Ch. 1

The wave function and Schrödinger equation

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QM - Overview

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Lưu ý 'format' email nộp bài

21VLH1TN - HoVaTen - Tuần N
(với N=1, 2, 3...)

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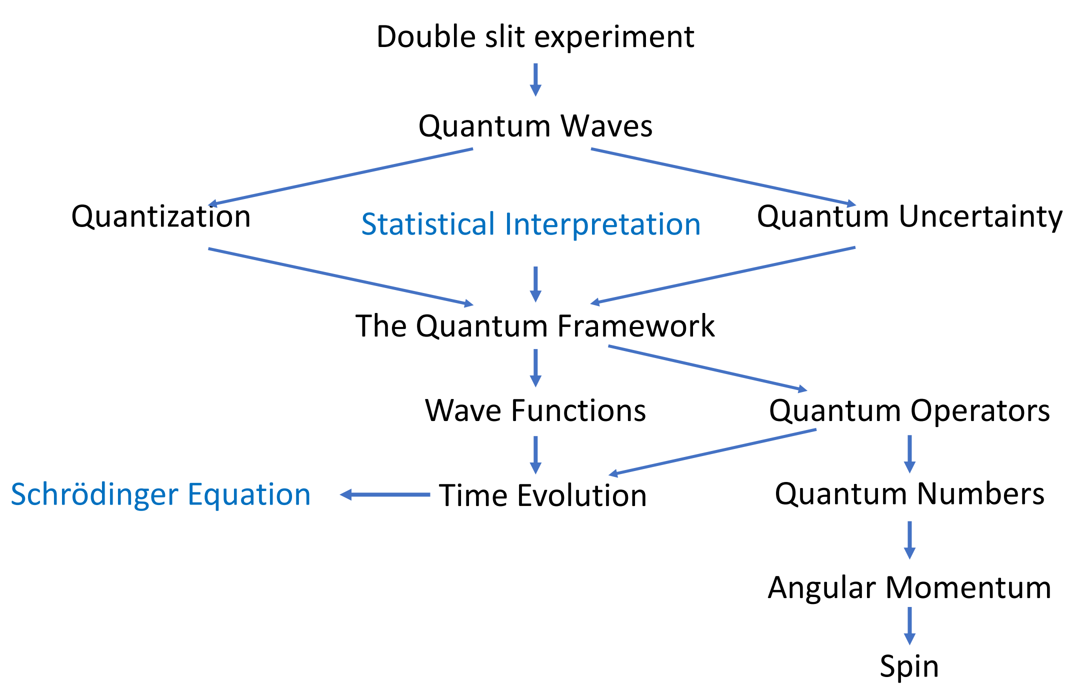

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Quantum Mechanics

Concepts	Equations	Tools
Wave functions State vectors Operators …	Schrödinger Equation …	Expectation values Eigenfunctions Eigenvalues …

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Ch. 1

The wave function and Schrödinger equation

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Lưu ý 'format' email nộp bài

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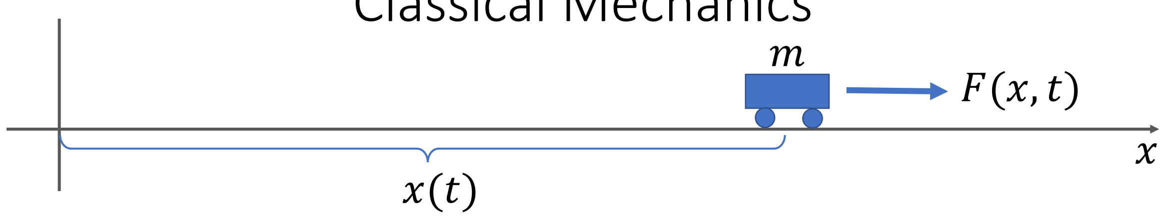
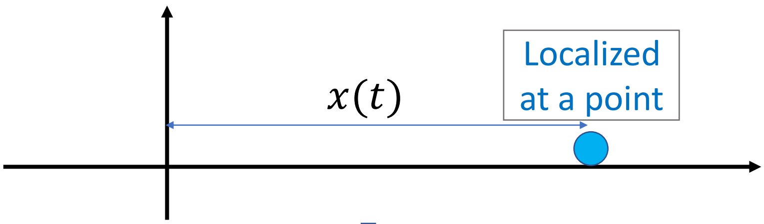
Classical Mechanics

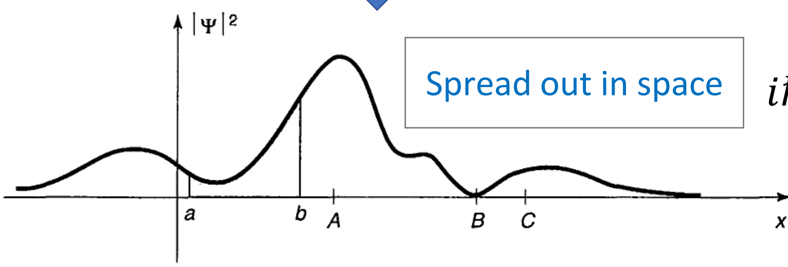


- The state (of the particle) is determined by: $x(t)$
- The velocity $v = \dot{x}(t)$, → $p = mv$, $\mathrm{T} = \frac{1}{2}mv^2$, ...
- How to determine $x(t)$?
- $F = ma = m\ddot{x} = m\frac{d^2x}{dt^2}$
- $F = -\frac{dV}{dx}$ (conservative system) $[F = -\frac{\partial V}{\partial x}]$. V: potential energy.
- → Equation of motion: $m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x} \xrightarrow{x(t=0)\ldots} x(t)$



$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x} \qquad x(t=0)$$

QUANTUM MECHANICS



Spread out in space

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

$$\hbar = \frac{h}{2\pi} = 1.054573 \times 10^{-34}\,\mathrm{J\,s}$$

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

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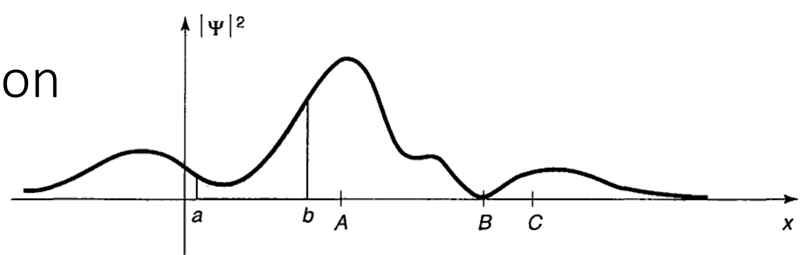
The wave function $\Psi(x,t)$



- The wave function is **the most important concept** in QM.
- Particle may be described as a wave → the wave function.

Born's statistical interpretation:

- A particle is described by a wave function $\Psi(x,t)$;
- $|\Psi(x,t)|^2$ **($= \Psi^*\Psi$) gives the probability of finding the particle at point x, at time t**.
- The wave function is also called the state function, or the state.

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Hàm sóng $\Psi(x, t)$

- $|\Psi(x, t)|^2$ ($= \Psi^* \Psi$) **gives the probability of finding the particle at point x, at time t.**
- More precisely:

$$\int_a^b |\Psi(x,t)|^2 \, dx$$
$= \{$probability of finding the particle between *a* and *b*, at time $t\}$.

- Thus,

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \, dx = 1$$
$= \{$probability of finding the particle in the entire space, at time $t\}$.

- This is known as **the normalization condition** for the wave function.
- Chú ý: $\Psi(x,t) \to 0 \text{ khi } x \to \pm\infty$

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The wave function and Schrödinger equation

In general, the wave function $\Psi\,(x, t)$ is the solution to the time dependent Schrödinger equation

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

$V(x, t)$: position and time dependent potential energy.

m: mass of the particle.

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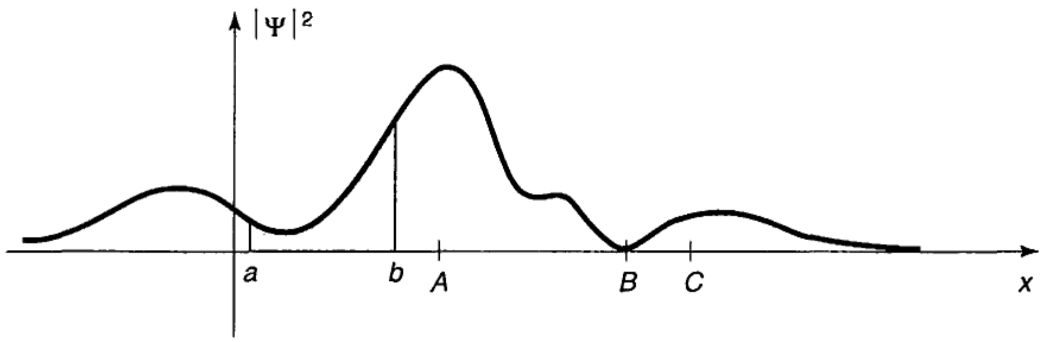
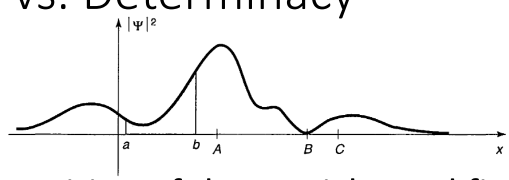
QM: Indeterminacy

- $|\Psi(x,t)|^2$: Probability
- → Indeterminacy: Quantum mechanics → ***statistical*** information about the ***possible*** results.



QM: Indeterminacy vs. Determinacy



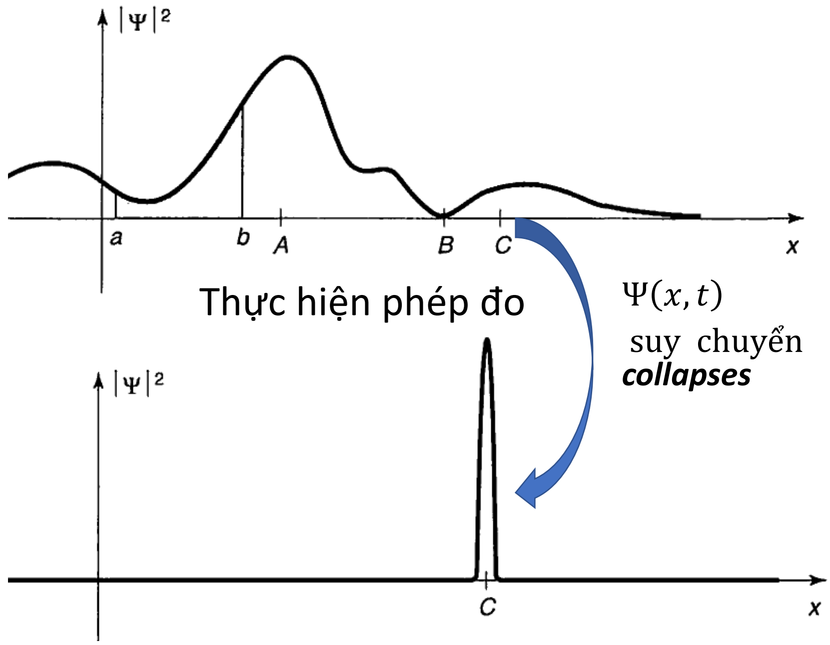
- Suppose we do measure the position of the particle, and find it to be at point C.
- Question:Where was the particle just before we made the measurement?

1. [Determinacy] It is at C!
   QM is an incomplete theory → unable to tell us where the particle is.
   Ψ is not the whole story. Some additional information (known as a HIDDEN VARIABLE) is needed to provide a complete description.
2. [Indeterminacy] The orthodox position: The particle wasn't really anywhere! It was the act of measurement that forced it to "take a stand" [Copenhagen interpretation]

What if we made a second measurement, *immediately* after the first?

We get C again!

The first measurement → Ψ ***collapses***, upon measurement, to a spike at the point *C*. And it soon spreads out again, in accordance with the Schrödinger equation, so the second measurement must be *made quickly*



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Links to “pilot – wave dynamics”

- http://math.mit.edu/~bush/wordpress/wp-content/uploads/2013/10/Gallery-Harris-2013.pdf
- https://www.youtube.com/watch?v=nmC0ygr08tE

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Probability

Continuous Variables

- The average of x:

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

$\rho(x)$ is probability density,

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

- The average of $f(x)$

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

Discrete Variables

- The average value of j

$$\langle j \rangle = \sum_{j=0}^{\infty} jP(j)$$

$P(j) = \frac{N(j)}{N}$ is the probability of getting *j*, and

$$\sum_{j=0}^{\infty} P(j) = 1$$

- The average value of function of j:

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j)P(j)$$

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Probability

Continuous Variables

- The standard deviation σ is given by the variance:
  $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$

Discrete Variables

- The standard deviation σ :
  $\sigma^2 = \langle (\Delta j)^2 \rangle$, với $\Delta j = j - \langle j \rangle$

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

- σ^2: The variance
- σ is a measure of the amount of variation or dispersion of a set of values.

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Normalization of the wave function

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

$=$ {probability of finding the particle in the entire space, at time t}.

- This is the normalization condition for the wave function
- It is proved that [see Griffiths' book]!

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

- → If the wave function is normalized at $t = 0$, it stays normalized for all $t > 0$ [all future time]

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Problem 1

At time $t = 0$ a particle is represented by the wave function

$$\Psi(x,0) = \begin{cases} A\dfrac{x}{a}, & \text{if } 0 \le x \le a, \\ A\dfrac{(b-x)}{(b-a)}, & \text{if } a \le x \le b, \\ 0, & \text{otherwise,} \end{cases}$$

where A, a, and b are constants.

(a) Normalize Ψ (that is, find A, in terms of a and b).

(b) Sketch $\Psi(x, 0)$, as a function of x.

(c) Where is the particle most likely to be found, at $t = 0$?

(d) What is the probability of finding the particle to the left of a? Check your result in the limiting cases $b = a$ and $b = 2a$.

(e) What is the expectation value of x?

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Bài tập 1

- Tại thời điểm ban đầu $t = 0$, 1 hạt được biểu diễn bởi hàm sóng [hoặc 1 hạt ở trạng thái được cho bởi]
- $\Psi(x, t=0) = \begin{cases} A\frac{x}{a} \text{ nếu } 0 \leq x \leq a \\ A\frac{(b-x)}{(b-a)} \text{ nếu } a \leq x \leq b \\ 0 \text{ trong những vùng khác} \end{cases}$.

  a, b là những hằng số đã biết. A là hằng số chưa biết
- Hãy xác định A. [Người ta còn thể nói: Hãy chuẩn hoá hàm sóng]
- Hãy phác vẽ hàm sóng $\Psi(x, t=0)$ theo biến x
- Tại $t = 0$, khả năng tìm thấy hạt ở đâu cao nhất?
- Tính xác suất tìm thấy hạt trong miền bên trái của điểm a [tức là $x \leq a$]. Hãy kiểm tra lại kết quả trong 2 trường hợp: $b = a$ và $b = 2a$.
- Hãy tìm giá trị trung bình của x.

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How to calculate the expectation value of any physical quantity in QM

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The expectation value of x, v, p (momentum)

- The expectation value (the average) of x:

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

- $|\Psi(x,t)|^2$ is probability density →

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

- The expectation value of $\langle x \rangle$ is the average of measurements performed on particles all in the state Ψ.

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The expectation value of x, v, p (momentum)

- $\langle x \rangle$ is the average of measurements performed on particles all in the state Ψ.
- → We must find some way of returning the particle to its original state after each measurement,
  or we have to prepare a whole ensemble of particles, each in the same state Ψ, and measure the positions of all of them.
- The expectation value is the average of measurements on an ensemble of identically-prepared systems [not the average of repeated measurements on one and the same system].

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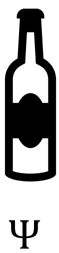
the average



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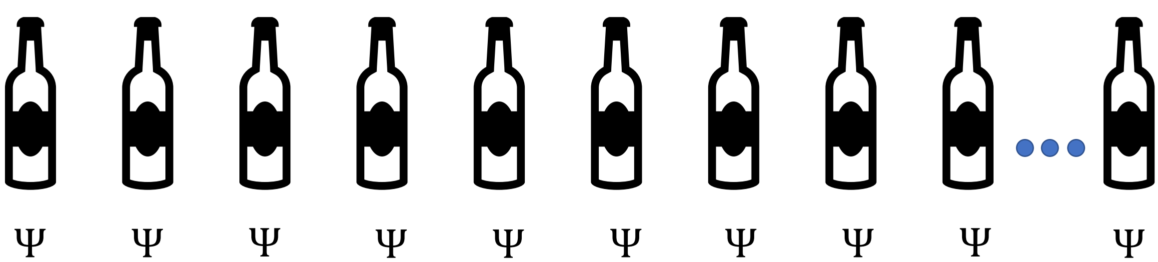
the average



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The expectation value of x, v, p (momentum)

- The expectation value of x

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

- Prove that [See Griffiths' book]

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m}\int_{-\infty}^{+\infty} \Psi^* \frac{\partial \Psi}{\partial x}\,dx$$

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The expectation value of x, v, p (momentum)

- Postulate that

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

- Momentum:

$$\langle p \rangle = m\langle v \rangle = m\frac{d\langle x \rangle}{dt} = -i\hbar\int_{-\infty}^{+\infty} \Psi^* \frac{\partial \Psi}{\partial x}\,dx$$

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The expectation value of x, v, p (momentum)

- Rewrite $\langle x \rangle$ and $\langle p \rangle$:

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

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi\, dx = \int_{-\infty}^{+\infty} \Psi^* \frac{\hbar}{i}\frac{\partial}{\partial x} \Psi\, d = \int_{-\infty}^{+\infty} \Psi^*\, p\, \Psi\, dx$$

- →

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

- Momentum p is an **operator** (toán tử)! [One often let an operator "wear a hat" $\hat{p}$ to distinguish an operator to a number]. Position x is also an **operator.**

The expectation value of a physical quantity

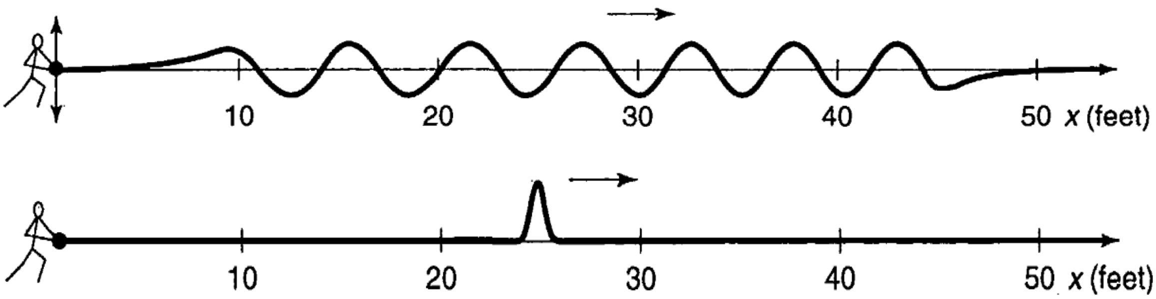
- The expectation value of a quantity $Q(x,p)$

$$\langle Q(x,p) \rangle = \int_{-\infty}^{+\infty} \Psi^*\, Q(\hat{x}, \hat{p})\, \Psi\, dx = \int_{-\infty}^{+\infty} \Psi^*\, Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi\, dx$$

- Calculate the expectation value of the kinetic energy

$$\hat{T} = \frac{\hat{p}^2}{2m}$$

The Uncertainty Principle



The more precise a wave's position is, the less precise is its wavelength, and vice versa.

This applies also to the quantum mechanical wave function.

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The Uncertainty Principle

- de Broglie formuar:

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

- A change/spread in wavelength → a change/spread in momentum.
- ⇒ **The more precisely determined a particle's position is, the less precisely is its momentum, and vice versa**.

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The Uncertainty Principle

- **The more precisely determined a particle's position is, the less precisely is its momentum, and vice versa**.
- Mathematically,

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

(σ_x is the standard deviation in x, σ_p is the standard deviation in p.)

- This is Heisenberg's famous uncertainty principle..

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[Standard deviation]

- $\sigma^2 = \langle j^2 \rangle - \langle j \rangle^2$
- $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$
- $\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^* \, x \ \Psi \, dx$
- $\langle x^2 \rangle = \int_{-\infty}^{+\infty} \Psi^* \, x^2 \ \Psi \, dx$
- $\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \, \hat{p} \ \Psi \, dx$
- $\langle p^2 \rangle = \int_{-\infty}^{+\infty} \Psi^* \, \hat{p}^2 \ \Psi \, dx$

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