HERMITE POLYNOMIALS - GENERATION

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When we solve the Schrödinger equation for the harmonic oscillator we find that we can peel off an exponential factor and what remains to be solved is the differential equation:

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

We can solve this equation using a power series, and we find that in order for the solution to be normalizable, the power series must contain only a finite number of terms. The energy of the oscillator is determined by the number of terms we allow the series to have, and the energy levels for the harmonic oscillator turn out to be:

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

where $n = 0, 1, 2, \ldots$

The stationary states for the oscillator are then

$$\psi(y) = e^{-y^2/2} \sum_{j=0}^{\infty} a_j y^j \tag{3}$$

where y was introduced as a shorthand variable:

$$y \equiv \sqrt{\frac{m\omega}{\hbar}}x \tag{4}$$

and the coefficients a_j satisfy the recursion relation

$$a_{j+2} = \frac{2j+1-\epsilon}{(j+1)(j+2)} a_j \tag{5}$$

where ϵ is another shorthand variable for the energy:

$$\epsilon \equiv \frac{2E}{\hbar\omega} \tag{6}$$

Once we decide on how many terms the series will have, this fixes the energy E since all terms beyond a particular point in the recursion formula must vanish. Since the recursion formula relates every *second* coefficient, and for any given stationary state the energy must have only one value, the series can contain only even terms or only odd terms, but not both. That is, once we have chosen an energy level, the corresponding stationary state wave function will be either even or odd.

Let's have a look at the first few stationary states that are generated by this recursion relation. The ground state corresponds to a polynomial that contains only the zeroth degree term, so a_0 is non-zero and all higher coefficients are zero. From the recursion relation 5 with $j = 0$:

$$a_2 = \frac{1-\epsilon}{2}a_0 \tag{7}$$
$$= 0 \tag{8}$$
$$\epsilon = 1 \tag{9}$$
$$E = \frac{\hbar\omega}{2} \tag{10}$$

In this case, the complete wave function for the stationary ground state is

$$\psi_0 = a_0 e^{-y^2/2} \tag{11}$$

The next state is found by taking $a_0 = 0$ to eliminate all the even terms in the series, and then requiring that $a_1 y$ is the single term in the series. So we have

$$a_3 = \frac{3-\epsilon}{6}a_1 \tag{12}$$
$$= 0 \tag{13}$$
$$\epsilon = 3 \tag{14}$$
$$E = \frac{3}{2}\hbar\omega \tag{15}$$

with corresponding stationary state

$$\psi_1 = a_1 y e^{-y^2/2} \tag{16}$$

In both these cases, we must determine a_0 and a_1 by normalizing the wave functions as usual. So in the case of a_0 we must have

$$|a_0|^2 \int_{-\infty}^{\infty} e^{-y^2} dx = 1 \tag{17}$$

Notice that the variable we must integrate over is the original x but we have the exponential expressed in terms of the convenience variable

$y=\sqrt{\frac{m\omega}{\hbar}}x$, so we need to transform the differential. Since both limits are infinite, they remain the same after the transformation.

$$|a_0|^2\sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty}e^{-y^2}dy=1 \tag{18}$$

The integral is the Gaussian integral, and its value is known to be $\sqrt{\pi}$, so we get

$$a_0=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \tag{19}$$

For the other stationary states, we can show that equation 1 has as its solutions the Hermite polynomials H_n. Furthermore, these polynomials form an orthogonal set of functions when weighted by the factor e^{-x^2}, in the sense that

$$\int_{-\infty}^{\infty}e^{-x^2}H_n(x)H_m(x)dx=2^m m!\sqrt{\pi}\delta_{nm} \tag{20}$$

When $n=m$, then, normalizing the stationary states requires that

$$|a_n|^2\int_{-\infty}^{\infty}e^{-y^2}H_n(y)H_m(y)dx=1 \tag{21}$$

Changing the variable of integration from x to y and using equation 20, we get

$$\begin{aligned}|a_n|^2\sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty}e^{-y^2}H_n^2(y)dy &= 1 \qquad (22)\\ |a_n|^2\sqrt{\frac{\hbar}{m\omega}}2^n n!\sqrt{\pi} &= 1 \qquad (23)\\ a_n &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}} \qquad (24)\end{aligned}$$

The final form for the stationary states of the harmonic oscillator is therefore

$$\begin{aligned}\psi_n(y) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(y)e^{-y^2/2} \qquad (25)\\ \psi_n(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar} \qquad (26)\end{aligned}$$

In the last line we have replaced the convenience variable y by its original form in terms of the position variable x.

The general solution of the time dependent Schrödinger equation for the harmonic oscillator is then a linear combination of the stationary states multiplied by the complex energy term, as usual

$$\Psi(x,t)=\sum_{n=0}^{\infty}c_{n}\psi_{n}(x)e^{-iE_{n}t/\hbar} \tag{27}$$

Note that the sum starts at $n=0$, unlike most potentials where the sum starts at $n=1$.