HERMITE POLYNOMIALS – THE RODRIGUES FORMULA

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 \( n \)th 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
\[ v = e^{-x^2}y \]  
\[ v' = e^{-x^2}[y' - 2xy] \]  
\[ v'' = -2xe^{-x^2}[y' - 2xy] + e^{-x^2}[y'' - 2y - 2xy'] \]  
\[ = e^{-x^2}[y'' - 4xy' + (4x^2 - 2)y] \]  

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

\[ y'' - 4xy' + (4x^2 - 2)y + 2x(y' - 2xy) + 2(n + 1)y = 0 \]  
\[ y'' - 2xy + 2ny = 0 \]  

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

\[ \frac{d^2 f}{d\xi^2} - 2\xi \frac{df}{d\xi} + (\epsilon - 1)\xi = 0 \]  
\[ \epsilon = \frac{2E}{\hbar\omega} \]  
\[ \xi = \sqrt{\frac{m\omega}{\hbar}}x \]  

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

\[ f = y \]  
\[ = e^{\xi^2}v \]  
\[ = (-1)^n e^{\xi^2}u^{(n)} \]  
\[ = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \]  

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 \(-2\xi\), so the term with the highest power of \( \xi \) in the \( n \)th 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
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\[ H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \]  \hspace{1cm} (21)

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

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

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