Quantum Harmonic Oscillator

The probability density evolution in a one-dimensional harmonic trapping potential is governed by the partial differential equation:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} - V(x)\Psi(x,t) = 0. \quad (1)$$

where: $\Psi(x,t)$ is the probability density and $V(x) = \frac{kx^2}{2}$ is the harmonic confining potential. A typical solution technique for this problem is to assume a solution of the form:

$$\Psi(x,t) = \sum_{n=1}^{N} a_n \Phi_n(x) \exp\left(-i \frac{E_n t}{2\hbar}\right) \quad (2)$$

and is called an eigenfunction expansion solution where:

ϕ_n = eigenfunctions $\qquad$ $E_n > 0$ = eigenvalues.

Plugging in this ansatz into (1) gives the time-independent ordinary differential equation (or boundary value problem):

$$-\frac{\hbar^2}{2m} \frac{d^2\Phi_n(x)}{dx^2} + \frac{kx^2}{2}\Phi_n(x) = E_n \Phi_n(x). \quad (3)$$

We know from the classical mechanical oscillator how the spring constant (k) relates to the oscillation frequency (ω) and the mass (m) by:

$$\omega = \sqrt{\frac{k}{m}} \Rightarrow \omega^2 = \frac{k}{m} \Rightarrow k = m\omega^2$$

Putting this into Eq.(3) we get:

$$-\frac{\hbar^2}{2m} \frac{d^2\Phi_n(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \Phi_n(x) = E_n \Phi_n(x) \quad (4).$$

Eq (4) can be written as:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\Phi_n(x)=E_n\Phi_n(x) \Rightarrow \hat{H}\,\Phi_n(x)=E_n\Phi_n(x)$$

where: $\hat{H}$ is the Hamiltonian operator of the system and $V(x)$ is the harmonic trapping potential.

This problem is simplified by transforming Eq(4) into a dimensionless eigenvalue problem. A simple strategy is to define a dimensionless coordinate $q=\frac{x}{\xi}$, where $\xi=\sqrt{\frac{\hbar}{m\omega}}$ is the local harmonic oscillator length (or the length scale) $\Rightarrow$

$$-\frac{\hbar^2}{2m}\frac{d^2\Phi_n(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\Phi_n(x)=E_n\Phi_n(x)$$

$$\frac{d^2\Phi_n(x)}{dx^2}+\frac{m\omega^2x^2}{2}\left(\frac{-2m}{\hbar^2}\right)\Phi_n(x)=\frac{-2m}{\hbar^2}E_n\Phi_n(x)$$

$$\frac{d^2\Phi_n(x)}{dx^2}-\frac{m\omega^2}{\hbar^2}x^2\Phi_n(x)=\frac{-2mE_n}{\hbar^2}\Phi_n(x).$$

$$x=q.\xi \Rightarrow \frac{d^2\Phi_n(q\xi)}{d(q\xi)^2}-\frac{m\omega^2}{\hbar^2}(q\xi)^2\Phi_n(q\xi)=\frac{-2mE_n}{\hbar^2}\Phi_n(q\xi)$$

$$\Phi_n(q\xi)=u_n(q) \Rightarrow \frac{1}{\xi^2}\frac{d^2u_n(q)}{dq^2}-\frac{m\omega^2\xi^2}{\hbar^2}q^2u_n(q)=\frac{-2mE_n}{\hbar^2}u_n(q)$$

$$\frac{d^2u_n(q)}{dq^2}-\frac{m\omega^2\xi^4}{\hbar^2}q^2u_n(q)=\frac{-2m\xi^2E_n}{\hbar^2}u_n(q) \quad (5)$$

Assuming that: $\alpha = \frac{m\omega^2 \xi^4}{\hbar^2}$ $\quad \epsilon_n = \frac{2m\xi^2}{\hbar^2} E_n$.

Eq (5) becomes:

$$\frac{d^2 u_n(q)}{dq^2} - \alpha q^2 u_n(q) = -\epsilon_n u_n(q)$$

Using FDM, we can use the second order numerical derivative

as following:

$$-\frac{d^2 u_n(q)}{dq^2} + \alpha q^2 u_n(q) = \epsilon_n u_n(q)$$

$$-\left(\frac{u(q_{n+1}) - 2u(q) + u(q_{n+1})}{\Delta q^2}\right) + \alpha q^2 u(q_n) = \epsilon_n u(q_n)$$

$$-\frac{1}{\Delta q^2} u(q_{n+1}) + \frac{2}{\Delta q^2} u(q_n) - \frac{1}{\Delta q^2} u(q_{n+1}) + \alpha q^2 u(q_n) = \epsilon_n u(q_n)$$

$$\underbrace{\left(\frac{2}{\Delta q^2} + \alpha q^2\right)}_{\text{Diagonal}} u(q_n) - \underbrace{\frac{1}{\Delta q^2} u(q_{n+1}) - \frac{1}{\Delta q^2} u(q_{n-1})}_{\text{off-diagonal.}} = \epsilon_n u(q_n)$$