HERMITE POLYNOMIALS - THE RODRIGUES FORMULA

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There are several theorems concerning Hermite polynomials, which show up in the solution of the Schrödinger equation for the harmonic oscillator.

First, we'll look at the Rodrigues formula (which is a different formula from the Rodrigues formula for Legendre polynomials).

Suppose we start with $u = e^{-x^2}$ and take its derivative. We have

$$u' = -2xe^{-x^2} \tag{1}$$

$$u' + 2xu = 0 \tag{2}$$

We can now take the derivative of the second equation $n+1$ times and use Leibniz's formula for the nth derivative of a product, which is

$$(fg)^{(n)} = \sum_{k=0}^{n} \binom{n}{k} f^{(k)} g^{(n-k)} \tag{3}$$

We get

$$(xu)^{(n+1)} = \sum_{k=0}^{n+1} \binom{n+1}{k} x^{(k)} u^{(n+1-k)} \tag{4}$$

Since any derivative of x higher than the first gives zero, we have

$$(xu)^{(n+1)} = xu^{(n+1)} + (n+1)\,u^{(n)} \tag{5}$$

Applying this to the original equation, we get

$$u^{(n+2)} + 2xu^{(n+1)} + 2(n+1)\,u^{(n)} = 0 \tag{6}$$

Defining yet another variable $v \equiv (-1)^n u^{(n)}$ we get (the factor of $(-1)^n$ is inserted to make things come out right at the other end):

$$v'' + 2xv' + 2(n+1)\,v = 0 \tag{7}$$

Finally, defining $y \equiv e^{x^2} v$, we have

$$v = e^{-x^2} y \tag{8}$$

$$v' = e^{-x^2}\left[y' - 2xy\right] \tag{9}$$

$$v'' = -2xe^{-x^2}\left[y' - 2xy\right] + e^{-x^2}\left[y'' - 2y - 2xy'\right] \tag{10}$$

$$= e^{-x^2}\left[y'' - 4xy' + \left(4x^2 - 2\right)y\right] \tag{11}$$

Substituting this into 7 we get, after dividing out the common factor of e^{-x^2}:

$$y'' - 4xy' + \left(4x^2 - 2\right)y + 2x\left(y' - 2xy\right) + 2(n+1)y = 0 \tag{12}$$

$$y'' - 2xy + 2ny = 0 \tag{13}$$

This last equation is the same as that obtained from the Schrödinger equation earlier (with different variable names):

$$\frac{d^2 f}{d\xi^2} - 2\xi\frac{df}{d\xi} + (\epsilon - 1)\xi = 0 \tag{14}$$

$$\epsilon = \frac{2E}{\hbar\omega} \tag{15}$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \tag{16}$$

We can see by comparing the two forms of the equation that a solution to the latter is

$$f = y \tag{17}$$

$$= e^{\xi^2} v \tag{18}$$

$$= (-1)^n e^{\xi^2} u^{(n)} \tag{19}$$

$$= (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \tag{20}$$

Since this is a solution it must be a multiple of the Hermite polynomial. To see that it is actually the Hermite polynomial itself, consider the derivative term. Each derivative of $e^{-\xi^2}$ will have a term multiplying the previous derivative by -2ξ, so the term with the highest power of ξ in the nth derivative will be $(-2\xi)^n = (-1)^n 2^n \xi^n e^{-\xi^2}$. We now see why the factor of $(-1)^n$ was introduced earlier: by the usual convention, the coefficient of the highest power of a Hermite polynomial is 2^n, which is what we obtain from the formula above. Thus the Rodrigues formula for Hermite polynomials is

Rodrigues formula

$$\boxed{H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}} \tag{21}$$

We can apply this formula directly to get the first few polynomials. We get

$$H_0 = 1 \tag{22}$$
$$H_1 = 2x \tag{23}$$
$$H_2 = e^{x^2} \frac{d}{dx}\left(-2xe^{-x^2}\right) \tag{24}$$
$$= 4x^2 - 2 \tag{25}$$
$$H_3 = -e^{x^2} \frac{d}{dx}\left(-2e^{-x^2} + 4x^2 e^{-x^2}\right) \tag{26}$$
$$= 8x^3 - 12x \tag{27}$$
$$H_4 = e^{x^2} \frac{d}{dx}\left(4xe^{-x^2} + 8xe^{-x^2} - 8x^3 e^{-x^2}\right) \tag{28}$$
$$= e^{x^2} \frac{d}{dx}\left(12xe^{-x^2} - 8x^3 e^{-x^2}\right) \tag{29}$$
$$= 16x^4 - 48x^2 + 12 \tag{30}$$

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