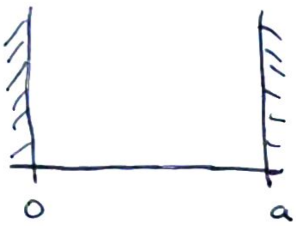
Infinite Square Well & Context



$$V(x) = \begin{cases} \infty & a < x < 0 \\ 0 & 0 < x < a \end{cases}$$

The wavefunctions obey the Schrodinger equation.

What are the stationary states?

$H\Psi = E\Psi$ time-independent S.E.

$\Rightarrow$ This is an eigenvalue equation.

$\Rightarrow$ This is useful because linear algebra helps.

H is the Hamiltonian, or energy operator.
Could write $H = \hat{E}$ if you want.

$\hat{E}\Psi = E\Psi$ $\hat{E}$: operator E: Eigenvalues
Ψ: Eigenfunctions

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

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

$$\frac{d^2\Psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\Psi(x) \qquad K^2 \equiv \frac{2mE}{\hbar^2}$$

$$\Rightarrow \frac{d^2\Psi}{dx^2} = -K^2\Psi(x)$$

$$\Psi(x) = A\sin(Kx + \phi)$$

B.C. $\Psi(0) = \Psi(a) = 0$ $\Psi(0) = A\sin(\phi) \Rightarrow \phi = 0$

$\Psi(a) = A\sin(Ka) \Rightarrow Ka = n\pi \quad n = 1, 2, \ldots$

$$\Rightarrow K = \frac{n\pi}{a}$$

But $k^2 = 2mE/\hbar^2$ $\Rightarrow$ $k^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$

$$\Rightarrow \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \Big\} \text{ Eigenvalues.}$$

$\psi_n(x) = A\sin\left(\frac{n\pi x}{a}\right)$ Normalized: $\underbrace{\psi_n(x) = \sqrt{\frac{2}{a}}\sin}_{\text{Eigenfunctions}}\left(\frac{n\pi x}{a}\right)$

In bra-ket notation:

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

or $\hat{E}|n\rangle = E_n|n\rangle$ or $\hat{E}|E_n\rangle = E_n|E_n\rangle$

What is the expectation value for $\hat{E}$?

$$\langle E_n|\hat{E}|E_n\rangle = \langle E_n|E_n|E_n\rangle$$
$$= E_n\cancelto{1}{\langle E_n|E_n\rangle}$$

$\langle E\rangle = E_n = \langle E_n|\hat{E}|E_n\rangle$ makes sense.

$\hat{E}$ is an operator and could be written like an infinite dimensional matrix.

$\hat{E} = \sum_{n,m} E_{nm}|E_n\rangle\langle E_m|$ $\qquad E_{nn} = \langle E_n|E|E_n\rangle = \langle E\rangle = E_n$

What about E_{nm}? $\langle E_n|\hat{E}|E_m\rangle$?

$$\Rightarrow \quad \langle E_n|\hat{E}|E_m\rangle = \langle E_n|E_n|E_m\rangle = E_n\cancelto{0}{\langle E_n|E_m\rangle}$$

$$\langle E_n|\hat{E}|E_m\rangle = 0 \quad \Rightarrow \quad E_{nm} = 0$$

$$\hat{E} = \begin{pmatrix} \frac{\pi^2\hbar^2}{2ma^2} & 0 & 0 & \cdots & \\ 0 & \frac{2^2\pi^2\hbar^2}{2ma^2} & 0 & \cdots & \\ 0 & 0 & \frac{3^2\pi^2\hbar^2}{2ma^2} & 0 & \cdots \\ \vdots & \vdots & 0 & \ddots & \\ & & \vdots & & \ddots \end{pmatrix}$$

*Every operator is diagonal in its own eigenbasis. *

You can do this for any operator. $\hat{x}$, $\hat{p}$, $\hat{x}^2$, $\hat{p}^2$, etc.

Ex: $A_{nn} = \langle E_n | \hat{A} | E_n \rangle = \int \psi_n^* \hat{A} \psi_n dx = \langle A \rangle$ } Expectation value

$A_{mn} = \langle E_m | \hat{A} | E_n \rangle = \int \psi_m^* \hat{A} \psi_n dx$

Completeness & Orthogonality are important!

$$\underbrace{g(x)}_{\text{any function}} = \sum_n \underbrace{c_n}_{\text{weights}} \underbrace{f_n(x)}_{\text{basis functions}}$$

In bra-ket notation: $\underbrace{|g\rangle}_{\text{still a function.}} = \sum_n \langle f_n | g \rangle | f_n \rangle$

$c_n = \langle f | g \rangle$

$c_n = \int f_n^* g \, dx$

Does a particle always have to be in an eigenstate?

No

Can be in any arbitrary state! If it starts in an eigenstate it will remain in an eigenstate.

If it is in an arbitrary state: $\Psi(x,0) = \underbrace{g(x)}_{\text{any function.}}$

Can write it as a linear sum of basis functions.

$$\Psi(x,0) = \sum_n c_n \psi_n(x) \qquad c_n = \int \psi_{n(x)}^* \Psi(x,0) \, dx$$

$$\Rightarrow \left(g(x) = \sum_n c_n f(x) \right)$$

↑ no label

In bra-ket notation: $|\Psi(x,0)\rangle = \sum_n \langle \psi_n | \Psi(x,0) \rangle | \psi_n \rangle$

Why does $c_n = \int f_n^* g \, dx$?

$g(x) = \sum_n c_n f_n(x)$ multiply by $f_m(x)$

$f_m(x) g(x) = \sum_n c_n f_m(x) f_n(x)$ integrate

$\int f_m(x) g(x) \, dx = \int \sum_n c_n f_m(x) f_n(x) \, dx$

$\Rightarrow \sum_n c_n \underbrace{\int f_m(x) f_n(x)}_{\substack{\text{if } n \neq m \\ = 0}} dx = \int f_m(x) g(x) dx$

$=0$, only non-zero if $m=n$, only those terms remain.

orthonormal !!

$\Rightarrow \quad c_m \overbrace{\int \cancel{f_m(x)} f_m(x) dx}^{1} = \int f_m(x) g(x) dx$

$c_m = \int f_m(x) g(x) dx$

or $c_n = \int f_n(x) g(x) dx$

index doesn't matter.

$|g\rangle = \sum_n c_n |f_n\rangle$

$\langle f_m | g \rangle = \sum_n c_n \langle f_m | f_n \rangle$

$\langle f_m | g \rangle = \sum_n c_n \delta_{mn}$

$\Rightarrow \quad c_m = \langle f_m | g \rangle$