Lecture #6 Time-Indep. Schrodinger Eq continued 9/11/98

Lecture #7 Particle in a box 9/14

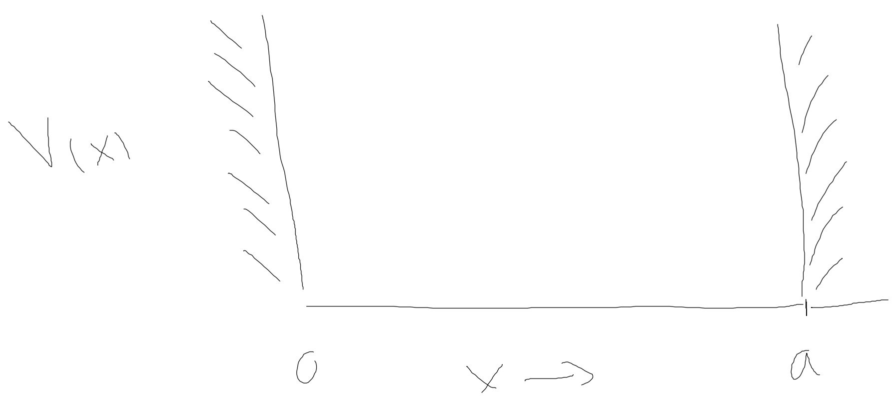
Solve space part of Schrodinger eq.

$\hat{H}\psi = E\psi$ or $\left[\frac{\hat{p}^2}{2m} + \hat{V}\right]\psi = E\psi$

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

Need to chose V. Consider simple model of a bound state Example nucleon (neutron or proton) bound in nucleus

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



Need $\psi(x) = 0$ outside otherwise $V\psi \to \infty$

<u>Boundary Conditions</u> at $x = 0$ and $x = a$

Wave function must be <u>continuous</u> (allways true)

Therefore $\psi(x) \to 0$ as $x \to 0$ or a inside

Inside $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x)$ $\quad k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$

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

$$\psi = A\sin kx + B\cos kx \qquad \text{inside}$$

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

and

$$\psi(a) = A\sin ka = 0$$

This gives an equation for allowed k

General Result the quantized energies in QM come from imposing B. Conditions on Wave Function

$$\sin ka = 0 \quad \Rightarrow \quad ka = \pm\pi, \pm 2\pi, \pm 3\pi \ldots$$

$$k = \frac{n\pi}{a} \qquad n = \text{integer} \qquad \boxed{E_n = \frac{\hbar^2\pi^2}{2ma^2}\, n^2}$$

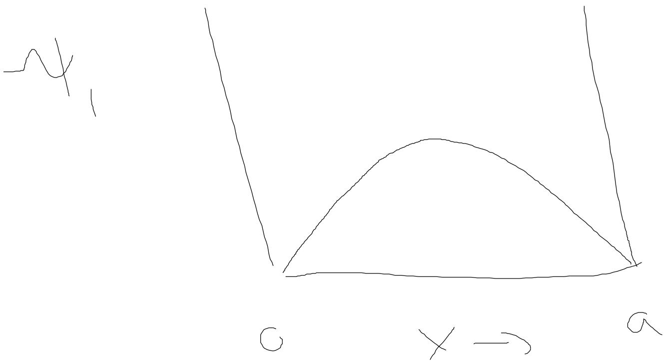
Normalize to find A

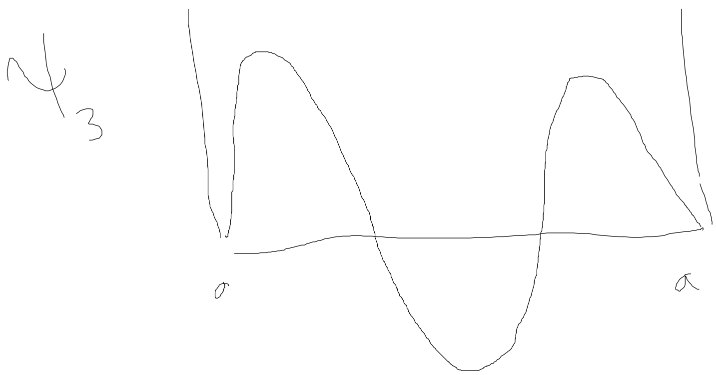
$$\psi(x) = \begin{cases} A\sin\left(\frac{n\pi}{a}x\right) & \text{inside} \\ 0 & \text{else} \end{cases}$$

$$\int_{-\infty}^{\infty} dx\, \psi^*\psi = A^2 \int_0^a \sin^2\left(\frac{n\pi}{a}x\right) dx = 1$$

$$\Rightarrow \qquad A = \sqrt{\frac{2}{a}}$$

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi x}{a}\right)} \qquad \text{inside}$$





General features

(i) Ground state (ψ_1) has minimum curvature (and still satisfy b.c.)

(ii) Number of nodes (zeros) increases as E increases

(iii) Wave functions are orthogonal

$$\int_{-\infty}^{\infty} dx \; \psi_m^*(x)\, \psi_n(x) = 0 \qquad m \neq n$$

[You show $\int_0^a \sin\left(\frac{n\pi}{a} x\right) \sin\left(\frac{m\pi}{a} x\right) dx = 0$

for $m \neq n$]

Can combine with normalization and say wave functions are ortho-normal

$$\boxed{\int_{-\infty}^{\infty} dx \; \psi_m^*(x)\, \psi_n(x) = \delta_{mn}}$$

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

(iv) Wave functions are <u>complete</u>.
Can expand any function $f(x)$ (which satisfies B.C.) as a sum over the ψ_n

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

Use orthogonality to find c_n

$$\int_{-\infty}^{\infty} \psi_m^*(x) f(x)\, dx = \sum_n c_n \underbrace{\int dx\, \psi_m^* \psi_n}_{\delta_{mn}}$$

$$\boxed{\int \psi_m^*(x) f(x)\, dx = c_m}$$