13|10|2025

Day 26. The Quantum Mechanical Simple Harmonic Oscillator

Problems where the position of a particle (or even collective coordinates of N-particles) move about a stable equilibrium are modelled, at a first degree of approximation as a simple harmonic oscillator.

Let us illustrate this by considering a classical particle, tied to the origin by a "restoring force", moving only along the x-direction.

The potential energy of the particle is a function of the position x. Therefore, for small displacements from the origin we could expand the potential energy $V(x)$ in a Taylor series.

$$V(x) = V(0) + \left.\frac{dV}{dx}\right|_{x=0} x + \frac{1}{2}\left.\frac{d^2V}{dx^2}\right| x^2 + O(x^3) \quad — ①$$

Now, if we assume that the potential energy function achieves its minimum value at $x=0$. In this case

$$\left.\frac{dV}{dx}\right|_{x=0} = 0 \qquad -(2)$$

Then the first non-trivial dependence on x (leading order term) comes from the quadratic term. To a good approximation then, for small displacements we have.

$$V(x) \simeq \quad + \frac{1}{2} \left.\frac{d^2V}{dx^2}\right|_0 x^2 \qquad -(3)$$

Let
$$\left.\begin{aligned} V_0 &\equiv V(x_0) = 0 \\ \& \ k &\equiv m\omega^2 = \left.\frac{d^2V}{dx^2}\right|_0 \end{aligned}\right\} -(4)$$

$m \rightarrow$ mass of particle

$\omega = \sqrt{\frac{k}{m}}$ = fundamental (angular) frequency of oscillation

The force acting on the particle at any instant, when its displacement is $x(t) \equiv x$, is:

$$F(t) = -\frac{dV(x(t))}{dx} \quad — (5)$$

In the present case this means

$$F(t) = -k\,x(t) \quad — (6)$$

If $x > 0$, F acts towards the origin. Hence, it is called a restoring force. From Newton's eqn of motion:

$$F = ma = m\frac{d^2x}{dt^2} = -m\omega^2 x \quad — (7)$$

or $$\frac{d^2x}{dt^2} + \omega^2 x = 0 \quad — (8)$$

$$\Rightarrow \quad x(t) = A\,e^{i\omega t} + B\,e^{-i\omega t} \quad — (9)$$

Also, $\dot{x}(t) = ik\left[Ae^{ikx} - Be^{-ikx}\right]$ — (10)

Suppose, $$\left.\begin{aligned} x(0) &= A_0 \\ \dot{x}(0) &= 0 \end{aligned}\right\} \quad (11)$$

$\Rightarrow$ $$A + B = A_0 \quad — (12)$$
$$ik(A - B) = 0 \quad — (13)$$

(13) $\Rightarrow$ $A = B$ — (14)

(12) & (14) $\Rightarrow$ $A = B = A_0/2$ — (15)

Putting it all together we get

$$\left.\begin{aligned} x(t) &= A_0 \cos(\omega t) \\ v(t) = \dot{x}(t) &= -A_0 \omega \sin(\omega t) \end{aligned}\right\} \quad (16)$$

Note that the K.E. is

$$T(t) = \frac{1}{2} m \dot{x}(t)^2 = \frac{1}{2} m A_0^2 \omega^2 \sin^2(\omega t)$$

P.E. is $$V(t) = \frac{1}{2} k x^2(t) = \frac{1}{2} m A_0^2 \omega^2 \cos^2(\omega t)$$

— (17)

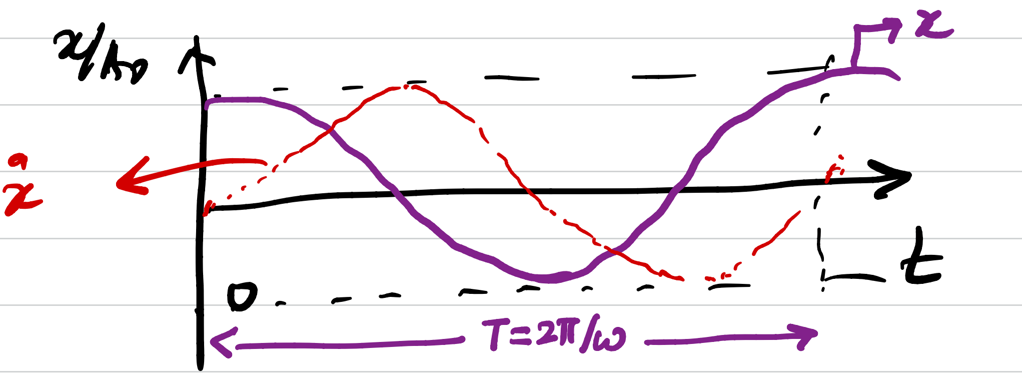
$\Rightarrow$ Total energy at any time is

$$E(t) = T(t) + V(t)$$
$$= \frac{1}{2} m\omega^2 A_0^2 \quad — (18)$$

i.e. Total energy is conserved.
and $E \propto A_0^2$ for a given m, ω.
— (19)

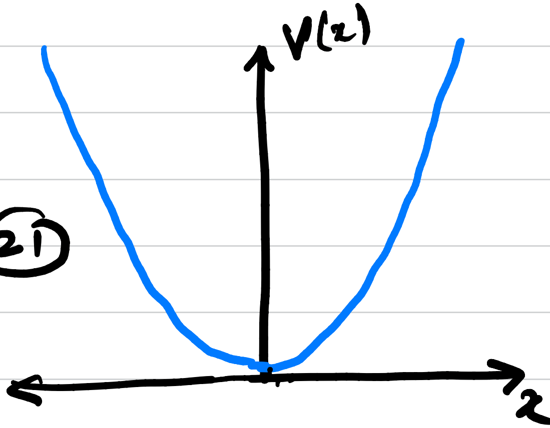
Also note at, $T=0 \Rightarrow x = \pm A_0$ — (20)

These are called "turning points".
The classical particle cannot take a larger amplitude than this since that would render $T<0$.



Now on to the quantum problem.
For the Harmonic potential we have

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \qquad (21)$$



$$V(-x) = V(x) \qquad (22)$$

$\Rightarrow$ eigenfunctions will have odd/even parity!

As always, solving the dynamical problem requires first solving the eigenvalue problem as $V(\hat{x})$ is time-independent.

TISE: $$\hat{H}|\psi\rangle = E|\psi\rangle \qquad (23)$$

Let's first look at the position basis solution.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x) \quad — (24)$$

Let $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ & $\xi = x/x_0$ — (25)

$$\Rightarrow \frac{d^2}{dx^2} = \frac{1}{x_0^2}\frac{d^2}{d\xi^2} \quad — (26)$$

Substituting (26) in (24)

$$\frac{\hbar\omega}{2}\left[-\frac{d^2}{d\xi^2}\psi(x_0\xi) + \xi^2\psi(x_0\xi)\right] = E\psi(x_0\xi) \quad — (27)$$

or letting $\psi(x_0\xi) = \tilde{\psi}(\xi)$ — (28)

$$\tilde{\psi}''(\xi) + (\lambda - \xi^2)\tilde{\psi}(\xi) = 0 \quad — (29)$$

where $\lambda = E/(\hbar\omega/2)$ — (30)

We are looking for bound state solutions for which $\lim_{|\xi|\to\infty} \tilde{\psi}(\xi) \to 0$ — (31)

In this limit ($|\xi| \to \infty$) the differential equation becomes

$$\tilde{\Psi}''(\xi) - \xi^2 \tilde{\Psi}(\xi) = 0 \quad - (32)$$

Consider $y(\xi) = \xi^p e^{\pm \xi^2} \quad - (33)$
for some finite $p > 0$.

$$y'(\xi) = \left(p \xi^{p-1} \pm \xi^{p+1}\right) e^{\pm \xi^2/2}$$

& $$y''(\xi) = \left(p(p-1)\xi^{p-2} \pm p\xi^p \pm (p+1)\xi^p + \xi^{p+2}\right) e^{\pm \xi^2/2}$$

$$= \left(p(p-1)\xi^{p-2} \pm (2p+1)\xi^p + \xi^{p+2}\right) e^{\pm \xi^2}$$

$$= \left(\frac{p(p-1)}{\xi^2} + (2p+1) + 4\xi^2\right) y(\xi)$$

$$\longrightarrow \xi^2 y(\xi) \quad (|\xi| \to \infty) \quad - (34)$$

Thus, a solution of the form (33) would satisfy the $|\xi| \to \infty$ behaviour of $\tilde{\psi}(\xi)$ required by (32). But for $\tilde{\psi}(\xi)$ to be bound we need to discard the $e^{\xi^2/2}$ possibility as it would blow up at $|\xi| \to \infty$.

So, we could write

$$\tilde{\psi}(\xi) = f(\xi)\, e^{-\xi^2/2} \quad — (35)$$

where $f(\xi)$ is representible by some polynomial ξ. Substituting (35) in (29) and eliminating the exponential from both sides yields:

$$f''(\xi) - 2\xi f'(\xi) + (\lambda - 1) f(\xi) = 0 \quad — (36)$$

The solutions to this 2nd order differential equation form a vector space.

Consider the set of polynomials.

$\mathbb{P} = \{1, \xi, \xi^2, \xi^3, \ldots\}$

These are clearly linearly independent. Now consider the set of all functions

$$f(\xi) = \sum_{n=0}^{\infty}{}' \, c_n \xi^n \quad \text{— (37)}$$

For $c_n \in \mathbb{R}$, and defined on $\xi \in (a,b)$

This set forms a vector space over real fields.

Let's define the notion of an inner product for these:

$$\langle f | g \rangle \equiv \int_a^b d\xi \; f(\xi) g(\xi) w(\xi) \quad \text{— (38)}$$

where $0 \leq w(\xi) \leq 1$ is a weighting function. This now forms a Hilbert space $\mathcal{L}^2((a,b); w)$.

Using the definition of the I.P. and the L.I. set Φ, we can come up with an orthogonalized set of "basis functions"

$$\Phi = \{ \phi_0(\xi), \phi_1(\xi), \phi_2(\xi), \cdots \}$$

such that

$$\langle \phi_i | \phi_j \rangle = N_i \, \delta_{ij} \quad \text{— (39)}$$

&

$$f(\xi) = \sum_{i=0}^{\infty} c_i \, \phi_i(\xi) \quad \text{— (40)}$$

for any $f \in \mathcal{L}^2([a,b]; w)$

Obviously $\{\phi_\xi\}$ are polynomial functions. They are called "orthogonal polynomials"

We can also ~~chose~~ to normalize the $\{\phi_i\}$ to get $\{\tilde{\phi}_i\}$ s.t.

$$\langle \tilde{\phi}_i | \tilde{\phi}_j \rangle = \delta_{ij} \quad \text{— (41)}$$

Let us choose $w(x) = e^{-\xi^2}$
and $a = -\infty$, $b = \infty$

Then, $\{\tilde{\phi}_i\}$ satisfy:

$$\int_{-\infty}^{\infty} d\xi \, \tilde{\phi}_i(\xi) \, \tilde{\phi}_j(\xi) \, e^{-\xi^2} = \delta_{ij} \quad \text{— (42)}$$

In this case, we get the orthogonal polynomials to be the Hermite polynomials defined through:

not normalized

$$\boxed{H_n(\xi) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)} \quad \text{— (43)}$$

which yields:

$$H_n(\xi) = \sum_{s=0}^{[n/2]} (-1)^s (2\xi)^{n-2s} \frac{n!}{(n-2s)!\,s!}$$

where $[\;]$ = greatest integer function (or floor function) — (44)

e.g. $[4.3] = 4 \qquad [-4.3] = -4$

These satisfy the recurrence relations

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi) \qquad \text{— (45)}$$

$$H_n'(\xi) = 2n H_{n-1}(\xi) \qquad \text{— (46)}$$

Using these two relations we can show that $H_n(\xi)$ satisfy the differential equation

$$\boxed{H_n''(\xi) - 2\xi H_n'(\xi) + 2n H_n(\xi) = 0} \qquad \text{— (47)}$$

Normalization:

$$\int_{-\infty}^{\infty} d\xi \; e^{-\xi^2} \left(H_n(\xi)\right)^2 = 2^n \pi^{1/2} n! \qquad \text{— (48)}$$

$$\Rightarrow \quad N_n = \frac{1}{2^{n/2} \pi^{1/4} \sqrt{n!}} \qquad \text{— (49)}$$

Normalization

Comparing (47) with the equation we had for our quantum Harmonic oscillator (36), we readily identify that

$$f(\xi) \equiv H_n(\xi) \qquad \text{— (49)}$$

if

$$(\lambda - 1) = 2n \qquad \text{— (50)}$$

$$(50) \Rightarrow \quad E\Big/\left(\frac{\hbar\omega}{2}\right) \quad (2n+1)$$

or

$$\boxed{E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega} \qquad \text{— (51)}$$

$$n = 0, 1, 2, 3, \ldots$$

$$\Rightarrow \boxed{\begin{gathered} \tilde{\psi}_n(\xi) = \frac{1}{2^{n/2}\pi^{1/4}\sqrt{n!}} H_n(\xi)\, e^{-\xi^2/2} \\ E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega \\ n = 0, 1, 2, \ldots \end{gathered}} \qquad \text{— (52)}$$

are the eigen solutions of the Q.H.O.