جامعة الانبار-كلية العلوم – قسم الفيزياء

Quantum Mechanics

The Time- Independent Schrödinger Equation (TISE) and its solutions:

أ.د. نبيل ابراهيم فواز

Ref.: Quantum Mechanics
Concepts and Applications
Second Edition
Nouredine Zettili
Jacksonville State University, Jacksonville, USA

The Simple Harmonic Oscillator Potential (S.H.O.): by Operators:

Simple Harmonic Oscillator (S.H.O.):

"Classical: $H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$ $\left[\omega = \sqrt{\frac{K}{m}} \Rightarrow K = m\omega^2\right]$

$= \frac{1}{2m}(p^2 + m^2\omega^2x^2)$

$= \frac{1}{2m}(ip + m\omega x)(-ip + m\omega x)$ ← Valide Classically

Dynamic Variables Changed to operators in Q.M.

In Q.M.:

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{1}{2m}(\hat{p}^2 + m^2\omega^2\hat{x}^2)$

$= \frac{1}{2m}(-i\hat{p} + m\omega\hat{x})(-i\hat{p} + m\omega\hat{x})$

$= \frac{1}{2m}(\hat{p}^2 + m^2\omega^2\hat{x}^2 - im\omega(\hat{x}\hat{p} - \hat{p}\hat{x}))$ $[\hat{x},\hat{p}] = i\hbar$

$= \frac{1}{2m}(\hat{p}^2 + m^2\omega^2\hat{x}^2 + \hbar m\omega)$

Schrö. Eqn.

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

From the shape of the potential, E must be real number and a non-negative value because the potential has an absolute minimum at $x = 0$. Because x^2 is not Constant so, we can not solve it as a

superposition of two exponentials.

In order to solve this equ. we need to put boundary conditions, in which we like to get a bound state and should be normalizable, so, they are:

1) $\phi(x) \longrightarrow 0$ as $x \longrightarrow \mp \infty$

2) $\int_{-\infty}^{\infty} |\phi(x)|^2 \, dx < \infty$ Normalization

The parameters in this case in m, ω & $\hbar$. From these parameters We can Construct a quantity of dimension x and dimension P.

$[\hbar] = ML^2T^{-1}$ $[\omega] = \frac{1}{T} = T^{-1}$ $[M] = M$

$\therefore \sqrt{\frac{\hbar}{m\omega}} = \sqrt{\frac{ML^2T^{-1}}{MT^{-1}}} = \sqrt{L^2}$ length

$p = mv = MLT^{-1} \Rightarrow \therefore \sqrt{m\hbar\omega} = \sqrt{M \, ML^2T^{-1}T^{-1}} = \sqrt{M^2L^2T^{-2}}$ Momentum

Define the dimensionless operators

$$\hat{a} = \frac{1}{\sqrt{2m\omega\hbar}}\left[m\omega\hat{x} + i\hat{p}\right] = \frac{\hat{x}}{\sqrt{2\hbar/m\omega}} + \frac{i\hat{p}}{\sqrt{2\hbar m\omega}}$$

$$= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} + \frac{i}{\sqrt{m\omega\hbar}}\,\hat{p}\right]$$

($\sqrt{m\omega/\hbar}$: length; $\hat{x}$: length; $\frac{i}{\sqrt{m\omega\hbar}}$: momentum; $\hat{p}$: momentum)

Known as annihilation or lowering operator

and

$$a^{\dagger} = \frac{\hat{x}}{\sqrt{2\hbar/m\omega}} - \frac{i\hat{p}}{\sqrt{\hbar m\omega}} = \frac{1}{\sqrt{2m\omega\hbar}}\left[m\omega\hat{x} - i\hat{p}\right]$$

$$= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} - \frac{i}{\sqrt{m\omega\hbar}}\,\hat{p}\right]$$

Known as Creation or raising operator.

Although $\hat{x}$ and $\hat{p}$ are Hermitian operators but a & $a^{\dagger}$ are not because the existance of i.

$a^{\dagger}\hat{a}$ - is Hermitian operator.

To find $\hat{a}a^{\dagger}$ [Ladder operator]

$$\hat{a}a^{\dagger} = \frac{1}{2m\omega\hbar}(i\hat{p} + m\omega\hat{x})(-i\hat{p} + m\omega\hat{x})$$

$$= \frac{1}{2m\omega\hbar}\left(\hat{p}^2 + m^2\omega^2\hat{x}^2 - 2m\omega(\hat{x}\hat{p} - \hat{p}\hat{x})\right) \qquad [\hat{x},\hat{p}] = i\hbar$$

$$= \frac{1}{\hbar\omega}\hat{H} + \frac{\frac{1}{\hbar\omega}\hat{H}}{2m\omega\hbar}\hbar m\omega = \frac{1}{\hbar\omega}\hat{H} + \frac{1}{2}$$

& $a^{\dagger}a = \frac{1}{\hbar\omega}H - \frac{1}{2}$

$\therefore \hat{H} = \hbar\omega(aa^{\dagger} - \frac{1}{2}\mathbb{1})$ ($\mathbb{1}$: unit operator)

$\hat{H} = \hbar\omega(a^{\dagger}a + \frac{1}{2}\mathbb{1})$

$\therefore \hat{H}\Psi = E\Psi$ Can be written as:

$\hbar\omega(a^{\dagger}a + \frac{1}{2})\Psi = E\Psi$

or $\hbar\omega(aa^{\dagger} - \frac{1}{2})\Psi = E\Psi$

To see what happen when $a^\dagger$ acts before the $\hat{H}$ $(\hat{H}(\hat{a}^\dagger\psi))$

$$\hbar\omega(\hat{a}^\dagger\hat{a}+\tfrac{1}{2})(a^\dagger\psi) = \hbar\omega(\hat{a}^\dagger\hat{a}\hat{a}^\dagger+\tfrac{1}{2}a^\dagger)\Psi$$
$$= \hbar\omega\, a^\dagger(aa^\dagger+\tfrac{1}{2})\Psi$$
$$= \hbar\omega\, a^\dagger(aa^\dagger-\tfrac{1}{2}+1)\Psi$$
$$= a^\dagger(\hat{H}+\hbar\omega)\Psi \overset{\hat{H}}{=} a^\dagger(E+\hbar\omega)\Psi$$
$$= (E+\hbar\omega)\,a^\dagger\Psi$$

$\therefore \hat{H}(a^\dagger\Psi) = (E+\hbar\omega)(a^\dagger\Psi)$

also $\hat{H}(a\Psi) = (E-\hbar\omega)(a\Psi)$

So, if Ψ is a solution, then $a^\dagger\Psi$ is also solution with $E+\hbar\omega$ eigenvalue

$a\Psi$ " " " " $E-\hbar\omega$ eigenvalue

$$\Psi_{n-2} \xleftarrow{a} \Psi_{n-1} \xleftarrow{a} \Psi_n \xrightarrow{a^\dagger} \Psi_{n+1} \xrightarrow{a^\dagger} \Psi_{n+2} \cdots$$

So, we cannot have solutions with very low E. There should be a function that gives zero, we call it $a|0\rangle = 0$ or $a\phi_0(x) = 0$

This can be used to find the W.F. of the S.H.O., by starting From

$$a|0\rangle = 0 \Rightarrow \left(\frac{\hat{x}}{\sqrt{2\hbar/m\omega}} + \frac{i\hat{p}}{\sqrt{2m\omega\hbar}}\right)|0\rangle = 0$$

$$\frac{1}{\sqrt{2m\omega\hbar}}\left[m\omega\hat{x}+i\hat{p}\right]|0\rangle = 0 \Rightarrow (m\omega\hat{x}+i\hat{p})|0\rangle = 0$$

For the ground state W.F. $\phi_0(x)$

By definition $\phi_0(x) = \langle x|0\rangle$ which it is the representative in the position basis of the g.S. vector.

$\therefore \langle x|(m\omega\hat{x}+i\hat{p})|0\rangle = 0$

$$m\omega x\,\phi_0(x) + \hbar\frac{d}{dx}\phi_0(x) = 0 \quad \left[ip = i(-i\hbar)\frac{d}{dx} = \hbar\frac{d}{dx}\right]$$

$$\left[m\omega x + \hbar\frac{d}{dx}\right]\phi_0(x) = 0$$

$$\frac{d\phi_0(x)}{dx} = -\frac{m\omega x}{\hbar}\phi_0(x) \Rightarrow \frac{d\phi_0(x)}{\phi_0(x)} = -\frac{m\omega x}{\hbar}dx$$

integrating

$$\ln\phi_0(x) = -\frac{m\omega x^2}{2\hbar} + C \Rightarrow \boxed{\phi_0(x) = C_0\, e^{-\frac{m\omega x^2}{2\hbar}}}$$

$$\int_{-\infty}^{\infty}|\phi_0(x)|^2dx = 1 = C_0^2\sqrt{\frac{2\pi\hbar}{m\omega}} \Rightarrow C_0 = \left(\frac{m\omega}{2\pi\hbar}\right)^{1/4}$$

$$\therefore \phi_0(x) = \left(\frac{m\omega}{2\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$$

So, we cannot have solutions with very low E.

So, there should be a function that gives zero, we call it

$\hat{a}_- \psi_0 = 0$ The lowest energy state

So, we can find

$\hat{a}_- \psi_0 = 0$

$\hat{p} = \frac{\hbar}{i}\left(-2\pi \frac{d}{dx}\right) = \hbar \frac{d}{dx}$

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar \frac{d}{dx} + m\omega x\right)\psi_0 = 0$$

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar} x\, \psi_0 \Rightarrow \int \frac{d\psi_0}{\psi_0} = \int -\frac{m\omega}{\hbar} x\, dx$$

$$\therefore \psi_0 = C\, e^{-\frac{m\omega}{2\hbar}x^2} \Rightarrow C = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\therefore \psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

What is the value of energy for the ground state $|0\rangle$?

To find

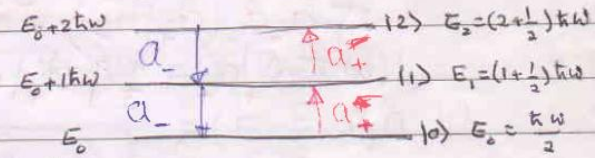
$$\hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)|0\rangle = E_0|0\rangle$$

$$\hbar\omega\, \hat{a}_+\hat{a}_-|0\rangle + \frac{1}{2}\hbar\omega|0\rangle = E_0|0\rangle$$

$\hat{a}_-|0\rangle = 0$

$$\therefore \frac{1}{2}\hbar\omega|0\rangle = E_0|0\rangle$$

$$\therefore E_0 = \frac{\hbar\omega}{2}$$



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

or

label for any state