

HARMONIC OSCILLATOR: HERMITE POLYNOMIALS AND ORTHOGONALITY OF EIGENFUNCTIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercises 7.3.2 - 7.3.3.

The eigenfunctions of the harmonic oscillator are given by

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{-m\omega x^2/2\hbar} \quad (1)$$

where $H_n(u)$ is a Hermite polynomial. The Hermite polynomials obey the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (2)$$

The first few Hermite polynomials are given in Shankar's equation 7.3.21, and we may use these to verify this relation for a couple of cases. Taking $n = 2$ we have

$$H_3(x) = 2xH_2(x) - 4H_1(x) \quad (3)$$

$$= 2x[-2(1-2x^2)] - 4(2x) \quad (4)$$

$$= -12x + 8x^3 \quad (5)$$

The last line agrees with H_3 as given in Shankar.

For $n = 3$ we have

$$H_4(x) = 2xH_3(x) - 6H_2(x) \quad (6)$$

$$= 2x[-12x + 8x^3] - 6[-2(1-2x^2)] \quad (7)$$

$$= 12 - 48x^2 + 16x^4 \quad (8)$$

which again agrees with Shankar's equation.

When deriving the solution in terms of Hermite polynomials, we followed Griffiths and found that we could write the polynomials in the form

$$H_n(y) = \sum_{j=0}^n a_j y^j \quad (9)$$

where the coefficients a_j obey the recursion relation

$$a_{j+2} = \frac{2j+1-\varepsilon}{(j+1)(j+2)} a_j \quad (10)$$

The ε used by Griffiths is equivalent to 2ε in Shankar, so using Shankar's notation, we see that this recursion relation is the same as Shankar's equation 7.3.15:

$$C_{n+2} = C_n \frac{2n+1-2\varepsilon}{(n+1)(n+2)} \quad (11)$$

Here, we have

$$\varepsilon = \frac{E}{\hbar\omega} \quad (12)$$

where E is the energy of the oscillator state.

Looking at the polynomials in Shankar's equation 7.3.21, we have

$$H_3(y) = -12 \left(y - \frac{2}{3}y^3 \right) \quad (13)$$

so

$$C_1 = -12 \quad (14)$$

$$C_3 = 8 \quad (15)$$

With $n = 1$, we get from 11

$$C_3 = -12 \frac{3-2\varepsilon}{6} \quad (16)$$

However, for this state, $E = (3 + \frac{1}{2}) \hbar\omega$ so $2\varepsilon = 7$ and $C_3 = 8$ as required. For H_4 we have

$$H_4(y) = 12 \left(1 - 4y^2 + \frac{4}{3}y^4 \right) \quad (17)$$

This means

$$C_0 = 12 \quad (18)$$

$$C_2 = -48 \quad (19)$$

$$C_4 = 16 \quad (20)$$

Here $E = (4 + \frac{1}{2}) \hbar\omega$, so $2\varepsilon = 9$ and

$$C_2 = 12 \frac{(-8)}{2} = -48 \quad (21)$$

$$C_4 = -48 \frac{5-9}{12} = 16 \quad (22)$$

We can see from the relation 2 that, given that $H_0 = 1$ and $H_1 = 2x$, all Hermite polynomials of even index contain only even powers of x , and all polynomials of odd index contain only odd powers of x . This means that all even Hermite polynomials are even functions of x , in the sense that $H_{2n}(-x) = H_{2n}(x)$, and all odd Hermite polynomials are odd functions of x , so that $H_{2n+1}(-x) = -H_{2n+1}(x)$.

If $\psi(x)$ is even and $\phi(x)$ is odd, then

$$\psi(-x)\phi(-x) = -\psi(x)\phi(x) \quad (23)$$

That is, the product $\psi(x)\phi(x)$ is an odd function. Since the integral of any odd function over an interval symmetric about $x = 0$ is zero, we have

$$\int_{-\infty}^{\infty} \psi(x)\phi(x) dx = 0 \quad (24)$$

Looking at the eigenfunctions 1, we see that the exponential factor is a Gaussian centred at $x = 0$ and is therefore even, so that ψ_n will be even or odd depending on whether n is even or odd. In particular, the integral of any even ψ_n multiplied by any odd ψ_n over all x will be zero.

To show that pairs of even functions are also orthogonal is a bit trickier, but we can do it in the simplest case, where we consider the functions ψ_0 and ψ_2 .

$$\int_{-\infty}^{\infty} \psi_0(x)\psi_2(x) dx = \sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{8}} \int_{-\infty}^{\infty} H_0\left(\sqrt{\frac{m\omega}{\hbar}}x\right) H_2\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/\hbar} dx \quad (25)$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{8}} \int_{-\infty}^{\infty} (1) \left[-2\left(1 - 2\frac{m\omega}{\hbar}x^2\right)\right] e^{-m\omega x^2/\hbar} dx \quad (26)$$

$$= -\sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2}} \left[\sqrt{\frac{\pi\hbar}{m\omega}} - \sqrt{\frac{\pi\hbar}{m\omega}} \right] \quad (27)$$

$$= 0 \quad (28)$$

The two Gaussian integrals can be done using standard formulas as given in Shankar's Appendix A.2. (I used Maple.)

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