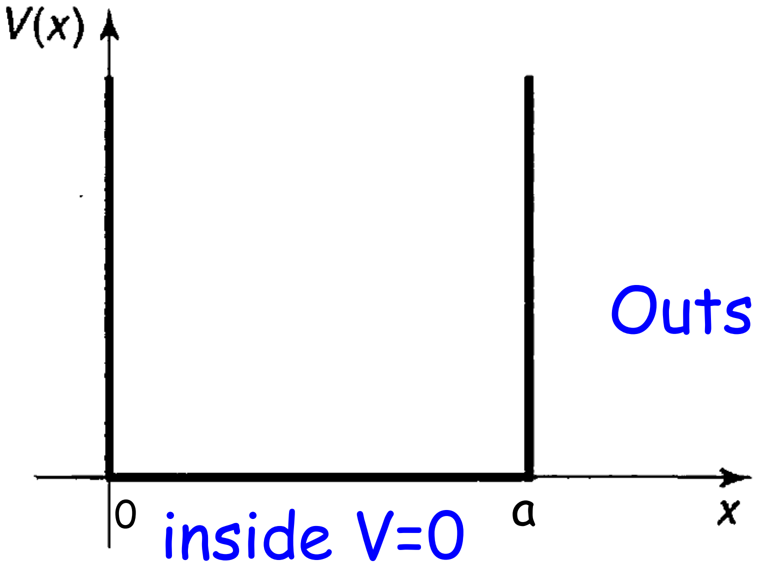
2.2 The infinite square well



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

Outside V=∞ → $\psi(x) = 0$

inside V=0

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

$$k \equiv \frac{\sqrt{2mE}}{\hbar}$$

E is is determined by boundary conditions. It can't be any number, as in classical physics! "Inside" the potential *E* will be discrete.

The diff. eq. $\frac{d^2\psi}{dx^2} = -k^2\psi$ has as solution:

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

Check!

A and *B* are constants fixed by boundary conditions.

In this case, the only bound. conditions are

$$\psi(0) = \psi(a) = 0$$

The first one is easy:

$$\psi(0) = A\underbrace{\sin 0}_{=0} + B\underbrace{\cos 0}_{=1} = \boxed{B = 0}$$

The second one becomes:

Reminder:
"a" is width of well

$$\psi(a) = A \sin ka \quad \text{or} \quad \sin ka = 0$$

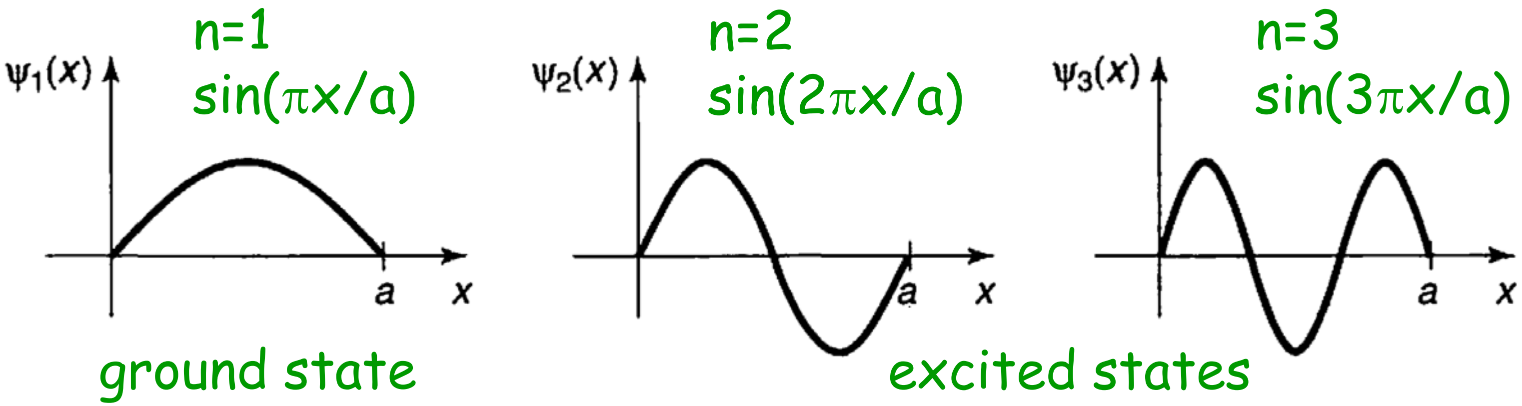
$$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \ldots$$

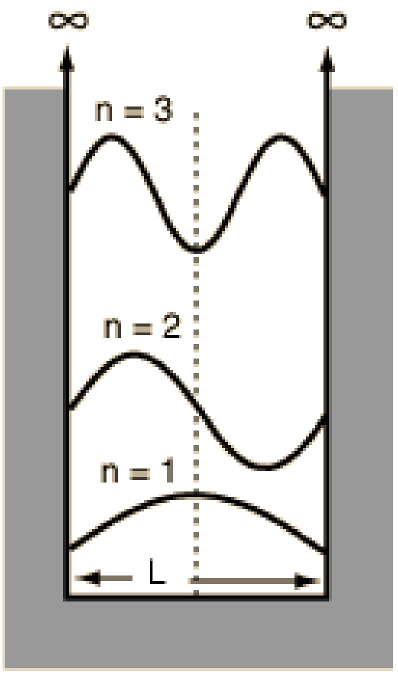
A=0 or k=0 leads to zero wave function. Not good b.c. not normalizable.
The "-" solutions are redundant because sin(x) is odd.

Only solutions are then:

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

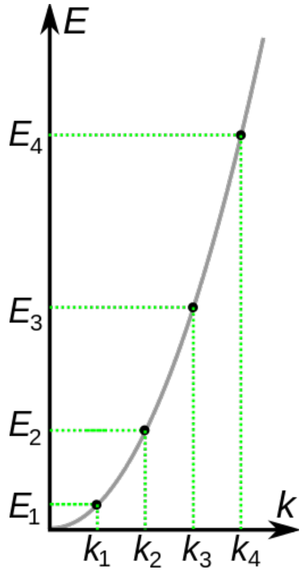
Note that this is a discrete set of solutions, thus energies will be discrete.





x = 0 at left wall of box.

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



Energies are quantized in QM, while in classical mechanics inside the well you can have any energy (if no gravity, no friction, elastic collisions with walls).

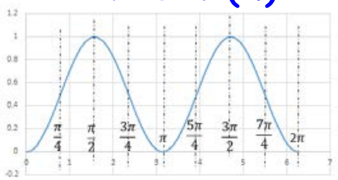
To finish the problem neatly, find A such that the wave function is normalized to 1.

k=nπ/a, use u=kx. Check!
Careful with limits of integration

$$\int_0^a |A|^2 \sin^2(kx)\,dx = |A|^2 \frac{a}{2} = 1$$

Result is n independent

Y=sin²(u)

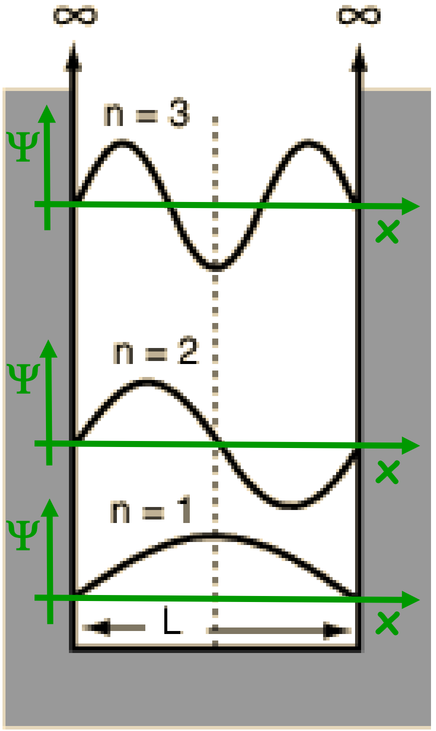


The final complete solution then is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad , \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Learn to identify "symmetries"! This one is invariant under reflection.

Separating in even-odd is valid only for even V(x)=V(-x) potentials



x = 0 at left wall of box.

2^{nd} excited state	even	2 nodes
1^{st} excited state	odd	1 node
ground state	even	0 node

Remember there is a $e^{-iE_n t/\hbar}$ multiplying always.

Thus, Re Ψ and Im Ψ parts are oscillating with time. But $|\Psi|^2$ is time independent.

For even odd functions see https://www.youtube.com/watch?v=lKaV03ZznN0

Two neat properties of the solutions.
(I) They are orthonormal.

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

Kronecker delta
=1 if m equal to n
=0 if m diff from n

If m=n this is obvious from normalization done.

If m≠n , left as exercise (please check):

$$\int \psi_m(x)^* \psi_n(x)\, dx = \frac{2}{a} \int_0^a \sin\left(\frac{m\pi}{a}x\right) \sin\left(\frac{n\pi}{a}x\right) dx$$

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

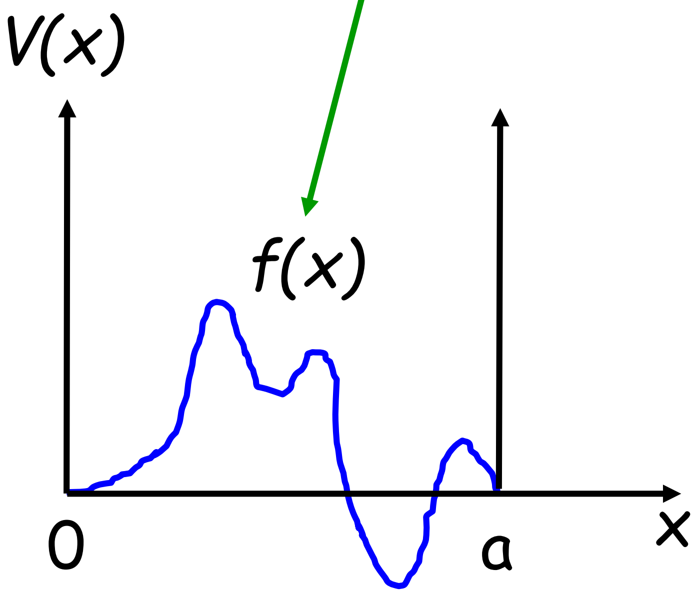
$$= \left\{\frac{1}{(m-n)\pi} \sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi} \sin\left(\frac{m+n}{a}\pi x\right)\right\}\Bigg|_0^a$$

$$= \frac{1}{\pi}\left\{\frac{\sin[(m-n)\pi]}{(m-n)} - \frac{\sin[(m+n)\pi]}{(m+n)}\right\} = 0.$$

(II) They are complete. This means coefficients c_n can always be found such that any wave function inside the square well can be written as

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

This expression is not surprising. This is just the sine Fourier series of *f*(x).



Arbitrary example

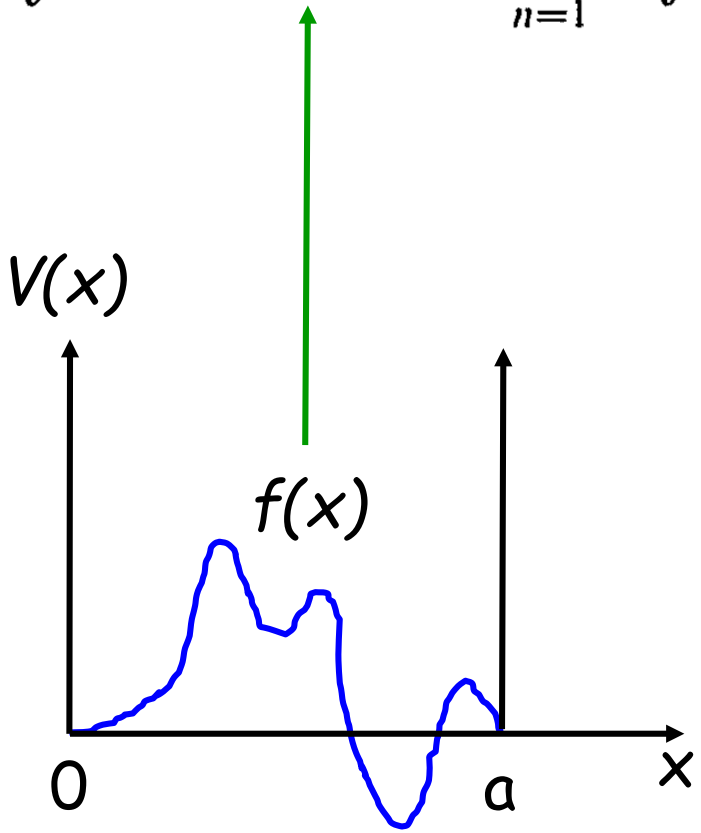
(1) *f*(x) can be **ANY function that is 0 outside the infinite well**. If not, then it is not acceptable.

(2) It could be discontinuous inside the well.

(3) *f*(x) does NOT have a sharp energy but an average energy.

How do we find the coefficients?

$$\int \psi_m(x)^* f(x)\,dx = \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \psi_n(x)\,dx = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$



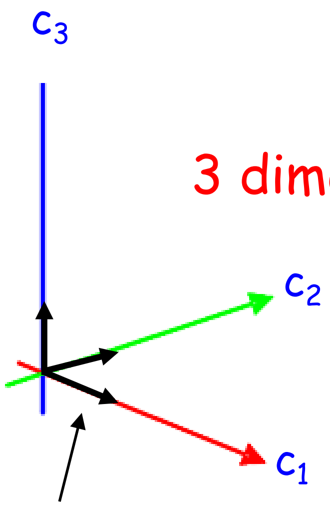
$$c_n = \int \psi_n(x)^* f(x)\,dx.$$

The integration can be done analytically or numerically.

This page not in book, just FYI. More details in Ch. 3.

Cartesians axes

$$\boldsymbol{r} = \sum_{n=1}^{3} c_n \, \boldsymbol{e}_n$$



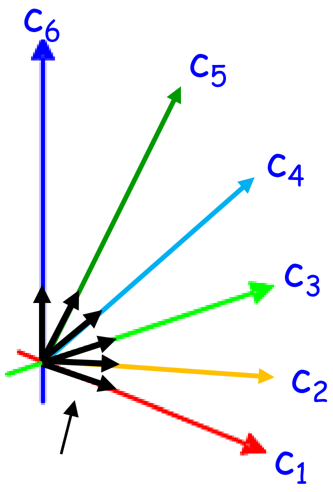
3 dimensions

Unit vectors are e_1,e_2,e_3.

Any **vector** can be expanded in the orthonormal basis e_1,e_2,e_3.
E.g. (2,0,-3)

Square-well solutions

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$



∞ dimensions

"Unit vectors" are ψ_1,ψ_2,ψ_3,ψ_4,ψ_5,...

Any **wave function** can be expanded in the orthonormal basis ψ_n
E.g. (1,2,0,-4,10,0.1,...)

All these properties are not pathological of the square well but very generic.