equation and a power series Ansatz which requires truncation. An alternative approach is presented here.

Hermite's differential equation is

$$\frac{\partial^2 y}{\partial x^2} - 2x\frac{\partial y}{\partial x} + 2\alpha y = 0 \tag{2.1}$$

which we rewrite as

$$y'' - 2xy' + 2\alpha y = 0$$

using the "prime" notation scheme, i.e.,

$$y' = \frac{\partial y}{\partial x}$$

$$y'' = \frac{\partial^2 y}{\partial x^2}$$

etc.. Dividing both sides by y' and transposing one term one obtains

$$\frac{y''}{y'} - 2x\frac{y'}{y'} + 2\alpha\frac{y}{y'} = 0$$

i.e.,

$$\frac{y''}{y'} - 2x = -2\alpha\frac{y}{y'}$$

which we solve for $\frac{y'}{y}$ thusly:

$$\frac{y'}{y} = \frac{\partial \ell n y}{\partial x} = (-2\alpha)\frac{1}{\frac{y''}{y'} - 2x}$$

$$\frac{\partial \ell n y}{\partial x} = \frac{2\alpha}{2x - \frac{y''}{y'}} \tag{2.2}$$

Next, taking the derivative of Equation 2.1

$$\frac{\partial\left(\frac{\partial^2 y}{\partial x^2} - 2x\frac{\partial y}{\partial x} + 2\alpha y = 0\right)}{\partial x} = \frac{\partial\left(y'' - 2xy' + 2\alpha y = 0\right)}{\partial x} \tag{2.3}$$

we obtain

$$y''' - 2y' - 2xy'' + 2\alpha y' = 0 \tag{2.4}$$

and dividing byy'' we obtain

$$\frac{y'''}{y''} + (2\alpha - 2)\frac{y'}{y''} - 2x = 0$$

which we solve for $\frac{y''}{y'}$ which we need in the denominator of Equation 2.2:

$$\frac{y''}{y'} = \frac{2(\alpha - 1)}{2x - \frac{y'''}{y''}}$$

Substituting into Equation 2.2, we have

$$\frac{\partial \ell n y}{\partial x} = \frac{2\alpha}{2x - \frac{2(\alpha-1)}{2x - \frac{y'''}{y''}}} \tag{2.5}$$

Is it clear that we will now take the derivative of Equation 2.4, i.e.,

$$\frac{d\left(y''' + (2\alpha - 2)y' - 2xy''\right)}{dx} = 0 \tag{2.6}$$

obtaining

$$y^{iv} + (2\alpha - 2)y'' - 2y'' - 2xy''' = 0 \tag{2.7}$$

i.e.,

$$y^{iv} + (2\alpha - 4)y'' - 2xy''' = 0$$

which we solve

$$\frac{y^{iv}}{y'''} + (2\alpha - 4)\frac{y''}{y'''} - 2x = 0$$

so,

$$\frac{y'''}{y''} = \frac{2\alpha - 4}{2x - \frac{y^{iv}}{y''}}$$

*Electronic address: Carl.David@uconn.edu

Typeset by REVTEX

Using this in Equation 2.5 we obtain

$$\frac{\partial \ell ny}{\partial x} = \frac{2\alpha}{2x - \frac{2(\alpha-1)}{2x - \frac{2\alpha-4}{2x - \frac{y^{iv}}{y''}}}} \tag{2.8}$$

It is obvious what is going on. The process is going to continue forever. It is also obvious, the numerators in each cascading term can individually be set equal to zero, thereby terminating the continued fraction. There is an infinite set of such terminating conditions, i.e., $\alpha = 0$, $\alpha = 1$, $\alpha = 2$, etc., etc., etc..

If $\alpha = 0$ we have

$$\frac{\partial \ell ny}{\partial x} = 0 \tag{2.9}$$

which means, upon integration

$$\ell ny = \ell n C_1 \tag{2.10}$$

where C_1' is a constant of integratation (so that $\ell n C_1$ is also a constant).

If $\alpha = 1$ then we have

$$\frac{\partial \ell ny}{\partial x} = \frac{2}{2x - 0} \tag{2.11}$$

which means that, integrating

$$\ell ny = \ell nx + \ell n C_1$$

or

$$y = C_1 x$$

again, where C_1 is some constant of integration.

We will do one more, just to make sure all is clear. If $\alpha = 2$ we have

$$\frac{\partial \ell ny}{\partial x} = \frac{2\alpha}{2x - \frac{2(\alpha-1)}{2x - \frac{2\times 2-4}{2x - \frac{y^{iv}}{y''}}}} \tag{2.12}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{2\alpha}{2x - \frac{2(\alpha-1)}{2x-0}} \tag{2.13}$$

which is

$$\frac{\partial \ell ny}{\partial x} = \frac{(2\alpha)(2x)}{(2x)^2 - 2(1)} \tag{2.14}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{4\alpha x}{2(2x^2 - 1)} \tag{2.15}$$

which is, defining $u = 2x^2 - 1$, so that $du = 4xdx$, we have

$$\frac{\partial \ell ny}{\partial x} = \frac{\alpha}{2}\frac{4x}{(2x^2 - 1)} \tag{2.16}$$

$$\int d\ell ny = \frac{\alpha}{2}\int \frac{4xdx}{(2x^2 - 1)} = \frac{\alpha}{2}\int \frac{du}{u} \tag{2.17}$$

which leads to

$$\ell ny = \frac{\alpha}{2}\ell nu + \ell n C = \frac{\alpha}{2}\ell n(2x^2 - 1) + \ell n C \tag{2.18}$$

i.e.,

$$y = \frac{\alpha C}{2}(2x^2 - 1) = C'(2x^2 - 1)$$

which is Hermite's Polynomial of Order 2. To make sure that this is true, we substitute this solution into Hermite's differential equation, (Equation 2.1):

$$\begin{aligned} y'' &= 4 \\ -2xy' &= -2x(4x) \\ 2\alpha y &= 2\alpha(2x^2 - 1) \\ 0 &= ? \end{aligned}$$

which, of course, equals zero upon adding. Not so fast. What we have is, on the l.h.s. $y'' - 2xy' + 2\alpha y = 0$ but, on the r.h.s we have

$$4 - 2x(4x) + 2\alpha(2x^2 - 1)$$

which is

$$4 - 8x^2 + 4\alpha x^2 - 2\alpha$$

which, if $\alpha = 2$ is zero! Note also, that the constant, C', is irrelevant for this demonstration. (Why?)

III. LEGENDRE'S DIFFERENTIAL EQUATION

Legendre polynomials are usually generated using the differential equation and a power series Ansatz which requires truncation. An alternative approach is presented here.

Legendre's differential equation is

$$(1 - x^2)\frac{\partial^2 y}{\partial x^2} - 2x\frac{\partial y}{\partial x} + \ell(\ell + 1)y = 0 \tag{3.1}$$

which we rewrite as

$$(1 - x^2)y'' - 2xy' + \ell(\ell + 1)y = 0$$

using the "prime" notation scheme, i.e.,

$$y' = \frac{\partial y}{\partial x}$$

$$y'' = \frac{\partial^2 y}{\partial x^2}$$

etc.. Dividing both sides by y' and transposing one term one obtains

$$(1-x^2)\frac{y''}{y'} - 2x\frac{y'}{y'} + \ell(\ell+1)\frac{y}{y'} = 0$$

i.e.,

$$(1-x^2)\frac{y''}{y'} - 2x = -\ell(\ell+1)\frac{y}{y'}$$

which we solve for $\frac{y'}{y}$ thusly:

$$\frac{y'}{y} = \frac{\partial \ell n(y)}{\partial x} = \frac{(-\ell(\ell+1))}{(1-x^2)\frac{y''}{y'} - 2x} \tag{3.2}$$

Next, taking the derivative of Equation 3.1

$$= \frac{\partial\left((1-x^2)y'' - 2xy' + \ell(\ell+1)y = 0\right)}{\partial x} \tag{3.3}$$

we obtain

$$(1-x^2)y''' - 2xy'' - 2y' - 2xy'' + \ell(\ell+1)y' = 0 \tag{3.4}$$

i.e.,

$$(1-x^2)y''' - 4xy'' + (\ell(\ell+1)-2)y' = 0$$

and dividing byy'' we obtain

$$(1-x^2)\frac{y'''}{y''} + (\ell(\ell+1)-2)\frac{y'}{y''} - 4x = 0$$

which we solve for $\frac{y''}{y'}$ which we need in the denominator of Equation 3.2:

$$\frac{y''}{y'} = \frac{\ell(\ell+1)-2)}{4x - (1-x^2)\frac{y'''}{y''}}$$

Substituting into Equation 3.2, we have

$$\frac{\partial \ell ny}{\partial x} = \frac{\ell(\ell+1)}{2x - (1-x^2)\frac{\ell(\ell+1)-2}{4x-(1-x^2)\frac{y'''}{y''}}} \tag{3.5}$$

Is it clear that we will now take the derivative of Equation 3.4, i.e.,

$$\frac{d\left((1-x^2)y''' - 4xy'' + (\ell(\ell+1)-2)y' = 0\right)}{dx} = 0 \tag{3.6}$$

obtaining

$$(1-x^2)y^{iv} - 2xy''' + (\ell(\ell+1)-2)y'' - 4y'' - 4xy''' = 0 \tag{3.7}$$

i.e.,

$$(1-x^2)y^{iv} + (\ell(\ell+1)-2)y'' - 4y'' - 6xy''' = 0$$

i.e.,

$$(1-x^2)y^{iv} + (\ell(\ell+1)-4)y'' - 6xy''' = 0$$

which we solve

$$(1-x^2)\frac{y^{iv}}{y'''} + (\ell(\ell+1)-6)\frac{y''}{y'''} - 6x = 0$$

so,

$$\frac{y'''}{y''} = \frac{\ell(\ell+1)-6}{6x - (1-x^2)\frac{y^{iv}}{y''}}$$

Using this in Equation 3.5 we obtain

$$\frac{\partial \ell ny}{\partial x} = \frac{\ell(\ell+1)}{2x - (1-x^2)\frac{\ell(\ell+1)-2}{4x-(1-x^2)\frac{\ell(\ell+1)-6}{6x-(1-x^2)\frac{y^{iv}}{y'''}}}} \tag{3.8}$$

It is obvious what is going on. The process is going to continue forever. It is also obvious, the numerators in each cascading term can individually be set equal to zero, thereby terminating the continued fraction. There is an infinite set of such terminating conditions, i.e., $\ell(\ell+1) = 0$, $\ell(\ell+1) = 1$, $\ell(\ell+1) = 2$, etc., etc., etc.. If $\ell(\ell+1) = 0$ we have

$$\frac{\partial \ell ny}{\partial x} = 0 \tag{3.9}$$

which means, upon integration

$$\ell ny = \ell nC_2 \tag{3.10}$$

where C_2 is a constant of integratation (so that ℓnC_2 is also a constant).

If $\ell(\ell+1) = 2$ (i.e., ℓ=1) then we have

$$\frac{\partial \ell ny}{\partial x} = \frac{2}{2x - 0(1-x^2)}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{1}{x} \tag{3.11}$$

which means that, integrating

$$\ell ny = \ell nx + \ell nC_2$$

or

$$y = C_2 x$$

again, where C_2 is some constant of integration.

We will do one more, just to make sure all is clear. If $\ell(\ell+1) = 6$ (i.e., $\ell = 2$), we have

$$\frac{\partial \ell ny}{\partial x} = \frac{6}{2x - (1-x^2)\frac{(2(2+1)-2)}{4x-(1-x^2)\frac{2\times 3-6}{6x-\frac{y^{iv}}{y''}}}}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{6}{2x - (1-x^2)\frac{(6-2)}{4x-(1-x^2)\frac{0}{6x-\frac{y^{iv}}{y'''}}}} \tag{3.12}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{6}{4x - (1-x^2)\frac{4}{4x-0}} \tag{3.13}$$

which is (moving to common denominators)

$$\frac{\partial \ell ny}{\partial x} = \frac{(6)(4x)}{(2x)(4x) - 4(1-x^2)} \tag{3.14}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{24x}{12x^2 - 4} \tag{3.15}$$

which is, defining $u = 3x^2 - 1$ so that $du = 6xdx$, we have

$$\frac{\partial \ell ny}{\partial x} = \frac{du}{u} \tag{3.16}$$

which leads to

$$\ell ny = \ell n(3x^2 - 1) + \ell nC \tag{3.17}$$

i.e.,

$$y = C(3x^2 - 1)$$

which is Legendre's Polynomial of Order 2. To make sure that this is true, we substitute this solution into Legendre's differential equation, (Equation 3.1):

$$\begin{aligned}
(1-x^2)y'' &= (1-x^2)6 = 6 - \cancel{6x^2} \\
-2xy' &= -2x(6x) = -\cancel{12x^2} \\
2\ell(\ell+1)y &= 2(1)(2+1)(3x^2-1) = \cancel{18x^2} - 6 \\
0 &= ?
\end{aligned}$$

which equals zero upon adding (when ℓ=2).. Note also, that the constant, C, is irrelevant for this demonstration. (Why?)

IV. LAGUERRE'S DIFFERENTIAL EQUATION

Laguerre polynomials associated with the radial solution to the Schrödinger Equation for the H atom's electron are usually generated using the differential equation and a power series Ansatz which requires truncation.

Laguerre's differential equation is

$$x\frac{\partial^2 y}{\partial x^2} + (1-x)\frac{\partial y}{\partial x} + \alpha y = 0 \tag{4.1}$$

which we rewrite as

$$xy'' + (1-x)y' + \alpha y = 0 \tag{4.2}$$

Dividing both sides by y'

$$x\frac{y''}{y'} + (1-x)\frac{y'}{y'} + \alpha\frac{y}{y'} = 0$$

and transposing one obtains

$$\frac{y'}{y} = \frac{\alpha}{(x-1) - x\frac{y''}{y'}} \tag{4.3}$$

Next, taking the derivative of Equation 4.2

$$\frac{\partial\left(xy'' + (1-x)y' + \alpha y = 0\right)}{\partial x} \tag{4.4}$$

we obtain

$$\begin{aligned}
xy''' + y'' - y' + (1-x)y'' + \alpha y' &= 0 \\
= xy''' + (2-x)y'' + (\alpha-1)y' &= 0
\end{aligned} \tag{4.5}$$

and dividing by y'' we obtain

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

which we solve for $\frac{y''}{y'}$ which we need in the denominator of Equation 4.3:

$$\frac{y''}{y'} = \frac{(1-\alpha)}{(2-x) + x\frac{y'''}{y''}} = \frac{(\alpha-1)}{(x-2) - x\frac{y'''}{y''}}$$

Substituting into Equation 4.3, we have

$$\frac{y'}{y} = \frac{\alpha}{(x-1) - x\frac{(\alpha-1)}{(x-2)-x\frac{y'''}{y''}}} \tag{4.6}$$

Is it clear that we will now take the derivative of Equation 4.5, i.e.,

$$\frac{d\left(xy''' + (2-x)y'' + (\alpha-1)y'\right)}{dx} = 0 \tag{4.7}$$

obtaining

$$xy^{iv} + y''' - y'' + (2-x)y''' + (\alpha-1)y'' = 0 \tag{4.8}$$

i.e.,

$$xy^{iv} + (3-x)y'''(\alpha-2)y'' = 0$$

which we solve

$$\frac{y^{iv}}{y'''} + (\alpha-2)\frac{y''}{y'''} + 3 - x = 0$$

so,

$$\frac{y'''}{y''} = \frac{\alpha-2}{(x-3) - x\frac{y^{iv}}{y''}}$$

Using this in Equation 4.6 we obtain

$$\frac{y'}{y} = \frac{\alpha}{(x-1) - x\frac{(\alpha-1)}{(x-2)-x\frac{(\alpha-2)}{(x-3)-x\frac{y''}{y'''}}}} \tag{4.9}$$

It is obvious what is going on. The process is going to continue forever. It is also obvious, the numerators in each cascading term can individually be set equal to zero, thereby terminating the continued fraction. There is an infinite set of such terminating conditions, i.e., $\alpha = 0$, $\alpha = 1$, $\alpha = 2$, etc., etc., etc..

If $\alpha = 0$ we have

$$\frac{\partial \ell ny}{\partial x} = 0 \tag{4.10}$$

which means, upon integration

$$\ell ny = \ell nC \tag{4.11}$$

where C is a constant of integratation (so that ℓnC is also a constant).

If $\alpha = 1$ then we have

$$\frac{\partial \ell ny}{\partial x} = \frac{1}{(x-1)} \tag{4.12}$$

which means that, integrating

$$\ell ny = \ell n(x-1) + \ell nC$$

or

$$y = C(x-1)$$

again, where C is some constant of integration.

We will do one more, just to make sure all is clear. If $\alpha = 2$ we have

$$\frac{y'}{y} = \frac{2}{(x-1) - x\frac{(2-1)}{(x-2)-x\frac{(2-2)}{(x-3)-x\frac{y''}{y'''}}}} = \frac{2}{(x-1) - x\frac{(2-1)}{(x-2)}} \tag{4.13}$$

$$\frac{y'}{y} = \frac{2(x-2)}{(x-1)(x-2) - x} \tag{4.14}$$

which is

$$\frac{d\ell ny}{dx} = \frac{2(x-2)}{x^2 - 4x + 2} \tag{4.15}$$

$$\frac{\partial \ell ny}{\partial x} = \frac{du}{u} \tag{4.16}$$

which is, defining $u = x^2 - 4x + 2$ so that $du = (2x-4)dx$, we have

$$\int d\ell ny = \int \frac{du}{u} \tag{4.17}$$

which leads to

$$\ell ny = \ell nu + \ell nC = \ell nC((x^2 - 4x + 2)) \tag{4.18}$$

i.e.,

$$y = C(x^2 - 4x + 2)$$

which is Laguerre's Polynomial of Order 2. To make sure that this is true, we substitute this solution into Laguerre's differential equation, (Equation 4.2):

$$\begin{aligned} xy'' &= 2x \\ (1-2)y' &= (1-x)(2x-4) = 2x - 4 - 2x^2 + 4x \\ \alpha y &= 2(x^2 - 4x + 2) = 2x^2 - 8x + 4 \end{aligned}$$

which, of course, equals zero upon adding.

$$\begin{aligned} xy'' &= 2x \\ (1-2)y' &= (1-x)(2x-4) = 2x - 4 - \cancel{2x^2} + 4x \\ \alpha y &= \cancel{2x^2} - 8x + 4 \end{aligned}$$

which, equals zero upon adding. Note also, that the constant, C', is irrelevant for this demonstration. (Why?)

V. REMARKS

You will have noted how similar the wording is in the three sections treated here. In the original online version(s), using Computer Assisted Reading, they were separated, cloned from an original text with equations changed, but with the layouts left intact. With my retirement, the Computer Assisted Reading sites will be (eventually) dismantled, and to prevent their loss, I've created this document. Readers should be aware that this corresponds to an article I wrote [1] which corresponds to the same material, presented in yet still a different arrangement.

[1] C. W. David, Am. J. Phys., **42**, *228*, 1974