Time-independent Schrödinger Equation [TISE]

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The Schrödinger equation

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

Let us consider the case of time-independent potentials, $V(x,t) = V(x)$

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

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The Schrödinger equation

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

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{\hat{L}_t}\Psi = \underbrace{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]}_{\hat{L}_x}\Psi$$

In this case, the Schrödinger equation can be solved by the method of *separation of variables*: $\Psi(x,t) = \varphi(t)\,\psi(x)$.

Substituting $\Psi = \varphi(t)\,\psi(x)$ into the Sch. eq., and dividing both sides by $\varphi(t)\,\psi(x)$, we obtain:

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- $\hat{L}f(x,y) = 0$
- If: $\hat{L} = \hat{L}_x + \hat{L}_y$
- $\Rightarrow f(x,y) = X(x)Y(y)$
- $[\hat{L}_x + \hat{L}_y]X(x)Y(y) = 0$
- $\frac{1}{X(x)Y(y)}[\hat{L}_x + \hat{L}_y]X(x)Y(y) = 0$
- …

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$$\overbrace{i\hbar\frac{\partial}{\partial t}}^{\hat{L}_t}\Psi = \overbrace{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]}^{\hat{L}_x}\Psi$$

$$\hat{L}_t\Psi(x,t) = \hat{L}_x\Psi(x,t)$$

$$\hat{L}_t\varphi(t)\psi(x) = \hat{L}_x\varphi(t)\psi(x)$$

$$\frac{\hat{L}_t\varphi(t)\psi(x)}{\varphi(t)\psi(x)} = \frac{\hat{L}_x\varphi(t)\psi(x)}{\varphi(t)\psi(x)}$$

$$\Longrightarrow \frac{\psi(x)\hat{L}_t\varphi(t)}{\varphi(t)\psi(x)} = \frac{\varphi(t)\hat{L}_x\psi(x)}{\varphi(t)\psi(x)}$$

$$\frac{\hat{L}_t\varphi(t)}{\varphi(t)} = \frac{\hat{L}_x\psi(x)}{\psi(x)} \qquad \left(\frac{1}{\varphi(t)}\hat{L}_t\varphi(t) = \frac{1}{\psi(x)}\hat{L}_x\psi(x)\right)$$

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The Schrödinger equation

$$i\hbar\frac{1}{\varphi(t)}\frac{\partial\varphi(t)}{\partial t} = \frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x)$$

$$\underbrace{i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt}}_{A(t)} = \underbrace{\frac{1}{\psi}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi}_{B(x)}$$

$$A(t) = B(x)\ \forall\ t,x \quad \to A(t) = B(x) = \text{const.} \equiv E$$

$$\Rightarrow \begin{cases} A(t) = E \\ B(x) = E \end{cases} \quad \Rightarrow \begin{cases} i\hbar\dfrac{d\varphi}{dt} = E\varphi \\ -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}\psi + V\psi = E\psi \end{cases}$$

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The Schrödinger equation

$$i\hbar\frac{\partial\varphi}{\partial t} = E\varphi \longrightarrow \varphi(t) = Ce^{-iEt/\hbar}$$

$$\rightarrow \Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

$\psi(x)$ satisfies the equation

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

This equation is known as the *time-independent* Schrödinger equation [TISE] for a particle of mass *m* moving in a time-independent potential $V(x)$.

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Stationary state (Trạng thái dừng)

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

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

This particular solution of the Schrödinger equation (*) for a *time-independent potential* is called a *stationary state*.

Why is this state called *stationary*?

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Stationary state (Trạng thái dừng)

$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

$\Psi(x,t)$ depends on time t.

Calculate $|\Psi(x,t)|^2$!

$|\Psi(x,t)|^2 = |\psi(x)|^2$: time - independent

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Stationary state (Trạng thái dừng)

$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

Calculate the expectation value of $\mathrm{Q}(x,p)$!

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

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

Every expectation value is constant in time.

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Stationary state – Definite total energy

Classical Mechanics: The total energy (kinetic + potential energy) is called the Hamiltionian H :

$$H(x,p) = \frac{p^2}{2m} + V(x)$$

CM → QM:

Hamiltionian function→ Hamiltionian operator

$$H(x,p) \to \hat{H}\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)$$

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Definite total energy

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

The time-independent Schrödinger Eq. [TISE]

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

can be written

$$\hat{H}\psi = E\psi$$

The TISE is an Eigenvalue Eq. (phương trình trị riêng)

Each eigenvalue E_n corresponds to one (or more) eigenfunctions (hàm riêng) ψ_n : $E_n \leftrightarrow \psi_n$

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Definite total energy

Calculate $\langle H \rangle$!

$\langle H \rangle = E \quad \rightarrow E$ is the total energy.

Calculate $\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2$!

$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = 0$

$\sigma_H^2 = 0$ → The total energy is definite !

Every measurement of the total energy is certain to return the value E.

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Definite total energy

- E (eigenvalue) is the total energy.
  → $\{\text{Eigenvalue}\} = \{\text{Energy}\}$
- → Each $E_n \leftrightarrow$ Energy level.
- The set of *energy levels* that are solutions to the TISE are called the *energy spectrum* of the system.
- The states ψ_n (eigenfunction – "wave function") corresponding to discrete and continuous spectra are called *bound* and *unbound* states, respectively.

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The general solution

The TISE $\hat{H}\psi = E\psi$ → an infinite set of eigenfunctions $\psi_1(x), \psi_2(x), \ldots$ corresponding to eigenvalues $E_1, E_2, \ldots : \{\psi_n\} \leftrightarrow \{E_n\}$

→ $\Psi_n(x,t) = \psi_n(x)e^{-iE_n t/\hbar}$

The general solution is a *linear combination* of separable solutions (eigenfunctions) to Schrödinger Eq.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(\boldsymbol{r},t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$

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The TISE (Time-independent Schrödinger Eq)

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

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

$$k = \frac{\sqrt{2mE}}{\hbar}$$

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

Solution: $\psi(x) = Ae^{ikx} + Be^{-ikx}$

Or $\psi(x) = C\sin(kx) + Dcos(kx)$

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$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \;\;, E < 0$$

with $\kappa = \frac{\sqrt{-2mE}}{\hbar}$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

Solutions: $\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$

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