3. APPLICATION OF QUANTUM MECHANICS IN 1-D :—

3.1 The Time-independent Schrödinger Equation :—

Let us consider the time-dependent Schrödinger equation : (in 1-D)

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\,\Psi(x,t) \equiv \underbrace{\hat{H}}_{\text{Hamiltonian operator.}}\Psi(x,t) \quad \text{—— (1)}$$

Now, to solve this, we shall assume that the potential V is independent of t. Then it is possible to reduce that partial differential equation to two ordinary differential equations by the method of "separation of variables." We write

$$\Psi(x,t) = \psi(x)\,T(t)$$

which implies that,

$$i\hbar\,\psi(x)\frac{dT(t)}{dt} = \left[-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x)\right]T(t)$$

Division by $\psi(x)T(t)$ gives —

$$i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt} = \frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x)\right].$$

Since the two sides of the equation depend on different variables (that's why, we cannot apply this separation of variables if $V = V(x,t)$), this can only be satisfied if both sides are constant. We denote the constant by E. Then,

$$i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt} = E$$

$$\Rightarrow d\ln T(t) = -\frac{iE}{\hbar}\,dt.$$

$$\Rightarrow \ln T(t) = -\frac{iE}{\hbar}t + c_1$$

$$\Rightarrow \boxed{T(t) = C\,e^{-iEt/\hbar}} \quad \text{—— (2)}$$

If V does depend on t, then the energy is not conserved, so it is no longer a constant of the motion.

The other eq^n :

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)} \quad \text{—— (3)}$$

↳ time-independent Schrödinger eq^n.

In classical mechanics, the motion of a particle is determined by the force $F(x) = -\frac{dV(x)}{dx}$, so that adding a constant V_0 to the potential has no effect. We can see that, the same holds in quantum mechanics. If $V(x)$ is replaced by $V(x) + V_0$ then all we need to do is to replace the label E by $E + V_0 \Rightarrow$

$$T(t) = C e^{-i(E+V_0)t/\hbar}$$

and
$$(E+V_0)\,\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + (V(x)+V_0)\,\psi(x)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)$$

So, the time-independent eq^n remains unchanged. The presence of V_0 merely changes the sol^n $\psi(x,t)$ by a phase factor of $e^{-iV_0t/\hbar}$

Equation ③ is an "eigenvalue equation":

- An "operator" acting on a function maps it into another function like: $\mathcal{O}f(x) = f(x) + x^2$ or $\mathcal{O}f(x) = [f(x)]^2$ etc.
- A special case of operators, called "linear operators" have the property that:
$$L[f_1(x) + f_2(x)] = Lf_1(x) + Lf_2(x)$$
and, $L\,c\,f(x) = c\,Lf(x) \rightarrow c$ being an arbitrary complex number.
like: $\mathcal{O}f(x) = f(3x^2+1)$ or $\mathcal{O}f(x) = \frac{df(x)}{dx} - 2f(x)$.
- If a linear operator has this property:
$$Lf(x) = \lambda f(x)$$ then it's called eigenvalue eq^n.

The equation ③ may be written in the form

$$\boxed{\hat{H}\psi(x) = E\,\psi(x)}$$

where, $\hat{H}$ is the Hamiltonian operator: $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

The eigenvalue E is called "energy eigenvalue" and the eigenfunction $\psi(x)$ corresponding to the eigenvalue E of the operator $\hat{H}$ is called "energy eigenfunction" or "energy eigenstate".

• The probability density doesn't depend on t:

$$\boxed{\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar}}$$

then the probability density

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{iEt/\hbar}\, \psi e^{-iEt/\hbar} = \psi^*(x)\,\psi(x) = |\psi(x)|^2$$

→ the time dependence cancels out.

Similarly, every expectation values are "constant in time":

$$\langle \hat{Q}(x,p)\rangle = \int \psi^*(x)\, \hat{Q}\left(x, \frac{\hbar}{i}\frac{d}{dx}\right)\psi(x)\, dx .$$

The expectation value of the total energy is:

$$\langle \hat{H}\rangle = \int \psi^*(x)\, \hat{H}\, \psi(x) dx = E\int |\psi|^2 dx = E$$

and,

$$\langle \hat{H}^2\rangle = \int \psi^*(x)\, \hat{H}^2 \psi(x)\, dx = \int \psi^* \hat{H}(\hat{H}\psi)\, dx$$

$$= \int \psi^*\, \hat{H}\,(E\psi)\, dx = E\int \psi^* \hat{H}\,\psi\, dx = E^2\int |\psi|^2 dx = E^2$$

Then the standard deviation in $\hat{H}$ is:

$$\sigma_{\hat{H}}^2 = \langle \hat{H}^2\rangle - \langle \hat{H}\rangle^2 = E^2 - E^2 = 0 .$$

$\sigma = 0$ means that the distribution has zero spread, that is every member of the sample has the same value.

Thus, ~~the~~ every measurement of the total energy will surely gives the value E.

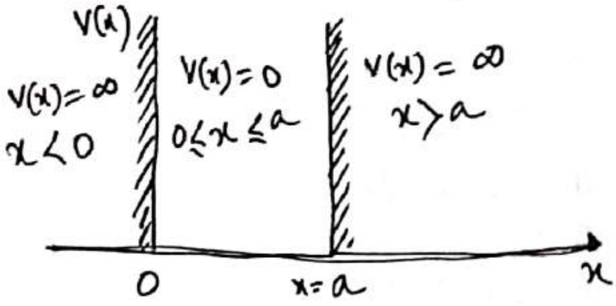
• The solution of eq^n ① [time-dependent Schrödinger eq^n] is of the form $\psi(x)\, e^{-iEt/\hbar}$, but eq^n ① itself is a linear equation. So, a sum of the solution of the above form is also a solution. Permissible values of E may be discrete, E_n ($n = 1, 2, 3, \ldots$) or continuous. If we describe the eigenfunctions corresponding to the discrete eigenvalues E_n by $\psi_n(x)$ and those corresponding to continuous eigenvalues E by $\psi_E(x)$, then the most general sol^n of the Schrödinger eq^n will be —

$$\boxed{\Psi(x,t) = \sum_n c_n \psi_n(x)\, e^{-iE_n t/\hbar} + \int dE\; C(E)\, \psi_E(x)\, e^{-iEt/\hbar}}$$

→ c_n are arbitrary constants and the $C(E)$ are arbitrary functions of E, only constrainted by the condition that $\Psi(x,t)$ be square-integrable.

3.2 One-dimensional Potential Problems:

3.2.1 The infinite well:
(Particle in a box)



Consider a potential as —

$$V(x) = \infty, \quad x < 0$$
$$= 0, \quad 0 \le x \le a$$
$$= \infty, \quad x > a$$

Outside the well, the probability of finding the particle is zero.
So,
$$\psi(x) = 0, \quad x < 0$$
$$= 0, \quad x > a$$

Inside the well/box, where $V(x) = 0$, we have

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$\Rightarrow$ Now, if $E < 0$, then the eq^n takes the form —

$$\frac{d^2\psi(x)}{dx^2} - k^2\psi(x) = 0,$$

where, $k^2 = \frac{2m|E|}{\hbar^2}$. The most general sol^n to this eq^n is $\psi(x) = Ae^{kx} + Be^{-kx} \longrightarrow$ this sol^n doesn't vanish at $x = a$, so we cannot have $E < 0$. E must be > 0.

So, $\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$, where, $k^2 = \frac{2mE}{\hbar^2}$ $(E > 0)$.

Most general sol^n to this —

$$\psi(x) = A\sin kx + B\cos kx$$

Now, $\psi(0) = 0 \longrightarrow B = 0$.

$$\psi(x) = A\sin kx$$

The condition $\psi(a) = 0 \Rightarrow A\sin ka = 0$.

$$\Rightarrow ka = n\pi, \quad n = 1, 2, 3, \ldots$$

[n=0 excluded, otherwise the wavefunction would vanish everywhere]

Thus, the energy eigenvalues are —

$$\boxed{E_n = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2\pi^2n^2}{2ma^2}}, \quad n = 1, 2, 3, \ldots$$

The wavefunction is:

$$\psi_n(x) = A\sin\frac{n\pi x}{a}$$

Now, check for normalization:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_0^a |A|^2 \sin^2 \frac{n\pi x}{a}\, dx = 1$$

$$\Rightarrow |A|^2 \cdot \frac{1}{2} \int_0^a \left[1 - \cos \frac{2n\pi x}{a}\right] dx = 1 \quad [\text{as } 2\sin^2 x = 1 - \cos 2x]$$

$$\Rightarrow |A|^2 \cdot \frac{a}{2} = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{a}}$$ [we take only the positive real value, as the phase of A doesn't carry any physical significance]

So, $$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}} \quad \text{for } 0 \le x \le a$$

$$= 0 \quad \text{for } x < 0,\ x > a$$

- **Some properties of infinite well wave functions:** —

1. **Orthonormality:**

$$\int_{-\infty}^{+\infty} dx\, \psi_m^*(x)\, \psi_n(x) = \int_0^a dx.\ \frac{2}{a} \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a}$$

$$= \frac{1}{a} \int_0^a dx \left[\cos \frac{(m-n)\pi x}{a} - \cos \frac{(m+n)\pi x}{a}\right]$$

[As, $\sin x \sin y = \frac{1}{2}[\cos(x-y) - \cos(x+y)]$]

$$= \frac{1}{a}\left[\frac{a}{(m-n)\pi} \sin \frac{(m-n)\pi x}{a} - \frac{a}{(m+n)\pi} \cdot \sin \frac{(m+n)\pi x}{a}\right]\Bigg|_0^a$$

$$= \frac{\sin[(m-n)\pi]}{(m-n)\pi} - \frac{\sin[(m+n)\pi]}{(m+n)\pi}$$

$$= 0 \quad \text{when } m \neq n$$

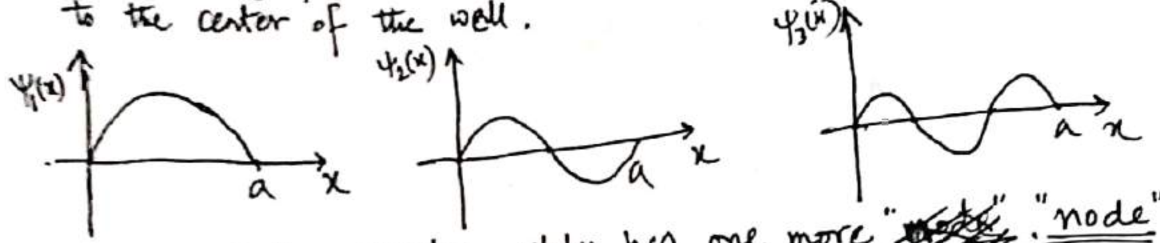
When $m = n$, the integral can be written as: $\int_{-\infty}^{+\infty} |\psi_n|^2 dx = 1$ from normalization.

So, $$\boxed{\int_{-\infty}^{+\infty} dx\, \psi_m^*(x)\, \psi_n(x) = \delta_{mn}}$$

i.e. the eigenfunctions corresponding to different eigenvalues are orthogonal. They are also "complete", i.e. any other function $f(x)$ can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1} c_n \sin \frac{n\pi x}{a}.$$

2. These eigenfunctions are alternatively even and odd with respect to the center of the well.



each successive state has one more "node".

3. The expectation value of the position & momentum:

$$\langle x \rangle = \int_{-\infty}^{+\infty} dx\, \psi_n^*(x)\, x\, \psi_n(x)$$

$$= \frac{2}{a}\int_0^a x \sin^2\frac{n\pi x}{a}\, dx$$

$$= \frac{2}{a}\left[\left(x . \int \sin^2\frac{n\pi x}{a}\, dx\right)\Big|_0^a - \int_0^a\left[\int \sin^2\frac{n\pi x}{a}\, dx\right]dx\right]$$

integration by parts:
$\int f(x) g(x)\, dx$
$= f(x)\int g(x)\, dx - \int\left[f'(x)\int g(x)\, dx\right]dx$

$$\cancel{= \frac{2}{a}\left[\frac{a^2}{2} - \int_0^a \ldots dx\right]}$$

$$= \frac{2}{a}\left[\frac{x}{2}\int\left(1-\cos\frac{2n\pi x}{a}\right)dx - \frac{1}{2}\int\left\{\int\left(1-\cos\frac{2n\pi x}{a}\right)dx\right\}dx\right]_0^a$$

$$= \frac{2}{a}\left[\frac{x}{2}\left[x - \frac{a}{2n\pi}\sin\frac{2n\pi x}{a}\right] - \frac{1}{2}\int\left(x - \frac{a}{2n\pi}\cdot\sin\frac{2n\pi x}{a}\right)dx\right]_0^a$$

$$= \frac{2}{a}\left[\frac{x^2}{2} - \frac{ax}{4n\pi}\sin\frac{2n\pi x}{a} - \frac{x^2}{4} + \frac{a}{4n\pi}\cdot\left(-\frac{a}{2n\pi}\cdot\cos\frac{2n\pi x}{a}\right)\right]_0^a$$

$$= \frac{2}{a}\left[\frac{a^2}{4}\right] = \frac{a}{2}.$$

As the probability distribution is symmetric about $x = a/2$, this is expected to find the particle at middle of the box.

$$\langle x^2 \rangle = \frac{2}{a}\int_0^a x^2 \sin^2\frac{n\pi x}{a}\, dx. = a^2\,\frac{2n^2\pi^2 - 3}{6n^2\pi^2} \quad \text{[Check it!]}$$

Now,

$$\langle p \rangle = \int_0^a dx\, \psi_n(x)\left(-i\hbar\frac{d\psi_n(x)}{dx}\right)$$

$$= -i\hbar\int_0^a dx\,\frac{1}{2}\frac{d}{dx}\left(\psi_n(x)\right)^2 \quad [\text{as } \psi_n(x) \text{ is real}]$$

$$= -\frac{i\hbar}{2}\left[\psi_n^2(a) - \psi_n^2(0)\right] = 0$$

Alternatively, as $\langle p \rangle = \frac{d\langle x \rangle}{dt}$ & $\langle x \rangle = \text{const.}$ so $\langle p \rangle = 0$

$\langle p^2 \rangle = 2mE_n$ [inside the box]

$= \frac{\hbar^2 \pi^2 n^2}{a^2}$

So, $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$

$= a^2 \frac{2n^2\pi^2 - 3}{6n^2\pi^2} - \frac{a^2}{4}$

$= a^2 \left(\frac{4n^2\pi^2 - 6 - 3n^2\pi^2}{12n^2\pi^2} \right) = a^2 \left(\frac{n^2\pi^2 - 6}{12n^2\pi^2} \right)$

$\Rightarrow \sigma_x = a\sqrt{\frac{n^2\pi^2 - 6}{12n^2\pi^2}} = \frac{a}{2n\pi}\sqrt{\frac{n^2\pi^2-6}{3}}$.

& $\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$

$= \frac{\hbar^2 \pi^2 n^2}{a^2}$

$\Rightarrow \sigma_p = \frac{\hbar \pi n}{a}$.

$\sigma_x \sigma_p = \frac{\hbar}{2}\sqrt{\frac{n^2\pi^2 - 6}{3}} > \frac{\hbar}{2}$ [As for $n=1$, this value is $\sqrt{\frac{\pi^2-6}{3}} > 1$ & for $n>1$, this value is even greater than its $n=1$ value]

↳ uncertainty principal satisfied.

4. If we put the boundaries of the box at $x = -a/2$ and $x = +a/2$.

⟶ This shift is accomplished by the change of variables

$x \to x - a/2$.

We then get,

$\sin\frac{n\pi x}{a} \longrightarrow \sin\left(\frac{n\pi x}{a} - \frac{n\pi}{2}\right)$

$= \sin\frac{n\pi x}{a}\cos\frac{n\pi}{2} - \cos\frac{n\pi x}{a}\sin\frac{n\pi}{2}$.

So, for $n = 1, 3, 5, \ldots$ the solutions are proportional to $\cos\frac{n\pi x}{a}$ which are "even functions" of x. [the '$-$'ve sign will be absorbed as overall phase factor]

for $n = 2, 4, 6, \ldots$ the solutions are proportional to $\sin\frac{n\pi x}{a}$ which are "odd functions" of x.

So, the solutions will be (for the infinite well bounded by $x = \pm a/2$):

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad \text{with } n = 2, 4, 6, \ldots$$

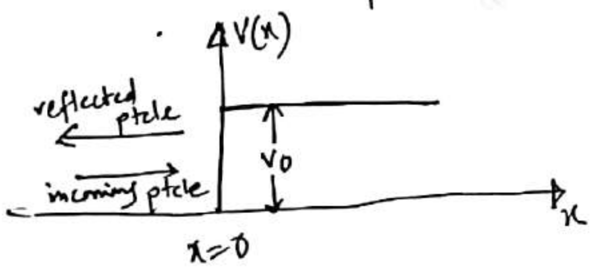
$$= \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a}, \quad \text{with } n = 1, 3, 5, \ldots$$

Energy eigenvalues remain same as earlier.

(3.2.2.) The Potential Step:

Consider a potential of the form:

$$V(x) = 0 \quad \text{if } x < 0$$
$$= V_0 \quad \text{if } x > 0.$$



The time-independent Schrödinger eq^n:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$$

We take, $\frac{2mE}{\hbar^2} = k^2$ [$E > 0$, as E must be greater than V_{min}]

and $\frac{2m(E - V_0)}{\hbar^2} = -q^2$ (for $E < V_0$)

$= q^2$ (for $E > V_0$)

(i) For $x < 0$, $V(x) = 0$. $\rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0$ [As $E > V_{min}$ to get normalizable sol^n, so, have $E > 0$]

Then the solution will be.

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{For } x < 0$$

Ae^{ikx}: wave associated with the particle heading towards the barrier

Be^{-ikx}: wave associated with particle reflected from the barrier.

(ii) for $x > 0$ $\quad V(x) = V_0$.

There could be two different cases:

(a) if $E > V_0$, then $q^2 = \frac{2m(E - V_0)}{\hbar^2} \rightarrow \frac{d^2\psi}{dx^2} + q^2\psi = 0.$

Then the solution will be –

$$\psi(x) = Ce^{iqx} + De^{-iqx}$$

Now, we shall assume that only a wave from left is incoming (like in an experiment), then at right or $x > 0$ region the only transmitted wave will be of the form e^{iqx}.

So, $\psi(x) = C e^{iqx}$, for $x > 0$.

Now the constants A, B, C cannot be all arbitrary. The continuity of the wave function at $x=0$ implies that:

$$A + B = C \quad \text{--- (1)}$$

And the continuity of its first derivative at $x=0$ implies that:

$$ik(A-B) = iqC$$

$$\Rightarrow k(A-B) = qC \quad \text{--- (2)}$$

solving eq^{n}s (1) & (2) gives.

$q \times (1) - (2) \longrightarrow \quad B = \frac{k-q}{k+q} A.$

$k \times (1) + (2) \longrightarrow \quad C = \frac{2k}{k+q} A.$

So,
$$\psi(x) = Ae^{ikx} + \frac{k-q}{k+q} \cdot Ae^{-ikx}. \quad \text{at } x<0$$

$$= \frac{2k}{k+q} A e^{iqx}, \quad \text{at } x>0.$$

We may view this as Ae^{ikx} is the incident or incoming wave, $\left(\frac{k-q}{k+q}\right) Ae^{-ikx}$ is the reflected wave and $\frac{2k}{k+q} Ae^{iqx}$ is the transmitted wave.

Now, we want to calculate the flux associated with each of these corresponding waves.

- The incoming flux (J_i) will be:

$$J_i = \frac{\hbar}{2mi}\left[\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[e^{-ikx}(ik)e^{ikx} - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[ik + ik\right]$$

$$= \frac{\hbar}{2mi}|A|^2 \cdot 2ik$$

$$\Rightarrow \boxed{J_i = \frac{\hbar k}{m}|A|^2}$$

• The reflected flux will be:

$$J_r = \frac{\hbar}{2mi}|A|^2\left[\left(\frac{k-q}{k+q}\right)^2 e^{ikx}(-ik)e^{-ikx} - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2 \cdot [-ik - ik]\cdot\left(\frac{k-q}{k+q}\right)^2$$

$$\Rightarrow \boxed{J_r = -\frac{\hbar k}{m}|A|^2 \cdot \left(\frac{k-q}{k+q}\right)^2}$$

↳ this '−'ve sign corresponds to a flux moving in the '−'ve x direction.

• The transmitted flux will be:

$$J_t = \frac{\hbar}{2mi}|A|^2\left[\frac{2k}{k+q}e^{-iqx}\cdot\frac{2k}{k+q}\cdot(iq)e^{iqx} - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[\left(\frac{2k}{k+q}\right)^2\cdot iq + \left(\frac{2k}{k+q}\right)^2\cdot iq\right]$$

$$= \frac{\hbar}{2mi}|A|^2\cdot 2iq\cdot\left(\frac{2k}{k+q}\right)^2$$

$$\Rightarrow \boxed{J_t = \frac{\hbar q}{m}|A|^2\left(\frac{2k}{k+q}\right)^2}$$

Now the "reflection coefficient" (i.e. the fraction of incoming beam of particles that will be bounce back) is defined as:

$$R = \left|\frac{J_r}{J_i}\right| = \left(\frac{k-q}{k+q}\right)^2 = \frac{(k-q)^4}{(k^2-q^2)^2} = \frac{\left(\sqrt{E}-\sqrt{E-V_0}\right)^4}{V_0^2}$$

As, for $E > V_0$, we have:

$$k^2 = \frac{2mE}{\hbar^2},\quad q^2 = \frac{2m(E-V_0)}{\hbar^2}$$

So, $k-q = \frac{\sqrt{2m}}{\hbar}\left[\sqrt{E}-\sqrt{E-V_0}\right]$

& $k^2-q^2 = \frac{2m}{\hbar^2}V_0$

And the "transmission coefficient" is defined similarly as:

$$T = \left|\frac{J_t}{J_i}\right| = \frac{q}{k}\left(\frac{2k}{k+q}\right)^2 = \frac{4kq}{(k+q)^2}$$

$$= \frac{4kq(k-q)^2}{(k^2-q^2)^2} = \frac{4\sqrt{E}\cdot\sqrt{E-V_0}\cdot\left(\sqrt{E}-\sqrt{E-V_0}\right)^2}{V_0^2}.$$

Now,

$$R+T = \left(\frac{k-q}{k+q}\right)^2 + \frac{4kq}{(k+q)^2}$$

$$= \frac{(k+q)^2}{(k+q)^2} = 1.$$

Sum of the reflection and transmitted probability must be 1.
— i.e. conserved.

⊛⊛ ⇒ In contrast to the classical mechanics, according to which a particle or beam of particles going over a potential step would slow down to conserve energy but never be reflected back, since $E > V_0$. But here we do see some fraction of these particles ~~are~~ is being reflected — This is a direct consequence of the "wave properties" of the particle, ~~where~~ as we see reflection of light as a common thing.

⇒ For $E \gg V_0$, $q \to k$, so the reflection coefficient $R \to 0$.
→ This agrees with intuition.

(b) Now if $E < V_0$, then $q^2 = \frac{2m(V_0 - E)}{\hbar^2}$.

$$\rightarrow \frac{d^2\psi}{dx^2} - q^2\psi = 0$$

Sol^n:
for $x < 0$, same as before:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

for $x > 0$, $\psi(x) = Ce^{+qx} + De^{-qx}$.
But ψ must vanish at $x = +\infty$
so, $C = 0$ & $\boxed{\psi(x) = De^{-qx}}$ → also known as "Evanescent wave"

The continuity of the wave function at $x=0$ gives —

$$A + B = D \quad \text{——— (1)}$$

And the continuity of its first derivative at $x=0$ gives —

$$ik(A - B) = -qD \quad \text{——— (2)}$$

which can be solved to give:

$$(1) \times q + (2) \longrightarrow B = \frac{ik+q}{ik-q} A$$

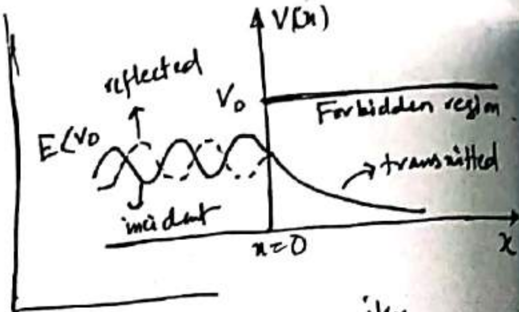
$$(1) \times ik + (2) \longrightarrow D = \frac{2ik}{ik-q} A.$$

Hence,

$$\psi(x) = Ae^{ikx} + \frac{ik+q}{ik-q} Ae^{-ikx}, \quad x < 0$$

$$= \frac{2ik}{ik-q} Ae^{-qx} \quad x > 0.$$

- The incoming flux (J_i) will be :



$$J_i = \frac{\hbar}{2mi}\left[\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right]$$

$$= \frac{\hbar k}{m}|A|^2 \text{ [same as before]}$$

- The reflected flux :

$$J_r = \frac{\hbar}{2mi}|A|^2\left[\frac{-ik+q}{-ik-q}\cdot e^{-ikx} \cdot \frac{ik+q}{ik-q}(-ik)\cdot e^{ikx} - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[\frac{ik-q}{ik+q}\cdot\frac{ik+q}{ik-q}\cdot(-ik) - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[-ik - ik\right]$$

$$= -\frac{\hbar k}{m}|A|^2$$

- The transmitted flux :

$$J_t = \frac{\hbar}{2mi}|A|^2\left[\frac{-2ik}{-(ik+q)}\cdot e^{-qx}\cdot\frac{2ik}{ik-q}(-q)e^{-qx} - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[\frac{(2ik)^2}{(ik+q)(ik-q)}(-q).\ e^{-2qx} - c.c.\right]$$

$$= \frac{\hbar}{2mi}|A|^2\left[\frac{4k^2}{k^2+q^2}\cdot q e^{-2qx} - c.c.\right]$$

$$= 0.$$

so, reflection coefficient, $R = \left|\frac{J_r}{J_i}\right|^2 = 1.$ $\longrightarrow$ total reflection like Classical mechanics.

& transmission coefficient, $T = \left|\frac{J_t}{J_i}\right|^2 = 0.$

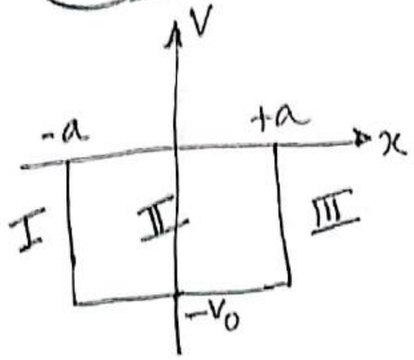
But, if we calculate the probability density of finding the particle at $x>0$, we get:

$$|\psi(x)|^2_{x>0} = |A|^2\left|\frac{2ik}{ik-q}\right|^2 e^{-2qx}$$

$$= |A|^2 \cdot \frac{4k^2}{k^2+q^2}\cdot e^{-2qx}$$

This probability is exponentially decreasing, but "non-zero" ! This permits a ~~tunne~~ "tunneling" through barriers that would totally block particles in a classical description., Although, there is no flux to the right (as $J_t = 0$) and a total reflection happens, there is an exponentially decaying field that penetrates into the forbidden region. This phenomena is known as "quantum tunneling".

3.2.3 The finite potential well :—



Consider a finite potential well by:

$$V(x) = \begin{cases} -V_0 & \text{if } |x| \leq a \\ 0 & \text{if } |x| > a \end{cases}$$

- First consider the bound states $(E<0)$ only.

$\Rightarrow$ Schrödinger eq^n (time-indep.):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{2m(E-V(x))}{\hbar^2}\psi(x) = 0$$

Now define:

$$\boxed{\alpha^2 = -\frac{2mE}{\hbar^2}} \quad \& \quad \boxed{k^2 = \frac{2m(E+V_0)}{\hbar^2}}$$

[as $E<0$ and $E > V_{min} = -V_0$]

$\Rightarrow E+V_0$ is positive

in region I & III (i.e. $|x|>a$):

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} - \alpha^2\psi(x) = 0$$

sol^n: $\boxed{\psi_1(x) = A_1 e^{\alpha x} + B_1 e^{-\alpha x} \quad (\text{say, for } x<-a)}$

& $\boxed{\psi_3(x) = A_3 e^{\alpha x} + B_3 e^{-\alpha x} \quad (\text{for } x>a)}$

in region II (i.e. $|x| \leq a$):

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m(E+V_0)}{\hbar^2}\psi(x) = 0$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0.$$

sol^n: $\boxed{\psi_2(x) = A_2\cos(kx) + B_2\sin(kx) \quad (\text{for } |x| \leq a)}$

so,

(I) $\psi_1(x) = A_1 e^{\alpha x} + B_1 e^{-\alpha x}$ $\quad [x < -a]$

(II) $\psi_2(x) = A_2 \cos(kx) + B_2 \sin(kx)$ $\quad [-a \le x \le a]$

(III) $\psi_3(x) = A_3 e^{\alpha x} + B_3 e^{-\alpha x}$ $\quad [x > a]$

• Now apply the boundary conditions:

(i) $\psi_1(-\infty) = 0 \Rightarrow B_1 = 0$

(ii) $\psi_3(\infty) = 0 \Rightarrow A_3 = 0$

Furthermore, $\psi(x)$ & $\frac{d\psi}{dx}$ must be continuous at the boundary

(iii) $\psi_1(-a) = \psi_2(-a)$; $\frac{d\psi_1}{dx}(-a) = \frac{d\psi_2}{dx}(-a)$

$$\Rightarrow A_1 e^{-\alpha a} = A_2 \cos(ka) - B_2 \sin(ka) \quad \text{—— (1)}$$

and, $$\alpha A_1 e^{-\alpha a} = A_2 k \sin(ka) + B_2 k \cos(ka) \quad \text{—— (2)}$$

(iv) $\psi_2(a) = \psi_3(a)$; $\frac{d\psi_2}{dx}(a) = \frac{d\psi_3}{dx}(a)$.

$$\Rightarrow B_3 e^{-\alpha a} = A_2 \cos(ka) + B_2 \sin(ka) \quad \text{—— (3)}$$

and, $$-\alpha B_3 e^{-\alpha a} = -A_2 k \sin(ka) + B_2 k \cos(ka) \quad \text{—— (4)}$$

Now, (1) + (3) : $(A_1 + B_3) e^{-\alpha a} = 2 A_2 \cos(ka)$ —— (5)

(2) − (4) : $\alpha (A_1 + B_3) e^{-\alpha a} = 2 A_2 k \sin(ka)$ —— (6)

(1) − (3) : $(A_1 - B_3) e^{-\alpha a} = -2 B_2 \sin(ka)$ —— (7)

(2) + (4) : $\alpha (A_1 - B_3) e^{-\alpha a} = 2 B_2 k \cos(ka)$ —— (8)

• Now, assuming $A_1 + B_3 \neq 0$ and $A_2 \neq 0$, eqⁿs (5) & (6) gives

$$\boxed{\alpha = k \tan(ka)} \quad \text{—— (9)}$$

so, $\sin(ka) = \frac{\alpha}{\sqrt{\alpha^2 + k^2}}$; $\cos(ka) = \frac{k}{\sqrt{\alpha^2 + k^2}}$

from eqⁿ (8), $(A_1 - B_3) e^{-\alpha a} = 2 B_2 \frac{k}{\alpha} \cdot \cos(ka)$

from eq^n (7), $(A_1 - B_3)e^{-\alpha a} = -2B_2 \cdot \frac{\alpha}{k} \cos(ka)$ [As, $\sin(ka) = \frac{\alpha}{k}\cos(ka)$]

equating both of the above eq^{n}s:

$$2B_2\left(\frac{k}{\alpha} + \frac{\alpha}{k}\right)\cos(ka) = 0$$

$$\Rightarrow 2B_2 \cdot \left(\frac{k^2+\alpha^2}{\alpha k}\right) \cdot \frac{k}{\sqrt{k^2+\alpha^2}} = 0$$

$$\Rightarrow 2B_2 \cdot \frac{\sqrt{k^2+\alpha^2}}{\alpha} = 0$$

So, $B_2 = 0$ [As $\frac{\sqrt{k^2+\alpha^2}}{\alpha} \neq 0$]

put this into eq^n (7) or (8):

$$A_1 = B_3$$

So, the sol^n becomes:

(I) $\psi_1(x) = A_1 e^{\alpha x}$ $[x < -a]$

(II) $\psi_2(x) = A_2 \cos(kx)$ $[-a \leq x \leq a]$

(III) $\psi_3(x) = A_1 e^{-\alpha x}$ $[x > a]$

As a result, we get a symmetric solution with $\psi(x) = \psi(-x)$
$\longrightarrow$ "positive parity"/even parity.

- If we assume $A_1 - B_3 \neq 0$ and $B_2 \neq 0$, we get

$$\boxed{\alpha = -k\cot(ka)} \longrightarrow (10)$$

and similarly: $A_1 = -B_3$ and $A_2 = 0$

the sol^n becomes:

(I) $\psi_1(x) = A_1 e^{\alpha x}$ $[x < -a]$

(II) $\psi_2(x) = B_2 \sin(kx)$ $[-a \leq x \leq a]$

(III) $\psi_3(x) = -A_1 e^{-\alpha x}$ $[x > a]$

thus, we get an anti-symmetric sol^n with $\psi(x) = -\psi(-x)$.
$\longrightarrow$ "negative parity"/ odd parity.

Now ~~denote~~ introduce two new variables:

$$\xi = ka \quad \text{and} \quad \eta = \alpha a$$

So, $\xi^2 + \eta^2 = (k^2 + \alpha^2)a^2 = \dfrac{2mV_0 a^2}{\hbar^2} = r^2 \text{ (say)}$ — (11)

$\left[\text{as, } \alpha^2 = -\dfrac{2mE}{\hbar^2} \text{ \& } k^2 = \dfrac{2m(E+V_0)}{\hbar^2}\right]$

eq^n of a circle with radius $r = \dfrac{a}{\hbar}\sqrt{2mV_0}$.

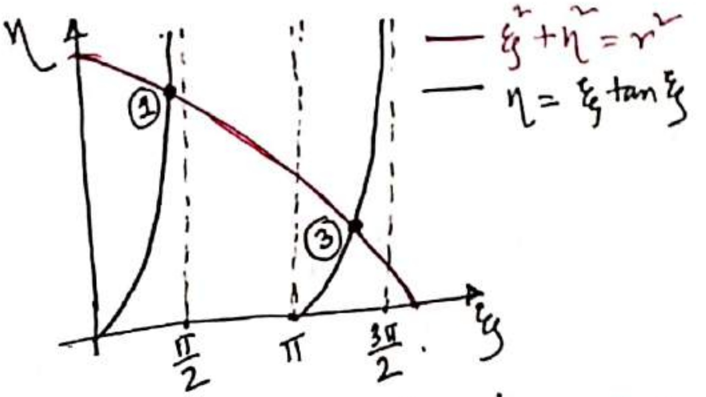
On the other hand, from eq^n (9) & (10):

$\alpha = k\tan(ka)$ $\qquad\qquad$ $\alpha = -k\cot(ka)$

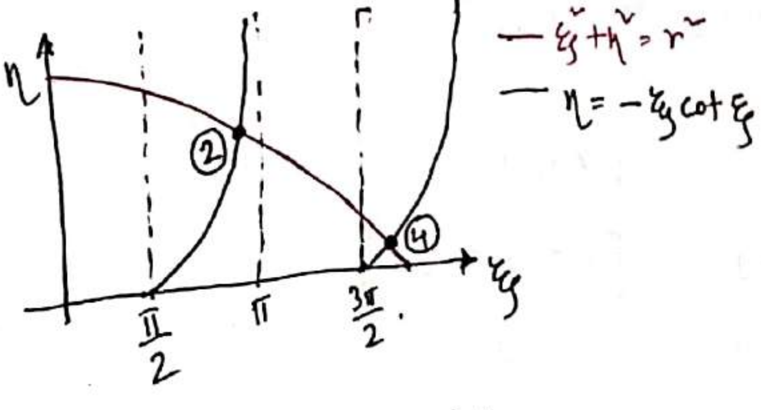
$\Rightarrow \alpha a = ka\tan(ka)$ $\qquad$ $\Rightarrow \alpha a = -ka\cot(ka)$

$\Rightarrow \eta = \xi\tan(\xi)$ $\qquad\qquad$ $\Rightarrow \eta = -\xi\cot(\xi)$

So, to get the solutions for η and ξ, we will try graphical solution. That is, the desired energy ~~states~~ values can be obtained by constructing the intersection of those two curves (i.e. $\eta = \xi\tan(\xi)$ ~~and~~ or $\eta = -\xi\cot(\xi)$) with the circle defined in eq^n (11), within the (ξ, η) plane.



For positive parity, at least one solution must exist for any arbitrary value of V_0, as the tan-function intersects the origin.



For negative parity, the radius of the circle needs to be larger than a minimum value so that the two curves can at least intersect once.

The number of solutions or equivalently the number of energy levels increases with the radius r (the bigger the radius, more no. of intersecting points appear), i.e. with V_0, a and mass m.

In the limiting case $mV_0a^2 \to \infty$, the intersections are found at

$$\left.\begin{aligned} \tan(ka) &= \infty \Rightarrow ka = \frac{2n-1}{2}\pi = n\pi - \pi/2 \\ -\cot(ka) &= \infty \Rightarrow ka = n\pi \end{aligned}\right\} n = 1, 2, 3, \ldots$$

or combined

$$k(2a) = n\pi \quad (n = 1, 2, 3, \ldots)$$

$$\Rightarrow k = \frac{n\pi}{2a}.$$

So, $k^2 = \left(\frac{n\pi}{2a}\right)^2$

$$\Rightarrow \frac{2m(E_n + V_0)}{\hbar^2} = \left(\frac{n\pi}{2a}\right)^2$$

$$\Rightarrow \boxed{E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2 - V_0} \quad (\text{for } n = 1, 2, 3, \ldots)$$

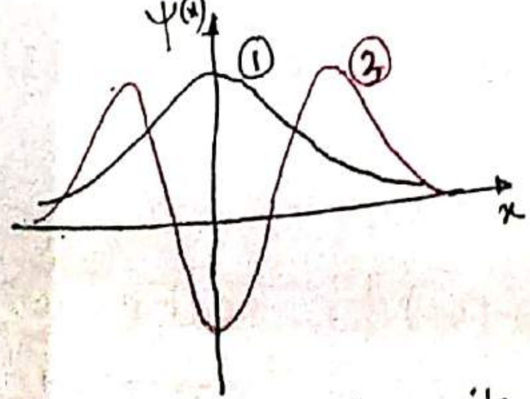
Now, for $n=1$, i.e. the lowermost state or ground state is:

$E_1 = \frac{\hbar^2}{2m}\cdot\left(\frac{\pi}{2a}\right)^2 - V_0$ (is not located at $(-V_0)$, but a little higher).

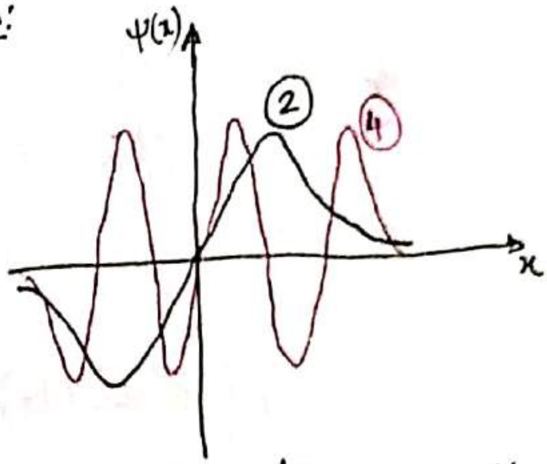
This difference $\left[\text{i.e. } \frac{\hbar^2}{2m}\left(\frac{\pi}{2a}\right)^2\right]$ is called the "zero-point energy".
[We'll see same thing happens also for harmonic oscillator later]

If we enlarge the potential well (i.e. increase a) and/or particle's mass m, the difference between two neighbouring energy eigenvalues will decrease.

- The shape of the bound-state wavefunction:



wave-func. with positive parity

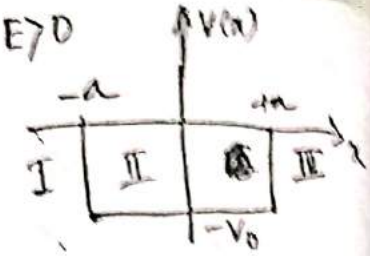


wave-func. with negative parity.

- Similarly, solve for the scattering state $(E>0)$ wavefunction!

Scattering state ($E>0$) solution:

for $E>0$



At region (I), and (III), $V(x)=0$

(I) $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$ (for $x<-a$)

We'll get a reflected part as well even though $E>0$ in contrast to classical physics, as in the wave-phenomena we see a reflection from the sharp edges (here $x=-a$ and $x=+a$)

(III) $\psi_{III}(x) = Fe^{ikx}$ (for $x>a$)

(assuming there is no incoming wave from the right side.)

(II) $\psi_{II}(x) = C\sin(lx) + D\cos(lx)$ (for $-a<x<a$)

$V(x) = -V_0$

where, $\boxed{k = \frac{\sqrt{2mE}}{\hbar}}$ (as $E>0$)

and $\boxed{l = \frac{\sqrt{2m(E+V_0)}}{\hbar}}$

A is "incident amplitude", B is the "reflected amplitude" and F is the "transmitted amplitude".

Boundary conditions;

→ $\psi_I(x=-a) = \psi_{II}(x=-a)$

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \quad \text{(1)}$$

→ $\left.\frac{d\psi_I}{dx}\right|_{x=-a} = \left.\frac{d\psi_{II}}{dx}\right|_{x=-a}$

$$ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right] \quad \text{(2)}$$

→ $\psi_{II}(x=a) = \psi_{III}(x=a)$

$$C\sin(la) + D\cos(la) = Fe^{ika} \quad \text{(3)}$$

→ $\left.\frac{d\psi_{II}}{dx}\right|_{x=a} = \left.\frac{d\psi_{III}}{dx}\right|_{x=a}$

$$l\left[C\cos(la) - D\sin(la)\right] = ikFe^{ika} \quad \text{(4)}$$

Now multiplying eq^n 3 by $\sin(la)$ and eq^n 4 by $\frac{1}{l}\cos(la)$ and add:

$$C\sin^2(la) + D\sin(la)\cos(la) = Fe^{ika}\sin(la)$$

$$C\cos^2(la) - D\sin(la)\cos(la) = \frac{ik}{l}Fe^{ika}\cos(la)$$

$$C = Fe^{ika}\left[\sin(la) + \frac{ik}{l}\cos(la)\right] \quad \text{—— (5)}$$

Then multiplying eq^n 3 by $\cos(la)$ and eq^n 4 by $\frac{1}{l}\sin(la)$ and subtract:

$$C\sin(la)\cos(la) + D\cos^2(la) = Fe^{ika}\cos(la)$$

$$C\sin(la)\cos(la) - D\sin^2(la) = \frac{ik}{l}Fe^{ika}\sin(la)$$

$$D = Fe^{ika}\left[\cos(la) - \frac{ik}{l}\sin(la)\right] \quad \text{—— (6)}$$

put eq^n 5 & 6 into eq^n 1:

$$Ae^{-ika} + Be^{ika} = -Fe^{ika}\left[\sin(la) + \frac{ik}{l}\cos(la)\right]\sin(la)$$
$$+ Fe^{ika}\left[\cos(la) - \frac{ik}{l}\sin(la)\right]\cos(la)$$

$$= Fe^{ika}\left[\cos^2(la) - \frac{ik}{l}\sin(la)\cos(la) - \sin^2(la) - \frac{ik}{l}\sin(la)\cos(la)\right]$$

$$= Fe^{ika}\left[\cos(2la) - \frac{ik}{l}\sin(2la)\right] \quad \text{—— (7)}$$

likewise, put eq^n 5 & 6 into eq^n 2:

$$Ae^{-ika} - Be^{ika} = -\frac{il}{k}Fe^{ika}\left[\left(\sin(la) + \frac{ik}{l}\cos(la)\right)\cos(la) + \left(\cos(la) - \frac{ik}{l}\sin(la)\right)\sin(la)\right]$$

$$= -\frac{il}{k}Fe^{ika}\left[\sin(la)\cos(la) + \frac{ik}{l}\cos^2(la) + \sin(la)\cos(la) - \frac{ik}{l}\sin^2(la)\right]$$

$$= -\frac{il}{k}Fe^{ika}\left[\sin(2la) + \frac{ik}{l}\cos(2la)\right]$$

$$= Fe^{ika}\left[\cos(2la) - \frac{il}{k}\sin(2la)\right] \quad \text{—— (8)}$$

Add eq^n 7 & 8 :

$$2Ae^{-ika} = Fe^{ika}\left[2\cos(2la) - i\left(\frac{k}{l} + \frac{l}{k}\right)\sin(2la)\right]$$

$$\Rightarrow F = \frac{Ae^{-2ika}}{\cos(2la) - i\frac{\sin(2la)}{2kl}(k^2+l^2)} \quad \text{——— } (9)$$

Subtract 8 from 7 :

$$2Be^{ika} = Fe^{ika}\left[i\left(\frac{l}{k} - \frac{k}{l}\right)\sin(2la)\right]$$

$$\Rightarrow B = iF\frac{\sin(2la)}{2kl}(l^2-k^2) \quad \text{——— } (10)$$

Thus, the transmission coefficient will be

$$T = \frac{|F|^2}{|A|^2}$$ (relative probability that an incident particle will be transmitted)

or, $$T^{-1} = \left|\frac{A}{F}\right|^2 = \left|\cos(2la) - i\frac{\sin(2la)}{2kl}(k^2+l^2)\right|^2$$ (using eq^n 9)

$$= \underbrace{\cos^2(2la)}_{=} + \frac{\sin^2(2la)}{(2kl)^2}(k^2+l^2)^2$$

$$= \underline{1 - \sin^2(2la)} + \frac{\sin^2(2la)}{(2kl)^2}(k^2+l^2)^2$$

$$= 1 + \sin^2(2la)\left[\frac{(k^2+l^2)^2}{(2kl)^2} - 1\right]$$

$$= 1 + \frac{(k^2-l^2)^2}{(2kl)^2}\sin^2(2la)$$

But, $k = \frac{\sqrt{2mE}}{\hbar}$, $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

So, $k^2 - l^2 = -\frac{2mV_0}{\hbar^2}$ and $2la = \frac{2a}{\hbar}\sqrt{2m(E+V_0)}$

and $$\frac{(k^2-l^2)^2}{(2kl)^2} = \frac{\left(\frac{2m}{\hbar^2}\right)^2 V_0^2}{4\left(\frac{2m}{\hbar^2}\right)^2 E(E+V_0)} = \frac{V_0^2}{4E(E+V_0)}$$

So, $$\boxed{T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}$$

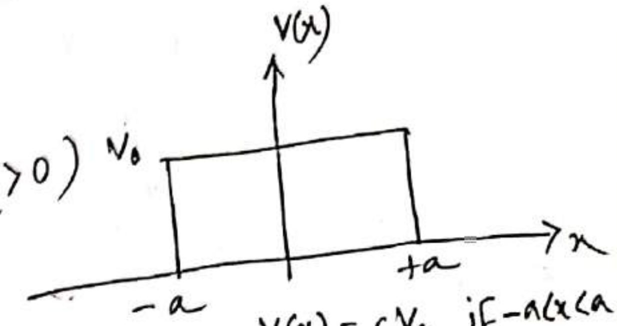
Notice that, $T = 1$ (the well becomes "transparent") whenever the argument of the sine is zero, i.e.,

$$\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi \quad (n \text{ is any integer})$$

Then the energies for "perfect transmission" is

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} - V_0}$$ ← same as the allowed energies for the infinite square well.

Rectangular Barrier:



(but E is always > 0)

Case 1: $\boxed{E < V_0}$

$$V(x) = \begin{cases} V_0 & \text{if } -a<x<a \\ 0 & \text{if } |x|>a \end{cases}$$

$$\psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<-a) \\ Ce^{\alpha x} + De^{-\alpha x} & (-a \le x < a) \\ Fe^{ikx} & (x>a) \end{cases}$$

$$k = \frac{\sqrt{2mE}}{\hbar}, \qquad \alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

In our earlier example, we choose $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

and got, $$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right) \quad \text{—— (1)}$$

So, if we switch the sign of V_0 $(V_0 \to -V_0)$ in that eq (1) [then α becomes $\alpha \to il$]

$$T^{-1} = 1 + \frac{V_0^2}{4E(E-V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E-V_0)}\right)$$

$$= 1 - \frac{V_0^2}{4E(V_0-E)} \sin^2\left(\frac{2ai}{\hbar}\sqrt{2m(V_0-E)}\right) \quad (\text{as } E<V_0)$$

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Now, $\sinh x = -i\sin(ix)$

$\Rightarrow \sinh^2 x = -\sin^2(ix)$.

So, $$\boxed{T^{-1} = 1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\right)}$$

Case II: $\boxed{\boxed{E = V_0}}$ $\quad \psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<-a) \\ C + Dx & (-a<x<a) \\ Fe^{ikx} & (x>a) \end{cases}$

$\left(\text{as } \frac{d^2\psi}{dx^2} = 0\right)$

Now, in eq^n 1, if we change $V_0 \to -V_0$, then

$$T^{-1} = 1 + \frac{V_0^2}{4E(E-V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E-V_0)}\right)$$

then take the limit $E \to V_0$ and using $\sin x \simeq x$ if $x \to 0$

$$T^{-1} \simeq 1 + \frac{V_0^2}{\cancel{4}E(E-V_0)}\frac{\cancel{4}a^2}{\hbar^2}\cdot 2m(E-V_0)$$

$$= 1 + \frac{V_0^2}{V_0\hbar^2}\cdot 2ma^2 \cdot (\text{as } E = V_0)$$

$$\Rightarrow \boxed{T^{-1} = 1 + \frac{2mV_0}{\hbar^2}a^2}$$

Case III $\boxed{\boxed{E > V_0}}$ for this case, $\psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<-a) \\ C\sin lx + D\cos lx & (-a<x<a) \\ Fe^{ikx} & (x>a) \end{cases}$

identical with the earlier problem of finite potential well, but now with $l = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

So, changing $V_0 \to -V_0$ in eq^n 1:

$$\boxed{T^{-1} = 1 + \frac{V_0^2}{4E(E-V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E-V_0)}\right)}$$

3.24 The Harmonic Oscillator :—

Harmonic oscillator potential is of great interest because many complicated potentials can be approximated in the vicinity of their equilibrium points by a harmonic oscillator.

Expanding a potential $V(x)$ in one dimension in a Taylor series gives :

$$V(x) = V(a + (x-a))$$

$$= V(a) + V'(a)(x-a) + \frac{1}{2} V''(a)(x-a)^2 + \cdots$$

If a stable equilibrium exists for $x = a$, $V(x)$ has a minimum at $x = a$ [i.e. $V'(a) = 0$ and $V''(a) > 0$].
Next if we choose a as the origin of the coordinate system and set $V(a) = 0$, then an oscillator potential is indeed a first approximation of any potential in the vicinity of $x = a$, i.e. in the vicinity of the equilibrium point.

We will consider only the one-dimensional case. The classical hamiltonian for this is

$$H = \frac{p^2}{2m} + \frac{1}{2} kx^2 \; (= T + V)$$

where the spring constant $k = m\omega^2$, ω being the angular freq. of the oscillator.

[classically, the motion is governed by Hooke's law:

$$F = -kx = m\frac{d^2x}{dt^2} \quad \text{(Ignoring the friction)}$$

the sol^n is : $x(t) = A\sin(\omega t) + B\cos(\omega t)$.

and potential energy $V = \frac{1}{2}kx^2 = \frac{1}{2} m\omega^2 x^2$ [as $F = -\frac{dV}{dx}$]

Using this, the time-independent Schrödinger equation is

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

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) - \frac{m^2\omega^2 x^2}{\hbar^2}\psi(x) = 0 \quad \text{—— (1)}$$

To solve this differential equation, we'll use "trial solution" method.
The solution must vanish at $\pm\infty$ (for square-integratable wave function).
The potential term goes like $x^2\psi(x)$, whereas the E-term goes like $\psi(x)$. Therefore, at large x the potential term should dominate the Schrödinger equation →

$$\frac{d^2\psi(x)}{dx^2} - \frac{m^2\omega^2 x^2}{\hbar^2}\psi(x) = 0 \quad \text{—— (2)}$$

Note that, the second derivative of the wave function must result in some constant times x^2 times $\psi(x)$. This suggests that we can choose the trial function as:

$$\psi(x) = e^{-\alpha x^\beta}$$ [We take this '−'ve sign in exp, as at $x \to \infty$, we want $\psi(x) \to 0$]

So, $$\frac{d\psi}{dx} = -\alpha\beta x^{\beta-1} e^{-\alpha x^\beta}$$

and $$\frac{d^2\psi}{dx^2} = -\alpha\beta(\beta-1)x^{\beta-2}e^{-\alpha x^\beta} + \alpha^2\beta^2 x^{2\beta-2} \cdot e^{-\alpha x^\beta}$$

At large x, the 2nd term grows more rapidly than the first term. So, we can drop the 1st term.

$$\frac{d^2\psi}{dx^2} \approx \alpha^2\beta^2 x^{2\beta-2} e^{-\alpha x^\beta}$$

Substituting the trial function into eq^n (2):

$$\alpha^2\beta^2 x^{2\beta-2} e^{-\alpha x^\beta} - \frac{m^2\omega^2 x^2}{\hbar^2} e^{-\alpha x^\beta} = 0$$

$$\Rightarrow \alpha^2\beta^2 x^{2\beta-2} = \frac{m^2\omega^2}{\hbar^2} x^2 \quad (\text{as } e^{-\alpha x^\beta} \neq 0) \text{ —— (3)}$$

Now, as this eq^n should be true for any value of x, the powers of x must be same in the both sides.

$$2\beta - 2 = 2$$

$$\Rightarrow \boxed{\beta = 2}$$

Substituting this into eq^n (3):

$$4\alpha^2 = \frac{m^2\omega^2}{\hbar^2}$$

$$\Rightarrow \boxed{\alpha = \frac{1}{2}\frac{m\omega}{\hbar}}$$

So, we have determined that for large x, the wave function looks like –

$$\boxed{\psi(x) \sim e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}}$$

Now introduce another variable $y = \sqrt{\frac{m\omega}{\hbar}}\, x$ (to express the differential eq^n in terms of dimensionless quantities) $\left[dy = \sqrt{\frac{m\omega}{\hbar}}\, dx \right]$

Changing variables in eq^n (1) from x to y gives:

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$$\frac{m\omega}{\hbar}\frac{d^2}{dy^2}\psi(y) + \frac{2mE}{\hbar^2}\psi(y) - \frac{m^2\omega^2}{\hbar^2}\cdot\frac{\hbar}{m\omega}y^2\psi(y) = 0$$

$$\Rightarrow \frac{d^2\psi(y)}{dy^2} + \frac{2E}{\hbar\omega}\psi(y) - y^2\psi(y) = 0$$

Now, define another dimensionless variable

$$\epsilon = \frac{2E}{\hbar\omega}$$

So, $$\frac{d^2\psi(y)}{dy^2} + \epsilon\psi(y) - y^2\psi(y) = 0 \quad \text{—— (4)}$$

The next step is to remove the asymptotic behaviour of the wave function from the differential equation. To do this we write

$$\boxed{\psi(y) = f(y)\, e^{-\frac{1}{2}y^2}}$$ [without the normalization const. We'll take that in the final step]

So, $$\frac{d\psi}{dy} = f'(y)\, e^{-\frac{1}{2}y^2} - y f(y)\, e^{-\frac{1}{2}y^2}$$

and, $$\frac{d^2\psi}{dy^2} = f''(y)\, e^{-\frac{1}{2}y^2} - 2y f'(y)\, e^{-\frac{1}{2}y^2} - f(y) e^{-\frac{1}{2}y^2} + y^2 f(y) e^{-\frac{1}{2}y^2}$$

Now, substitute all these into eq^n (4):

$$f''(y)\, e^{-\frac{1}{2}y^2} - 2y f'(y)\, e^{-\frac{1}{2}y^2} - f(y)\, e^{-\frac{1}{2}y^2} + \cancel{y^2 f(y)\, e^{-\frac{1}{2}y^2}}$$
$$+ \epsilon f(y)\, e^{-\frac{1}{2}y^2} - \cancel{y^2 f(y)\, e^{-\frac{1}{2}y^2}} = 0$$

$$\Rightarrow f''(y) - 2y f'(y) + (\epsilon - 1) f(y) = 0 \quad \text{—— (5)}$$

• The final step is to see if we can find a solution of eq^n (5) in terms of the power series:

$$\boxed{f(y) = \sum_{i=0}^{\infty} a_i y^i}$$

So, $$f'(y) = \sum_{i=0}^{\infty} i a_i y^{i-1} = \sum_{i=1}^{\infty} i a_i y^{i-1}$$

and $$f''(y) = \sum_{i=1}^{\infty} i(i-1) a_i y^{i-2} = \sum_{i=2}^{\infty} i(i-1) a_i y^{i-2}$$

Substituting those into eq^n (5) gives:

$$\sum_{i=2}^{\infty} i(i-1) a_i y^{i-2} - 2y \sum_{i=1}^{\infty} i a_i y^{i-1} + (\epsilon - 1) \sum_{i=0}^{\infty} a_i y^i = 0$$

$$\Rightarrow \sum_{i=2}^{\infty} i(i-1) a_i y^{i-2} - 2 \sum_{i=1}^{\infty} i a_i y^i + (\epsilon - 1) \sum_{i=0}^{\infty} a_i y^i = 0$$

The a_i can be found by requiring the coefficients of like powers of y vanish. So make slight re-adjustment to the above eq^n: (substitute $i \to i+2$ in the first term)

$$\sum_{i=0}^{\infty} (i+2)(i+1) a_{i+2} y^i - 2 \sum_{i=0}^{\infty} i a_i y^i + (\epsilon - 1) \sum_{i=0}^{\infty} a_i y^i =$$

$$\Rightarrow \sum_{i=0}^{\infty} \left[(i+2)(i+1) a_{i+2} - [2i - \epsilon + 1] a_i \right] y^i = 0$$

$$\Rightarrow \boxed{a_{i+2} = \frac{2i - \epsilon + 1}{(i+2)(i+1)} a_i} \quad \text{——— (6)}$$

This is a "recursion relation" for generating the coefficients of the power series.

Since this recursion relation connects $i+2$ to i, we can ~~independently~~ independently choose a_0 and a_1!

If we choose $a_1 = 0$ and a_0 to be finite, then the series will only have even powers of y, i.e.

$$F_{even}(y) \equiv a_0 + a_2 y^2 + a_4 y^4 + \cdots$$

and if we choose, $a_0 = 0$ and a_1 to be finite, then the series contains only odd powers of y i.e.

$$F_{odd}(y) \equiv a_1 y + a_3 y^3 + a_5 y^5 + \cdots$$

So, $F(y) = F_{even}(y) + F_{odd}(y)$

One can determine $F(y)$ in terms of only two arbitrary constants — a_0 and a_1, which is expected for a 2nd-order differential eq^n.

Note that, for large values of i,

$$\frac{a_{i+2}}{a_i} = \frac{2i - \epsilon + 1}{(i+2)(i+1)} \sim \frac{2}{i}$$

This indicates that the infinite series cannot converge over the entire region $-\infty < x < \infty$. The only way the series solution can be valid only if a finite number of terms have non-zero coefficients (not all terms can ~~be~~ have non-zero coefficients, then the series couldn't converge). This will happen if the recursion relation will cause one of the coefficients to vanish for some value of i, then all higher coefficients will vanish automatically and the series will <u>truncate to a finite number of terms</u>.

Let 'n' be the value of i for which the coefficient $a_{n+2} = 0$. This requires –

$$2n - \epsilon + 1 = 0$$

$$\text{or} \quad \epsilon = 2n+1$$

$$\Rightarrow \frac{2E}{\hbar\omega} = 2n+1$$

$$\Rightarrow \boxed{E_n = \hbar\omega\left(n+\tfrac{1}{2}\right)}$$ → energy eigen-values for quantum H.O.

where $n = 0, 1, 2, ----$

$\frac{1}{2}\hbar\omega$ is called <u>"zero-point energy" (E_0)</u>.

Then the recursion relation becomes (eq^n 6):

$$a_{i+2} = \frac{2(i-n)}{(i+2)(i+1)} a_i$$

n=0 gives the <u>ground-state wave function</u>, for which the energy is minimum. Now for n=0, there is only one term in the series which is a_0.

$$f_0(y) = a_0$$

$$\Rightarrow \boxed{\psi_0(y) = a_0 e^{-\frac{1}{2}y^2}}$$

Now for $n=1$, $i=1$, then from recursion relation, $a_3 = 0$ and a_0 must be chosen as $a_0 = 0$ (because either $a_0 = 0$ and $a_1 \neq 0$ or $a_0 \neq 0$ and $a_1 = 0$)

So, $f_1(y) = a_1 y$

$$\Rightarrow \boxed{\psi_1(y) = a_1 y e^{-\frac{1}{2}y^2}}$$

For $n=2$, i could be 0 or 2. (as there are only three ~~term~~ non-zero terms in the series).

For $i=0$ and $n=2$, $a_2 = -2a_0$ ⎫
and for $i=2$ and $n=2$, $a_4 = 0$ ⎭ from the recursion relation.

So, $F_2(\gamma) = a_0(1-2\gamma^2)$

and $\boxed{\psi_2(\gamma) = a_0(1-2\gamma^2)e^{-\frac{1}{2}\gamma^2}}$

and so on.

So, $F_n(\gamma)$ will be a polynomial of degree n in γ, involving even powers only, if n is an even integer; and odd powers only, if n is an odd integer.

Now, if we make the choice that,

$$a_0 = (-1)^{\frac{n}{2}} \frac{n!}{\left(\frac{n}{2}\right)!} \quad \text{for even } n$$

and $$a_1 = 2n(-1)^{\frac{n-1}{2}} \frac{(n-1)!}{\left(\frac{n-1}{2}\right)!} \quad \text{for odd } n,$$

then $\boxed{F_n(\gamma) = H_n(\gamma)}$, where $H_n(\gamma)$ are the Hermite polynomials.

[Now, check for $n=0$, $a_0 = 1 \Rightarrow F_0(\gamma) = 1$

For $n=1$, $a_1 = 2 \Rightarrow F_1(\gamma) = 2y$

for $n=2$, $a_0 = (-1).\frac{2!}{1} = -2 \Rightarrow F_2(\gamma) = -2(1-2y^2)$
$= 4y^2 - 2$]

....

The first few of these polynomials are:

$$\boxed{\begin{aligned} H_0(y) &= 1 \\ H_1(\gamma) &= 2y \\ H_2(\gamma) &= 4y^2 - 2 \\ H_3(\gamma) &= 8y^3 - 12y \end{aligned}}$$

"Rodrigues formula" for Hermite polynomial:

$$\boxed{H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}}$$

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So, we can finally write the eigenfunctions for the one-dimensional harmonic oscillator as:

$$\psi_n(y) = \underset{\wedge}{\text{Normalization Constant}} \times f(y)\, e^{-\frac{1}{2}y^2}$$

$$= N_n \times H_n(y)\, e^{-\frac{1}{2}y^2}$$

writing in terms of x,

$$\psi_n(x) = N_n\, H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \qquad \left[\text{as } y = \sqrt{\frac{m\omega}{\hbar}}\, x\right]$$

The normalization constant N_n can be determined from:

$$\int_{-\infty}^{+\infty} dx\, |\psi_n(x)|^2 = 1$$

$$\Rightarrow N_n = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \qquad (\text{check it } b)$$

The eigenfunction are then given by:

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \cdot \frac{1}{\sqrt{2^n n!}}\, H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}}$$

$$\int_{-\infty}^{+\infty} dx\, |\psi_n(x)|^2 = 1$$

$$\Rightarrow N_n^2 \int_{-\infty}^{+\infty} dx\, H_n^2\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega}{\hbar}x^2} = 1$$

$$\Rightarrow N_n^2 \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{+\infty} dy\, H_n^2(y)\, e^{-y^2} = 1$$

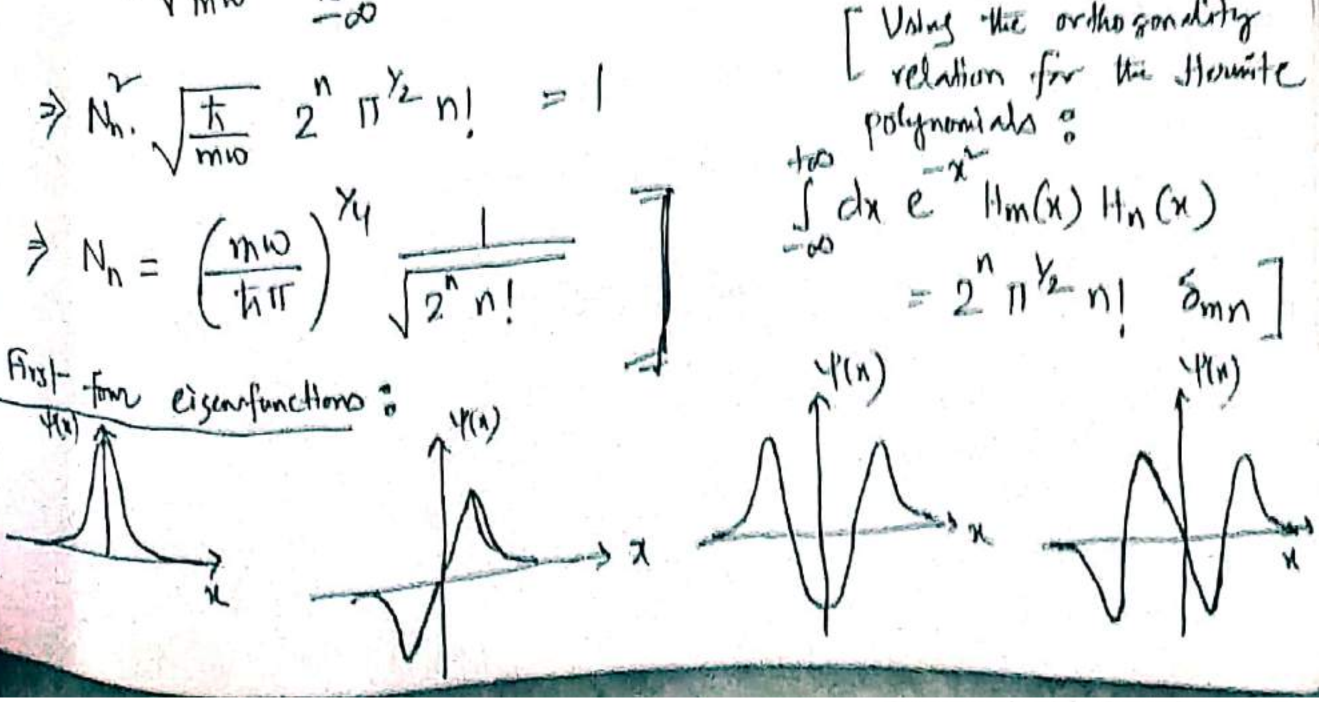
$$\Rightarrow N_n^2 \cdot \sqrt{\frac{\hbar}{m\omega}}\, 2^n \pi^{1/2} n! = 1$$

$$\Rightarrow N_n = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}$$

[Using the orthogonality relation for the Hermite polynomials:

$$\int_{-\infty}^{+\infty} dx\, e^{-x^2} H_m(x)\, H_n(x) = 2^n \pi^{1/2} n!\, \delta_{mn}]$$

First four eigenfunctions:



APPENDIX OF CHAPTER - 3

(4) Solving Linear Harmonic Oscillator in Operator Method :

Time-independent Schrödinger eq^n for one-dimensional harmonic oscillator :

$$\left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right]\psi_n(x) = E_n\psi_n(x)$$

In Dirac notation :

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

where $|\psi_n\rangle$ is the "ket" vector associated with the eigenf^{n}s $\psi_n(x)$ and the Hamiltonian operator is written as :

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

- Factorizing the Hamiltonian :

Let's factor out $\hbar\omega$ in the $\hat{H}$:

$$\hat{H} = \hbar\omega\left[\frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar}\hat{x}^2\right]$$

Checking the dimension of the constants :

$[\hbar\omega]$ = energy

$[2m\omega\hbar]$ = momentum^2 $\left(\text{as } [\hbar\omega] = \text{energy and } \frac{\text{momentum}^2}{2m} \equiv \text{energy}\right)$

$\left[\frac{2\hbar}{m\omega}\right]$ = length^2 $\left[\text{as } [\hbar] = \text{angular momentum } (\sim m\omega r^2)\right]$

Now introducing the dimensionless quantities :

$$\hat{\xi} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}$$

$$\hat{\eta} = \frac{\hat{p}}{\sqrt{2m\hbar\omega}}$$

So, the Hamiltonian becomes:

$$\hat{H} = \hbar\omega\left[\hat{\eta}^2 + \hat{\xi}^2\right]$$

The operators $\hat{\xi}$ and $\hat{\eta}$ are simply the position and the momentum operator rescaled by some real constants, therefore both of them are Hermitian.

$$[\hat{\xi}, \hat{\eta}] = \frac{1}{2\hbar}[\hat{x}, \hat{p}] = \frac{i}{2} \quad \left(\text{as } [\hat{x}, \hat{p}] = i\hbar\right)$$

So, $\hat{\xi}$ and $\hat{\eta}$ ~~doesn't~~ doesn't commute with each other.

If they were commuting variables, we could have written as:

$$\hat{H} = \hbar\omega\left(\hat{\xi} + i\hat{\eta}\right)\left(\hat{\xi} - i\hat{\eta}\right)$$

But we "can't write" the above eq^n as the operators $\hat{\xi}$ and $\hat{\eta}$ do not commute. So, let us introduce:

$$\left.\begin{aligned} \hat{a} &= \hat{\xi} + i\hat{\eta} \\ \hat{a}^\dagger &= \hat{\xi} - i\hat{\eta} \end{aligned}\right\} \quad \left(\text{as } \hat{\xi}, \hat{\eta} \text{ are Hermitian, } \hat{\xi}^\dagger = \hat{\xi} \ \& \ \hat{\eta}^\dagger = \hat{\eta}\right)$$

So, in terms of $\hat{x}$ and $\hat{p}$:

$$\boxed{\begin{aligned} \hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\,\hat{p} \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\,\hat{p} \end{aligned}}$$

We can then compute:

$$\begin{aligned} \hat{a}\hat{a}^\dagger &= (\hat{\xi} + i\hat{\eta})(\hat{\xi} - i\hat{\eta}) \\ &= \hat{\xi}^2 + i\hat{\eta}\hat{\xi} - i\hat{\xi}\hat{\eta} + \hat{\eta}^2 \\ &= \hat{\xi}^2 + i[\hat{\eta}, \hat{\xi}] + \hat{\eta}^2 \quad (\text{as } \hat{\eta} \ \& \ \hat{\xi} \text{ don't commute}) \quad \text{—— (1)} \end{aligned}$$

and $\hat{a}^\dagger\hat{a} = \hat{\xi}^2 - i[\hat{\eta}, \hat{\xi}] + \hat{\eta}^2$ —— (2)

So, $\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 2(\hat{\xi}^2 + \hat{\eta}^2)$

So, $\boxed{\hat{H} = \frac{\hbar\omega}{2}\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right)}$

and eq^n ① − ②:

$$\hat{a}\hat{a}^\dagger - a^\dagger\hat{a} = 2i[\hat{x}, \hat{\xi}]$$
$$= -2i \cdot \frac{i}{2} \quad \left(\text{as } [\hat{\xi}, \hat{x}] = i/2\right)$$
$$= 1$$

$\Rightarrow \boxed{[\hat{a}, \hat{a}^\dagger] = 1} \quad \Rightarrow \hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$

An alternative, and more useful, expression for $\hat{H}$ is:

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

$$\Rightarrow \boxed{\hat{H} = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega}$$

- Creation and annihilation:

We are now going to find the eigenvalues of $\hat{H}$ using the operators $\hat{a}$ and $\hat{a}^\dagger$.

First let us calculate the commutators $[\hat{H}, \hat{a}]$ and $[\hat{H}, \hat{a}^\dagger]$:

$$[\hat{H}, \hat{a}] = \left[\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega, \hat{a}\right]$$
$$= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}] \quad \left(\text{as } [\tfrac{1}{2}, \hat{a}] = 0\right)$$
$$= \hbar\omega\left(\underline{\hat{a}^\dagger\hat{a}}\hat{a} - \underline{\hat{a}\hat{a}^\dagger}\hat{a}\right)$$
$$= \hbar\omega[\hat{a}^\dagger, \hat{a}]\hat{a} \quad \left(\text{as } [\hat{a}, \hat{a}^\dagger] = 1\right)$$

$$\boxed{[\hat{H}, \hat{a}] = -\hbar\omega\hat{a}}$$

Similarly, $[\hat{H}, \hat{a}^\dagger] = \left[\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega, \hat{a}^\dagger\right]$
$$= \hbar\omega[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hbar\omega\left(\hat{a}^\dagger\underline{\hat{a}a^\dagger} - \hat{a}^\dagger\underline{\hat{a}^\dagger\hat{a}}\right)$$
$$= \hbar\omega\hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger$$

$$\boxed{[\hat{H}, \hat{a}^\dagger] = \hbar\omega \hat{a}^\dagger}$$

Let us now compute:

$$\hat{H}(\hat{a}|\psi_n\rangle) = \hat{a}\hat{H}|\psi_n\rangle + [\hat{H}, \hat{a}]|\psi_n\rangle$$

$$= E_n \hat{a}|\psi_n\rangle - \hbar\omega \hat{a}|\psi_n\rangle$$

$$\boxed{\hat{H}\hat{a}|\psi_n\rangle = (E_n - \hbar\omega)\hat{a}|\psi_n\rangle}$$

The above eq^n is an eigenvalue eq^n where $\hat{a}|\psi_n\rangle$ is an eigenfunction of $\hat{H}$ with the eigenvalue $(E_n - \hbar\omega)$, unless $\hat{a}|\psi_n\rangle = 0$. We say that, the operator $\hat{a}$ is called "lowering operator", as its action on an energy eigensate is to turn it into another energy eigenstate of lower energy. It is also called an "annihilation operator", because it removes one quantum of energy $\hbar\omega$ from the system.

Similarly, it's straightforward to show that:

$$\boxed{\hat{H}\hat{a}^\dagger|\psi_n\rangle = (E_n + \hbar\omega)\hat{a}^\dagger|\psi_n\rangle}$$

The operator $\hat{a}^\dagger$ is a "raising operator" or "creation operator".

We can summarise the result by denoting the states with energy $(E_n \pm \hbar\omega)$ by $|\psi_{n\pm1}\rangle$ and writing:

$$\boxed{\hat{a}|\psi_n\rangle = c_n|\psi_{n-1}\rangle} \quad \text{and} \quad \boxed{\hat{a}^\dagger|\psi_n\rangle = d_n|\psi_{n+1}\rangle}$$

where c_n and d_n are constants of proportionality.

Then,

$$\left.\begin{aligned} \hat{H}|\psi_{n-1}\rangle &= E_{n-1}|\psi_{n-1}\rangle = (E_n - \hbar\omega)|\psi_{n-1}\rangle \\ \hat{H}|\psi_{n+1}\rangle &= E_{n+1}|\psi_{n+1}\rangle = (E_n + \hbar\omega)|\psi_{n+1}\rangle \end{aligned}\right\} \text{—} (3)$$

- **Eigenvalue & Eigenvectors:**

So, the repeated application of the lowering operator, $\hat{a}$, generates states of successively lower energy unless there is a state with lowest energy. (There cannot be any state with negative energy, as $E > V_{min}$ or $E > 0$, here $V = \frac{1}{2}m\omega^2 x^2$)

We denote the state of lowest energy, or ground state, by $|\psi_0\rangle$, since there cannot be a state of lower energy than this, we can write:

$$\hat{a}|\psi_0\rangle = 0$$

Applying the Hamiltonian to this state gives:

$$\hat{H}|\psi_0\rangle = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right)|\psi_0\rangle$$
$$= \tfrac{1}{2}\hbar\omega|\psi_0\rangle$$
$$= E_0|\psi_0\rangle$$

Thus, the ground state energy: $\boxed{E_0 = \frac{1}{2}\hbar\omega}$

Applying the raising operator $\hat{a}^\dagger$ on ground state generates the 1st exited state $|\psi_1\rangle$ with energy $\boxed{E_1 = \frac{3}{2}\hbar\omega}$.

One can see that from eq^n 3:

$$\hat{H}|\psi_{n+1}\rangle = E_{n+1}|\psi_{n+1}\rangle = (E_n + \hbar\omega)|\psi_{n+1}\rangle$$

now if $n = 0$,

$$\hat{H}|\psi_1\rangle = E_1|\psi_1\rangle = (E_0 + \hbar\omega)|\psi_1\rangle$$
$$\Rightarrow E_1 = E_0 + \hbar\omega = \tfrac{3}{2}\hbar\omega.$$

Similarly, with n applications of raising operator generates the state $|\psi_n\rangle$ with energy:

$$\boxed{E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, 3, \ldots}$$

↳ energy eigenvalues for 1-D quantum harmonic oscillator.

• Now we want to determine the proportionality constants c_n and d_n of eq^n (3). For that, we require $|\psi_n\rangle$ and $|\psi_{n-1}\rangle$ to be normalized.

Consider,

$$\langle\psi_n|\hat{a}^\dagger\hat{a}|\psi_n\rangle = c_n\langle\psi_n|\hat{a}^\dagger|\psi_{n-1}\rangle \quad [\text{as } \hat{a}|\psi_n\rangle = c_n|\psi_{n-1}\rangle]$$

$$= c_n\langle\psi_{n-1}|\hat{a}|\psi_n\rangle^* \quad [\text{as } |\psi_n\rangle = \langle\psi_n|^* \text{ and } (\hat{a}^\dagger)^\dagger = \hat{a}\,]$$

$$= c_n c_n^*\langle\psi_{n-1}|\psi_{n-1}\rangle^* \quad [\text{as } (\hat{a}|\psi_n\rangle)^* = c_n^*|\psi_{n-1}\rangle^*]$$

$$= |c_n|^2, \text{ since } \langle\psi_{n-1}|\psi_{n-1}\rangle = 1, \text{ normalized.}$$

Now, we note that $\hat{a}^\dagger\hat{a} = (\hat{H}/\hbar\omega) - \frac{1}{2}$.

So, $$\langle\psi_n|\hat{a}^\dagger\hat{a}|\psi_n\rangle = \langle\psi_n|\left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)|\psi_n\rangle$$

$$= \frac{1}{\hbar\omega}\langle\psi_n|\hat{H}|\psi_n\rangle - \frac{1}{2}\langle\psi_n|\psi_n\rangle$$

$$= \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)\langle\psi_n|\psi_n\rangle$$

$$= \left[\frac{(n+\frac{1}{2})\hbar\omega}{\hbar\omega} - \frac{1}{2}\right] \cdot (\text{as } \psi_n \text{ is normalized})$$

$$= n$$

So, $|c_n|^2 = n$ and if we choose the phase so that, c_n is real, then we can write:

$$c_n = \sqrt{n}$$

Similarly, $\langle\psi_n|\hat{a}\hat{a}^\dagger|\psi_n\rangle = |d_n|^2 = (n+1)$

$$\Rightarrow d_n = \sqrt{n+1}$$

Thus,

$$\boxed{\hat{a}|\psi_n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle} \text{ and } \boxed{\hat{a}^\dagger|\psi_n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle}$$

- **Wave-functions:**

Finally, we'll determine the analytic expression for the eigenfunctions.

The ground state is defined by:

$$\hat{a}|\psi_0\rangle = 0$$

So, in our usual wavefunction notation:

$$\hat{a}\psi_0(x) = \left[\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\,\hat{p}\right]\psi_0(x)$$

$$= \left[\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{\hbar}{\sqrt{2m\omega\hbar}}\frac{d}{dx}\right]\psi_0(x) \qquad \left(\text{as } \hat{p} = \frac{\hbar}{i}\frac{d}{dx}\right)$$

$$= 0$$

$$\Rightarrow \frac{\hbar}{\sqrt{2m\omega\hbar}}\frac{d}{dx}\psi_0(x) = -\sqrt{\frac{m\omega}{2\hbar}}\,x\psi_0(x) \quad (\text{as } \hat{x} = x)$$

$$\Rightarrow \frac{d\psi_0(x)}{dx} = -\sqrt{\frac{2m\omega}{\hbar}}\cdot\sqrt{\frac{m\omega}{2\hbar}}\,x\psi_0(x)$$

$$= -\frac{m\omega}{\hbar}x\psi_0(x)$$

$$= -\alpha^2 x\psi_0(x) \quad \left[\text{where } \alpha^2 = \frac{m\omega}{\hbar}\right]$$

$$\Rightarrow \frac{1}{\psi_0(x)}d\psi_0(x) = -\alpha^2 x\,dx$$

$$\int d(\ln\psi_0(x)) = -\alpha^2\int x\,dx + C$$

$$\Rightarrow \ln\psi_0(x) = -\alpha^2 x^2/2 + C$$

$$\Rightarrow \psi_0(x) = c_0 e^{-\alpha^2x^2/2}$$

$$\Rightarrow \psi_0(x) = c_0 e^{-\frac{m\omega x^2}{2\hbar}}$$

normalizing this:

$$\int_{-\infty}^{+\infty} dx\,|\psi_0(x)|^2 = |c_0|^2\int_{-\infty}^{+\infty} dx\, e^{-\frac{m\omega x^2}{2\hbar}}$$

$$= |c_0|^2\sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

as $\int_{-\infty}^{+\infty} e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{2\alpha}}$

$$\Rightarrow \quad C_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

So,
$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)} \leftarrow \text{normalized ground-state wave function}$$

Every other eigenfunctions are obtained by repeatedly applying the creation operator $\hat{a}^\dagger$ to the ground state:

$$\left(\text{as} \quad \hat{a}^\dagger |\psi_n\rangle = \sqrt{n+1}\, |\psi_{n+1}\rangle\right)$$

$$|\psi_{n+1}\rangle = \frac{1}{\sqrt{n+1}} \hat{a}^\dagger |\psi_n\rangle$$

put $n=0$: $|\psi_1\rangle = \frac{1}{\sqrt{1}} \hat{a}^\dagger |\psi_0\rangle$

put $n=1$, $|\psi_2\rangle = \frac{1}{\sqrt{2}} \hat{a}^\dagger |\psi_1\rangle = \frac{1}{\sqrt{1.2}} \left(\hat{a}^\dagger\right)^2 |\psi_0\rangle$

put $n=2$, $|\psi_3\rangle = \frac{1}{\sqrt{3}} \hat{a}^\dagger |\psi_2\rangle = \frac{1}{\sqrt{1.2.3}} \left(\hat{a}^\dagger\right)^3 |\psi_0\rangle$

$\vdots$

in general,
$$\boxed{\psi_n(x) = \frac{1}{\sqrt{n!}} \left(\hat{a}^\dagger\right)^n \psi_0(x)}$$

Now, if we express this in terms of the dimensionless quantity: $\boxed{y = \sqrt{\frac{m\omega}{\hbar}}\, x}$

$$\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}} \frac{d}{dy}$$

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

$$\hat{a}^\dagger = \left(\sqrt{\frac{m\omega}{2\hbar}}\, x - \frac{i}{\sqrt{2m\omega\hbar}} \frac{\hbar}{i} \frac{d}{dx}\right) \leftarrow \text{expressed in functional form.}$$

$$= \frac{1}{\sqrt{2}} \left(y - \frac{d}{dy}\right).$$

Thus,
$$\psi_n(y) = \frac{1}{\sqrt{n!}} \cdot \frac{1}{\sqrt{2^n}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left(y - \frac{d}{dy}\right)^n e^{-y^2/2}$$

$$= \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-y^2/2}\, e^{y^2/2} \left(y - \frac{d}{dy}\right)^n e^{-y^2/2}$$

$$\boxed{H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}}$$

It can be shown, from "Rodrigues formula" for Hermite polynomials, that,

$$H_n(y) = e^{y^2/2} \left(y - \frac{d}{dy}\right)^n e^{-y^2/2}$$

So,

$$\psi_n(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-y^2/2} H_n(y)$$

or,

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right)}$$

↳ same as we got earlier by solving the differential eq^n.

Schrödinger equation in momentum space:

In coordinate space, we write Schrödinger eq^n as:

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

the usual operators look like: $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$

$\hat{x} = x$ (just a number)

It's equally possible to use alternate operator correspondence:

$$\boxed{\begin{aligned} \hat{p} &= p \text{ (just a number)} \\ \hat{x} &= i\hbar \frac{d}{dp} \end{aligned}}$$

called "momentum representation".

Note that, in both representation one should obey

$$[\hat{x}, \hat{p}] = i\hbar$$

Now, we are looking for S.E. in terms of momentum representation of wave function i.e. $\phi(p,t)$

Using the Fourier Transform, one can easily move from coordinate representation of wave function to the momentum representation.

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{ipx/\hbar}\, \Phi(p,t)}$$

put this into Schrödinger eq^n: $\quad i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)$

$$\Rightarrow \frac{i\hbar}{\sqrt{2\pi\hbar}}\frac{\partial}{\partial t}\int dp\, e^{ipx/\hbar}\,\Phi(p,t) = -\frac{\hbar^2}{2m}\cdot\frac{1}{\sqrt{2\pi\hbar}}\frac{\partial^2}{\partial x^2}\int dp\, e^{ipx/\hbar}\,\Phi(p,t)$$
$$+ \frac{V(x)}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\,\Phi(p,t) \quad \text{— (1)}$$

Note that, the inverse Fourier transform reads as:

$$\boxed{\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int dx\, e^{-ipx/\hbar}\,\Psi(x,t)}$$

Thus, the last term simplifies as:

$$\frac{V(x)}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\,\Phi(p,t)$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\cdot\underbrace{\frac{1}{\sqrt{2\pi\hbar}}\int dx'\, e^{-ipx'/\hbar}\, V(x')\,\Psi(x',t)}$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\cdot \underbrace{V(p) * \Phi(p,t)}_{\text{convolution}}$$

From eq^n (1),

$$\frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\left[i\hbar\frac{\partial}{\partial t}\Phi(p,t) + \frac{\hbar^2}{2m}\cdot\left(\frac{ip}{\hbar}\right)\cdot\left(\frac{ip}{\hbar}\right)\Phi(p,t) - V(p) * \Phi(p,t)\right] = 0$$

So, $$\boxed{i\hbar\frac{\partial}{\partial t}\Phi(p,t) = \frac{p^2}{2m}\Phi(p,t) + V(p) * \Phi(p,t)}$$

↳ Schrödinger eq^n in momentum space representation.