

VP390 RECITATION CLASS

FOUR

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Wave function

In quantum mechanics the state of a particle is represented by a **wave-function**. The wave function is in general complex-valued. For the wave function in the position representation in 1D and in 3D, respectively:

$$\psi(x, t)$$

$$\psi(\vec{r}, t)$$

How to interpretate the wave function?

The square of the magnitude of the wave function represents the **probability** of finding the particle at some position in 1D or 3D at some instant of time.



Max Born
(1882-1970)

Wave function

Functions satisfying the following condition are said to be **normalized**:

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

$$\iiint_{R^3} |\psi(\vec{r}, t)|^2 d^3r = 1$$

Functions satisfying the following condition are said to be **square-integrable**:

$$\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx < \infty$$

$$\iiint_{R^3} |\psi(\vec{r}, t)|^2 d^3r < \infty$$

Wave function

average position of the particle:

$$\langle x \rangle_{\psi} = \int_{-\infty}^{\infty} x |\psi(x, t)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x, t) x \psi(x, t) dx$$

variance of the position of the particle:

$$\begin{aligned} (\Delta_x^{(\psi)})^2 &= \langle (x - \langle x \rangle_{\psi})^2 \rangle_{\psi} = \langle x^2 - 2x \langle x \rangle_{\psi} + \langle x \rangle_{\psi}^2 \rangle_{\psi} \\ &= \langle x^2 \rangle_{\psi} - 2 \langle x \rangle_{\psi} \langle x \rangle_{\psi} + \langle x \rangle_{\psi}^2 = \langle x^2 \rangle_{\psi} - \langle x \rangle_{\psi}^2 \end{aligned}$$

standard deviation of the position of the particle:

$$\Delta_x^{(\psi)} = \sqrt{\langle x^2 \rangle_{\psi} - \langle x \rangle_{\psi}^2}$$

Stationary state

If the modulus square does not depend on time, then the state represented by Ψ is called a **stationary state**:

$$|\psi(x, t)|^2 = \phi(x)$$

For a stationary state, the **average** and the **standard deviation** of the particle is **time-independent**.

Example: $\psi(x, t) = e^{-\frac{i}{\hbar}Et} f(x)$

Inner product

In the linear space formed by the square-integrable functions, the inner product can be introduced as:

$$\langle \psi, \phi \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) \phi(x, t) dx$$

For such inner products, they have the following properties:

$$\langle \psi, \phi_1 + \phi_2 \rangle = \langle \psi, \phi_1 \rangle + \langle \psi, \phi_2 \rangle$$

$$\langle \psi, \alpha \phi \rangle = \alpha \langle \psi, \phi \rangle$$

$$\langle \psi, \phi \rangle = \langle \phi, \psi \rangle^*$$

$$\langle \psi, \psi \rangle \geq 0; \quad \langle \psi, \psi \rangle = 0 \Leftrightarrow \psi \equiv 0$$

Hermitian operators

In quantum mechanics, physical quantities are represented by **Hermitian operators**.

What are operators?

What kind of operators are Hermitian?

Are the following operators Hermitian?

$$\hat{x}, \hat{p}, \hat{K}, \hat{V}, \hat{H}$$

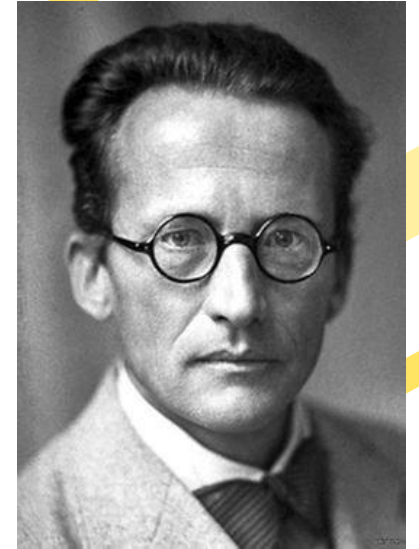
Schrödinger equation

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

Schrödinger equation is a linear 2nd order differential equation. What does its linearity imply?

stationary Schrödinger equation:

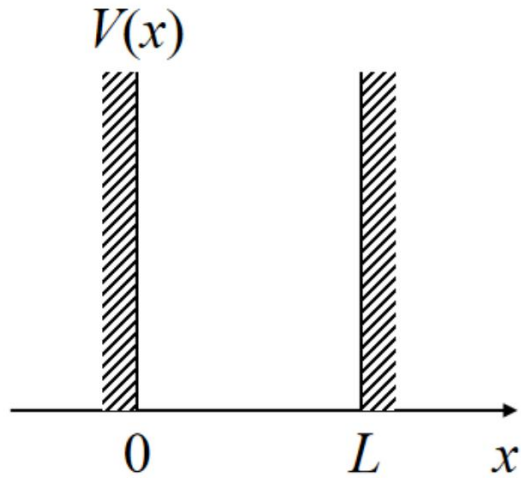
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \varphi(x) + V(x)\varphi(x) = E\varphi(x)$$



Erwin Schrödinger
(1887-1961)

How is stationary Schrödinger equation derived from the time-dependent one?

Infinite Potential Well



Potential distribution:

$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

Stationary Schrödinger equation:

$$\begin{cases} -\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} = E \varphi(x) \\ \varphi(0) = \varphi(L) = 0 \end{cases}$$

What kind of problem is it and how to solve it?

Exercise 1

An electron moving in a thin metal wire is a reasonable approximation of a particle in a one-dimensional infinite well. The potential inside the wire is constant on average but rises sharply at each end. Suppose the electron is in a wire 1.0 cm long.

- (a). Compute the ground-state energy for the electron.
- (b). If the electron's energy is equal to the average kinetic energy of the molecules in a gas at $T=300$ K, about 0.03 eV, what is the electron's quantum number n ?

Exercise 2

Suppose that the electron in Exercise 1 could be “seen” while in its ground state.

- (a) What would be the probability of finding it somewhere in the region $0 < x < L/4$?
- (b) What would be the probability of finding it in a very narrow region $\Delta x < 0.01L$ wide centered at $x = 5L/8$?



Thank you very much!!!