

SOLVE NEWTON'S EQ. , INITIAL CONDITIONS

$x(0), v(0)$



POSITION $x(t)$



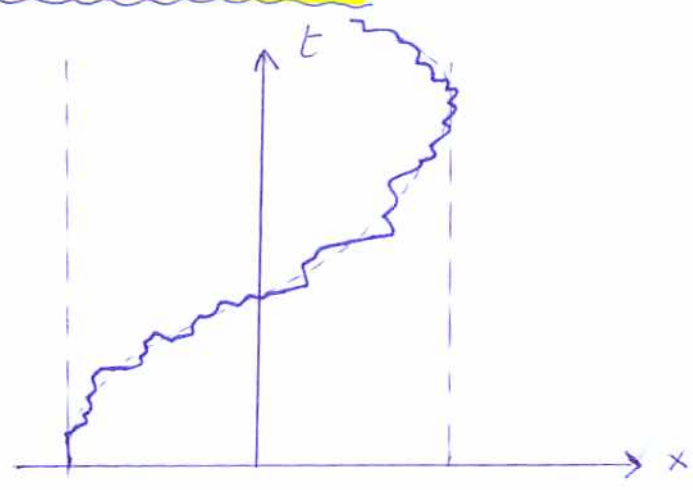
VELOCITY $v(t) = \frac{dx}{dt}$



MOMENTUM $p = m v$

KINETIC ENERGY $T = \frac{1}{2} m v^2 = \frac{p^2}{2m}$

QUANTUM MECHANICS



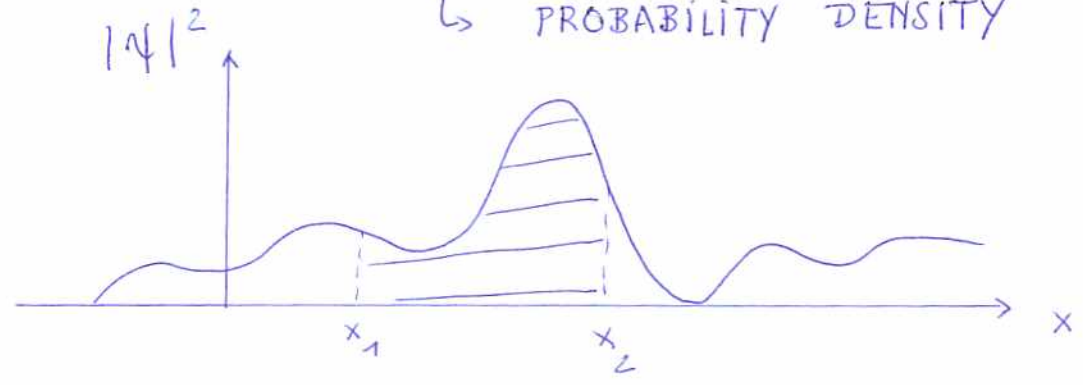
- POSITION CAN NOT BE DETERMINED TO ARBITRARY ACCURACY
- FLUCTUATIONS (ON MICROSCOPIC SCALE) AROUND CLASSICAL PATH / TRAJECTORY

→ WE CAN ONLY SPEAK OF PROBABILITY
 TO FIND } PARTICLE AT A GIVEN TIME t
 } OBJECT
 AT A GIVEN POSITION x

→ BASIC CONCEPT : WAVE FUNCTION $\Psi(x, t)$

INTERPRETATION : $|\Psi(x, t)|^2 = \Psi^*(x, t) \cdot \Psi(x, t)$

↳ PROBABILITY DENSITY



$\int_{x_1}^{x_2} dx |\Psi(x, t)|^2$ IS PROBABILITY TO FIND
 PARTICLE AT TIME t
 OBJECT
 BETWEEN x_1 AND x_2 .

→ WAVE FUNCTION SATISFIES SCHRÖDINGER EQ.

$$\boxed{
 \begin{aligned}
 - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi &= i \hbar \frac{\partial \Psi}{\partial t} \\
 \uparrow & \quad \uparrow \quad \quad \quad \uparrow \\
 \text{KINETIC} & \quad \text{POTENTIAL} & \quad \text{TOTAL} \\
 \text{ENERGY} & \quad \text{ENERGY} & \quad \text{ENERGY}
 \end{aligned}
 }$$

SOLUTION [+ { BOUNDARY INITIAL CONDITIONS } $\Psi(x, 0)$]
 $\hookrightarrow \Psi(x, t)$

$$\hbar = \frac{h}{2\pi} = 1.054572 \cdot 10^{-34} \text{ J}\cdot\text{s}$$

h : PLANCK'S CONSTANT } RECALL : LIGHT OF FREQUENCY ν
 ENERGY PACKETS \downarrow $E = h\nu$ (PHOTON)

→ SMALLNESS OF h : FOR MACROSCOPIC OBJECTS

FLUCTUATIONS AROUND CLASSICAL TRAJECTORY

VERY TINY \Rightarrow TO GOOD APPROXIMATION :
 WE CAN APPLY NEWTON'S EQ.

1.3 PROBABILITY

DISCRETE VARIABLES

GROUP OF PEOPLE N = TOTAL # PERSONS

$j = 0, 1, 2, \dots$ AGE OF PERSON IN GROUP

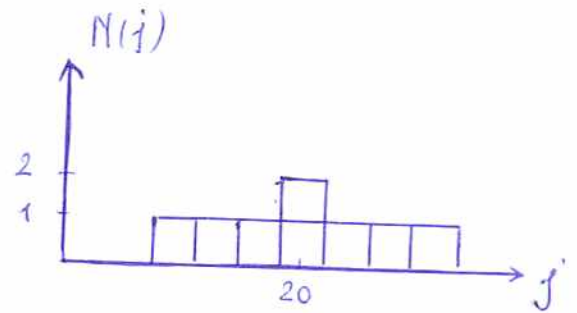
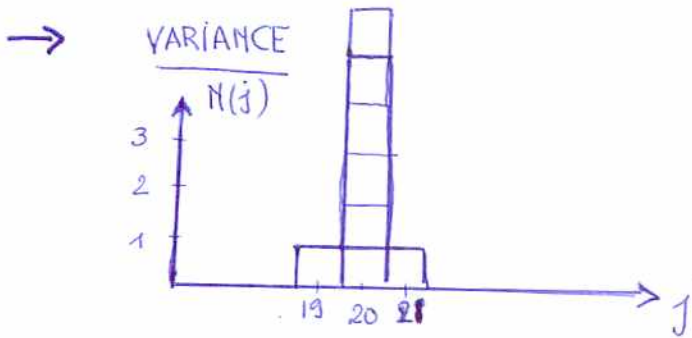
$N(j)$ = # PERSONS WITH AGE j

→ PROBABILITY TO FIND PERSON WITH AGE j

$$P(j) = \frac{N(j)}{N}$$

→ AVERAGE AGE

$$\langle j \rangle = \sum_{j=0}^{\infty} j P(j) = \frac{1}{N} \sum_{j=0}^{\infty} j N(j)$$



2 DISTRIBUTIONS HAVE SAME AVERAGE BUT DIFFERENT SPREAD



MEASURE OF SPREAD: VARIANCE σ^2

$$\begin{aligned}\sigma^2 &\equiv \langle (j - \langle j \rangle)^2 \rangle \\ &= \langle j^2 - 2j\langle j \rangle + \langle j \rangle^2 \rangle \\ &= \langle j^2 \rangle - 2\langle j \rangle^2 + \langle j \rangle^2 \\ &= \langle j^2 \rangle - \langle j \rangle^2\end{aligned}$$

→ STANDARD DEVIATION

$$\sigma = \sqrt{\sigma^2} = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$$

• CONTINUOUS VARIABLES

e.g. HEIGHT OF PERSON x

→ PROBABILITY DENSITY $p(x)$

* INFINITESIMAL INTERVAL

PROBABILITY TO FIND SOMEONE WITH HEIGHT BETWEEN x AND $x + dx$

$$\hookrightarrow p(x) dx$$

* FINITE INTERVAL

PROBABILITY TO FIND SOMEONE WITH HEIGHT BETWEEN a AND b

$$\hookrightarrow P_{ab} = \int_a^b dx p(x)$$

* NORMALIZATION

$$1 = \int_{-\infty}^{+\infty} dx p(x)$$

→ AVERAGE

$$\langle x \rangle = \int_{-\infty}^{+\infty} dx x p(x)$$

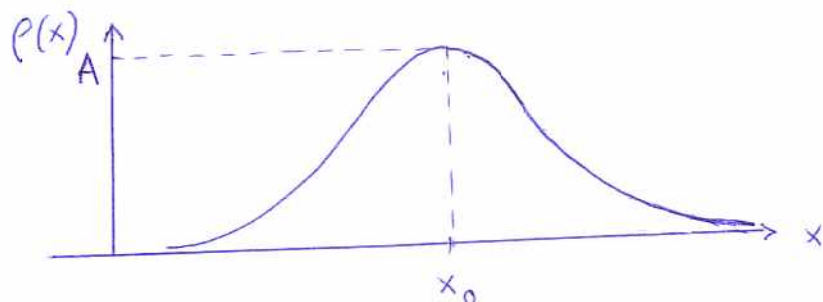
$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} dx f(x) p(x)$$

→ VARIANCE

$$\begin{aligned}\sigma^2 &= \langle (x - \langle x \rangle)^2 \rangle \\ &= \int_{-\infty}^{+\infty} dx (x - \langle x \rangle)^2 \rho(x) \\ &= \langle x^2 \rangle - \langle x \rangle^2\end{aligned}$$

→ EXAMPLE: GAUSSIAN DISTRIBUTION.

* $\rho(x) = A e^{-\lambda(x-x_0)^2}$



* NORMALIZATION

$$\int_{-\infty}^{+\infty} dx \rho(x) = 1$$

$$1 = A \int_{-\infty}^{+\infty} dx e^{-\lambda(x-x_0)^2} = A \underbrace{\int_{-\infty}^{+\infty} dx' e^{-\lambda x'^2}}_{\substack{\parallel \\ \sqrt{\frac{\pi}{\lambda}} \text{ GAUSSIAN} \\ \text{INTEGRAL}}}}$$

↑
 $x' = x - x_0$
 $dx' = dx$

$$1 = A \cdot \sqrt{\frac{\pi}{\lambda}}$$

⇓

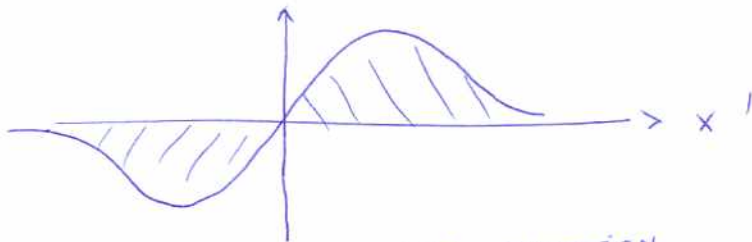
$$\underline{\underline{A = \sqrt{\frac{\lambda}{\pi}}}}$$

* AVERAGE

$$\langle x \rangle = A \int_{-\infty}^{+\infty} dx \ x \ e^{-\lambda(x-x_0)^2}$$

$$x' = x - x_0 \quad \Rightarrow \quad A \int_{-\infty}^{+\infty} dx' (x' + x_0) e^{-\lambda x'^2}$$

$$= A \left\{ \underbrace{\int_{-\infty}^{+\infty} dx' x' e^{-\lambda x'^2}}_0 + x_0 \underbrace{\int_{-\infty}^{+\infty} dx' e^{-\lambda x'^2}}_{\sqrt{\frac{\pi}{\lambda}}} \right\}$$



ODD FUNCTION
INTEGRATED BETWEEN
SYMMETRIC INTEGRATION BOUNDS

$$= A x_0 \sqrt{\frac{\pi}{\lambda}}$$

$$\underline{\underline{\langle x \rangle = x_0}}$$

* VARIANCE

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$= \langle (x - \langle x \rangle)^2 \rangle$$

$$= \langle (x - x_0)^2 \rangle$$

$$= A \int_{-\infty}^{+\infty} dx (x - x_0)^2 e^{-\lambda (x - x_0)^2}$$

$$= A \int_{-\infty}^{+\infty} dx' x'^2 e^{-\lambda x'^2}$$

$$= A \frac{1}{2} \sqrt{\frac{\pi}{\lambda}} \frac{1}{\lambda}$$

$$\underline{\underline{\sigma^2 = \frac{1}{2\lambda}}}$$

$$\underline{\underline{\sigma = \frac{1}{\sqrt{2\lambda}}}}, \quad \lambda = \frac{1}{2\sigma^2}$$

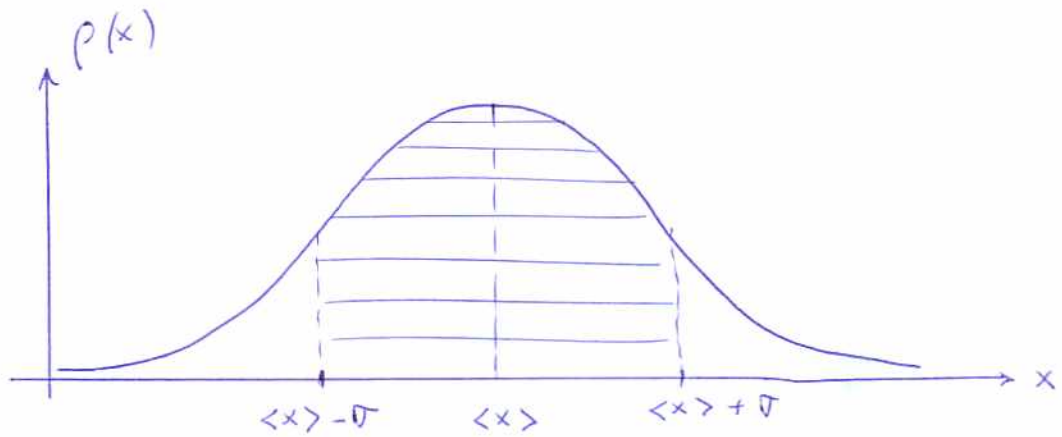
MATH HELP:

$$\int_{-\infty}^{+\infty} dx e^{-\lambda x^2} = \sqrt{\frac{\pi}{\lambda}}$$

$$\int_{-\infty}^{+\infty} dx x^2 e^{-\lambda x^2} = -\frac{d}{d\lambda} \int_{-\infty}^{+\infty} dx e^{-\lambda x^2}$$

$$= -\frac{d}{d\lambda} \sqrt{\frac{\pi}{\lambda}}$$

$$= \frac{1}{2} \sqrt{\frac{\pi}{\lambda}} \frac{1}{\lambda}$$



$$p(x) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} e^{-\frac{1}{2\sigma^2} (x - \langle x \rangle)^2}$$

PROBABILITY $x \in [\langle x \rangle - \sigma, \langle x \rangle + \sigma]$

$P_{1\sigma}$ "1 σ " DEVIATION FROM AVERAGE

$$P_{1\sigma} = A \int_{\langle x \rangle - \sigma}^{\langle x \rangle + \sigma} dx \cdot e^{-\frac{1}{2\sigma^2} (x - \langle x \rangle)^2}$$

$$\downarrow x' = x - \langle x \rangle$$

$$= A \int_{-\sigma}^{+\sigma} dx' \cdot e^{-\frac{1}{2\sigma^2} x'^2}$$

$$\downarrow A = \sqrt{\frac{\lambda}{\pi}} = \frac{1}{\sqrt{2\pi} \sigma}$$

$$P_{1\sigma} = 0.68 \quad (68\%)$$

$$P_{1\sigma} = 68\%$$

$$P_{2\sigma} = 95\%$$

$$P_{3\sigma} = 99.7\%$$

1.4 NORMALIZATION

→ WAVE FUNCTION $\Psi(x, t)$: INTERPRET AS "PROBABILITY AMPLITUDE"
SOLUTION OF SCHRÖDINGER EQUATION

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

→ PROBABILITY DENSITY

$$\rho(x, t) = |\Psi(x, t)|^2 = \Psi^* \Psi$$

↳ PROBABILITY TO FIND PARTICLE AT POINT x
AT TIME t

Ψ is COMPLEX

$$\Psi = |\Psi| e^{i\phi}$$

$|\Psi|$: AMPLITUDE

ϕ : PHASE

$$\text{Re } \Psi = |\Psi| \cos \phi$$

$$\text{Im } \Psi = |\Psi| \sin \phi$$

→ NORMALIZATION

$|\Psi(x, t)|^2 dx$: PROB. TO FIND PARTICLE BETWEEN x & $x+dx$

PROB. TO FIND PARTICLE BETWEEN $-\infty$ & $+\infty = 1$

$$1 = \int_{-\infty}^{+\infty} dx |\Psi(x, t)|^2$$



IF Ψ IS SOLUTION OF SCHRÖDINGER EQ.

$A\Psi$ IS ALSO SOLUTION OF SCHRÖDINGER EQ.

- NON-NORMALIZABLE SOLUTION $\int_{-\infty}^{+\infty} dx |\Psi(x,t)|^2 \neq 1$

↳ DOES NOT DESCRIBE A PHYSICAL STATE

- NORMALIZABLE SOLUTION $\int_{-\infty}^{+\infty} dx |\Psi(x,t)|^2 = 1$.

SQUARE, INTEGRABLE SOLUTION

↳ DESCRIBES PHYSICAL STATES, PARTICLES

→ NORMALIZATION IS TIME - INDEPENDENT

$$\int_{-\infty}^{+\infty} dx |\Psi(x,t)|^2 = 1$$

$$\frac{d}{dt} \int_{-\infty}^{+\infty} dx |\Psi(x,t)|^2 = 0$$

$$\int_{-\infty}^{+\infty} dx \frac{\partial}{\partial t} |\Psi(x,t)|^2 = 0.$$

PROOF THAT A SOLUTION OF SCHRÖDINGER EQ.
PRESERVES THE NORMALIZATION

1.14

$$\begin{aligned} \hookrightarrow \frac{\partial}{\partial t} |\Psi|^2 &= \frac{\partial}{\partial t} (\Psi^* \Psi) \\ &= \left(\frac{\partial \Psi^*}{\partial t} \right) \Psi + \Psi^* \left(\frac{\partial \Psi}{\partial t} \right) \end{aligned}$$

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

↪ POTENTIAL
V IS REAL

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

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

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

+

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

$$= \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right)$$

$$\hookrightarrow \int_{-\infty}^{+\infty} dx \frac{\partial}{\partial t} |\Psi(x, t)|^2$$

$$= \frac{i\hbar}{2m} \int_{-\infty}^{+\infty} dx \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right)$$

$$\downarrow \int_a^b dx \frac{\partial F(x)}{\partial x} = F(b) - F(a)$$

$$= \frac{i\hbar}{2m} \left[\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right]_{-\infty}^{+\infty}$$

\downarrow

FOR A NORMALIZABLE WAVE FUNCTION

$$\Psi(x = +\infty, t) = \Psi(x = -\infty, t) = 0.$$

$$= 0$$

■ QED

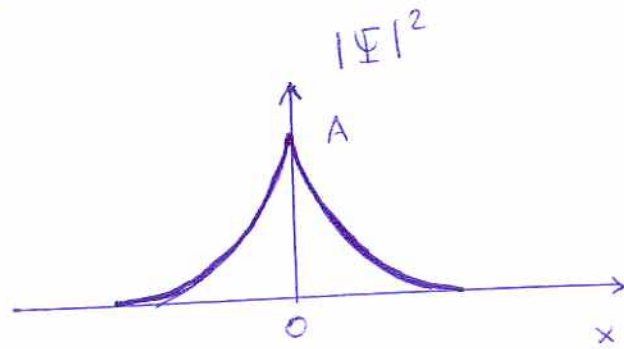
∴ IF $\Psi(x, t)$ IS NORMALIZED AT $t=0$

IT STAYS NORMALIZED AT ALL TIMES.

→ EXAMPLE : PROBLEM 1.5

$$\Psi(x,t) = A e^{-\lambda|x|} e^{-i\omega t}$$

$$|\Psi(x,t)|^2 = A^2 e^{-2\lambda|x|}$$



• NORMALIZATION

$$\int_{-\infty}^{+\infty} dx |\Psi(x,t)|^2 = 1$$

$$\downarrow$$
$$A^2 \int_{-\infty}^{+\infty} dx e^{-2\lambda|x|} = 1.$$

$$2A^2 \int_0^{+\infty} dx e^{-2\lambda x} = 1.$$

$$\left[-\frac{1}{2\lambda} e^{-2\lambda x} \right]_0^{+\infty}$$

$$\frac{2A^2}{2\lambda} = 1 \quad \Rightarrow \quad \underline{\underline{A = \sqrt{\lambda}}}$$

• $\langle x \rangle = 0$

• $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$

$$= \langle x^2 \rangle = A^2 \int_{-\infty}^{+\infty} dx x^2 e^{-2\lambda|x|}$$

$$= 2A^2 \int_0^{+\infty} dx x^2 e^{-2\lambda x}$$

MATH HELP

$$\begin{aligned}
 & \int_0^{+\infty} dx \, x^2 e^{-2\lambda x} \\
 &= \frac{1}{4} \frac{d^2}{d\lambda^2} \int_0^{+\infty} dx \, e^{-2\lambda x} \\
 &= \frac{1}{4} \frac{d^2}{d\lambda^2} \left(\frac{1}{2\lambda} \right) \\
 &= \frac{1}{4} \cdot \frac{2}{2\lambda^3}
 \end{aligned}$$

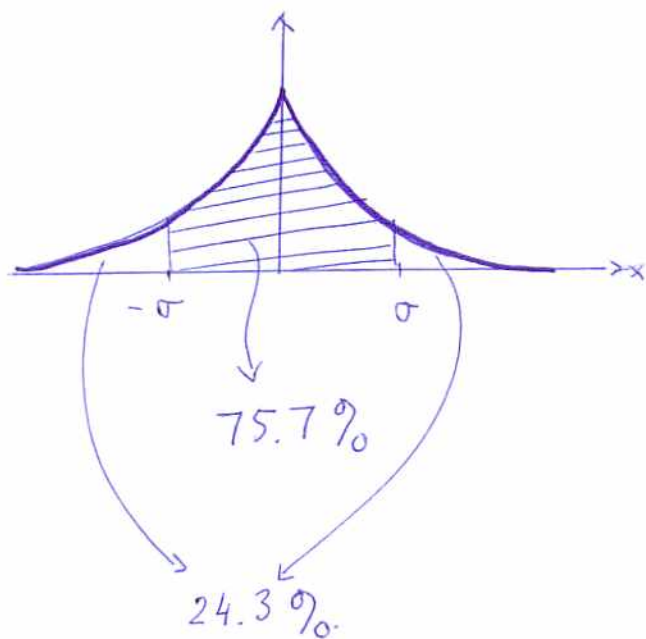
$$\sigma^2 = 2A^2 \cdot \frac{1}{4\lambda^3} = \frac{1}{2\lambda^2}$$

$$\underline{\underline{\sigma = \frac{1}{\sqrt{2}\lambda}}}$$

$$\bullet \, P(x \in [-\sigma, \sigma])$$

$$\begin{aligned}
 &= \int_{-\sigma}^{\sigma} dx \, |\Psi(x, t)|^2 \\
 &= 2A^2 \int_0^{\sigma} dx \, e^{-2\lambda x} \\
 &= -\frac{2A^2}{2\lambda} e^{-2\lambda x} \Big|_0^{\sigma}
 \end{aligned}$$

$$= 1 - \underbrace{e^{-\sqrt{2}}}_{0.243} = \underline{\underline{0.757}} \quad (75.7\%)$$



1.5 MOMENTUM

1-18

→ EXPECTATION VALUE

$\Psi(x, t)$ DESCRIBES STATE OF SYSTEM

IMAGINE AN ENSEMBLE OF SYSTEMS

↳ AVERAGE POSITION $\langle x \rangle$ OVER THIS ENSEMBLE

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

↳ TIME EVOLUTION OF $\langle x \rangle$

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

$$= \frac{i\hbar}{2m} \int_{-\infty}^{+\infty} dx \ x \ \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right)$$

SEE P. 1.14

↓ INTEGRATION BY PARTS

$$= -\frac{i\hbar}{2m} \int dx \ \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) + \text{BOUNDARY TERM}$$

@
-∞ AND +∞

↓
INTEGRATION
BY
PARTS

0
 $\Psi(x = \pm\infty, t) = 0$

$$= -\frac{i\hbar}{m} \int dx \ \Psi^* \frac{\partial \Psi}{\partial x}$$

$\langle v \rangle$ EXPECTATION VALUE OF VELOCITY

$$\langle v \rangle = \frac{d}{dt} \langle x \rangle$$

↳ $\langle p \rangle$ EXPECTATION VALUE OF MOMENTUM

$$\langle p \rangle = m \langle v \rangle = -i\hbar \int dx \Psi^* \frac{\partial \Psi}{\partial x}$$

↳ ' OPERATORS '

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

↑
POSITION 'OPERATOR'

$$\langle p \rangle = \int dx \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi$$

↑
MOMENTUM 'OPERATOR'

$\langle T \rangle$: KINETIC ENERGY

$$T = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\langle T \rangle = \int dx \Psi^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \Psi$$

↑
KINETIC ENERGY 'OPERATOR'

$$\langle V \rangle = \int dx \Psi^* V \Psi$$

↳ POTENTIAL ENERGY 'OPERATOR'

↳ SCHRÖDINGER EQ

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

↳ MULTIPLY ON LEFT BY Ψ^* AND $\int dx$

$$\underbrace{\int dx \Psi^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \Psi}_{\langle T \rangle} + \underbrace{\int dx \Psi^* V \Psi}_{\langle V \rangle} = \underbrace{\int dx \Psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \Psi}_{\langle E \rangle}$$

EXPECTATION VALUE
OF TOTAL ENERGY

↳ TIME EVOLUTION OF $\langle p \rangle$

$$\frac{d}{dt} \langle p \rangle = \frac{d}{dt} \int dx \Psi^* \left(-i\hbar \frac{\partial \Psi}{\partial x} \right)$$

$$= -i\hbar \int dx \left(\frac{\partial \Psi^*}{\partial t} \cdot \frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial}{\partial x} \cdot \frac{\partial \Psi}{\partial t} \right)$$

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

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

$$\frac{d}{dt} \langle P \rangle = \int dx \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} \cdot \frac{\partial \Psi}{\partial x} + V \Psi^* \frac{\partial \Psi}{\partial x} + \frac{\hbar^2}{2m} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} - \Psi^* \frac{\partial}{\partial x} (V \Psi) \right)$$

INTEGRATION BY PARTS TWICE ON FIRST TERM



$$\int_{-\infty}^{+\infty} dx \frac{\partial^2 \Psi^*}{\partial x^2} \cdot \frac{\partial \Psi}{\partial x} = - \int_{-\infty}^{+\infty} dx \frac{\partial \Psi^*}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} = + \int_{-\infty}^{+\infty} dx \Psi^* \frac{\partial^3 \Psi}{\partial x^3}$$

$$\frac{d}{dt} \langle P \rangle = \int dx \left(-\frac{\hbar^2}{2m} \cancel{\Psi^* \frac{\partial^3 \Psi}{\partial x^3}} + \cancel{V \Psi^* \frac{\partial \Psi}{\partial x}} + \frac{\hbar^2}{2m} \cancel{\Psi^* \frac{\partial^3 \Psi}{\partial x^3}} - \Psi^* \frac{\partial V \Psi}{\partial x} - \cancel{V \Psi^* \frac{\partial \Psi}{\partial x}} \right)$$

$$\frac{d}{dt} \langle P \rangle = \int dx \Psi^* \left(-\frac{\partial V}{\partial x} \right) \Psi$$

$$= \left\langle -\frac{\partial V}{\partial x} \right\rangle$$

EHRENFEST'S THEOREM

↳ EXPECTATION VALUES OBEY CLASSICAL LAWS
(e.g. NEWTON'S LAWS)

1.6 UNCERTAINTY PRINCIPLE

→ WAVE FUNCTION Ψ

WAVELENGTH λ



PARTICLE MOMENTUM p



PARTICLE - WAVE
DUALITY IN Q.M.

DE BROGLIE FORMULA:

$$p = \frac{h}{\lambda} = \frac{2\pi \hbar}{\lambda}$$

$$\hbar = \frac{h}{2\pi}$$

→ HEISENBERG'S UNCERTAINTY PRINCIPLE

THE MORE PRECISE WE KNOW POSITION,
THE LESS PRECISE WE KNOW ITS MOMENTUM
AND VICE VERSA

$$\sigma_x \cdot \sigma_p \geq \frac{\hbar}{2}$$

SOMETIMES ONE ALSO DENOTES

$$\sigma_x = \Delta x$$

$$\sigma_p = \Delta p$$

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$