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Eigenenergy values and Eigenfunctions of a one-dimensional quantum mechanical harmonic oscillator

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Abstract: Quantum mechanics is one of the branches of physics. In this mechanics, physical problems are solved by algebraic and analytic methods. By applying a simple procedure we can find the general solutions of Schrodinger's time - independent wave equation of one dimensional quantum mechanical harmonic oscillator without making any approximation. In this paper, we will discuss the Eigenenergy values and Eigenfunctions of one of the most important physical models of quantum mechanics, namely the one-dimensional Quantum mechanical Harmonic Oscillator by modifying the Hermite differential equation.

Key words: Eigenfunctions, Eigenvalues, harmonic oscillator, Hermite polynomials.

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I. INTRODUCTION

Quantum mechanical harmonic oscillator problem is often encountered in many fields of science and engineering. This problem can be solved by a variety of proposed analytical and algebraic methods but they are tedious and apply massive computation. The Quantum mechanical harmonic oscillator is a quantum mechanical analogue of classical harmonic oscillator and is one of the most important physical models in quantum mechanics. An advantage of finding Eigenenergy values and Eigenfunctions of one-dimensional Quantum mechanical Harmonic Oscillator by modifying Hermite differential equation is that it can provide analytical solutions without approximation. Hermite differential equation is a second order linear differential equation. The solution to this equation are referred to as special functions. They are called 'special' as they are different from the standard functions like sine, cosine, exponential, logarithmic etc. To define Eigen values and Eigenfunctions, let us suppose that an operator Ô is applied on the function f to produce same function f multiplied by some constant α i.e.Ô f = α f. In this equation, f is called the Eigenfunction of operator Ô and the constant α is called the Eigen value of the operator Ô associated with the Eigenfunction f. This Equation is called Eigen value equation. The Eigenfunctions are selected from a special class of functions. For example, in bound state problem, all wave functions and their derivatives must be continuous, single valued and finite everywhere. They must also vanish at infinity. Such functions are called as well-behaved functions [1-6]. As an example, to illustrate the Eigen value of an operator, consider the operator $(\frac{\mathrm{d}}{\mathrm{dz}})$ operating on a well – behaved function$\mathrm{e}^{-5\mathrm{z}}$. The result is

$$\frac{\mathrm{d}}{\mathrm{dz}}(\mathrm{e}^{-5\mathrm{z}}) = -5\mathrm{e}^{-5\mathrm{z}}$$

Comparing this equation with standard Eigen value equation Ô f = α f, we find that (-5) is the Eigen value of operator$(\frac{\mathrm{d}}{\mathrm{dz}})$ associated with the Eigenfunction$\mathrm{e}^{-5\mathrm{z}}$.

Hermite differential equation and Hermite polynomials

Consideringadifferential equation of the form:

$$D_z^2 £\,(z) – 2z\, D_z\, £(z) + 2n£\,(z) = 0, \quad D_z \equiv \frac{\partial}{\partial z} \quad (1)$$

Here, £ (z) is a function of real number z.

This equation is second order differential equation and isknown as Hermite differential equation.The solutions of this equation are called Hermite polynomials. These polynomials can be obtained from the function e^{2zh-h^2}. This function isknown as generating function of Hermite polynomials [7-10]. Hermite polynomial is the coefficient of h^n in the expansion of the function e^{2zh-h^2} i.e.

$$e^{2zh-h^2} = \sum_{n=0}^{\infty} \frac{\mathrm{H_n(z)}}{n!} h^n \quad (2)$$

We can prove that Hermite polynomial is the coefficient of h^n in the expansion of the function e^{2zh-h^2} as follows:

We have $e^{2zh-h^2}=e^{2zh}.e^{-h^2}$

Expanding e^{2zh} and e^{-h^2}, we can write

$$e^{2zh-h^2}=\{1+2zh+\frac{(2zh)^2}{2!}+\ldots\ldots+\frac{(2zh)^j}{j!}+\cdots\}.\{1-h^2+\frac{(h^2)^2}{2!}-\ldots\ldots+(-1)^i\frac{(h^2)^i}{i!}+\cdots\}$$

Or

$$e^{2zh-h^2} = \sum_{j,i=0}^{\infty}(-1)^i\frac{(2z)^j}{j!\ i!}h^{j+2i}$$

The coefficient of h^n on right hand side of this equation can be obtained by substituting j +2i = n or j = n – 2i and is given by

$$(-1)^i\frac{(2z)^{n-2i}}{(n-2i)!\ i!}$$

As j ≥ 0, therefore, n – 2i ≥ 0 or i ≥ $\frac{n}{2}$.

Now we can obtain the total coefficient of h^n by summing over all allowed values of i.

Thus coefficient of h^n = $\sum_{i=0}^{\frac{n}{2}}(-1)^i\frac{(2z)^{n-2i}}{(n-2i)!\,i!}$

$$= \sum_{i=0}^{\frac{n}{2}}(-1)^i\frac{n!}{(n-2i)!\ i!}\frac{(2z)^{n-2i}}{n!}$$

$$= \frac{H_n(z)}{n!}$$

Hence we can write:

$$e^{2zh-h^2} = \sum_{n=0}^{\infty}\frac{H_n(z)}{n!}h^n$$

From above discussion, we find that the Hermite polynomial of degree n can be obtained from the formula given by

$$H_n(z) = \sum_{i=0}^{\frac{n}{2}}(-1)^i\frac{n!}{(n-2i)!\ i!}(2z)^{n-2i}$$

Here, n is a positive integer.

This formula can be relabeled as

$$H_n(z) = \sum_{i=0}^{m}(-1)^i\frac{n!}{(n-2i)!\ i!}(2z)^{n-2i}$$

Here, m = n/2 for n even and $\frac{n-1}{2}$ for n odd.

Hermite polynomials can also be directly deduced from an important formula known as Rodrigue's formula [7-10]. This formula is written as

$$H_n(z) = (-1)^n e^{z^2}D_z^n e^{-z^2} (3)$$

Here n is an integer.

We can derive Rodrigue's formula as follows:

Rewrite the generating function (2) as

$$e^{z^2-z^2+2zh-h^2} = \sum_{n=0}^{\infty}\frac{H_n(z)}{n!}h^n$$

$$or \qquad e^{z^2-(z-h)^2} = \sum_{n=0}^{\infty}\frac{H_n(z)}{n!}h^n (4)$$

If we differentiate both sides of this equation partially n times with respect to h and then substitute h =0, we get

$$H_n(z) = [e^{z^2}D_z^n e^{-(z-h)^2}]_{h=0}\ (5)$$

Leth – z = v such that at h=0, v = - z and $D_z^n = D_v^n$, then we can rewrite equation (4) as

$$H_n(z) = [e^{z^2}D_v^n e^{-v^2}]_{v=-z}$$

$$\text{or } H_n(z) = (-1)^n e^{z^2}D_z^n e^{-z^2}$$

This is Rodrigue's formula for Hermite polynomials $H_n(z)$.

Some Hermite polynomials for n=0, 1, 2, 3 are written below:

$$H_0(z) = 1,\ H_1(z) = 2z,\ H_2(z) = 4z^2 - 2,\ H_3(z) = 8z^3 - 12z$$

Hermite polynomials are mutually orthogonal[10-13]with respect to the density or weight function $e^{-z^2}$and the orthogonality of these polynomials can be expressed as:

$$\int_{-\infty}^{\infty} H_n(z)H_m(z)e^{-z^2}dz = 0, \text{for } m \neq n \qquad (6)$$

$$\int_{-\infty}^{\infty} H_n(z)H_m(z)e^{-z^2}dz = \pi^{\frac{1}{2}}2^n n!, \text{for } m = n \qquad (7)$$

Since Hermite polynomials $H_n(z)$ satisfy the equation (1), therefore we can write

$D_z^2 H_n(z) - 2z\, D_z H_n(z) + 2n\, H_n(z) = 0 \qquad (8)$

This equation (8) is known as recurrence relation that Hermite polynomials will satisfy.

Modification of Hermite differential equation

Now consider a well-behaved function of the form:

$$\Psi_n(z) = e^{\frac{-z^2}{2}} H_n(z) \qquad (9)$$

This function approaches to zero when z approaches to infinity. The orthogonality property satisfied by this function is given below:

We can rewrite equations (6) and (7) as

$$\int_{-\infty}^{\infty} e^{\frac{-z^2}{2}} H_n(z) e^{\frac{-z^2}{2}} H_m(z)dz = 0, \text{for } m \neq n$$

$$\int_{-\infty}^{\infty} e^{\frac{-z^2}{2}} H_n(z) e^{\frac{-z^2}{2}} H_m(z)\, dz = \pi^{\frac{1}{2}}2^n n!, \text{for } m = n$$

Or

$$\int_{-\infty}^{\infty} \psi_n^*(z)\psi_m(z)\, dz = 0, \text{for } m \neq n$$

$$\int_{-\infty}^{\infty} \psi_n^*(z)\psi_m(z)\, dz = \pi^{\frac{1}{2}}2^n n!, \text{for } m = n$$

Now we can rewrite equation (9) as

$$H_n(z) = e^{\frac{z^2}{2}} \Psi_n(z) \qquad (10)$$

Differentiate equation (10) with respect to z, we get

$$D_z H_n(z) = e^{\frac{z^2}{2}} [D_z \Psi_n(z) + z\, \Psi_n(z)] \qquad (11)$$

Again, differentiate this equation with respect to z, we get

$$D_z^2 H_n(z) = e^{\frac{z^2}{2}} [D_z^2 \Psi_n(z) + 2z\, D_z \Psi_n(z) + (1 + z^2)\, \Psi_n(z)] = 0 \qquad (12)$$

If we substitute equations (10), (11), (12) in equation (8), we get a second- order differential equation of the form:

$$e^{\frac{z^2}{2}} [D_z^2 \Psi_n(z) + (1 - z^2 + 2n)\, \psi_n(z)] = 0$$

Relabel the equation, we get

$$D_z^2 \Psi_n(z) + (1+2n-z^2)\, \psi_n(z) = 0 \qquad (13)$$

We will call this equation as a modified form of Hermite differential equation.It plays a key role in obtaining the Eigenenergy values and Eigenfunctions of one-dimensional quantum mechanical harmonic oscillator.The solutions of equation (13) are given by equation (9).

One-dimensional quantum mechanical harmonic oscillator problem

Now we willdiscuss thoroughly how Eigenenergy values and Eigenfunctions of one-dimensional quantum mechanical harmonic oscillator are obtained by using equation (13).

The time - independent Schrodinger equation[1-4] in one-dimensions is written as:

$$D_z^2 \psi_n(z) + \frac{2m}{\hbar^2}(E - V(z))\, \psi_n(z) = 0 \qquad (14)$$

This equation is second-order linear differential equation. In this equation, $\psi_n(z)$ is probability wave function of the oscillator and V(z) is the potential energy.

For a harmonic oscillator, thepotential energyV(z) is given by [1-4]

$$V(z) = ½\, kz^2 = ½\, m\omega^2 z^2$$

Substitute this value of potential in equation (13), we get

$$D_z^2\psi_n(z) \;+\; \frac{2m}{\hbar^2}(E - ½\, m\omega^2 z^2)\; \psi_n(z) = 0$$

$$\text{Or}\, D_z^2\psi_n(z) \;+ (\frac{2m}{\hbar^2}E - (\frac{m\omega}{\hbar}z)^2)\; \psi_n(z) = 0 \qquad (14)$$

For convenience, let us substitute $\frac{m\omega}{\hbar} = \alpha$

Therefore, equation (14) becomes

$$D_z^2\psi_n(z) \;+ (\frac{2m}{\hbar^2}E - \alpha^2 z^2)\; \psi_n(z) = 0 \qquad (15)$$

To make thisequation similar to equation (13), Let us substitute a dimensionless constant

$y = \sqrt{\alpha}z$

$$\text{Or } z = y/\sqrt{\alpha} \qquad (16)$$

Such that $D_z y \;=\; \sqrt{\alpha}$

Now we can write $D_z\Psi_n(z)$ as

$$D_z\Psi_n(z) = (D_y\Psi_n(z)).\,(D_z y)$$

$$or \qquad D_z\Psi_n(z) = \sqrt{\alpha}D_y\Psi_n(z)$$

Now $D_z^2\psi_n(z)$ can be written as

$$D_z^2\psi_n(z) = \; D_z(D_z\Psi_n(z))$$

$$or \qquad D_z^2\psi_n(z) \;\; = D_y(\sqrt{\alpha}D_y\Psi_n(z)).D_z y$$

$$or \qquad D_z^2\psi_n(z) \; = \alpha D_y^2\psi_n(z) \qquad (17)$$

Substituting equations (16) and (17) in equation (15), we get

$$\alpha D_y^2\psi_n(z) \;\; + (\frac{2m}{\hbar^2}E - \alpha^2 y^2/\alpha)\; \psi_n(z) = 0$$

Divide both sides of this equation by α, we get

$$D_y^2\psi_n(z) \;\; + (\frac{2m}{\alpha\hbar^2}E - y^2)\; \psi_n(z) = 0 \qquad (18)$$

This equation looks similar to equation (13). Only those solutions of this equation are acceptable for which

$$\frac{2m}{\alpha\hbar^2}E = 1 + 2n,$$

$$\text{Or} \qquad E = (n+\tfrac{1}{2})\,\frac{\alpha\hbar^2}{2m}$$

Put the value of α, we get

$$\text{Or} \qquad E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega \qquad (19)$$

Where n is a non- negative integer.

Here we have written E as E_n because the Eigenenergy values are quantized. Therefore, the energy $E_n$corresponds to the n^{th} state.

For n = 0, equation (19) gives

$$E_0 = \tfrac{1}{2}\hbar\omega$$

This value of Eigenenergy corresponds to the ground state energy of quantum mechanical one-dimensional harmonic oscillator. For n = 1, 2, 3… n, we can find first, second, third…………..n^{th}excited states energies.

The solutions or Eigenfunctions of the equation (18) are given by

$$\Psi_n(z) = A\, e^{\frac{-y^2}{2}} H_n(y) \qquad (20)$$

Where A is normalizing constant and $H_n(y)$ is Hermite polynomial.

The constant A can be obtained by applying normalization condition[1-3]:

$$\int_{-\infty}^{\infty} \psi_n^*(z)\psi_n(z)\; dz = 1$$

Here $\psi_n^*(z)$ is complex conjugate of $\psi_n(z)$.

$$\text{As } y = \sqrt{\alpha}z, \text{ we have}$$

$$dz = \frac{dy}{\sqrt{\alpha}}$$

We can write

$$\int_{-\infty}^{\infty} A\, e^{\frac{-y^2}{2}} H_n(y) A\, e^{\frac{-y^2}{2}} H_n(y) \;\; \frac{dy}{\sqrt{\alpha}} = 1$$

$$\text{Or}\frac{A^2}{\sqrt{\alpha}}\int_{-\infty}^{\infty} e^{-y^2}[H_n(y)]^2 dy = 1$$

Applying orthogonality property of Hermite polynomials, we get

$$\frac{A^2}{\sqrt{\alpha}}\pi^{\frac{1}{2}}2^n n! = 1$$

$$\text{Or} \qquad A = \left[\frac{\sqrt{\alpha}}{\pi^{\frac{1}{2}}2^n n!}\right]^{1/2} \qquad (21)$$

On substituting the equation (21) in equation (20), we get the Eigenfunctions of the one-dimensional harmonic oscillator as

$$\Psi_n(z) = \left[\frac{\sqrt{\alpha}}{\pi^{\frac{1}{2}}2^n n!}\right]^{1/2} \; e^{\frac{-y^2}{2}} H_n(y)$$

Relabel the equation, we get

$$\Psi_n(z) = \left[\frac{\sqrt{\alpha}}{\pi^{\frac{1}{2}}2^n n!}\right]^{1/2} \; e^{\frac{-\alpha z^2}{2}} H_n(\sqrt{\alpha} z)$$

$$\text{Or} \quad \Psi_n(z) = \left[\frac{\sqrt{\frac{m\omega}{\hbar}}}{\pi^{\frac{1}{2}}2^n n!}\right]^{1/2} \; e^{\frac{-\sqrt{\frac{m\omega}{\hbar}}z^2}{2}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}z\right) \qquad (22)$$

Where n is a non- negative integer
For n=0, equation (22) gives

$$\Psi_0(z) = \left[\frac{\sqrt{\frac{m\omega}{\hbar}}}{\pi^{\frac{1}{2}}}\right]^{1/2} \; e^{\frac{-\sqrt{\frac{m\omega}{\hbar}}z^2}{2}}$$

This Eigenfunction corresponds to the ground state wave function of quantum mechanical one-dimensional harmonic oscillator. For n = 1, 2, 3… n, we will find first, second, third…………..nth excited states Eigenfunctions.

II. CONCLUSIONS

In this paper an attempt is made to find the Eigenenergy values and Eigenfunctions of one-dimensional quantum mechanical harmonic oscillator by comparing Schrodinger time - independent equation of one-dimensional quantum mechanical harmonic oscillator with modified form of the Hermite differential equation. By the method, we obtained the Eigen values and Eigenfunctions of one dimensional quantum mechanical harmonic oscillator. This method can be an effective method for the quantum mechanical harmonic oscillator problem as through simple computation we have obtained Eigenenergy values and Eigenfunctions one-dimensional quantum mechanical harmonic oscillator.

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