Hermite polynomials in Quantum Harmonic Oscillator

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Introduction

In quantum mechanics and in other branches of physics, it is common to approach physical problems using algebraic and analytic methods. Examples include the use of differential equations for many interesting models, the use of quantum groups in quantum physics, and of differential geometry in relativity theory. In this article, we discuss the Hermite polynomials, some of their properties and a brief description of their applications to the Quantum Harmonic Oscillator.

Hermite Polynomials

Hermite polynomials, named after the French mathematician Charles Hermite, are orthogonal polynomials, in a sense to be described below, of the form

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \tag{1}$$

for $n = 0, 1, 2, 3, \ldots$.
The first few Hermite polynomials are

- for $n = 0$ we have $H_0(x) = 1$
- for $n = 1$ we have $H_1(x) = 2x$
- for $n = 2$ we have $H_2(x) = 4x^2 - 2$.

Definition 1. For $n \in \mathbb{N}$, we define Hermite polynomials $H_n(x)$ by

$$\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} r^n = e^{2xr-r^2}, \quad \text{for } |r| < \infty. \tag{2}$$

To find $H_n(x)$, expand the right hand side of (2) as a Maclaurin series in r and equate coefficients. From Equation (2) we derive the closed expression

$$H_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k n!}{k!(n-2k)!} (2x)^{n-2k} \tag{3}$$

where $\lfloor x \rfloor$ denotes the largest integer less than or equal to x. Checking with $n = 0, 1, 2, ...$, we find that (3) yields the expected Hermite polynomials. To prove that (3) holds in general, one can use induction (see [2]).

Recurrence Relations

Next we discuss recurrence relations that Hermite polynomials satisfy. We start with

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0, \qquad n = 1, 2, \ldots, \tag{4}$$

which follows from the fact that the generating function $w(x, r) = e^{2xr-r^2}$ satisfies the differential equation $\partial w/\partial r - (2x - 2r)w = 0$.

The next recurrence relation connects $H_n'(x)$ and $H_{n-1}(x)$. From (2), we have

$$H_n'(x) = 2nH_{n-1}(x), \qquad n = 1, 2, \ldots. \tag{5}$$

Now, after a moment's thought, and combining the above two recurrence relations we have another relation

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0, \qquad n = 1, 2, \ldots. \tag{6}$$

From a mathematician's viewpoint, relation (6) is a second-order linear differential equation, which is called *Hermite's differential equation*. From a physicist's point of view, differential equation (6) plays a central role in one of the most important physical models, namely the one-dimenisional *Quantum Harmonic Oscillator*. For both mathematicians and physicists, solutions of (6) are the Hermite polynomials.

Orthogonality

Next, we turn to a common topic for polynomials such as Hermite polynomials, the *orthogonality*. Our goal is to prove that the family of Hermite polynomials $\{H_n\}$ for $n = 0, 1, 2, ...$ is orthogonal with respect to the *weight* e^{-x^2}. In other words, we will prove that

$$\int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x) dx = 0 \tag{7}$$

for $m \neq n$. To prove this we will use a technique from [2]. It is easy to show by direct differentiation and using (6) that

$$u_n = e^{-\frac{x^2}{2}} H_n(x) \qquad \text{and} \qquad u_m = e^{-\frac{x^2}{2}} H_m(x)$$

satisfy

$$u_n'' + (2n + 1 - x^2) u_n = 0 \tag{8}$$

and

$$u_m'' + (2m + 1 - x^2) u_m = 0. \tag{9}$$

Multiplying (8) by u_m and (9) by u_n transforms each into

$$u_m u_n'' + (2n + 1 - x^2) u_m u_n = 0 \tag{10}$$

and

$$u_n u_m'' + (2m + 1 - x^2) u_n u_m = 0, \tag{11}$$

respectively. Subtracting (11) from (10) we have

$$(u_m u_n'' - u_n u_m'') + 2(n - m) u_m u_n = 0. \tag{12}$$

Finally, integrating (12) from $-\infty$ to $+\infty$ shows that

$$(n - m) \int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x) dx = 0.$$

Therefore, (7) follows if $m \neq n$.

When $m = n$, we have

$$\int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi},$$

a result which takes more work than the $m \neq n$ case – for a detailed proof, see [2].

Connection with Quantum Harmonic Oscillator

In this final part of our paper, we will show the connection of Hermite Polynomials with the Quantum Harmonic Oscillator. First of all, the analogue of the classical Harmonic Oscillator in Quantum Mechanics is described by the *Schrödinger* equation

$$\psi'' + \frac{2m}{\hbar^2}(E - V(y))\psi = 0,$$

where ψ is the *state* of a particle of mass m in the potential $V(y)$, with energy E.

We will suppose that the potential has the form $V(y) = y^2$, and therefore we consider the following equation

$$\psi'' + \frac{2m}{\hbar^2}(E - y^2)\psi = 0. \tag{13}$$

In order to simplify this equation, we make a change of variable $y = kx$. Equation (13) is transformed to

$$\psi'' - \frac{2mk^4}{\hbar^2}x^2\psi = -\frac{2mk^2}{\hbar^2}E\psi,$$

where the differentiation is now with respect to the new variable x. Choosing the constant k appropriately our equation becomes

$$\psi'' - x^2\psi = -\beta\psi, \tag{14}$$

where

$$\beta := \sqrt{\frac{2m}{\hbar^2}}E.$$

Equation (14) is a second order differential equation with variable coefficients. To solve this equation, we first notice that $\psi_*(x) = e^{-x^2/2}$ is a solution of the differential equation $\psi'' - x^2\psi = -\psi$. Using the method of variation of parameters (see [3]) we find the following solutions of Equation (14):

$$\psi_n(x) = \psi_*(x)H(x). \tag{15}$$

Here, $\psi_*(x)$ is the solution defined above, and $H(x)$ is a function to be determined. To find the form of $H(x)$, we substitute $\psi_n(x)$ given by (15) into equation (14) and we obtain the following equation:

$$H'' - 2xH' + (\beta - 1)H = 0. \tag{16}$$

Setting $\beta - 1 = 2n \Leftrightarrow \beta = \beta_n := 2n + 1$ in (16) we obtain none other than the Hermite differential equation (6) whose solutions are $H(x) := H_n(x)$, the Hermite polynomials.

References

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