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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 points.

II. WRITING THE SCHRÖDINGER EQUATION IN DIMENSIONLESS FORM

The relevant Schrödinger Equation is

$$-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial z^2} \psi + \frac{k}{2} z^2 \psi = E \psi \quad (2.1)$$

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

$$\frac{\partial^2}{\partial z^2} \psi - \frac{k\mu}{\hbar^2} z^2 \psi = -\frac{2\mu}{\hbar^2} E \psi \quad (2.2)$$

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

$$\frac{\partial}{\partial z} = \frac{\partial x}{\partial z} \frac{\partial}{\partial x} = \frac{1}{\alpha} \frac{\partial}{\partial x}$$

so

$$\left(\frac{1}{\alpha^2} \right) \frac{\partial^2}{\partial x^2} \psi - \frac{k\mu}{\hbar^2} \alpha^2 x^2 \psi = -\frac{2\mu}{\hbar^2} E \psi \quad (2.3)$$

and

$$\frac{\partial^2}{\partial x^2} \psi - \frac{k\mu}{\hbar^2} \alpha^4 x^2 \psi = -\alpha^2 \frac{2\mu}{\hbar^2} E \psi \quad (2.4)$$

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

$$\frac{\partial^2 \psi}{\partial x^2} - x^2 \psi = -\epsilon \psi \quad (2.5)$$

where

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

III. GUESSWORK FOR THE GROUND STATE

The easiest solution to this differential equation is

$$e^{-\frac{x^2}{2}}$$

which leads to

$$E = \frac{\hbar}{2} \sqrt{\frac{k}{\mu}}$$

IV. A GENERATING FUNCTION SCHEME

Given

$$\psi_0 = |0\rangle = e^{-\frac{x^2}{2}}$$

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

$$N^+ = -\frac{\partial}{\partial x} + x \quad (4.1)$$

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 ψ_0 obtaining

$$N^+ \psi_0 = N^+ |0\rangle = \left(-\frac{\partial}{\partial x} + x \right) e^{-\frac{x^2}{2}} = -(-x) \psi_0 + x \psi_0 = 2x e^{-x^2/2} = \psi_1 = |1\rangle \quad (4.2)$$

Doing this operation again, one has

$$N^+\psi_1 = N^+|1\rangle = \left(-\frac{\partial}{\partial x} + x\right)2xe^{-x^2/2} = (-2 + 4x^2)e^{-x^2/2} \quad (4.3)$$

etc., etc., etc..

where $H(x)$ is going to become a Hermite polynomial. One then has

V. HERMITE POLYNOMIAL DEFINITION

Assuming

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

and

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

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

From Equation 2.5 one has,

$$\frac{\partial^2\psi}{\partial x^2} - x^2\psi = -e^{-x^2/2}H(x) - 2xe^{-x^2/2}\frac{dH(x)}{dx} + e^{-x^2/2}\frac{d^2H(x)}{dx^2} = -\epsilon e^{-x^2/2}H(x) \quad (5.1)$$

or

$$-H(x) - 2x\frac{dH(x)}{dx} + \frac{d^2H(x)}{dx^2} = -\epsilon H(x) \quad (5.2)$$

one has

$$\frac{dy}{y} = -2xdx$$

which we re-write in normal lexicographical order

$$\frac{d^2H(x)}{dx^2} - 2x\frac{dH(x)}{dx} - (1 - \epsilon)H(x) = 0 \quad (5.3)$$

so, integrating each side separately, one has

$$\ln y = -x^2 + \ln C$$

This is Hermite's differential equation.

or, inverting the logarithm,

$$y = Ce^{-x^2}$$

VI. GENERATING HERMITE'S DIFFERENTIAL EQUATION

Starting with

$$\frac{dy}{dx} + 2xy = 0 \quad (6.1)$$

We now differentiate Equation 6.1, obtaining

$$\frac{d^2y}{dx^2} + 2\frac{d(xy)}{dx} = \frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + 2y\frac{dx}{dx} = \frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + 2y = 0; n = 0 \quad (6.2)$$

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

$$\frac{d^2\frac{dy}{dx}}{dx} + \frac{d2x\frac{d(y)}{dx}}{dx} + 2\frac{dy}{dx} = \frac{d^2\left(\frac{dy}{dx}\right)}{dx^2} + 2x\frac{d\left(\frac{dy}{dx}\right)}{dx} + 4\left(\frac{dy}{dx}\right) = 0; n = 1$$

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:

$$\frac{d \left(\frac{d^2 \frac{dy}{dx}}{dx^2} + 2x \frac{d \frac{dy}{dx}}{dx} + 4 \frac{dy}{dx} \right)}{dx} = 0$$

i.e.,

$$\frac{d^2 \left(\frac{d^2 y}{dx^2} \right)}{dx^2} + 2x \frac{d \left(\frac{d^2 y}{dx^2} \right)}{dx} + 6 \left(\frac{d^2 y}{dx^2} \right) = 0$$

$$\frac{d^2 f(x)}{dx^2} + 2x \frac{df(x)}{dx} + 6f(x) = 0; n = 2$$

$f(x)$ 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.,

$$(g''(x) - 4xg'(x) - 2g(x) + 4x^2g(x) + 2xg'(x) - 4x^2g(x) + 2(n+1)g(x))e^{-x^2} = 0$$

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.,

$$\epsilon = 1 + 2n = \frac{2E\sqrt{\mu/k}}{\hbar}$$

i.e.,

$$E = \hbar \left(n + \frac{1}{2} \right) \sqrt{\frac{k}{\mu}}$$

VII. FROBENIUS, BRUTE FORCE, METHODOLOGY

The most straight forward 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.,

$$\psi = \sum_{i=0}^{\infty} a_i x^i$$

and substitute this into Equation 5.3, obtaining

$$\begin{aligned} \frac{\partial^2 \psi}{\partial x^2} &= \sum_{i=2}^{\infty} i(i-1)a_i x^{i-2} \\ -2x \frac{\partial \psi}{\partial x} &= -2 \sum_{i=1}^{\infty} i a_i x^i \\ (\epsilon - 1)\psi &= (\epsilon - 1) \sum_i a_i x^i = 0 \end{aligned}$$

i.e.,

$$\frac{\partial^2 \psi}{\partial x^2} = 2(1)a_2 + (3)(2)a_3 x + (4)(3)a_4 x^2 + \dots$$

$$-2x \frac{\partial \psi}{\partial x} = -2a_1 x^1 - 2a_2 x^2 - 2a_3 x^3 - \dots$$

$$(\epsilon - 1)\psi = (\epsilon - 1)a_0 + (\epsilon - 1)a_1 x + (\epsilon - 1)a_2 x^2 - \dots = 0$$

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.