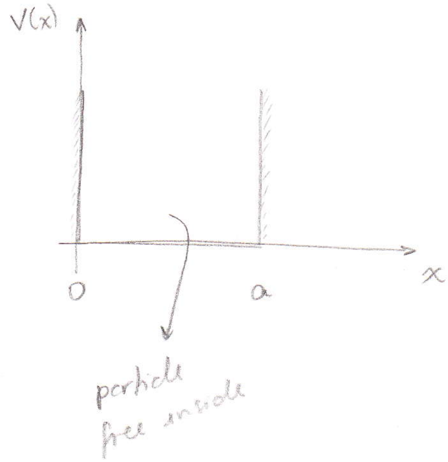
Infinite Square Well

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$



$\begin{cases} \text{outside}^{\text{well}} \ \psi(x) = 0 & \text{(zero probability)} \\ \text{inside}^{\text{well}} \ V = 0 \end{cases}$

Inside:

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

$$\frac{d^2\psi}{dx^2} = -\underbrace{\left(\frac{2mE}{\hbar^2}\right)}_{k^2}\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

finding roots $\lambda^2 + k^2 = 0$ → $\lambda_1 = +ik$, $\lambda_2 = -ik$

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

to find A and B → boundary conditions

$\psi(0) = 0 \Rightarrow \boxed{B = 0}$

$\psi(a) = 0 \Rightarrow A\sin ka = 0 \Rightarrow ka = 0, \pm\pi, \pm 2\pi, \ldots$

$k = 0 \rightarrow$ bad choice $\Rightarrow \psi(x) = 0$

$\oplus$ or $\ominus$ → just a global phase

$\Rightarrow ka = \pi, 2\pi, 3\pi, \ldots \Rightarrow \boxed{k_n = \frac{n\pi}{a}}$

2-2-02

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

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \boxed{\frac{n^2 \pi^2 \hbar^2}{2ma^2}}$$ → energy is quantized

how about A ?
↳ from normalization

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1 \Rightarrow \int_0^a |A|^2 \sin^2(kx)\, dx = 1$$

$$\left(\begin{array}{l} \cos 2x = \cos^2 x - \sin^2 x = 1 - 2\sin^2 x \\ \Rightarrow \sin^2 x = (1 - \cos 2x)/2 \end{array} \right)$$

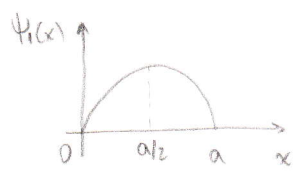
$$|A|^2 \int_0^a \left(\frac{1}{2} - \frac{\cos 2kx}{2} \right) dx = |A|^2 \left(\frac{a}{2} - \cancel{\frac{\sin(2kx)}{2(2k)}\Bigg|_0^a} \right) = A^2 \frac{a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\boxed{\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x \right)}$$ ← infinite set of solutions for the time indep Schröd. eq.

$$\left\{ \begin{array}{l} \Psi_1 \rightarrow \text{ground state} \\ \Psi_{2,3,\ldots} \rightarrow \text{excited states} \end{array} \right.$$

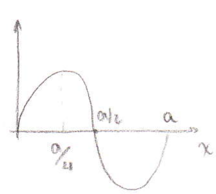
Properties

1) They are alternately even and odd with respect to center of well



$\Psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$

(even with respect to a/2)



$\Psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$

(odd with respect to a/2)

2) Go up in energy ⇒ one more <u>node</u>

3.) They are <u>orthonormal</u>

orthogonal + normalized

$$\int \psi_n^* \psi_n \, dx = 1$$

$$\int \psi_m^*(x)\, \psi_n(x)\, dx = 0 \quad \text{whenever } m \neq n$$

$$\frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)dx = \frac{2}{a}\int_0^a \frac{\left[\cos\left((m-n)\frac{\pi x}{a}\right) - \cos\left((m+n)\frac{\pi x}{a}\right)\right]}{2}dx =$$

$\cos(a+b) = \cos a \cos b - \sin a \sin b$

$\cos(a-b) = \cos a \cos b + \sin a \sin b$

$$= \frac{1}{a}\left\{\frac{\sin[(m-n)\pi x/a]}{(m-n)\pi/a} - \frac{\sin[(m+n)\pi x/a]}{(m+n)\pi/a}\right\}\Bigg|_0^a = \boxed{0}$$

$$\boxed{\int \psi_m^*(x)\, \psi_n(x)\, dx = \delta_{mn}}$$

<u>Kronecker delta</u>

$$\delta_{mn} \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$$

4) They are <u>complete</u>

= any function $f(x)$ can be written as a linear combination of them

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

{ <u>Fourier series</u> of $f(x)$

Use orthonormality to find coefficients c_n

multiply both sides by $\psi_m^*(x)$ and integrate

$$\int \psi_m^*(x)\, f(x)\, dx = \sum_n c_n \underbrace{\int \psi_m^*(x)\, \psi_n(x)\, dx}_{\delta_{nm}} = \boxed{c_m}$$

$$\boxed{c_n = \int \psi_n^*(x)\, f(x)\, dx}$$

1st property - valid when V is symmetric
2nd - universal
3rd, 4th - very general

⇒) Stationary states of the infinite square well

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

⇒) Most general solution

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

⇒) $$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \underbrace{\Psi(x,0)}_{\text{initial condition}} dx$$

With $\Psi(x,t)$ can find any dynamical quantity
any observable in time

Example 2.2

Particle in the infinite square well has the initial wave function

$$\Psi(x,0) = Ax(a-x) \qquad 0 \le x \le a$$

Find $\Psi(x,t)$

1st) find A

2nd) find c_n, given $\Psi(x,0)$

3rd) find $\Psi(x,t)$

$$\Rightarrow \int_0^a |A|^2 (ax-x^2)^2\, dx = \int_0^a |A|^2 (a^2x^2 - 2ax^3 + x^4)\, dx = |A|^2 \underbrace{\left(a^2 \frac{a^3}{3} - 2a\frac{a^4}{4} + \frac{a^5}{5}\right)}_{a^5 \underbrace{\left(\frac{1}{3} - \frac{1}{2} + \frac{1}{5}\right)}_{\frac{10-15+6}{30} = \frac{1}{30}}} = |A|^2 \frac{a^5}{30}$$

$$\boxed{A = \sqrt{\frac{30}{a^5}}}$$

$$\Rightarrow c_n = \int \psi_n^*(x)\, \Psi(x,0)\, dx = \sqrt{\frac{2}{a}}\sqrt{\frac{30}{a^5}} \int_0^a \sin\left(\frac{n\pi x}{a}\right) x(a-x)\, dx$$

$$= \frac{2\sqrt{15}}{a^3} \left\{ a \underbrace{\int_0^a x \sin\left(\frac{n\pi x}{a}\right) dx}_{\text{(by parts)}} - \int_0^a x^2 \sin\left(\frac{n\pi x}{a}\right) dx \right\} = \boxed{\begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{8\sqrt{15}}{n^3\pi^3} & \text{if } n \text{ is odd} \end{cases}} //$$

$$\Rightarrow \Psi(x,t) = \sum_{n=1}^{\infty} \frac{8\sqrt{15}}{n^3\pi^3} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar}$$

$$\boxed{\Psi(x,t) = \sqrt{\frac{30}{a}} \left(\frac{2}{\pi}\right)^3 \sum_{n=1}^{\infty} \frac{1}{n^3} \sin\left(\frac{n\pi x}{a}\right) e^{-in^2\pi^2\hbar t/2ma^2}} //$$

For orthonormal solutions $\int \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn}$,

we have

① $$\boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

② $$\boxed{\langle H\rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n}$$

$\Big\{$ $|c_n|^2$ is the probability of getting E_n when you measure energy

① ↳ follows from normalization

$$\int |\Psi(x,t)|^2\,dx = 1 \longrightarrow \boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

$$\int \left(\sum_{m=1}^{\infty} c_m^* \psi_m^* e^{+iE_m t/\hbar}\right)\left(\sum_{n=1}^{\infty} c_n \psi_n e^{-iE_n t/\hbar}\right) dx$$

$$= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_m^* c_n\, e^{-i(E_n-E_m)t/\hbar} \underbrace{\int \psi_m^*(x)\,\psi_n(x)\,dx}_{\delta_{mn}} = \sum_{n=1}^{\infty} |c_n|^2$$

② ↳ time indep Schröd eq $\hat{H}\psi = E\psi$

$H\psi_n = E_n\psi_n$

$$\langle H\rangle = \int \Psi^* H \Psi\,dx = \int\left(\sum c_m^* \psi_m^*(x)\right) H\left(\sum c_n \psi_n(x)\right) dx$$

$$= \sum_m \sum_n c_m^* E_n c_n \underbrace{\int \psi_m^* \psi_n\,dx}_{\delta_{mn}} = \sum |c_n|^2 E_n$$

$$\Rightarrow \boxed{\langle H\rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n}$$

expectation value of H is indep. of time ⇒ conservation of energy