Postulates and particle-in-a-box

Note Title 01-10-2009

Administrative stuff

Last opportunity to collect Minor 1 papers - Tuesday, Oct. 6 at 5 pm in Dr Deep's office (MS731).

Find the first quantum tutorial and more kinetics pratice problems in SCOOPS.

Quantum lectures will be on the web (URL to be announced later) early next week.

Recap

$$\lambda = \frac{h}{p}$$

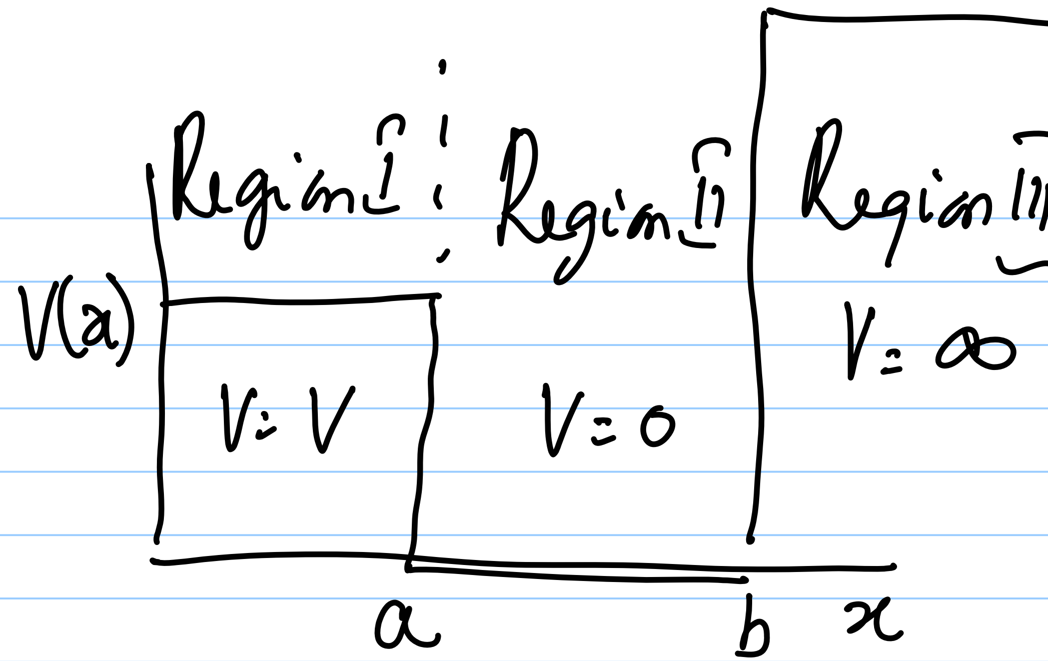
Schrödinger equation

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

↳ Probability amplitude

Conditions on $\psi(x,t)$

m



$V = 0 \quad -\infty \leq x \leq \infty$

S. E $\quad i\hbar \dfrac{\partial \psi}{\partial t} = -\dfrac{\hbar^2}{2m} \dfrac{d^2 \psi}{dx^2}$]

Region I :

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \Psi$$

Region II :

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x,t)$$

Region III :

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \overset{\infty}{V} \right) \underline{\underline{\Psi}}$$

$\Psi^* \Psi(x)\, dx \rightarrow$ Probability of finding the particle between x & $x + dx$

$|\Psi|^2$

Probability amplitude

Probability distribution

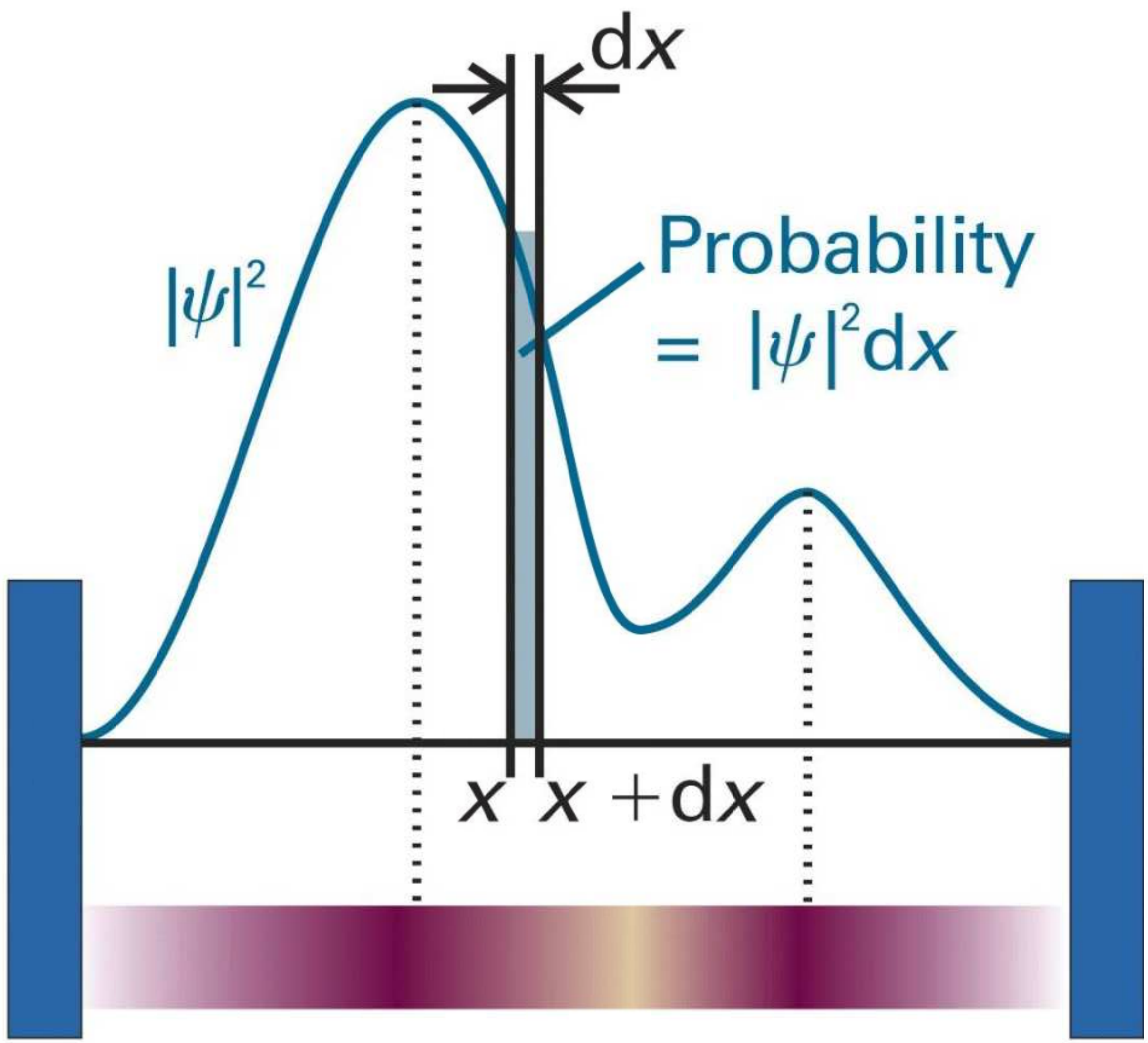


Figure 8-19
Atkins Physical Chemistry, Eighth Edition

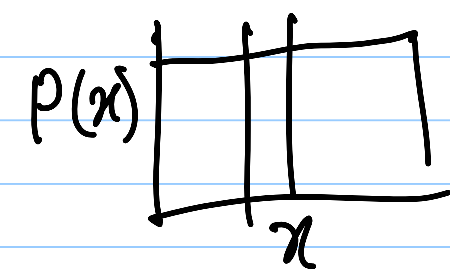
$$\int P(x)\, dx = 1$$

Mark distribution in CYL110 in Minor 1

(60 — 100)

30	60
	70
30	80
30	90
30 30	100

$\frac{30}{150}$



On solving the SE

$$\left[\int \psi'^{*} \psi' \, d\tau \neq 1\right]$$

ψ square integrable

$$\psi = c\psi'$$

c = normalization constant

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi$$

$$\int (c\psi')^{*} (c\psi') \, d\tau = 1$$

$$c^2 = \frac{1}{\int \psi'^{*} \psi' \, d\tau}$$

$$i\hbar \frac{\partial \Psi^{(x,t)}}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\Psi$$

Separation of variables

$$E = T = \frac{p^2}{2m} \qquad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x) \text{ for } V = 0$$

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

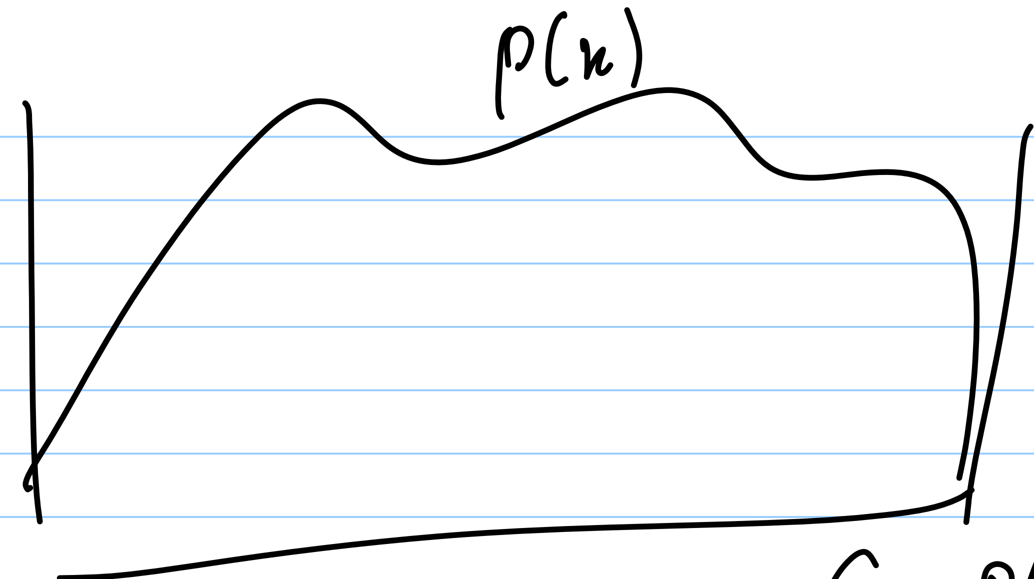
m	60	70	80	90	100
$P(m)$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$

$$\bar{m} = \cancel{\frac{\int m\, P(m)\, dm}{\int P(m)\, dm}}$$

$$\bar{m} = 80 = \sum_{m_i} m_i \, P(m_i)$$

$$\bar{m} = \int m \, P(m) \, dm \rightarrow \psi^* \psi$$

$$\langle x \rangle = \frac{\int x \, P(x) \, dx}{\int P(x) \, dx}$$



$\bar{x} = \underline{\langle x \rangle} = \int x P(x)\, dx$

↳ Average value

ASS U ME

"second moment" $\overline{m^2}$

$$\langle x^2 \rangle = \int x^2 \, P(x)\, dx$$

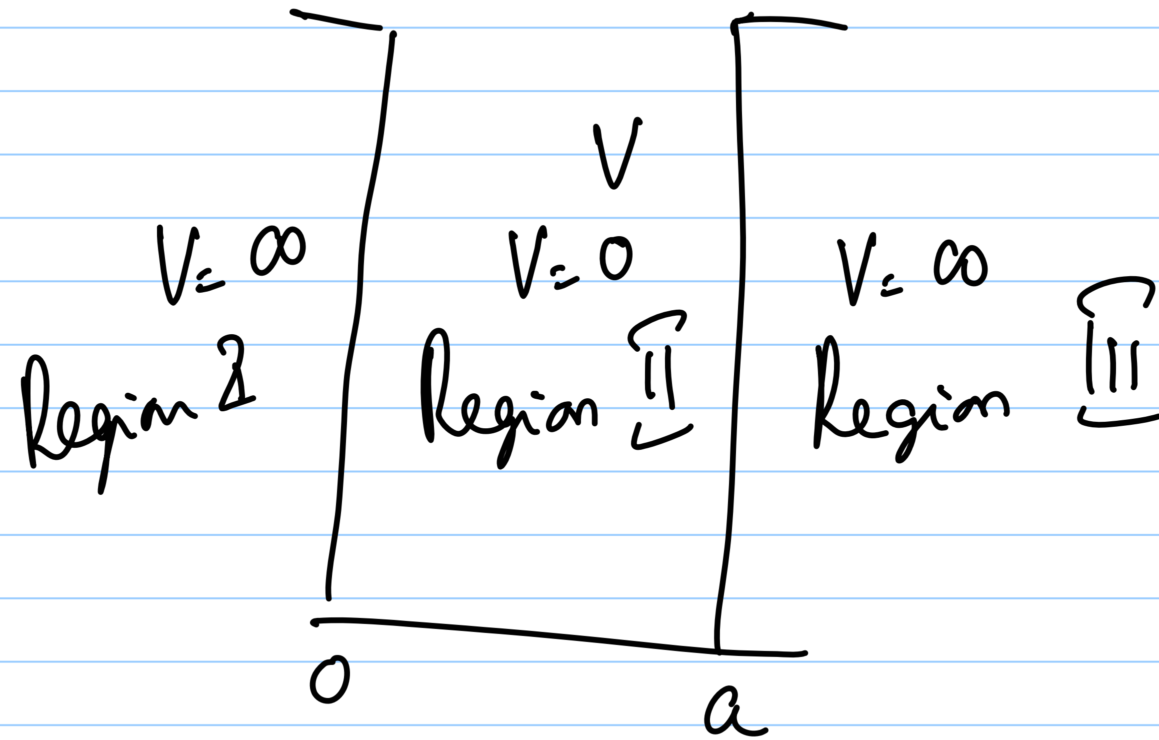
$$\sqrt{\underbrace{\langle x^2 \rangle}_{} - \underbrace{\langle x \rangle}_{}^2}$$

$$\int \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi^* \, \psi \, dx$$

$$\langle x \rangle = \int \Psi^* \, x \, \Psi \, dx$$

$$\langle \hat{E} \rangle = \int \Psi^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi \right) dx$$

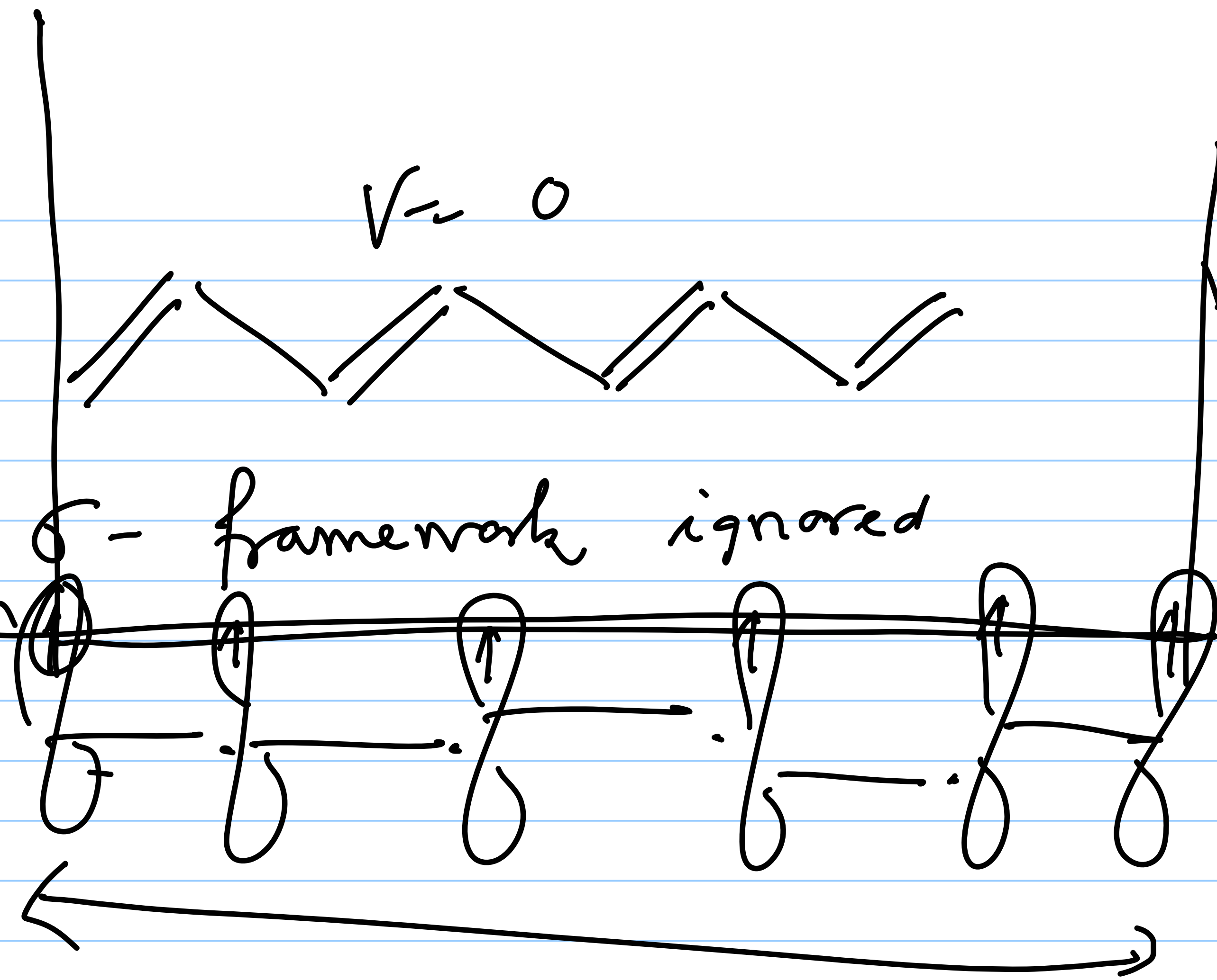
Particle-in-a-box



$V = \infty$

$V = 0$

$V = \infty$



1) σ - framework ignored

Free electron model

e^{ikx}

Region I & III : $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\infty\right)\psi_{I/III}=E\psi_{I/III}$

k & $k=\sqrt{\frac{2mE}{\hbar^2}}$ $\quad \psi_{I}=\psi_{III}=0$

Region II

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

$\therefore$

$$\frac{d^2\psi_{II}}{dx^2}+\frac{2mE}{\hbar^2}\psi_{II}=0$$

$\therefore$ $\psi_{II}=A\sin kx+B\cos kx$

$B = 0$

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

$$k = \frac{n\pi}{a}$$

$$\psi = A \sin\left(\frac{n\pi x}{a}\right)$$

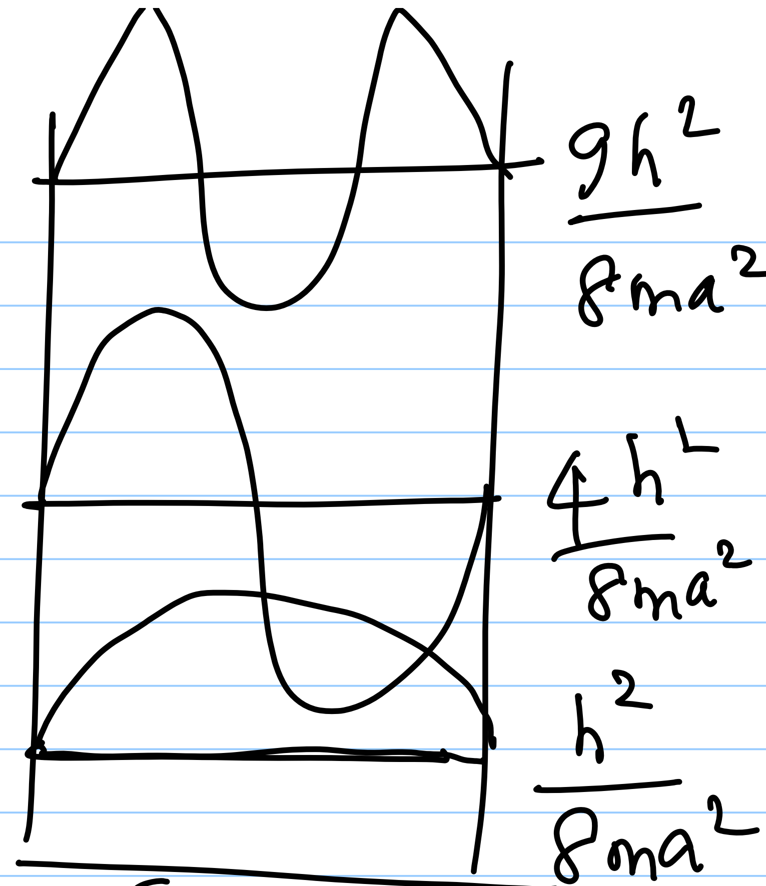
$$n = 1, 2, 3, \ldots$$

$$E_n = \frac{n^2 h^2}{8ma^2} \qquad k = \boxed{\sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}} \qquad n = 1, 2, 3$$

$$E_n = \frac{n^2 h^2}{8ma^2}$$

$$\psi_n = A \sin\left(\frac{n\pi x}{a}\right)$$

E



$$\psi_1 = A \sin \frac{\pi x}{a}$$

What is the position of a particle if it is in the state ψ_1?

$n = 1$, $\psi_n = A\sin\left(\frac{n\pi x}{a}\right)$

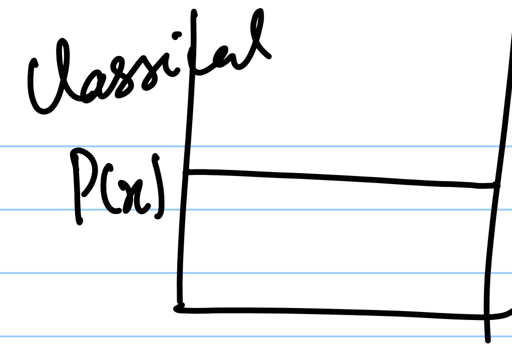
$$\psi_1 = A\sin\left(\frac{\pi x}{a}\right)$$

$$P(x) = \psi_1^* \psi_1 \qquad \psi^* \psi$$

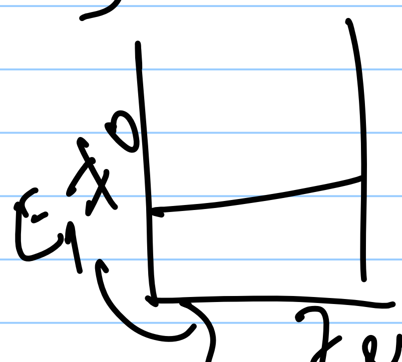
$$\langle x \rangle = \int A\sin\left(\frac{\pi x}{a}\right) x \, A\sin\left(\frac{\pi x}{a}\right) dx$$

$$\int A^2 \sin^2\left(\frac{\pi x}{a}\right) dx$$

$$\langle x \rangle = \frac{a}{2}$$



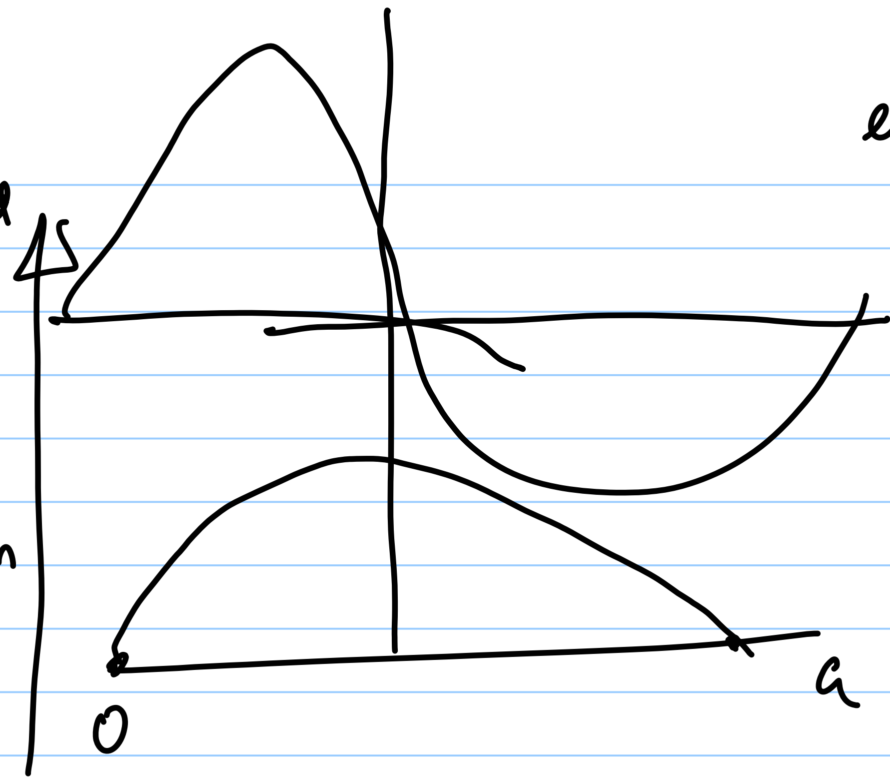
$$\int A \sin\left(\frac{\pi x}{a}\right) A \sin\left(\frac{\pi x}{a}\right) dx = 1$$



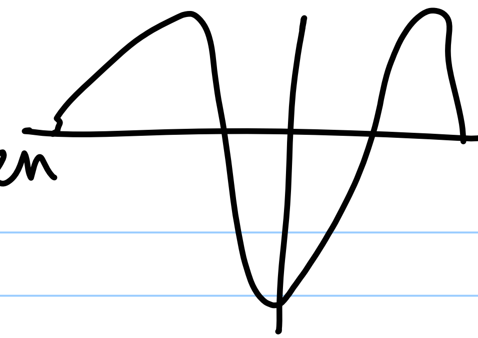
$$A = \sqrt{\frac{2}{a}}$$

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

symmetry $\begin{cases} \text{odd} \\ \text{even} \end{cases}$

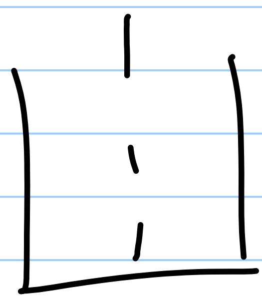


even



$n = 1, 3, \ldots$ even

$n = 2, 4, 6, \ldots$ odd



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

ψ_1

$$\langle E \rangle = \int \psi_1^* \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi_1 \, dx$$

$$\int \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) dx$$

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} = \frac{h^2}{8ma^2} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

$$\int \left(\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \frac{h^2}{8ma^2} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) dx \right)$$

$$= \frac{h^2}{8ma^2}$$

What is the momentum?

$\langle p \rangle = 0$ (physically)

$$p = mv$$

$$= m \frac{dx}{dt}$$

Ehrenfest theorem

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

Operator

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

Position, energy, momentum are some examples of classical observables.

Represented as operators in quantum mechanics.