

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

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

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

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

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

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

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

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

The last line agrees with H_3 as given in Shankar.

For $n = 3$ we have

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

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

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

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

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

where the coefficients a_j obey the recursion relation

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

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:

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

Here, we have

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

where E is the energy of the oscillator state.

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

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

so

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

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

With $n = 1$, we get from 11

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

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

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

This means

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

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

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

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

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

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

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

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

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

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

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 .

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

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

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

$$(28) \quad = 0$$

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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