

Quantum harmonic oscillator

This is the Schrodinger equation for a quantum harmonic oscillator. The system is an “harmonic oscillator” because the potential energy is proportional to distance squared. The system is a “quantum” harmonic oscillator because $n \in \mathbb{N}_0$ hence the total energy is quantized.

$$\underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n}{\partial x^2}}_{\text{kinetic energy}} + \underbrace{\frac{1}{2} m \omega^2 x^2 \psi_n}_{\text{potential energy}} = \underbrace{\hbar \omega \left(n + \frac{1}{2} \right)}_{\text{total energy}} \psi_n$$

The equation can also be written as

$$\hat{H} \psi_n = E_n \psi_n$$

where \hat{H} is the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2$$

and E_n is the observed energy

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

Wave functions ψ_n are composed of an exponential times a Hermite polynomial H_n .

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

Hermite polynomials can be computed using the formula

$$H_n(z) = (-1)^n \exp(z^2) \frac{d^n}{dz^n} \exp(-z^2)$$

or the recurrence relation

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

Ladder operators

It can be shown that

$$\frac{d}{dx} H_n(x) = 2nH_{n-1}(x)$$

Hence the recurrence relation for Hermite polynomials can be written as

$$H_{n+1}(x) = 2xH_n(x) - \frac{d}{dx} H_n(x)$$

This suggests that there is an operator \hat{O} of the form

$$\hat{O} = ax - \frac{d}{dx}$$

such that

$$\psi_{n+1} \propto \hat{O} \psi_n$$

As a convenience of notation, factor $\psi_n = AB$ as follows.

$$\begin{aligned} A &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \frac{1}{\sqrt{2^n n!}} \\ B &= H_n(z) \\ z &= \sqrt{\frac{m\omega}{\hbar}}x \end{aligned}$$

Apply provisional operator \hat{O} to wave function ψ_n .

$$\begin{aligned} \hat{O}\psi_n &= \left(ax - \frac{d}{dx}\right) AB \\ &= axAB - B\frac{dA}{dx} - A\frac{dB}{dz}\frac{dz}{dx} \\ &= axAB + \frac{m\omega x}{\hbar}AB - A\frac{dB}{dz}\sqrt{\frac{m\omega}{\hbar}} \\ &= A\left(axB + \frac{m\omega x}{\hbar}B - \frac{dB}{dz}\sqrt{\frac{m\omega}{\hbar}}\right) \end{aligned}$$

Let

$$a = \frac{m\omega}{\hbar}$$

so that

$$ax + \frac{m\omega x}{\hbar} = \frac{2m\omega x}{\hbar} = 2z\sqrt{\frac{m\omega}{\hbar}}$$

Returning to the expansion of $\hat{O}\psi_n$ we now have

$$\hat{O}\psi_n = \sqrt{\frac{m\omega}{\hbar}}A\left(2zB - \frac{dB}{dz}\right)$$

From the recurrence relation for Hermite polynomials we have

$$2zB - \frac{dB}{dz} = H_{n+1}(z)$$

Expanding A and substituting H_{n+1} for the expression in B we have

$$\hat{O}\psi_n = \sqrt{\frac{m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \frac{1}{\sqrt{2^n n!}} H_{n+1}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

Noting that

$$\psi_{n+1} = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \frac{1}{\sqrt{2^{n+1}(n+1)!}} H_{n+1}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

we conclude that

$$\psi_{n+1} = \frac{1}{\sqrt{2(n+1)}}\sqrt{\frac{\hbar}{m\omega}}\hat{O}\psi_n$$

The standard notation for a raising operator is \hat{a}^\dagger . Define \hat{a}^\dagger as

$$\hat{a}^\dagger = \sqrt{\frac{\hbar}{2m\omega}} \hat{O} = \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{m\omega x}{\hbar} - \frac{d}{dx} \right)$$

It follows that

$$\psi_{n+1} = \frac{1}{\sqrt{n+1}} \hat{a}^\dagger \psi_n$$

A lowering operator follows directly from the derivative of ψ_n .

$$\begin{aligned} \frac{d\psi_n}{dx} &= B \frac{dA}{dx} + A \frac{dB}{dz} \frac{dz}{dx} \\ &= -\frac{m\omega x}{\hbar} \psi_n + 2nA H_{n-1}(z) \sqrt{\frac{m\omega}{\hbar}} \\ &= -\frac{m\omega x}{\hbar} \psi_n + \sqrt{2n} \psi_{n-1} \sqrt{\frac{m\omega}{\hbar}} \end{aligned}$$

Hence

$$\psi_{n-1} = \frac{1}{\sqrt{n}} \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{m\omega x}{\hbar} + \frac{d}{dx} \right) \psi_n$$

The standard notation for a lowering operator is \hat{a} . Define \hat{a} as

$$\hat{a} = \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{m\omega x}{\hbar} + \frac{d}{dx} \right)$$

It follows that

$$\psi_{n-1} = \frac{1}{\sqrt{n}} \hat{a} \psi_n$$

Probability density

A wave function squared is a probability density hence

$$\int_{-\infty}^{\infty} (\psi_n)^2 dx = 1$$

The expectation value for the Hamiltonian of the n th energy state is

$$\langle \hat{H} \rangle_n = \int_{-\infty}^{\infty} (\hat{H} \psi_n) \psi_n dx = \int_{-\infty}^{\infty} E_n (\psi_n)^2 dx = E_n$$