Chapter 2: time-indep Sch. Eq.

Now the real work starts: how do we solve the Sch. Eq.?

In general, the Sch. Eq. has a *time-dependent* potential:

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi$$

where V=V(x,t). For example, the V(x,t) of an oscillating electric field **E**(x,t).

Start with something *simpler*: a *time independent* potential V=V(x). Then use "separation of variables". Assume:

$$\Psi(x,t)=\psi(x)\,\varphi(t)$$

$$\frac{\partial\Psi}{\partial t}=\psi\frac{d\varphi}{dt},\qquad\frac{\partial^2\Psi}{\partial x^2}=\frac{d^2\psi}{dx^2}\varphi$$

$$i\hbar\psi\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\varphi + V\psi\varphi.$$

Divide by $\psi\varphi$ to get:

$$i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x) \quad = E$$

(constant with important physical meaning)

Function of t only

Function of x only

Time dependence is easy here!

$$i\hbar \frac{1}{\varphi}\frac{d\varphi}{dt} = E \quad \Rightarrow \quad \frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi$$

$$\varphi(t) = e^{-iEt/\hbar}$$

Coordinate dependence is not easy! ☹

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x) = E$$

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

Constant to be found

The solutions of this time-indep. Sch. Eq. are important for three reasons [(1,2) given here, (3) later in this presentation]:

(1) They are stationary states: $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar}\psi e^{-iEt/\hbar} = |\psi(x)|^2$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2\,dx$$

Constant in time

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt} = 0$$

All expectation values of operators O(x,p) are constant in time.

operators are denoted by ^

(2) They have "sharp" energies.

$$H(x,p) = \frac{p^2}{2m} + V(x) \xrightarrow[\text{rules}]{\text{QM}} \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

Classical "Hamiltonian"

$$\hat{p} \rightarrow (\hbar/i)(\partial/\partial x)$$

Now the time-indep. Sch. Eq. looks "simple":

$$\boxed{\hat{H}\psi = E\psi}$$

Then, the constant E is the energy !

$$\langle \hat{H} \rangle = \int \psi^* \underbrace{\hat{H}\psi}_{E\psi} dx = E \int |\psi|^2 dx = E \underbrace{\int |\Psi|^2 dx}_{=1} = E$$

Why E is "sharp"?

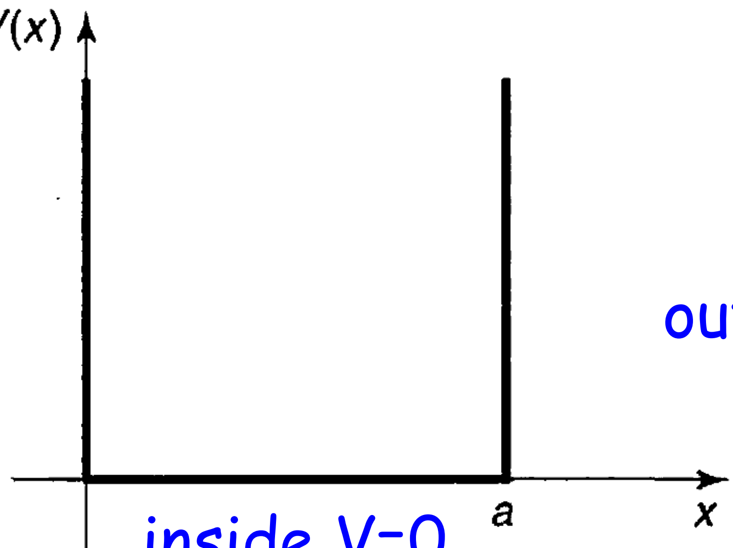
$$\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E(\hat{H}\psi) = E^2\psi$$

$$\langle \hat{H}^2 \rangle = \int \psi^* \hat{H}^2 \psi \, dx = E^2 \underbrace{\int |\psi|^2 dx}_{=1} = E^2$$

Thus: $\sigma_H^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = E^2 - E^2 = 0$

sharp!

2.2 The infinite square well



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

outside → $\psi(x) = 0$

inside V=0

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

E is to be determined by boundary conditions. It can't be any number! "Inside" the potential E will be discrete.

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

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

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

A and B are constants fixed by boundary conditions.

In this case, the only bound. cond. we know 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:

"a" is width of well

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

$$ka = \cancel{0},\ \pm\pi,\ \pm 2\pi,\ \pm 3\pi,\ \ldots$$

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

Only solutions are then:

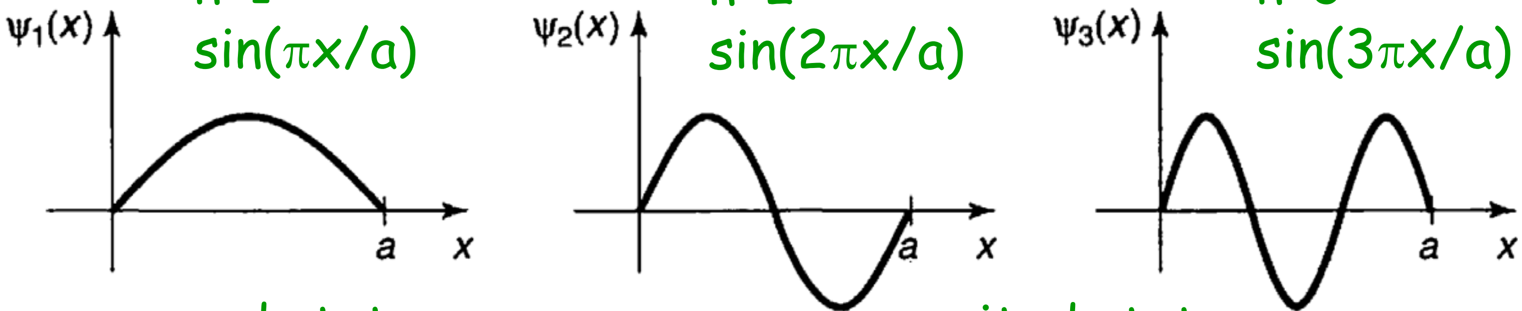
$$k_n = \frac{n\pi}{a}, \quad \text{with } n = 1, 2, 3, \ldots$$

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

n=1 $\sin(\pi x/a)$

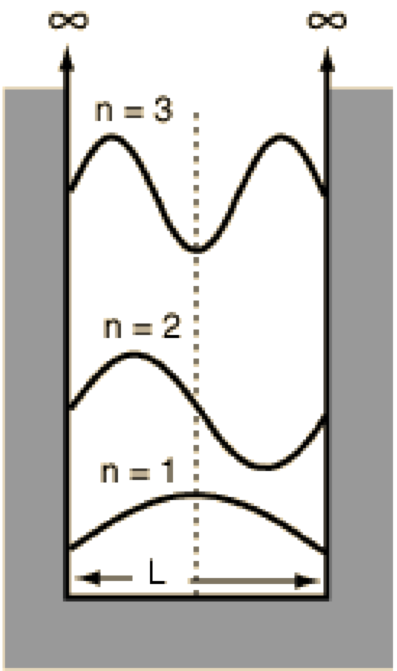
n=2 $\sin(2\pi x/a)$

n=3 $\sin(3\pi x/a)$



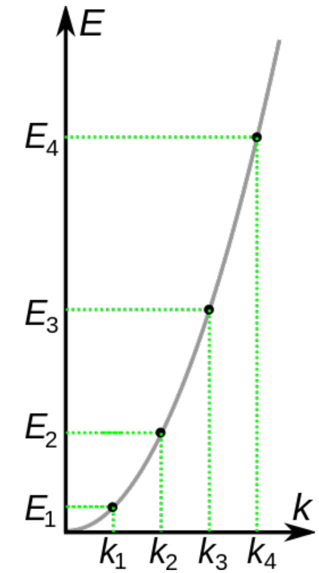
ground state

excited states



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 (no gravity, no friction, elastic collisions with walls).

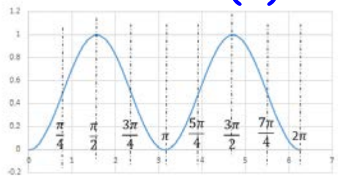
To finish the problem neatly, find A such that the wave function is normalized to 1.

k=nπ/a, use u=kx,
careful limits of integration

result n independent

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

Y=sin²(u)



The final complete solution then is:

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