The Harmonic Oscillator's Frobenius Solution

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

Follow this and additional works at: https://opencommons.uconn.edu/chem_educ

Recommended Citation
https://opencommons.uconn.edu/chem_educ/73
I. SYNOPSIS

The Frobenius solution to the differential equation associated with the Harmonic Oscillator is carried out in detail.

II. INTRODUCTION

The Harmonic Oscillator differential equation is (in dimensionless, i.e., textbook, form):

\[ \frac{\partial^2 \psi}{\partial z^2} + (\epsilon - z^2) \psi = 0 \]

and with \( \psi = H(z)e^{-z^2/2} \) we obtain a new differential equation for \( H(z) \) of the form:

\[ \frac{\partial^2 H(z)}{\partial z^2} - 2\epsilon \frac{\partial H(z)}{\partial z} + (\epsilon - 1)H(z) = 0 \]

If \( \epsilon - 1 \equiv n \) then this is called Hermite's differential equation. Assuming

\[ H(z) = \sum_{n=0}^{\infty} a_n z^n \]

i.e.,

\[ H(z) = a_0 + a_1 z + a_2 z^2 + \cdots + a_n z^n + \cdots \]

one obtains a recurrence relation in the standard manner of the form:

\[ \frac{a_{n+2}}{a_n} = \frac{2n - (\epsilon - 1)}{(n + 1)(n + 2)} \quad (2.1) \]

which leads to a solution of the form:

\[ H(z) = a_0 \left( 1 + (1 - \epsilon) \frac{z^2}{2!} + (1 - \epsilon)(5 - \epsilon) \frac{z^4}{4!} + \cdots \right) + a_1 \left( z + (3 - \epsilon) \frac{z^3}{3!} + (3 - \epsilon)(7 - \epsilon) \frac{z^5}{5!} + \cdots \right) \quad (2.2) \]

There are two separate and distinct solutions based on whether \( a_0 \) or \( a_1 \) is chosen to be zero. In other words, we have either an even or an odd solution. In either case, if \( \epsilon = 2n + 1 \) where \( n \) is an integer, the series terminates.

Otherwise, Equation 2.1 shows that

\[ \frac{a_{n+2}}{a_n} \sim \frac{2}{n} \]

as \( n \) grows large, so either series behaves as \( e z^2 \). To see this, create the power series for \( e z^2 \), i.e.,

\[ e^{z^2} = e^{z^2} \mid_{z=0} + \frac{1}{1!} \frac{\partial e^{z^2}}{\partial z} \mid_{z=0} z + \frac{1}{2!} \frac{\partial^2 e^{z^2}}{\partial z^2} \mid_{z=0} z^2 + \frac{1}{3!} \frac{\partial^3 e^{z^2}}{\partial z^3} \mid_{z=0} z^3 + \cdots \]

which, evaluating the partial derivatives,

\[ e^{z^2} = e^{z^2} \mid_{z=0} + \frac{1}{1!} (2z e^{z^2}) \mid_{z=0} z + \frac{1}{2!} (2 + (2z)^2 e^{z^2}) \mid_{z=0} z^2 + \frac{1}{3!} \left( 2z(2 + (2z)^2) + (d (2 + 4z^2) / dz) e^{z^2} \right) \mid_{z=0} z^3 + \cdots \quad (2.3) \]

(for the first step) followed by

\[ e^{z^2} = e^{z^2} \mid_{z=0} + \frac{1}{1!} ((2z) e^{z^2}) \mid_{z=0} z + \frac{1}{2!} ((2 + (2z)^2) e^{z^2}) \mid_{z=0} z^2 + \frac{1}{3!} \left( 2z(2 + (2z)^2) + (d^2 (2 + 4z^2) / dz^2) \right) e^{z^2} \mid_{z=0} z^3 + \cdots \quad (2.4) \]

and then, for the fourth term, we have

\[ e^{z^2} = e^{z^2} \mid_{z=0} + \frac{1}{1!} (2z) e^{z^2} \mid_{z=0} z + \frac{1}{2!} (2 + (2z)^2) e^{z^2} \mid_{z=0} z^2 + \frac{1}{3!} (2z(2 + (2z)^2) + 8z) e^{z^2} \mid_{z=0} z^3 \]
\[ \frac{1}{4!} \left( 2z (2z(2 + (2z)^2) + 8) + \frac{d [12z + 8z^3]}{dz} \right) e^z \bigg|_{z=0} z^4 + \ldots \] 

(2.5)

while for the fifth term, we have

\[ e^z = 1 + \frac{1}{1!} (0)z + \frac{1}{2!} 2z^2 + \frac{1}{3!} (4z + (2z)^3) e^z \bigg|_{z=0} z^3 \]

\[ \frac{1}{4!} \left( 2z (2z(2 + (2z)^2)) + [12 + (3)(8z^2)] \right) e^z \bigg|_{z=0} z^4 \]

\[ \frac{1}{5!} \left( 2z (6(2z)^2 + 4(2z)^3 + 12) + \frac{d [2z (8z + 2z(2 + 4z^2)) + (8 + 4 + 16z)]}{dz} \right) e^z \bigg|_{z=0} z^5 \]

\[ \frac{1}{6!} \left( 2z (2z(2z (8z + 2z(2 + 4z^2)) + (8 + 4 + 16z)) + 32 + 18z + 168z^2 + 16) e^z \right) \bigg|_{z=0} z^6 + \ldots \] 

(2.6)

At this point, it is getting complicated, and, in fact, if some reader can show me a better typographical way of showing the progression of terms which properly points to the \((2z)^n\) terms dominating, I would greatly appreciate it. For what it’s worth, here is my attempt, clearly faulty(!):

\[ e^z = 1 + \frac{1}{1!} 2z^2 + \frac{1}{3!} (0)e^z \bigg|_{z=0} z^3 \]

\[ \frac{1}{4!} \left( 12 + 48z^2 + 16z^4 \right) e^z \bigg|_{z=0} z^4 \]

\[ \frac{1}{5!} \left( 2z(2z (8z + 2z(2 + 4z^2)) + (8 + 4 + 16z)) + 32 + 18z + 168z^2 + 16 \right) e^z \bigg|_{z=0} z^5 \]

\[ \frac{1}{6!} \left( 2z(2z(2z (8z + 2z(2 + 4z^2)) + (8 + 4 + 16z)) + 32 + 18z + 168z^2 + 16) e^z \right) \bigg|_{z=0} z^6 + \ldots \] 

(2.7)

or

\[ e^z = 1 + 0z + \frac{1}{2!} 2z^2 + \frac{1}{3!} (0)e^z \bigg|_{z=0} z^3 \]

\[ \frac{1}{4!} (12) z^4 \]

\[ \frac{1}{5!} \left( 4(az)^3 + 2(2z)^4 + (2z)^5 \right) e^z \bigg|_{z=0} z^5 \]

\[ \frac{1}{6!} \left( 2z(2z(2z (8z + 2z(2 + 4z^2)) + (8 + 4 + 16z)) + 32 + 18z + 168z^2 + 16) e^z \right) \bigg|_{z=0} z^6 + \ldots \] 

(2.8)

which becomes, when looking solely at the highest powers of 2z,

\[ e^z = 1 + \frac{1}{1!} 0z + \frac{1}{2!} 2z^2 + \frac{1}{3!} 0z^3 + \frac{1}{4!} 12z^4 + \ldots + \frac{1}{k!} 2^k z^k + \ldots \]

where \(k\) is even. Adjacent terms of this expansion would now appear as

\[ \frac{1}{(k+2)!} 2^{k+2} \rightarrow \frac{2^k}{k} \]

which is the same as the \(\frac{2}{n}\) term for \(H(z)\).

This result implies that the power series for \(H(z)\) would overpower the exponential decay term \(e^{-z^2/2}\) appended to \(H(z)\) to create \(\psi\). Thus we would have an un-normalizable wave function, which is prohibited by the rules.

We conclude that the infinite series can not be infinite, i.e., it must be truncated to a polynomial.

Then we might have, for the even terms, \((1 - \epsilon) = 0\) or \((1 - \epsilon)(5 - \epsilon) = 0\) or \((1 - \epsilon)(5 - \epsilon)(9 - \epsilon) = 0\) etc., while for the odd terms, we might have \((3 - \epsilon) = 0\) or \((3 - \epsilon)(7 - \epsilon) = 0\) or \((3 - \epsilon)(7 - \epsilon)(11 - \epsilon) = 0\), etc.

This implies that \(2n + 1 - \epsilon = 0\) with \(n = 0, 2, 4, 6\), etc.,
on the even side, and \( n = 1, 3, 5, 7, \) etc., on the odd side, would force the numerators (and all following terms) to zero, thereby truncating the series into a polynomial. 

Et Voila!