

Hermite Polynomials and the Quantum Harmonic Oscillator: An Algebraic Approach

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ABSTRACT

This study presents a complete algebraic formulation of the quantum harmonic oscillator, demonstrating that the Hermite polynomials, $H_n(x)$, emerge as the fundamental solution when the power-series method is applied to the Schrödinger equation. The physical requirement of square integrability enforces the truncation of the series, leading precisely to these polynomials, which constitute the polynomial part of the energy eigenfunctions, $\psi_n(x) = N_n H_n(\alpha x) e^{-\alpha^2 x^2/2}$, where n is the quantum number. This quantum number directly determines the quantized energy levels through $E_n = \hbar\omega(n + \frac{1}{2})$. The analysis based on creation and annihilation operators further reveals that the action of the creation operator on the ground state generates the excited states along with their corresponding Hermite functions. The orthogonality of these polynomials, given by $\int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} 2^n n! \delta_{mn}$, ensures the orthonormality of the complete set of eigenfunctions. Therefore, Hermite polynomials encapsulate both the mathematical structure and the physical essence of quantization in this fundamental system.

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Introduction

The quantum harmonic oscillator constitutes one of the fundamental systems of modern quantum mechanics, standing out for being exactly solvable and for serving as a conceptual and mathematical model for a wide variety of physical phenomena. Its importance transcends the didactic character, being widely employed in the description of molecular vibrations in spectroscopy, in the quantization of electromagnetic fields in quantum electrodynamics, in field theory, in the analysis of normal modes in crystalline solids, and in the approximation of real potentials around stable equilibrium points [1, 2].

Historically, the quantum harmonic oscillator is intimately linked to the emergence of quantum mechanics itself. The introduction of energy quantization by Planck, in the context of blackbody radiation, already anticipated the idea of discrete modes associated with harmonic oscillators. Subsequently, with the development of the Schrödinger equation, it became evident that this system admitted discrete, orthogonal, and physically interpretable solutions, playing a central role in the consolidation of the probabilistic interpretation of quantum theory [3].

From a formal point of view, the quantum harmonic oscillator admits two complementary and mathematically elegant approaches: the analytical formulation, based on the direct resolution of the Schrödinger differential equation, and the algebraic formulation, founded on the use of creation and annihilation operators. Although both lead to the same physical results, the algebraic

method highlights particularly clearly the underlying mathematical structure of the problem and its profound connections with the theory of orthogonal polynomials, especially Hermite polynomials [4].

Hermite polynomials arise naturally in the analytical treatment of the harmonic oscillator when adequate physical conditions are imposed on the solutions of the Schrödinger equation. The requirement that the wave functions be square-integrable, an indispensable condition for the probabilistic interpretation of the quantum formalism, imposes rigorous restrictions on the asymptotic behavior of the solutions, selecting only a discrete set of mathematically well-behaved functions. This procedure unequivocally leads to Hermite polynomials as the polynomial part of the system's eigenfunctions [5].

In this context, the degree of the Hermite polynomial is directly associated with the quantum state of the system, simultaneously determining the energy and the spatial form of the wave function. The ground state corresponds to the lowest-degree solution, characterized by a Gaussian distribution, while the excited states exhibit progressively more complex nodal structures, reflecting the energy hierarchy of the system. In the algebraic approach, this structure emerges naturally from the successive action of the creation operator on the ground state, establishing a direct correspondence between the ladder operators and the Hermite polynomials [6, 7].

The mathematical properties of Hermite polynomials, such as their recurrence relations, their operational representation, and their orthogonality, play a central role in the description of

the quantum harmonic oscillator. In particular, orthogonality ensures that the system's eigenfunctions form a complete set, allowing the expansion of arbitrary quantum states and ensuring the mathematical and physical consistency of the theory [8, 9].

In this work, a compact and rigorous analytical description of the quantum harmonic oscillator is developed, highlighting Hermite polynomials as the natural solution of the Schrödinger equation. The analysis is conducted predominantly within the algebraic formalism, in which creation and annihilation operators are constructed from the canonical position and momentum variables and used to reformulate the system's Hamiltonian. This approach allows a clear and systematic understanding of the origin of energy quantization and the central role of Hermite polynomials in the mathematical structure and physical interpretation of this fundamental system.

Theoretical Framework

The Classical Harmonic Oscillator

The classical harmonic oscillator is characterized by a quadratic potential $V(x) = \frac{1}{2}m\omega^2x^2$, where m represents the particle mass and ω the angular oscillation frequency. The classical equation of motion is given by Newton's second law [10]:

$$m \frac{d^2x}{dt^2} = -kx \quad (1)$$

where $k = m\omega^2$ is the force constant. This is a second-order linear differential equation with constant coefficients, whose solution can be obtained by the Frobenius method (power series solution) or more simply by assuming a complex exponential solution. Figure 1 shows a schematic diagram of the classical harmonic oscillator. This figure illustrates the mass-spring system with quadratic potential, where the mass m is attached to a spring of constant $k = m\omega^2$ and executes simple harmonic motion $x(t) = A\cos(\omega t - \delta)$ around the equilibrium position $x = 0$.

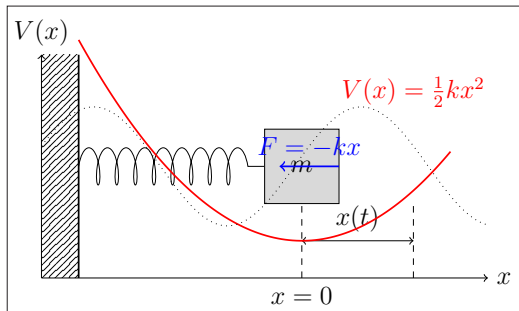


Figure 1: Classical harmonic oscillator: mass-spring system with quadratic potential. The mass m is attached to a spring of constant $k = m\omega^2$ and executes simple harmonic motion $x(t) = A\cos(\omega t - \delta)$ around the equilibrium position $x = 0$.

Source: Personal Archive.

Classical Solution via the Frobenius Method

In this subsection, the classical differential equation associated with the harmonic oscillator is generalized by means of a power series solution, employing the Frobenius method. Although the equation admits an elementary solution in terms of trigonometric functions, this approach is adopted for its conceptual value, as it anticipates the mathematical structure that emerges in the quantum treatment of the problem and establishes a direct parallel with the series method applied to the Schrödinger equation.

The classical harmonic oscillator equation can be rewritten as:

$$\frac{d^2x}{dt^2} + \omega^2x = 0 \quad (2)$$

Assuming a power series solution in time [11]:

$$x(t) = \sum_{n=0}^{\infty} a_n t^n \quad (3)$$

Differentiating term by term:

$$\frac{dx}{dt} = \sum_{n=1}^{\infty} n a_n t^{n-1} = \sum_{n=0}^{\infty} (n+1) a_{n+1} t^n \quad (4)$$

$$\frac{d^2x}{dt^2} = \sum_{n=2}^{\infty} n(n-1) a_n t^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} t^n \quad (5)$$

Substituting into the differential equation:

$$\sum_{n=0}^{\infty} [(n+2)(n+1) a_{n+2} + \omega^2 a_n] t^n = 0 \quad (6)$$

Since this equality must hold for all t , each coefficient must be zero:

$$(n+2)(n+1) a_{n+2} + \omega^2 a_n = 0 \quad (7)$$

$$a_{n+2} = -\frac{\omega^2}{(n+2)(n+1)} a_n \quad (8)$$

This is the recurrence relation that determines all coefficients from a_0 and a_1 . We note that there are two independent series: one for even n (depending on a_0) and another for odd n (depending on a_1). Developing the first terms:

Even series ($n = 2k$):

$$a_2 = -\frac{\omega^2}{2 \cdot 1} a_0 = -\frac{\omega^2}{2!} a_0 \quad (9)$$

$$a_4 = -\frac{\omega^2}{4 \cdot 3} a_2 = -\frac{\omega^4}{4!} a_0 \quad (10)$$

$$a_6 = -\frac{\omega^2}{6 \cdot 5} a_4 = -\frac{\omega^6}{6!} a_0 \quad (11)$$

$\vdots$

$$a_{2k} = \frac{(-1)^k \omega^{2k}}{(2k)!} a_0 \quad (12)$$

Odd series ($n = 2k + 1$):

$$a_3 = -\frac{\omega^2}{3 \cdot 2} a_1 = -\frac{\omega^2}{3!} a_1 \quad (13)$$

$$a_5 = -\frac{\omega^2}{5 \cdot 4} a_3 = -\frac{\omega^4}{5!} a_1 \quad (14)$$

$$a_7 = -\frac{\omega^2}{7 \cdot 6} a_5 = -\frac{\omega^6}{7!} a_1 \quad (15)$$

$\vdots$

$$a_{2k+1} = \frac{(-1)^k \omega^{2k}}{(2k+1)!} a_1 \quad (16)$$

The general solution is therefore [12]:

$$x(t) = a_0 \sum_{k=0}^{\infty} \frac{(-1)^k (\omega t)^{2k}}{(2k)!} + \frac{a_1}{\omega} \sum_{k=0}^{\infty} \frac{(-1)^k (\omega t)^{2k+1}}{(2k+1)!} \quad (17)$$

We recognize the series as the Taylor expansions of $\cos(\omega t)$ and $\sin(\omega t)$, respectively [13]:

$$x(t) = a_0 \cos(\omega t) + \frac{a_1}{\omega} \sin(\omega t) \quad (18)$$

Defining $A = \sqrt{a_0^2 + \left(\frac{a_1}{\omega}\right)^2}$ and $\delta = \arctan\left(\frac{a_1}{\omega a_0}\right)$,

we obtain the canonical form:

$$x(t) = A \cos(\omega t - \delta) \quad (19)$$

where A is the maximum oscillation amplitude and δ the initial phase.

The transition to quantum mechanics requires the canonical quantization of the dynamical variables, replacing classical quantities with operators that satisfy fundamental commutation relations. The classical Hamiltonian:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \quad (20)$$

becomes, in the quantum description, an operator acting on an appropriate Hilbert space, where x and p are Hermitian operators satisfying:

$$[x, p] = xp - px = i\hbar \quad (21)$$

This commutation relation is the foundation of quantum mechanics and will be essential for the development of creation and annihilation operators.

The Schrödinger Equation and the Quantum Harmonic Oscillator

The transition from classical to quantum mechanics is carried out through the process of canonical quantization, in which classical dynamical variables such as position x and momentum p are promoted to the category of Hermitian operators acting on a Hilbert space, obeying the fundamental commutation relation $[x, p] = i\hbar$. The time evolution and stationary states of a quantum system are governed by the time-independent Schrödinger equation [14, 15]:

$$\hat{H}\psi(x) = E\psi(x) \quad (22)$$

where $\hat{H}$ is the Hamiltonian operator of the system and $\psi(x)$ represents the wave function associated with the stationary state of energy E .

For the quantum harmonic oscillator, the Hamiltonian is obtained by directly substituting the classical variables with the corresponding quantum operators in the classical expression for the total energy. Starting from the classical Hamiltonian given by equation (23):

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \quad (23)$$

and applying canonical quantization, we obtain the quantum Hamiltonian operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 \quad (24)$$

In the position representation, we operate with $\hat{x} = x$ and $\hat{p} = -i\hbar \frac{d}{dx}$. Substituting these representations into the Schrödinger equation (22), we obtain the differential equation governing the eigenfunctions $\psi(x)$ of the harmonic oscillator [16]:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x) \quad (25)$$

This is a second-order linear differential equation with variable coefficients. To analyze it more clearly and highlight its essential mathematical structure, it is convenient to introduce dimensionless variables. We define:

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x = \alpha x, \quad \alpha = \sqrt{\frac{m\omega}{\hbar}} \quad (26)$$

and rewrite the energy as $E = \hbar\omega\varepsilon$, where ε is a dimensionless numerical parameter to be determined. In this case, equation (25) transforms into:

$$\frac{d^2\psi}{d\xi^2} + (2\varepsilon - \xi^2) \psi(\xi) = 0 \quad (27)$$

This form reveals that the asymptotic behavior of the solution for $|\xi| \rightarrow \infty$ is dominated by the term $-\xi^2$, suggesting a solution of the type $\psi(\xi) \sim e^{-\xi^2/2}$. We therefore seek solutions of the form [17]:

$$\psi(\xi) = h(\xi)e^{-\xi^2/2} \quad (28)$$

Substituting this ansatz into equation (27), we obtain the differential equation for $h(\xi)$:

$$\frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (2\varepsilon - 1)h(\xi) = 0 \quad (29)$$

Equation (29) is the Hermite differential equation. Its solution is obtained by the Frobenius method (power series). Assuming:

$$h(\xi) = \sum_{k=0}^{\infty} a_k \xi^k \quad (30)$$

and substituting into (29), we obtain the recurrence relation:

$$a_{k+2} = \frac{2k+1-2\varepsilon}{(k+1)(k+2)} a_k \quad (31)$$

Quantization Condition and Hermite Polynomials

The recurrence relation (31) connects coefficients of the same parity. For large values of k , we have $a_{k+2} \sim \frac{2}{k} a_k$, a behavior that, if not truncated, leads to $h(\xi) \sim e^{\xi^2}$ for $|\xi| \rightarrow \infty$ [18]. This solution would make $\psi(\xi) \sim e^{+\xi^2/2}$, which is not square-integrable and therefore not physically acceptable.

The physical condition that the wave function be square-integrable ($\int |\psi|^2 dx < \infty$) imposes that the series (30) be truncated, transforming into a polynomial of finite degree [19]. This truncation occurs when the numerator of the recurrence relation vanishes for some $k = n$, that is:

$$2n+1-2\varepsilon = 0 \implies \varepsilon = n + \frac{1}{2}, \quad n = 0, 1, 2, \dots \quad (32)$$

Substituting $\varepsilon = E/\hbar\omega$, we obtain the quantized energy eigenvalues:

$$E_n = \hbar\omega \left(n + \frac{1}{2}\right) \quad (33)$$

For each value of n , the series reduces to a polynomial of degree n , precisely the Hermite polynomial $H_n(\xi)$. The general solution of the Schrödinger equation for the quantum harmonic oscillator is therefore:

$$\psi_n(x) = N_n H_n(\alpha x) e^{-\alpha^2 x^2/2} \quad (34)$$

The constant N_n is determined by the normalization condition. This analytical procedure through the power series method combined with the physical boundary condition rigorously and directly establishes the origin of Hermite polynomials as the natural mathematical solution of the problem, unequivocally linking the degree n of the polynomial to the quantum number that indexes the energy levels of the system.

Definition and Derivation of Creation and Annihilation Operators

The algebraic formulation of the quantum harmonic oscillator introduces a canonical transformation of the variables x and p into new operators that simplify the structure of the Hamiltonian. These operators, called annihilation (or destruction) operators a and creation operators $a^\dagger$, are defined as dimensionless linear combinations of position and momentum [20].

Definition of the Operators

Consider the following linear combinations:

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}p \quad (35)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\omega\hbar}}p \quad (36)$$

Theorem 2.1: (Conjugate Hermiticity). *The operator $a^\dagger$ is the adjoint (Hermitian conjugate) operator of a .*

Proof. We note that x and p are Hermitian operators ($x = x^\dagger$, $p = p^\dagger$), and that the imaginary number i changes sign under Hermitian conjugation ($i^\dagger = -i$) [21]. Therefore:

$$\begin{aligned} a^\dagger &= \left(\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}p \right)^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x^\dagger - \frac{i}{\sqrt{2m\omega\hbar}}p^\dagger \\ &= \sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\omega\hbar}}p \end{aligned} \quad (37)$$

which coincides with definition (36).

Inversion of the Definitions

We can express x in terms of a and $a^\dagger$:

For position x :

Adding equations (35) and (36):

$$a + a^\dagger = 2\sqrt{\frac{m\omega}{2\hbar}}x = \sqrt{\frac{2m\omega}{\hbar}}x \quad (38)$$

Therefore:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad (39)$$

For momentum p :

Subtracting equation (36) from equation (35) [22]:

$$a - a^\dagger = \frac{2i}{\sqrt{2m\omega\hbar}}p = i\sqrt{\frac{2}{m\omega\hbar}}p \quad (40)$$

Therefore:

$$p = \frac{\sqrt{2m\omega\hbar}}{2i}(a - a^\dagger) = -i\sqrt{\frac{m\omega\hbar}{2}}(a - a^\dagger) \quad (41)$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a) \quad (42)$$

Demonstration of the Fundamental Commutation Relation
Theorem 2.2: The operators a and $a^\dagger$ satisfy the commutation relation [23]:

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1 \quad (43)$$

Proof. We calculate the commutator directly using definitions (35) and (36) [24]:

$$[a, a^\dagger] = \left[\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}p, \sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\omega\hbar}}p \right] \quad (44)$$

Expanding the bilinear commutator:

$$= \frac{m\omega}{2\hbar}[x, x] - \frac{i}{2\hbar}[x, p] + \frac{i}{2\hbar}[p, x] + \frac{1}{2m\omega\hbar}[p, p] \quad (45)$$

We know that $[x, x] = [p, p] = 0$ and $[p, x] = -[x, p] = -i\hbar$.

Therefore:

$$= 0 - \frac{i}{2\hbar}(i\hbar) + \frac{i}{2\hbar}(-i\hbar) + 0 = -\frac{i^2}{2} - \frac{i^2}{2} = \frac{1}{2} + \frac{1}{2} = 1 \quad (46)$$

$$\therefore [a, a^\dagger] = 1 \quad \text{Q.E.D.} \quad (47)$$

Reformulation of the Hamiltonian in Terms of Creation and Annihilation Operators

The canonical Hamiltonian of the harmonic oscillator is given by equation (23): **Theorem 2.3:** *The Hamiltonian can be rewritten as:*

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) = \hbar\omega \left(N + \frac{1}{2} \right) \quad (48)$$

where $N = a^\dagger a$ is the number operator.

Proof. We substitute expressions (39) and (42) for x and p into the Hamiltonian: For the kinetic term $\frac{p^2}{2m}$:

$$p^2 = \left[i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a) \right]^2 = -\frac{m\omega\hbar}{2}(a^\dagger - a)^2 \quad (49)$$

$$= -\frac{m\omega\hbar}{2}[(a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2] \quad (50)$$

$$\frac{p^2}{2m} = -\frac{\omega\hbar}{4}[(a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2] \quad (51)$$

For the potential term $\frac{1}{2}m\omega^2 x^2$:

$$x^2 = \left[\sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \right]^2 = \frac{\hbar}{2m\omega}(a + a^\dagger)^2 \quad (52)$$

$$= \frac{\hbar}{2m\omega}[a^2 + aa^\dagger + a^\dagger a + (a^\dagger)^2] \quad (53)$$

$$\frac{1}{2}m\omega^2 x^2 = \frac{\omega\hbar}{4}[a^2 + aa^\dagger + a^\dagger a + (a^\dagger)^2] \quad (54)$$

The sum of the terms: $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ (55)

$$= -\frac{\omega\hbar}{4}[(a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2] + \frac{\omega\hbar}{4}[a^2 + aa^\dagger + a^\dagger a + (a^\dagger)^2] \quad (56)$$

The $(a^\dagger)^2$ and a^2 terms cancel:

$$= \frac{\omega\hbar}{4}[a^\dagger a + aa^\dagger + aa^\dagger + a^\dagger a] = \frac{\omega\hbar}{4}[2a^\dagger a + 2aa^\dagger] = \frac{\omega\hbar}{2}(a^\dagger a + aa^\dagger) \quad (57)$$

Using $[a, a^\dagger] = aa^\dagger - a^\dagger a = 1$ from equation (43), we have $aa^\dagger = a^\dagger a + 1$:

$$H = \frac{\omega\hbar}{2}(a^\dagger a + a^\dagger a + 1) = \frac{\omega\hbar}{2}(2a^\dagger a + 1) = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \quad (58)$$

$$\therefore H = \hbar\omega\left(N + \frac{1}{2}\right) \quad \text{Q.E.D.} \quad (59)_{(59)}$$

Energy Spectrum and Stationary States

The algebraic structure of the quantum harmonic oscillator is particularly clearly revealed in the diagrammatic representation of the energy levels, presented in Figure 2. This diagram illustrates the action of the creation and annihilation operators on the stationary states of the system.

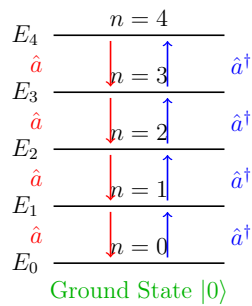


Figure 2: Energy level diagram of the quantum harmonic oscillator. Creation operators ($\hat{a}^\dagger$) raise the quantum state, while annihilation operators ($\hat{a}$) lower it. Each level corresponds to an eigenvalue $E_n = \hbar\omega(n + \frac{1}{2})$.

Source: Personal archive.

As shown in Figure 2, the creation operator $a^\dagger$ promotes upward transitions between energy levels, while the annihilation operator a induces downward transitions. This visual representation synthesizes the underlying algebraic structure of the system and provides an immediate physical intuition about the mechanism of energy quantization.

Theorem 2.4: The eigenvalues of the number operator N are non-negative integers $n = 0, 1, 2, \dots$, and the eigenvalues of the Hamiltonian are given by the equation:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad (60)$$

Proof. Let $|n\rangle$ be an eigenstate of N with eigenvalue n :

$$N|n\rangle = n|n\rangle \quad (61)$$

Lemma 2.1: $Na|n\rangle = (n-1)a|n\rangle$ (the operator a decreases the number of quanta by 1).

Proof.

$$Na = a^\dagger aa = (aa^\dagger - 1)a = aa^\dagger a - a = aN - a = a(N-1) \quad (62)$$

Therefore:

$$Na|n\rangle = a(N-1)|n\rangle = a(n-1)|n\rangle = (n-1)a|n\rangle \quad (63)$$

Lemma 2.2: $Na^\dagger|n\rangle = (n+1)a^\dagger|n\rangle$ (the operator $a^\dagger$ increases the number of quanta by 1).

Proof.

$$Na^\dagger = a^\dagger aa^\dagger = a^\dagger(a^\dagger a + 1) = a^\dagger(N+1) \quad (64)$$

Therefore:

$$Na^\dagger|n\rangle = a^\dagger(N+1)|n\rangle = a^\dagger(n+1)|n\rangle = (n+1)a^\dagger|n\rangle \quad (65)$$

Positivity Condition:

Since $N = a^\dagger a$ is a positive semi-definite operator, its eigenvalues must satisfy $n \geq 0$. If we apply a successively, we must eventually reach a state $|0\rangle$ such that:

$$a|0\rangle = 0 \quad (66)$$

Otherwise, we would obtain negative eigenvalues, violating the positivity of N .

For the ground state $|0\rangle$:

$$N|0\rangle = a^\dagger a|0\rangle = a^\dagger \cdot 0 = 0 \quad (67)$$

Hence, $n = 0$ for the ground state.

Applying $a^\dagger$ successively:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle \quad (68)$$

with eigenvalues $n = 0, 1, 2, \dots$ and energies:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad \text{Q.E.D.} \quad (69)$$

Connection with Hermite Polynomials

Ground State in the Position Representation

The ground state $|0\rangle$ is defined by condition (66), $a|0\rangle = 0$. In the position representation $\psi_0(x) = \langle x|0\rangle$, this condition becomes a differential equation.

Theorem 2.5: The ground state wave function is:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{\xi^2}{2}} = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha^2 x^2}{2}} \quad (70)$$

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ and $\xi = \alpha x$.

Proof.

$$a|0\rangle = 0 \quad (71)$$

$$\left[\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}p\right]|0\rangle = 0 \quad (72)$$

In the position representation, $p = -i\hbar\frac{d}{dx}$:

$$\sqrt{\frac{m\omega}{2\hbar}}x\psi_0(x) + \frac{i}{\sqrt{2m\omega\hbar}}(-i\hbar)\frac{d\psi_0}{dx} = 0 \quad (73)$$

$$\sqrt{\frac{m\omega}{2\hbar}}x\psi_0(x) + \sqrt{\frac{\hbar}{2m\omega}}\frac{d\psi_0}{dx} = 0 \quad (74)$$

Multiplying by $\sqrt{\frac{2m\omega}{\hbar}}$:

$$\frac{m\omega}{\hbar}x\psi_0(x) + \frac{d\psi_0}{dx} = 0 \quad (75)$$

Defining $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ and $\xi = \alpha x$:

$$\alpha^2 x \psi_0 + \frac{d\psi_0}{dx} = 0 \quad (76)$$

$$\frac{d\psi_0}{\psi_0} = -\alpha^2 x dx = -\xi d\xi \quad (77)$$

Integrating:

$$\ln |\psi_0| = -\frac{\xi^2}{2} + C \quad (78)$$

$$\psi_0(x) = A_0 e^{-\frac{\xi^2}{2}} = A_0 e^{-\frac{\alpha^2 x^2}{2}} \quad (79)$$

Normalization:

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = |A_0|^2 \int_{-\infty}^{\infty} e^{-\alpha^2 x^2} dx = |A_0|^2 \frac{\sqrt{\pi}}{\alpha} = 1 \quad (80)$$

$$|A_0|^2 = \sqrt{\frac{\alpha^2}{\pi}} = \sqrt{\frac{m\omega}{\pi\hbar}} \quad (81)$$

Therefore:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{\xi^2}{2}} = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha^2 x^2}{2}} \quad \text{Q.E.D.} \quad (82)$$

Excited States and Hermite Polynomials

Excited states are generated by the successive application of the creation operator according to equation (68):

$$\psi_n(x) = \langle x|n\rangle = \left\langle x \left| \frac{(a^\dagger)^n}{\sqrt{n!}} \right| 0 \right\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n \psi_0(x) \quad (83)$$

Theorem 2.6: The excited eigenfunctions take the form:

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}} \cdot \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} = N_n H_n(\alpha x) e^{-\frac{\alpha^2 x^2}{2}} \quad (84)$$

where $H_n(\xi)$ are the Hermite polynomials.

Proof by Induction. Base Case ($n = 0$):

$H_0(\xi) = 1$, consistent with $\psi_0(x)$ from equation (70).

Through the inductive step, we have the following:

Assuming it holds for n , we prove it for $n + 1$:

$$\psi_{n+1}(x) = \frac{1}{\sqrt{n+1}} a^\dagger \psi_n(x) \quad (85)$$

In the position representation:

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\omega\hbar}}(-i\hbar)\frac{d}{dx} = \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi} \right) \quad (86)$$

Therefore:

$$\psi_{n+1}(x) = \frac{1}{\sqrt{2(n+1)}} \left(\xi - \frac{d}{d\xi} \right) \left[N_n H_n(\xi) e^{-\frac{\xi^2}{2}} \right] \quad (87)$$

$$= \frac{N_n}{\sqrt{2(n+1)}} \left[\xi H_n(\xi) e^{-\frac{\xi^2}{2}} - \frac{d}{d\xi} (H_n(\xi) e^{-\frac{\xi^2}{2}}) \right] \quad (88)$$

$$\frac{N_n}{\sqrt{2(n+1)}} \left[\xi H_n(\xi) e^{-\frac{\xi^2}{2}} - H'_n(\xi) e^{-\frac{\xi^2}{2}} + \xi H_n(\xi) e^{-\frac{\xi^2}{2}} \right] \quad (89)$$

$$= \frac{N_n}{\sqrt{2(n+1)}} [2\xi H_n(\xi) - H'_n(\xi)] e^{-\frac{\xi^2}{2}} \quad (90)$$

By the property of Hermite polynomials:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - H'_n(\xi) \quad (91)$$

Therefore:

$$\psi_{n+1}(x) = \frac{N_n}{\sqrt{2(n+1)}} H_{n+1}(\xi) e^{-\frac{\xi^2}{2}} \quad (92)$$

With $N_{n+1} = \frac{N_n}{\sqrt{2(n+1)}}$, we complete the induction.

Actions of Creation and Annihilation Operators and Recurrence Relations

The action of the creation $a^\dagger$ and annihilation a operators on the eigenstates of the number operator $\hat{N} = a^\dagger a$ can be rigorously derived from the fundamental commutation relations. Consider the Hilbert space generated by the orthonormal states $|n\rangle$, with $n = 0, 1, 2, \dots$, which satisfy:

$$\hat{N} |n\rangle = n |n\rangle, \quad \langle m|n\rangle = \delta_{mn}. \quad (93)$$

Action of the Annihilation Operator

We compute $\hat{N}(a|n\rangle) = a^\dagger a(a|n\rangle)$. Using the commutator $[a, a^\dagger] = 1$, we have $a^\dagger a a = a(a^\dagger a - 1)$. Therefore,

$$\hat{N}(a|n\rangle) = a(\hat{N} - 1)|n\rangle = (n-1)(a|n\rangle). \quad (94)$$

Thus, $a|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $n-1$, which implies $a|n\rangle = c_n|n-1\rangle$, where c_n is a complex constant to be determined. The norm of this state is:

$$\|a|n\rangle\|^2 = \langle n|a^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = n. \quad (95)$$

On the other hand, $\|a|n\rangle\|^2 = |c_n|^2 \langle n-1|n-1\rangle = |c_n|^2$. Equating, we obtain $|c_n|^2 = n$. Adopting the standard phase convention (real and positive constants), we conclude:

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad \text{with } a|0\rangle = 0. \quad (96)$$

Action of the Creation Operator

Analogously, we consider $\hat{N}(a|n\rangle) = a^\dagger a(a|n\rangle)$. Using the commutator $[a, a^\dagger] = 1$, we have $a^\dagger a a = a(a^\dagger a - 1)$. Therefore,

$$\hat{N}(a|n\rangle) = a(\hat{N} - 1)|n\rangle = (n - 1)(a|n\rangle). \quad (94)$$

Thus, $a|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $n - 1$, which implies $a|n\rangle = c_n|n - 1\rangle$, where c_n is a complex constant to be determined. The norm of this state is:

$$\|a|n\rangle\|^2 = \langle n|a^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = n. \quad (95)$$

On the other hand, $\|a|n\rangle\|^2 = |c_n|^2 \langle n - 1|n - 1\rangle = |c_n|^2$. Equating, we obtain $|c_n|^2 = n$. Adopting the standard phase convention (real and positive constants), we conclude:

$$a|n\rangle = \sqrt{n}|n - 1\rangle, \quad \text{with } a|0\rangle = 0. \quad (96)$$

Action of the Creation Operator

Analogously, we consider $\hat{N}(a^\dagger|n\rangle) = a^\dagger a(a^\dagger|n\rangle)$. Using $aa^\dagger = a^\dagger a + 1$,

$$\hat{N}(a^\dagger|n\rangle) = a^\dagger(\hat{N} + 1)|n\rangle = (n + 1)(a^\dagger|n\rangle). \quad (97)$$

showing that $a^\dagger|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $n + 1$. Hence, $a^\dagger|n\rangle = d_n|n + 1\rangle$. Calculating the norm:

$$\|a^\dagger|n\rangle\|^2 = \langle n|aa^\dagger|n\rangle = \langle n|(\hat{N} + 1)|n\rangle = n + 1, \quad (98)$$

and comparing with $\|a^\dagger|n\rangle\|^2 = |d_n|^2$, we obtain $|d_n|^2 = n + 1$.

With the same phase convention:

$$a^\dagger|n\rangle = \sqrt{n + 1}|n + 1\rangle. \quad (99)$$

Immediate Consequence

The derived relations show that a and $a^\dagger$ act as lowering and raising operators, respectively, on the ladder of number states. Successive applications of $a^\dagger$ allow generating all states from the ground state $|0\rangle$:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (100)$$

This algebraic structure is directly reflected in the properties of the harmonic oscillator eigenfunctions in the position representation, where Hermite polynomials arise naturally from the action of the operators on the Gaussian ground state. The actions of the operators (96) and (99) translate into recurrence relations for the Hermite polynomials. In the position representation, the creation and annihilation operators are given by:

$$a = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right), \quad (101)$$

where $\xi = \sqrt{\frac{m\omega}{\hbar}}x$, and the normalized eigenfunctions are:

$$\psi_n(\xi) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(\xi) e^{-\xi^2/2}. \quad (102)$$

Recurrence Relations for Hermite Polynomials

From $a^\dagger \psi_n = \sqrt{n + 1} \psi_{n+1}$:

$$\frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right) \left[H_n(\xi) e^{-\xi^2/2} \right] = \sqrt{n + 1}.$$

$$\frac{1}{\sqrt{2^{n+1}(n+1)! \sqrt{\pi}}} H_{n+1}(\xi) e^{-\xi^2/2}. \quad (103)$$

Simplifying, we obtain:

$$\left(\xi - \frac{d}{d\xi}\right) H_n(\xi) = H_{n+1}(\xi), \quad (104)$$

that is,

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - H'_n(\xi). \quad (105)$$

From $a\psi_n = \sqrt{n}\psi_{n-1}$:

$$\frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right) \left[H_n(\xi) e^{-\xi^2/2} \right] = \sqrt{n} \cdot \frac{1}{\sqrt{2^{n-1}(n-1)! \sqrt{\pi}}} H_{n-1}(\xi) e^{-\xi^2/2}. \quad (106)$$

Simplifying:

$$\left(\xi + \frac{d}{d\xi}\right) H_n(\xi) = 2n H_{n-1}(\xi), \quad (107)$$

resulting in:

$$H'_n(\xi) = 2n H_{n-1}(\xi). \quad (108)$$

Combining (105) and (108), we obtain the classical recurrence formula:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi). \quad (109)$$

Rodrigues Formula and Properties of Hermite Polynomials

Rodrigues Formulation

Definition 2.1: (Rodrigues Formula). Hermite polynomials are defined by the equation:

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} (e^{-\xi^2}), \quad n = 0, 1, 2, \dots \quad (110)$$

Theorem 2.7: (Equivalence with the operator definition). The Rodrigues formula is equivalent to the definition via creation operators.

Proof. From the expression of excited states:

$$\psi_n(\xi) = \frac{1}{\sqrt{2^n n!}} \left(\xi - \frac{d}{d\xi}\right)^n \psi_0(\xi) \quad (111)$$

where $\psi_0(\xi) = \pi^{-1/4} e^{-\xi^2/2}$.

Note that:

$$\left(\xi - \frac{d}{d\xi}\right) e^{-\xi^2/2} = \xi e^{-\xi^2/2} + \xi e^{-\xi^2/2} = 2\xi e^{-\xi^2/2} \quad (112)$$

and more generally:

$$\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2} = H_n(\xi) e^{-\xi^2/2} \quad (113)$$

It can be shown by induction that:

$$H_n(\xi) = e^{\frac{\xi^2}{2}} \left(\xi - \frac{d}{d\xi} \right)^n e^{-\frac{\xi^2}{2}} = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \quad (114)$$

Verification for $n = 0$:

$$H_0(\xi) = (-1)^0 e^{\xi^2} e^{-\xi^2} = 1 \quad (115)$$

Verification for $n = 1$:

$$H_1(\xi) = (-1)^1 e^{\xi^2} \frac{d}{d\xi} (e^{-\xi^2}) = -e^{\xi^2} (-2\xi e^{-\xi^2}) = 2\xi \quad (116)$$

Verification for $n = 2$:

$$H_2(\xi) = (+1) e^{\xi^2} \frac{d^2}{d\xi^2} (e^{-\xi^2}) = e^{\xi^2} \frac{d}{d\xi} (-2\xi e^{-\xi^2}) \quad (117)$$

$$= e^{\xi^2} [-2e^{-\xi^2} + 4\xi^2 e^{-\xi^2}] = -2 + 4\xi^2 = 4\xi^2 - 2 \quad (118)$$

First Hermite Polynomials

Using the recurrence relation (109) with $H_0(\xi) = 1$ and $H_1(\xi) = 2\xi$:

$$\begin{aligned} H_0(\xi) &= 1 \\ H_1(\xi) &= 2\xi \\ H_2(\xi) &= 4\xi^2 - 2 \\ H_3(\xi) &= 8\xi^3 - 12\xi \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \end{aligned} \quad (119)$$

Orthogonality of Hermite Polynomials

Orthogonality Condition

Theorem 2.8: Hermite polynomials are orthogonal with respect to the weight function $w(\xi) = e^{-\xi^2}$ on the interval $(-\infty, \infty)$ according to the equation:

$$\int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} 2^n n! \delta_{mn} \quad (120)$$

where δ_{mn} is the Kronecker delta.

Proof. Consider the integral:

$$I_{mn} = \int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi \quad (121)$$

Using the Rodrigues formula (110) for H_m :

$$I_{mn} = \int_{-\infty}^{\infty} (-1)^m e^{\xi^2} \frac{d^m}{d\xi^m} (e^{-\xi^2}) H_n(\xi) e^{-\xi^2} d\xi \quad (122)$$

$$= (-1)^m \int_{-\infty}^{\infty} \frac{d^m}{d\xi^m} (e^{-\xi^2}) H_n(\xi) d\xi \quad (123)$$

Integrating by parts m times:

$$I_{mn} = \int_{-\infty}^{\infty} e^{-\xi^2} \frac{d^m H_n}{d\xi^m} d\xi \quad (124)$$

Case $m > n$:

Since H_n is a polynomial of degree n , its m -th derivative is zero for $m > n$.

Therefore, $I_{mn} = 0$.

Case $m = n$:

Since $H_n(\xi) = 2^n \xi^n$ lower-degree terms, we have:

$$\frac{d^n H_n}{d\xi^n} = 2^n n! \quad (125)$$

Therefore:

$$I_{nn} = 2^n n! \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = 2^n n! \sqrt{\pi} \quad (126)$$

$$\therefore \int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} 2^n n! \delta_{mn} \quad \text{Q.E.D.} \quad (127)$$

Orthogonality of Eigenfunctions

The eigenfunctions of the quantum harmonic oscillator form an orthogonal set, an essential property for the description of stationary states and for the spectral structure of the Hamiltonian.

Theorem 2.9:

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{mn} \quad (128)$$

Proof.

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = N_m N_n \int_{-\infty}^{\infty} H_m(\alpha x) H_n(\alpha x) e^{-\alpha^2 x^2} dx \quad (129)$$

Making the substitution

$$= N_m N_n \int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} \frac{d\xi}{\alpha} \quad (130)$$

$$= \frac{N_m N_n}{\alpha} \sqrt{\pi} 2^n n! \delta_{mn} \quad (131)$$

For normalization, we require:

$$\frac{N_n^2}{\alpha} \sqrt{\pi} 2^n n! = 1 \quad (132)$$

$$N_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} = \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} \quad (133)$$

Therefore:

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{mn} \quad (134)$$

The Kronecker delta, denoted by δ_{mn} , is defined as [14]:

$$\delta_{mn} = \begin{cases} 1, & \text{if } m = n, \\ 0, & \text{if } m \neq n. \end{cases} \quad (135)$$

This discrete function plays the role of the identity element in the space of integer indices, being widely used to express orthogonality conditions in vector and functional spaces. In the context of the quantum harmonic oscillator, the orthonormality of the eigenfunctions $\psi_n(\xi)$ can be represented, in the state space, by means of an identity matrix, as follows:

$$\left[\int_{-\infty}^{\infty} \psi_m(\xi) \psi_n(\xi) d\xi \right] = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \equiv I, \quad (136)$$

in which each matrix element corresponds directly to the Kronecker delta δ_{mn} , evidencing that distinct states are mutually orthogonal and that each eigenfunction has unit norm.

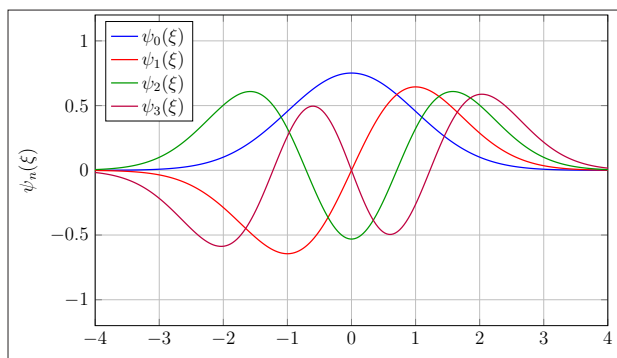
Results and Discussion

Wave Functions of the Quantum Harmonic Oscillator

The graphical representation of the quantum harmonic oscillator eigenfunctions is presented in Figure 3, constructed from the general expression given by [25]:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} H_n(\xi) e^{-\xi^2/2} \quad (137)$$

where $H_n(\xi)$ are the Hermite polynomials.



$$\xi = x \sqrt{\frac{m\omega}{\hbar}}$$

Figure 3: Dimensionless wave functions $\psi_n(\xi)$ of the quantum harmonic oscillator corresponding to the first stationary states, expressed as a function of the dimensionless variable $\xi = x \sqrt{\frac{m\omega}{\hbar}}$. Each curve results from the product of the Hermite polynomial $H_n(\xi)$ associated with state n and the Gaussian factor $e^{-\xi^2/2}$.

Source: Personal archive.

The dimensionless variable ξ is defined by $\xi = x \sqrt{m\omega/\hbar}$, which allows the solutions to be formulated in a universal manner, that is, independent of the specific physical parameters of the system. Full dimensionalization is recovered through the inverse relation $x = \xi \sqrt{\hbar/(m\omega)}$, fully preserving the physical content of the problem while, at the same time, highlighting its fundamental mathematical structure.

From a mathematical perspective, Figure 3 explicitly shows that the degree of the Hermite polynomial $H_n(\xi)$ controls the spatial complexity of the wave function. Each eigenfunction exhibits exactly n nodes, directly reflecting the quantum number associated with the state. The ground state ($n = 0$) corresponds to a purely Gaussian distribution, without nodes, while excited states show progressively more pronounced oscillations as n increases. The parity alternation is also observed: states with even n are symmetric about the origin, while states with odd n are antisymmetric, in full agreement with the symmetry of the harmonic potential. Furthermore, although Hermite polynomials exhibit polynomial growth for large values of $|\xi|$, the Gaussian exponential factor

dominates the asymptotic behavior, ensuring the decay of the eigenfunctions and their normalizability.

From a physical perspective, these graphical properties reflect the simultaneous increase in energy and spatial extent of quantum states with the growth of the quantum number n . The absence of nodes in the ground state and the inevitable presence of zeropoint energy evidence that the particle cannot remain at absolute rest, in accordance with the Heisenberg uncertainty principle. Thus, Figure 3 clearly synthesizes the correspondence between the mathematical structure of Hermite polynomials and the fundamental physical properties of the quantum harmonic oscillator, reinforcing their role as the natural analytical solution of this model system.

Conclusions

Hermite polynomials constitute the natural analytical solution of the quantum harmonic oscillator, emerging directly from the mathematical structure of the Schrödinger equation when the physical condition of square-integrability of the wave functions is imposed. The application of the power series method leads to a differential equation whose general solutions only remain normalizable when the series is truncated, precisely selecting Hermite polynomials of integer degree. This mechanism unequivocally establishes the quantization of energy levels and highlights the central role of these polynomials in the exact description of the system.

From an algebraic point of view, the same structure is recovered through the creation and annihilation operators, responsible for constructing the excited states from the ground state. The successive action of the creation operator generates wave functions whose polynomial part is described by Hermite polynomials, while the Gaussian envelope ensures the normalization of the solutions. The correspondence between the recurrence relations of Hermite polynomials and the algebra of ladder operators reveals a mathematical isomorphism that directly connects the analytical solution of the differential equation to the algebraic formalism of quantum mechanics.

Furthermore, the orthogonality of Hermite polynomials with Gaussian weight guarantees the orthonormality of the complete set of eigenfunctions of the quantum harmonic oscillator, allowing the expansion of arbitrary quantum states in this basis. The number of nodes of the wave functions, determined by the degree of the polynomial, is directly associated with the quantum number of the state and the respective energy level, establishing a clear link between mathematical properties and physical interpretation. Thus, Hermite polynomials not only provide the analytical solution of the quantum harmonic oscillator but also synthesize in a unified manner the quantization, symmetry, and spectral structure of this fundamental system.

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