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The Harmonic Oscillator, The Hermite Polynomial Solutions

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I. SYNOPSIS

The Harmonic Oscillator’s Quantum Mechanical solution involves Hermite Polynomials, which are introduced here in various guises any one of which the reader may find useful as a starting point.

II. WRITING THE SCHRÖDINGER EQUATION IN DIMENSIONLESS FORM

The relevant Schrödinger Equation is

\[-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial z^2} \psi + \frac{k}{2} z^2 \psi = E \psi\]  

(2.1)

where \(k\) is the force constant (dynes/cm) and \(\mu\) is the reduced mass (grams). Cross multiplying, one has

\[-\frac{\partial^2}{\partial z^2} \psi - \frac{k\mu}{\hbar^2} z^2 \psi = -\frac{2\mu}{\hbar^2} E \psi\]  

(2.2)

which would be simplified if the constants could be suppressed. To do this we change variable, from \(z\) to something else, say \(x\), where \(z = \alpha x\). Then

\[\frac{\partial}{\partial z} = \frac{\partial x \partial}{\partial z \partial x} = \frac{1}{\alpha} \frac{\partial}{\partial x}\]

so

\[\left(\frac{1}{\alpha^2}\right) \frac{\partial^2}{\partial x^2} \psi - \frac{k\mu}{\hbar^2} \alpha^2 x^2 \psi = -\frac{2\mu}{\hbar^2} E \psi\]  

(2.3)

and

\[\frac{\partial^2}{\partial x^2} \psi - \frac{k\mu}{\hbar^2} \alpha^4 x^2 \psi = -\alpha^2 \frac{2\mu}{\hbar^2} E \psi\]  

(2.4)

which demands that we treat

\[1 = \frac{k\mu}{\hbar^2} \alpha^4\]

\[\alpha = \left(\frac{1}{\frac{k\mu}{\hbar^2}}\right)^{1/4} = \left(\frac{\hbar^2}{k\mu}\right)^{1/4}\]

With this choice, the differential equation becomes

\[\frac{\partial^2 \psi}{\partial x^2} - x^2 \psi = -\epsilon \psi\]  

(2.5)

where

\[\epsilon = \frac{2\alpha^2 \mu E}{\hbar^2} = 2\sqrt{\frac{\epsilon}{k\mu \hbar^2}} = \frac{2E\sqrt{\epsilon}}{\hbar}\]

III. GUESSWORK FOR THE GROUND STATE

The easiest solution to this differential equation is

\[e^{-\frac{x^2}{\epsilon}}\]

which leads to

\[E = \frac{\hbar}{2\sqrt{\mu}} \frac{k}{\hbar}\]

IV. A GENERATING FUNCTION SCHEME

Given

\[\psi_0 = |0\rangle = e^{-\frac{x^2}{\epsilon}}\]

with \(\epsilon = 1\), it is possible to generate the next solution by using

\[N^+ = -\frac{\partial}{\partial x} + x\]  

(4.1)

as an operator, which ladders up from the ground \((n=0)\) state to the next one \((n=1)\) To see this we apply \(N^+\) to \(\psi_0\) obtaining

\[N^+ \psi_0 = N^+ |0\rangle = \left(-\frac{\partial}{\partial x} + x\right) e^{-\frac{x^2}{\epsilon}} = -(-x) \psi_0 + x \psi_0 = 2x e^{-x^2/2} = \psi_1 = |1\rangle\]  

(4.2)

Typeset by REVTEx
Doing this operation again, one has

\[
N^+\psi_1 = N^+|1 > = \left( -\frac{\partial}{\partial x} + x \right) 2xe^{-x^2} = (-2 + 4x^2)e^{-x^2/2}
\]

(4.3)

eq., etc., etc.

V. HERMITE POLYNOMIAL DEFINITION

Assuming

\[
\psi = e^{-x^2/2}H(x)
\]

one then has

\[
\frac{d\psi}{dx} = -xe^{-x^2/2}H(x) + e^{-x^2/2}\frac{dH(x)}{dx}
\]

From Equation 2.5 one has,

\[
\frac{\partial^2 \psi}{\partial x^2} - x^2\psi = -e^{-x^2/2}H(x) \left( -2 + 4x^2 \right) e^{-x^2/2} + e^{-x^2/2}\frac{d^2H(x)}{dx^2}
\]

(5.1)

or

\[
-H(x) - 2\frac{dH(x)}{dx} + \frac{d^2H(x)}{dx^2} = -\epsilon H(x)
\]

(5.2)

which we re-write in normal lexicographical order

\[
\frac{d^2H(x)}{dx^2} - 2\frac{dH(x)}{dx} - (1 - \epsilon)H(x) = 0
\]

(5.3)

This is Hermite’s differential equation.

VI. GENERATING HERMITE’S DIFFERENTIAL EQUATION

Starting with

\[
\frac{dy}{dx} + 2xy = 0
\]

(6.1)

We now differentiate Equation 6.1, obtaining

\[
\frac{d^2y}{dx^2} + 2\frac{d(xy)}{dx} = \frac{d^2y}{dx^2} + 2x \frac{dy}{dx} + 2y \frac{dx}{dy} = \frac{d^2y}{dx^2} + 2x \frac{dy}{dx} + 2y = 0 ; n = 0
\]

(6.2)

Doing this again, i.e., differentiating this (second) equation (Equation 6.2), one has

\[
\frac{d^3y}{dx^3} + 2\frac{d(xy)}{dx} + 2\frac{dy}{dx} = \frac{d^3y}{dx^3} + 2x \frac{dy}{dx} + 2y \frac{dx}{dy} = \frac{d^3y}{dx^3} + 2x \frac{dy}{dx} + 4 \frac{dy}{dx} = 0 ; n = 1
\]

(6.3)

which is the same equation, (but with a 4 multiplier of the last term) applied to the first derivative of y. Take
the derivative again:
\[
\frac{d}{dx} \left( d^2 \frac{dy}{dx^2} + 2x \frac{dy}{dx} + 4 \frac{dy}{dx} \right) = 0
\]
i.e.,
\[
\frac{d^2 y}{dx^2} + 2x \frac{dy}{dx} + 6 \left( \frac{dy}{dx} \right) = 0
\]
i.e.,
\[
\frac{d^2 f(x)}{dx^2} + 2x \frac{df(x)}{dx} + 6f(x) = 0; \quad n = 2
\]
which leads to
\[
(g''(x) - 4xg'(x) - 2g(x) + 4x^2g(x) + 2xg'(x) - 4x^2g(x) + 2(n+1)g(x)) e^{-x^2} = 0
\]
or
\[
g''(x) - 2xg'(x) + 2ng(x) = 0
\]
and we had
\[
H''(x) - 2xH'(x) - (1 - \epsilon)H(x) = 0
\]
which leads to
\[
2n = -1 + \epsilon
\]
i.e.,
\[
\epsilon = 1 + 2n = \frac{2E\sqrt{\mu/k}}{h}
\]
i.e.,
\[
E = h(n + \frac{1}{2}) \sqrt{\frac{k}{\mu}}
\]

VII. FROBENIUS, BRUTE FORCE, METHODOLOGY

The most straightforward technique for handling the Hermite differential equation is the method of Frobenius. We assume a power series Ansatz (ignoring the indicial equation argument here), i.e.,
\[
\psi = \sum_{i=0} a_i x^i
\]
and substitute this into Equation 5.3, obtaining
\[
\frac{\partial^2 \psi}{\partial x^2} = \sum_{i=2} i(i-1)a_i x^{i-2}
\]
\[-2x \frac{\partial \psi}{\partial x} = -2 \sum_{i=1} ia_i x^i
\]
\[(\epsilon - 1)\psi = (\epsilon - 1) \sum_i a_i x^i = 0
\]
f(x) has the form \( g(x)e^{-x^2} \) where \( g(x) \) is a polynomial in \( x \).
\[
\frac{d^2 g(x)e^{-x^2}}{dx^2} + 2x \frac{dg(x)e^{-x^2}}{dx} + 2(n+1)g(x)e^{-x^2} = 0
\]
i.e.,
\[
\frac{\partial^2 \psi}{\partial x^2} = 2(1)a_2 + (3)(2)a_3x + (4)(3)a_4x^2 + \cdots
\]
\[-2x \frac{\partial \psi}{\partial x} = -2a_1x - 2a_2x^2 - 2a_3x^3 - \cdots
\]
\[(\epsilon - 1)\psi = (\epsilon - 1)a_0 + (\epsilon - 1)a_1x + (\epsilon - 1)a_2x^2 - \cdots = 0
\]
which leads to
\[
(2)(1)a_2 + (\epsilon - 1)a_0 = 0 \text{ (even)}
\]
\[(3)(2)a_3 + (\epsilon - 1)a_1 - 2a_1 = 0 \text{ (odd)}
\]
\[(4)(3)a_4 - 2a_2 + (\epsilon - 1)a_2 = 0 \text{ (even)}
\]
\[(5)(4)a_5 - 2a_3 + (\epsilon - 1)a_3 = 0 \text{ (odd)}
\]
which shows a clear division between the even and the odd powers of \( x \). We can solve these equations sequentially.

We obtain
\[
a_2 = \frac{1 - \epsilon}{(2)(1)}
\]
\[
a_3 = \frac{2 + 1 - \epsilon}{(3)(2)} a_1
\]
\[
a_4 = \frac{2 + 1 - \epsilon}{(4)(3)} a_2 = \left( \frac{2 + 1 - \epsilon}{(4)(3)} \right) \left( \frac{1 - \epsilon}{(2)(1)} \right)
\]
i.e.,
\[
a_4 = \left( \frac{3 - \epsilon(1 - \epsilon)}{(4)(3)(2)(1)} \right)
\]
etc.

This set of even (or odd) coefficients leads to a series which itself converges unto a function which grows to positive infinity as $x$ varies, leading one to require that the series be terminated, becoming a polynomial.

We leave the rest to you and your textbook.