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.

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

The equation can also be written as

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

where $\hat{H}$ is the Hamiltonian operator

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

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.

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

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 nth energy state is

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