so that:

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

We say that the $\psi(x)$ function must be normalized - and the above equation expresses this "normalization requirement" mathematically.

APPLICATIONS OF TISE:

We will now discuss the application of Schrödinger Equation to several simple quantum-mechanical situations (but "simple" does not mean that they are not important!!!).

FREE PARTICLE:

The simplest of all conceivable quantum mechanical systems is certainly a free particle moving in the x direction, with no forces whatsoever acting on it. $F = 0$ means that the potential energy is constant: $U(x) = \text{const.}$

As you remember, in the case of potential energy we can arbitrarily choose where $U = 0$.

$$\boxed{\text{Question: when we talk about the potential energy due to Earth gravity, we often choose one special point to be that with } U=0. \text{ Where is this point located?}}$$

So, for the "free-particle" we can set $U=0$ and not worry any more about it!

Then, the TISE becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

or $$\frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{with} \quad k^2 = \frac{2mE}{\hbar^2}$$

This is a well-known equation, with a general solution:

$$\boxed{\psi = A\sin(kx) + B\cos(kx)}$$

where A and B are arbitrary constants.

This is an equation of a wave with $\lambda = \frac{k}{2\pi}$

The equation is satisfied for <u>any</u> value of k meaning that the energy is:

$$k^2 = \frac{2mE}{\hbar^2} \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

So, the free-particle equation describes essentially the motion of ~~any~~ a particle with <u>any</u> energy E.

Now, note that for non-relativistic particles:

$$\left.\begin{array}{l} E = K = \frac{mV^2}{2} = \frac{m^2V^2}{2m} = \frac{p^2}{2m} \\ \text{and} \quad E = \frac{\hbar^2 k^2}{2m} \end{array}\right\} \Rightarrow p = \hbar k$$

But $\hbar = \frac{h}{2\pi}$ and $k = \frac{2\pi}{\lambda}$

So: $p = \hbar k = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \frac{h}{\lambda}$, or $\lambda = \frac{h}{p}$

The latter is simply the de Broglie wavelength. So, the solution produced simply a de Broglie wave, which is not surprising!

<u>But there is a small problem...</u>

(not mentioned in the book!)

We said that $\psi(x)$ must be normalized!

And

$$\int_{-\infty}^{+\infty} |A\sin(kx) + B\cos(kx)|^2 \, dx$$

$$= \int_{-\infty}^{+\infty} \left[A^2\sin^2(kx) + B\cos^2(kx) + AB\sin(2kx)\right] dx = \infty \; !!!$$

So, did our very first encounter with the TISE produce an illegal solution?

Fortunately, ψ can be resqued!

Since $\psi(x) = A\sin(kx) + B\cos(kx)$ for any k is a "good" solution, any sum of those solutions ~~is also~~ with different k values is also a good solution. And by adding many such solutions, we can obtain a wave packet!

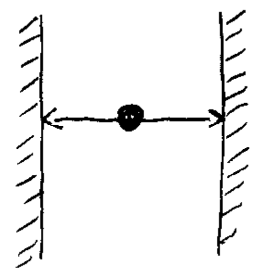
ψ:  $\int_{-\infty}^{+\infty} |\psi|^2 dx = \infty$

infinite wave

ψ:  finite wave-packet (Gaussian) $\int_{-\infty}^{+\infty} |\psi|^2 dx =$ finite value.

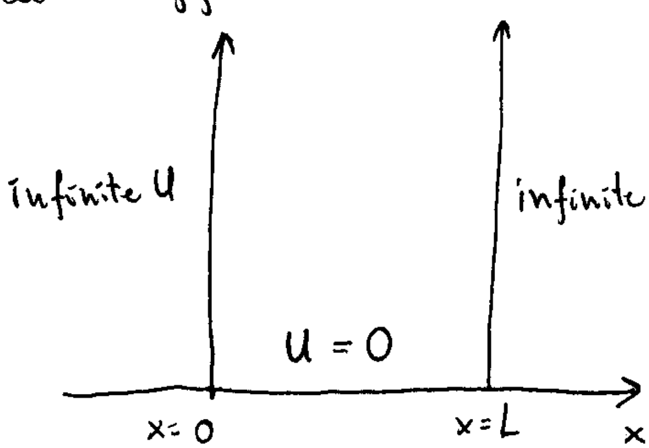
2. PARTICLE IN A BOX

Meaning: particle between two walls. The collisions with each wall are <u>elastic</u>, i.e., the particle is bounced back with no energy loss.



This is again a simple problem - but it has many impotant implications, and is used in many "serious" physical models.

We desribe this situation in terms of potential energy:



The particle cannot be in the regions $x < 0$ and $x > L$, so $\psi(x<0) = 0$ and $\psi(x>L) = 0$

Only for $0 \leq x \leq L$ the wavefunction can be $\psi(x) \neq 0$

The Schrödinger Eq. for the region between the walls is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

And, as was said before, the solution for ψ is:

$$\psi = A\sin(kx) + B\cos(kx) \quad \text{with } k^2 = \frac{2mE}{\hbar^2}$$

However, now there are some restrictions imposed on ψ. First, $\psi(x)$ must be a <u>continuous function</u>. For $x<0$, as we said, $\psi = 0$.
So, the ~~solution~~ "inside" solution also must be zero at $x=0$. And $\cos(kx)$ is <u>one</u> for $x=0$.
So, we conclude that B <u>must be zero</u>.

This leaves us with:

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

But, again, $\psi = 0$ for all $x > L$, so to assure the continuity of ψ, it must be:

$$\psi(L) = A\sin(kL) = 0$$

Meaning that:

$$kL = 0,\ \pi,\ 2\pi,\ 3\pi \ldots\ n\pi \ldots$$

$kL = 0$ would mean $\psi = 0$ everywhere, or no particle. So, it has to be rejected.
Other kL values are O.K. So we get:

$$k = \frac{n\pi}{L} \quad \text{with } n = 1, 2, 3, \ldots$$

and:

$$\psi = A \sin\left(\frac{n\pi}{L} x\right)$$

Still, we have to determine the value of A.
Here, the normalization condition becomes helpful:

$$\int_{-\infty}^{+\infty} |\psi(x)|\, dx = 1 \quad \xrightarrow[\text{present case}]{\text{in the}} \quad \int_0^L A^2 \sin^2\left(\frac{n\pi}{L} x\right) dx = 1$$

Use a dummy variable $z = \frac{n\pi}{L} x$: $\quad dx = \frac{L}{n\pi} dz$

$$\int_0^L A^2 \sin^2\left(\frac{n\pi}{L}\right) dx = A^2 \frac{L}{n\pi} \int_0^{n\pi} \sin^2(z)\, dz = A^2 \frac{L}{n\pi} \cdot \frac{n\pi}{2} = \frac{A^2 L}{2} = 1$$

so $A = \sqrt{\frac{2}{L}}$

Our wavefunction is then:

$$\psi = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) & \text{for } 0 \leq x \leq L \\ 0 & \text{for } x < 0 \text{ and } x > L \end{cases}$$

But we still have to find the energy E.

This is easy:

$$k^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad k = \frac{n\pi}{L}$$

So:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \quad \text{with } n = 1, 2, 3 \ldots$$

The <u>Lowest</u> allowed energy is for $n = 1$:

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

The other possible energies can be simply written as:

$$E_n = n^2 E_1$$

So $E_2 = 4E_1$, $E_3 = 9E_1$, $E_4 = 16E_1$, ...