

HERMITE POLYNOMIALS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Hermite polynomials turn up in the solution of the Schrödinger equation for the harmonic oscillator. Most quantum mechanics textbooks quote the properties of these polynomials and refer the reader to some other book on mathematics, so it is rare for a student to see where these properties come from. From a mathematical point of view, some of these properties seem almost magical, so it's interesting look at how they arise.

A *polynomial* in the single variable x is, in general, any sum of powers of x with constant coefficients. That is

$$P(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \dots + a_nx^n \quad (1)$$

$$= \sum_{j=0}^n a_jx^j \quad (2)$$

where the coefficients a_j are constant (independent of x).

The highest power of x (n in this case) is called the *degree* of the polynomial, and it is possible for the degree to be infinite.

There is nothing particularly remarkable about a general polynomial, but certain sets of polynomials have been discovered that do have notable properties. The Hermite polynomials are one such set.

There are several ways that Hermite polynomials can be defined, but the one used by physicists is this: the Hermite polynomial of degree n is defined as

$$H_n \equiv (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (3)$$

At first glance, this doesn't look like a polynomial at all, since it contains only exponentials. But if we calculate the first few, we can see that we get a sequence of polynomials:

$$H_0 = e^{x^2} e^{-x^2} \quad (4)$$

$$= 1 \quad (5)$$

$$H_1 = -e^{x^2} e^{-x^2} (-2x) \quad (6)$$

$$= 2x \quad (7)$$

$$H_2 = (-1)^2 e^{x^2} e^{-x^2} (4x^2 - 2) \quad (8)$$

$$= 4x^2 - 2 \quad (9)$$

$$H_3 = 8x^3 - 12x \quad (10)$$

$$H_4 = 16x^4 - 48x^2 + 12 \quad (11)$$

No matter how many derivatives of e^{-x^2} we take, the e^{-x^2} term always comes out the other end and is cancelled by the e^{x^2} term at the front, leaving the polynomial term as the only survivor. Note that polynomials of even degree (0, 2, 4, ...) are even functions, that is, $H(-x) = H(x)$ so they are symmetric about the origin, and polynomials of odd degree are odd functions ($H(-x) = -H(x)$). Note that the coefficient of the highest degree term in H_n is 2^n since every new derivative brings down a factor of $(-2x)$ from the exponential factor to multiply the previous polynomial.

The most remarkable property of the Hermite polynomials, and of vital importance for their use in quantum mechanics, is the fact that they are *orthogonal* functions when integrated over the interval $(-\infty, \infty)$, provided they are multiplied, or *weighted*, by e^{-x^2} . That is

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 0 \text{ if } n \neq m \quad (12)$$

To see this, we can use the definition 3 of the polynomials, and integration by parts. If we assume (without loss of generality) that $m < n$:

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = \int_{-\infty}^{\infty} (-1)^n \frac{d^n}{dx^n} e^{-x^2} H_m(x) dx \quad (13)$$

$$= (-1)^n \frac{d^{n-1}}{dx^{n-1}} e^{-x^2} H_m(x) \Big|_{-\infty}^{\infty} - (-1)^n \int_{-\infty}^{\infty} \frac{d^{n-1}}{dx^{n-1}} e^{-x^2} \frac{d}{dx} H_m(x) dx \quad (14)$$

The integrated term is zero, since the derivative in this term will always contain the factor e^{-x^2} and this goes to zero faster than any polynomial, so the in the limit of $\pm\infty$, the term vanishes.

The remaining integral can be integrated by parts again, with the same result for the integrated term, but with a remaining integral of

$$\int_{-\infty}^{\infty} \frac{d^{n-2}}{dx^{n-2}} e^{-x^2} \frac{d^2}{dx^2} H_m(x) dx \quad (15)$$

Since $H_m(x)$ is a degree- m polynomial, and since we took $m < n$, we will eventually reach the $(m+1)^{th}$ derivative of $H_m(x)$ at the same time as the other term becomes $\frac{d^{n-m-1}}{dx^{n-m-1}} e^{-x^2} = e^{-x^2} H_{n-m-1}(x)$ from equation 3. Now the $(m+1)^{th}$ derivative of a degree m polynomial is always zero, so the resulting integral is also zero.

When $n = m$, we stop the integration by parts when we reach the m^{th} derivative under the integral sign, since in that case, we will have $d^m H_m / dx^m = 2^m m!$. Remember from above that the coefficient of the degree- m term in H_m is 2^m . Taking the m^{th} derivative of $2^m x^m$ will give you $2^m m!$ since each derivative reduces the power of x by 1 and brings that power down as multiplicative factor out front. Thus we get

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_m(x) dx = 2^m m! \int_{-\infty}^{\infty} e^{-x^2} dx \quad (16)$$

$$= 2^m m! \sqrt{\pi} \quad (17)$$

(As to how we know that $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$, that's a topic for another post! Suffice it to say here that it's another of those magical moments when two seemingly unrelated fundamental constants in mathematics, e and π , turn out to be intimately related.)

We can combine these two results into one formula by saying:

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^m m! \sqrt{\pi} \delta_{nm} \quad (18)$$

where δ_{nm} is the Kronecker delta symbol, which is 1 if $m = n$ and 0 otherwise.

To make the connection with their usage in the quantum mechanics of the harmonic oscillator, we need to derive a recurrence relation for the polynomials, in which higher degree polynomials can be derived from lower degree ones. We'll introduce the notation

$$F(x) \equiv e^{-x^2} \quad (19)$$

From the definition 3, we have

$$\frac{d^n F}{dx^n} = F^{(n)}(x) \quad (20)$$

$$= (-1)^n H_n(x) e^{-x^2} \quad (21)$$

Starting with the $(n-1)^{th}$ derivative, we have

$$F^{(n)}(x) = \frac{dF^{(n-1)}(x)}{dx} \quad (22)$$

$$= (-1)^{n-1} H_{n-1}(x) (-2x) e^{-x^2} + (-1)^{n-1} \frac{dH_{n-1}(x)}{dx} e^{-x^2} \quad (23)$$

$$= (-1)^n \left[2xH_{n-1}(x) - \frac{dH_{n-1}(x)}{dx} \right] e^{-x^2} \quad (24)$$

$$= (-1)^n H_n(x) e^{-x^2} \quad (25)$$

where the last line comes from the definition 3. We therefore get our recursion relation:

$$H_n(x) = 2xH_{n-1}(x) - \frac{dH_{n-1}(x)}{dx} \quad (26)$$

PINGBACKS

Pingback: Harmonic oscillator - example starting state

Pingback: Harmonic oscillator - Hermite polynomials

Pingback: Harmonic oscillator: matrix elements using Hermite polynomials