$$\hat{U}(x,t;y,0) \equiv \sum_n \int dy\, \psi_n^*(y)\, \psi_n(x)\, e^{\left(\frac{-iE_n t}{\hbar}\right)}$$

$\hat{U}$ takes an initial wavefunction $\Psi(y,0) = \Psi_i(y)$ to $\Psi(x,t)$. Note the integral over y,

$\Rightarrow$ $\Psi(x,t)$ depends on all values of $\Psi_i(y)$ at $t=0$.

Applications in 1D.

The Infinite Square Well $\equiv$ Particle in a Box.

Consider a potential

$$V(x) = 0 \quad , \quad \forall\, 0 \le x \le a$$
$$\quad\;\; = \infty \quad , \quad \text{otherwise}$$

$$\therefore \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \quad , \quad \forall\, 0 \le x \le a$$
$$\quad\;\; = \infty \quad , \quad \text{otherwise}$$

We want to solve TISE $\hat{H}\Psi_E(x) = E\Psi_E(x)$

$E \neq \infty \Rightarrow \Psi_E(x) = 0 \; , \; \forall\, x > a \; , \; x < 0.$

Also $\quad -\frac{\hbar^2}{2m}\frac{d^2\Psi_E(x)}{dx^2} = E\Psi_E(x) \quad , \quad \forall\, 0 \le x \le a$

$\Rightarrow \quad \Psi_E''(x) = -k^2\Psi_E(x)$, where $k = \sqrt{\frac{2mE}{\hbar^2}}$

$\Psi_E'(x) \equiv \frac{d\Psi_E(x)}{dx}$.

$$\Rightarrow \psi_E(x) = A\sin(kx) + B\cos(kx).$$

Continuity of $\psi_E(x)$ at $x = a$ and $x = 0$

$$\Rightarrow A\sin(ka) + B\cos(ka) = 0$$

and $\qquad B\cos(0) = B = 0$

$$\Rightarrow \sin(ka) = 0$$

$$\Rightarrow k = \frac{n\pi}{a}, \quad n \in I.$$

We label k with n and ψ and E with n also. $\therefore$ $k_n = \frac{n\pi}{a}$, $E_n = \frac{\hbar^2 k_n^2}{2m}$

$$\Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$\psi_n(x) = A\sin(k_n x). \quad \int_{-\infty}^{\infty} |\psi_n|^2 dx = 1$$

$$\Rightarrow |A|^2 \int_0^a (\sin(k_n x))^2 dx = 1$$

$$\Rightarrow |A| = \sqrt{2/a}$$

We choose $A = |A|$

$$\therefore \psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right).$$

Note $\int_0^a \psi_m^*(x)\,\psi_n(x) = \delta_{m,n}$

The set $\{\psi_n,\ \underset{n>0}{n \in I,}\}$ are complete

Note $\psi_{-n}(x) = \psi_n(x)$, so they are linearly dependent. Hence we only need $n>0$ solutions.

$$\psi(x,t) = \sum_{n=1}^{\infty} \int_0^a dy \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi y}{a}\right) \psi(y,0) \times \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) \exp\left[\frac{-in^2\pi^2\hbar t}{2ma^2}\right]$$

$$= \left(\frac{2}{a}\right) \sum_{n=1}^{\infty} \left[\exp\left[\frac{-in^2\hbar\pi^2 t}{2ma^2}\right]\right] \sin\left(\frac{n\pi x}{a}\right) \int_0^a \sin\left(\frac{n\pi y}{a}\right) \psi(y,0)\,dy$$

Free particle $\Leftrightarrow$ $V(x) = 0$, $\forall x$

$$\hat{H} = \hat{T} + 0 = \hat{T} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

Again $\Rightarrow$ TISE becomes

$$\psi_E''(x) = -k^2\psi_E(x) \quad , \quad k = \sqrt{(2mE)/\hbar^2}$$

Solutions are Ae^{ikx}, Be^{-ikx}

Note these are linearly independent

$$\therefore \psi_E(x) = Ae^{ikx} + Be^{-ikx} \quad , \quad k > 0$$

$$\text{or} \quad \psi_k(x) = Ae^{ikx} \quad , \quad k \in R.$$

$$\therefore \quad \psi_k(x,t) = A\exp.\left[ikx - \frac{i\hbar^2k^2t}{2m\hbar}\right]$$

Let us normalize $\psi_k(x,t)$

$$\int_{-\infty}^{\infty} \psi_{k'}^*(x)\psi_k(x)dx = |A|^2\int_{-\infty}^{\infty} e^{ix(k-k')}dx$$

$$= 2\pi|A|^2\delta(k-k')$$

$$\Rightarrow |A| = 1/\sqrt{2\pi}$$

$$\therefore \psi_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}} \quad , \quad \psi_k(x,t) = \frac{e^{ikx - \frac{i\hbar k^2 t}{2m}}}{\sqrt{2\pi}}$$

The general solution of TDSE

$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$ is then

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k)\, \exp\left[ikx - \frac{i\hbar k^2 t}{2m}\right] \frac{dk}{\sqrt{2\pi}}$$

$\boxed{4\text{-}5}$

It should satisfy the initial condition $\Psi(x,0) = \Psi_i(x)$.

$$\therefore \quad \Psi_i(x) = \int_{-\infty}^{\infty} \phi(k) \frac{e^{ikx}}{\sqrt{2\pi}}\, dk$$

$$\Rightarrow \int_{-\infty}^{\infty} \frac{e^{-ik'x}}{\sqrt{2\pi}} \Psi_i(x)\, dx = \int_{-\infty}^{\infty} \frac{\phi(k)}{2\pi} dk \int_{-\infty}^{\infty} e^{i(k-k')x}\, dx$$

$$= \int_{-\infty}^{\infty} \phi(k)\, \delta(k-k')\, dk = \phi(k')$$

$$\Rightarrow \phi(k) = \int_{-\infty}^{\infty} \frac{e^{-ikx}}{\sqrt{2\pi}} \Psi_i(x)\, dx$$

$$\Rightarrow \Psi(x,t) = \left(\frac{1}{2\pi}\right) \int_{-\infty}^{\infty} \exp\left[ikx - \frac{i\hbar k^2 t}{2m}\right] dk \int_{-\infty}^{\infty} e^{-iky} \Psi_i(y)\, dy.$$

We have thus the general solution $\Psi(x,t)$ once we are given $\Psi(x,0) = \Psi_i(x)$ for the free particle.