Quantum harmonic oscillator is a system in Quantum Mechanics similar to the harmonic oscillation, given by $m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -kx$, in Classical Mechanics.

1. Why do we need to study quantum harmonic oscillator?

Although there's no perfect harmonic oscillator in the real world, when considering a second order Taylor Series expansion of the potential energy to approximate the potential energy of a system, we can see that the potential energy of a system can be approximated by a harmonic oscillator.

2. Analytic Method

2.1. Setup of the Problem

In Classical Mechanics, the potential energy of a harmonic oscillator is given by:

$$V(x) = \frac{1}{2}kx^2$$

By plugging this into the Schrödinger Equation, we have:

$$-\frac{\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}kx^2\psi = i\ \hbar\ \frac{\partial\Psi}{\partial t} \tag{1}$$

Since we know that general solutions to the Schrödinger Equation can be written as the linear combination of separable states, we have:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left(-iE_n\frac{t}{\hbar}\right)$$
$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

Our goal is to find $\psi_n(x)$ that satisfies the time-independent Schrödinger Equation:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}kx^2\psi = E\psi \tag{2}$$

2.2. Solving the differential equation

In order to solve Eq. 2, we first consider the Hermite differential equation:

$$y'' - 2xy' + 2ny = 0 \tag{3}$$

The solution [1] to Eq. 3 can be derived through series expansion, and is given by:

$$H_n(x) = n! \sum_{j=0}^{M} \frac{(-1)^j (2x)^{n-2j}}{j!(n-2j)!} \quad \text{where } M = \begin{cases} \frac{n}{2} \text{ if } n \text{ is even} \\ \frac{n+1}{2} \text{ if } n \text{ is odd} \end{cases} \tag{4}$$

For Eq. 3 to take a similar form as Eq. 2, we can consider the substitution $y = \exp\left(\frac{x^2}{2}\right)\varphi$. By making this substitution, we obtain:

$$\begin{aligned} y' &= \exp\left(\frac{x^2}{2}\right)(x\varphi + \varphi') \\ y'' &= x\exp\left(\frac{x^2}{2}\right)(x\varphi + \varphi') + \exp\left(\frac{x^2}{2}\right)(\varphi + x\varphi' + \varphi'') \\ &= \exp\left(\frac{x^2}{2}\right)\left[(1 + x^2)\varphi + 2x\varphi' + \varphi''\right] \end{aligned}$$

Plugging those into Eq. 3, we have:

$$\begin{aligned} \exp\left(\frac{x^2}{2}\right)\left[(1 + x^2)\varphi + 2x\varphi' + \varphi'' - 2x(x\varphi + \varphi') + 2n\varphi\right] &= 0 \\ \exp\left(\frac{x^2}{2}\right)\left[\varphi'' + (2n + 1 - x^2)\varphi\right] &= 0 \end{aligned}$$

$$\varphi'' + (2n + 1 - x^2)\varphi = 0 \tag{5}$$

Here, we can already see the similar second derivative, constant term, and x^2 term taking place in the differential equation.

Since we have $\varphi = \exp\left(-\frac{x^2}{2}\right)y$, using Eq. 4, we know that the solution to previous differential equation is:

$$\varphi_n(x) = \exp\left(-\frac{x^2}{2}\right) H_n(x) \tag{6}$$

2.3. Properties of $\varphi_n(x)$

We can now verify some properties of Eq. 6 to prove that it can be a solution to the time-independent Schrödinger equation.

1. Mutually Orthogonal

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \varphi_n(x)\varphi_m(x) = \int_{-\infty}^{\infty} H_n(x) H_m(x) \exp(-x^2)\, \mathrm{d}x$$

Since Hermite polynomials are orthogonal with respect to $\exp(-x^2)$, we have:

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) \exp(-x^2)\, \mathrm{d}x = 0$$

2. Normalizable

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}x\, \varphi_n^2(x) &= \int_{-\infty}^{\infty} \mathrm{d}x\, H_n^2(x) \exp(-x^2) \\ &= 2^n n! \sqrt{\pi}\end{aligned}$$

2.4. Back to time-independent Schrödinger equation

Going back to Eq. 2. Let $\omega := \sqrt{\frac{k}{m}}$, which means $k = m\omega^2$, we obtain:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2 \psi - E\psi = 0 \tag{7}$$

Let $s := \sqrt{\frac{m\omega}{\hbar}}x$, then $x = \sqrt{\frac{\hbar}{m\omega}}s$ and $\mathrm{d}x = \sqrt{\frac{\hbar}{m\omega}}\,\mathrm{d}s$

By Chain Rule for second derivative, we have:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) = \frac{\mathrm{d}}{\sqrt{\frac{\hbar}{m\omega}}\,\mathrm{d}s}\left(\frac{\mathrm{d}\psi}{\sqrt{\frac{\hbar}{m\omega}}\,\mathrm{d}s}\right) = \frac{m\omega}{\hbar}\frac{\mathrm{d}^2\psi}{\mathrm{d}s^2}$$

Then, we can plug this into Eq. 7:

$$-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{\mathrm{d}^2\psi}{\mathrm{d}s^2}+\frac{1}{2}m\omega^2\frac{\hbar}{m\omega}s^2\psi-E\psi=0$$
$$-\frac{\hbar\,\omega}{2}\frac{\mathrm{d}^2\psi}{\mathrm{d}s^2}+\frac{1}{2}\,\hbar\,\omega s^2\psi-E\psi=0$$
$$\frac{\mathrm{d}^2\psi}{\mathrm{d}s^2}-s^2\psi+\frac{2E}{\hbar\,\omega}\psi=0$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}s^2}+\left(\frac{2E}{\hbar\,\omega}-s^2\right)\psi=0 \tag{8}$$

As we verified already, Eq. 6 is a solution to Eq. 5 and satisfies the properties of solution to the time-independent Schrödinger equation.

Notice that the only difference between Eq. 8 and Eq. 5 is the $\frac{2E}{\hbar\,\omega}$ and $(2n+1)$ term. Therefore, we can consider:

$$E=E_n=\hbar\,\omega\left(n+\frac{1}{2}\right)\quad\text{where } n\in\mathbb{N}$$

Which allows Eq. 8 to take the same form as Eq. 5.

Putting all the substitutions together into Eq. 6, we have:

$$\psi_n(x)=A_n\varphi_n(s)=A_n\exp\left(-\frac{s^2}{2}\right)H_n(s)$$
$$=A_n\exp\left(-\frac{m\omega}{2\,\hbar}x^2\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

To solve for A_n, we normalize $\psi_n(x)$:

$$\int_{-\infty}^{\infty} \mathrm{d}x \, |\psi_n(x)|^2 = \int_{-\infty}^{\infty} \mathrm{d}x |A_n|^2 \; H_n^2\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\!\left(-\frac{m\omega}{\hbar} x^2\right)$$

$$1 = |A_n|^2 \sqrt{\frac{m\omega}{\hbar \; \pi}} 2^n n!$$

$$|A_n|^2 = \sqrt{\frac{\hbar \; \pi}{m\omega}} \frac{2^{-n}}{n!}$$

$$|A_n| = \sqrt{\frac{2^{-n}}{n!}} \left(\frac{\hbar \; \pi}{m\omega}\right)^{\frac{1}{4}}$$

$$\Psi(x,t) = \sqrt{\frac{2^{-n}}{n!}} \left(\frac{\hbar \; \pi}{m\omega}\right)^{\frac{1}{4}} \exp\!\left(-\frac{m\omega}{2 \; \hbar} x^2\right) \sum_{n=1}^{\infty} c_n H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\!\left(-i E_n \frac{t}{\hbar}\right)$$

$$\text{where } E_n = \hbar \; \omega\left(n + \frac{1}{2}\right) \text{ and } \omega = \sqrt{\frac{k}{m}}$$

$$\text{and } c_n = \sqrt{\frac{2^{-n}}{n!}} \left(\frac{\hbar \; \pi}{m\omega}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \mathrm{d}x \, \Psi(x,0) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\!\left(-\frac{m\omega}{2 \; \hbar} x^2\right)$$

3. Algebraic Method

Recall that we already define $\omega \coloneqq \sqrt{\frac{k}{m}}$, from Eq. 2 we have

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 + (m\omega x)^2\right]\psi = E\psi \tag{9}$$

3.1. Ladder Operators

Recall from Algebra 1, we have $u^2 + v^2 = (u + iv)(u - iv)$, we can consider [2]:

$$a_{\pm} \coloneqq \frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x} \pm i m\omega x\right)$$

$$a_-a_+ = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 + (m\omega x)^2\right] + \frac{1}{2}\,\hbar\,\omega$$

$$a_+a_- = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 + (m\omega x)^2\right] - \frac{1}{2}\,\hbar\,\omega$$

Therefore, we can rewrite Eq. 9 as:

$$\left(a_-a_+ - \frac{1}{2}\,\hbar\,\omega\right)\psi = E\psi \tag{10}$$

$$\left(a_+a_- + \frac{1}{2}\,\hbar\,\omega\right)\psi = E\psi \tag{11}$$

3.2. Properties of Ladder Operators

Now, we can consider $a_+\psi$ and $a_-\psi$. Replacing ψ with $a_+\psi$ in Eq. 10, we have:

$$\begin{aligned}
&\left(a_+a_- + \frac{1}{2}\,\hbar\,\omega\right)(a_+\psi) \\
&= a_+\left(a_-a_+ + \frac{1}{2}\,\hbar\,\omega\right)\psi \\
&= a_+\left(a_-a_+ - \frac{1}{2}\,\hbar\,\omega + \hbar\,\omega\right)\psi \\
&= a_+\left[\left(a_-a_+ - \frac{1}{2}\,\hbar\,\omega\right)\psi + \hbar\,\omega\psi\right] \\
&= (E + \hbar\,\omega)(a_+\psi)
\end{aligned}$$

We can prove this for $a_-\psi$ similarly that it gives energy $E - \hbar\,\omega$.

If we consider the state of energy of ψ, applying the ladder operators is increasing and decreasing the energy of ψ, like climbing up and down the ladder of energy. Therefore, a_+ is called the raising operator and a_- is called the lowering operator.

By instinct, we know that energy can't decrease infinitely, which means that there must be a "ground state", where applying a_- won't give us anything:

$$a_-\psi_0 = 0$$

3.3. Solving ψ_0

Expanding a_-, we have:

$$\begin{aligned}\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x} - im\omega x\right)\psi_0 &= 0 \\ \frac{\hbar}{i}\frac{\mathrm{d}\psi_0}{\mathrm{d}x} - im\omega x\psi_0 &= 0 \\ \frac{\mathrm{d}\psi_0}{\mathrm{d}x} + \frac{m\omega x}{\hbar}\psi_0 &= 0 \\ \int \frac{\mathrm{d}\psi_0}{\psi_0} &= -\int \frac{m\omega x}{\hbar}\,\mathrm{d}x \\ \ln(\psi_0) &= -\frac{m\omega}{\hbar}\frac{x^2}{2} + A_0 \\ \psi_0 &= A\exp\left(-\frac{m\omega}{2\,\hbar}x^2\right)\end{aligned}$$

Putting this into Eq. 10, we have:

$$\begin{aligned}\left(a_+a_- + \frac{1}{2}\,\hbar\,\omega\right)\psi_0 &= E_0\psi_0 \\ a_+(a_-\psi_0) + \frac{1}{2}\,\hbar\,\omega\psi_0 &= E_0\psi_0 \\ E_0 &= \frac{1}{2}\,\hbar\,\omega\end{aligned}$$

To get the excited states, we can continue to apply the raising operator a_+:

$$\psi_n = A_n(a_+)^n \exp\left(-\frac{m\omega}{2\,\hbar}x^2\right)$$

The corresponding energy is:

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

Bibliography

[1] N. Asmar, *Partial Differential Equations with Fourier Series and Boundary Value Problems*. Pearson Prentice Hall, 2005. [Online]. Available: https://books.google.com/books?id=2FonAQAAIAAJ

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