The Time – independent Schroedinger Equation (TISE)

The infinite square well

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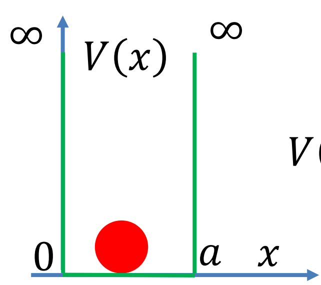
The infinite square well
(Giếng thế vuông vô hạn)



$$V(x) = \begin{cases} 0\,, & x \in (0, a) \\ \infty, & otherwise \end{cases}$$

A particle moves freely inside an infinite potential well.
At $0, a$: Potential → ∞ → An infinite force prevents the particle from escaping.

The partical is confined in the well → "quantum confinement"

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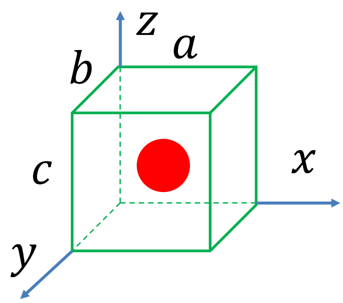
Quantum dot



$$V(\mathbf{r}) = V(x,y,z) = \begin{cases} 0, & x,y,z \in (0,a) \\ \infty, & otherwise \end{cases}$$

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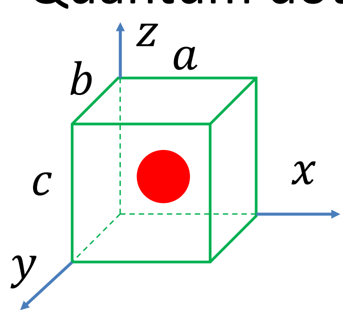
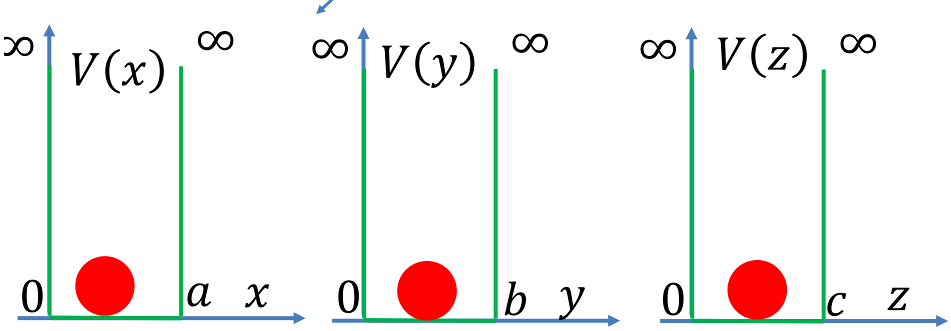
Quantum dot





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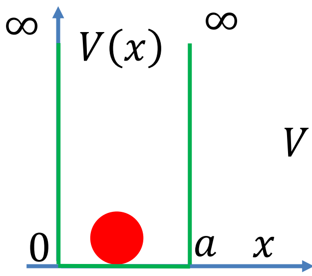
The infinite square well
(Giếng thế vuông vô hạn)



$$V(x) = \begin{cases} 0\,, & x \in (0, a) \\ \infty, & otherwise \end{cases}$$

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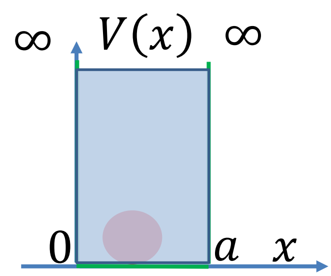
Consider different regions



Outside the well:

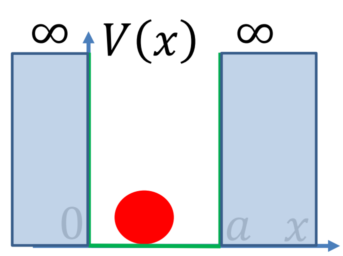
The particle does not exist.

$\rightarrow \psi(x) = 0$

Inside the well: $0 < x < a \rightarrow V(x) = 0$

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

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad [2.20]$$



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

$$\text{với } k = \frac{\sqrt{2mE}}{\hbar} \qquad [2.21] \qquad E \geq 0.$$

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$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi \qquad [2.21]$$

Solution: $\psi(x) = Asin(kx) + Bcos(kx)$ [2.22]

A and *B* are arbitrary constants. They are determined by the boundary conditions of the problem.

The appropriate boundary conditions for $\psi(x)$:

ψ and $d\psi/dx$ are continuous.

$\psi(x)$ at $x = 0$ and a → $\psi(0) = \psi(a) = 0$ [2.23]

$\psi(0) = Asin(0) + Bcos(0) = B \rightarrow B = 0$

$\rightarrow \psi(x) = Asin(kx)$ [2.24]

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$\psi(x) = Asin(kx)$

$\psi(a) = Asin(ka) = 0 \quad \rightarrow A = 0 \ \ or \ \ \sin(ka) = 0$

$A = 0 \ \rightarrow \psi(x) = 0$: The trivial (non-normalizable) solution!

$\sin(ka) = 0 \ \rightarrow ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi$... [2.25]

$k = 0 \ \rightarrow \psi(x) = 0$: The trivial solution!

$\sin(-\theta) = -\sin(\theta)$ → "–" can be inserted into A

→ $k_n = \frac{n\pi}{a}, n = 1, 2, 3,$... [2.26]

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

$$k_n = \frac{n\pi}{a}, n = 1, 2, 3, \ldots$$

$$\rightarrow E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \quad [2.27]$$

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

[CM!] $A = \sqrt{2/a}$ [2.28]

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

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

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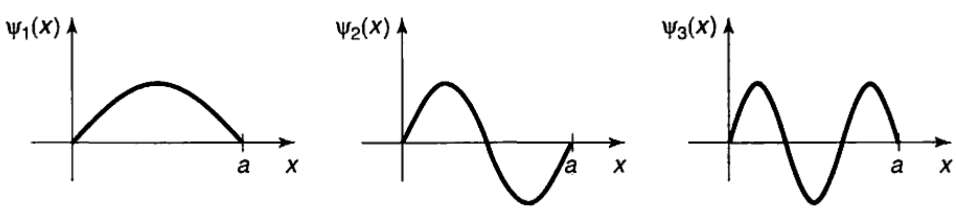

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Some properties of $\psi_n(x)$

1. The functions $\psi_n(x)$ (eigenfunctions, eigenstates) are alternatively even and odd, with respect to the center of the well ($a/2$): ψ_1 is even, ψ_2 is odd, ψ_3 is even, and so on.
2. Going up in energy, each successive state has one more node (zero-crossing): ψ_1 has no node, ψ_2 has one, ψ_3 has two, and so on.
3. They are mutually orthogonal (trực giao) and normal (chuẩn hóa) [= orthonormal: trực chuẩn]

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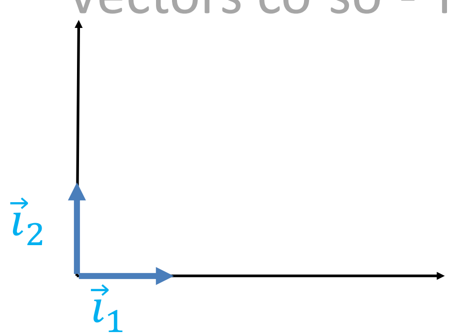
Vectors cơ sở - Trực chuẩn, đầy đủ



- ❖ Xét hệ toạ độ descarte 2 chiều.
- ❖ Gọi $\vec{i}_1$ và $\vec{i}_2$ là 2 vectors cơ sở theo trục x và y.
- ❖ Hai vectors này trực giao với nhau và có độ dài là 1. Tức là $\Leftrightarrow \vec{i}_1 \cdot \vec{i}_2 = 0$ và $\vec{i}_1 \cdot \vec{i}_1 = 1$.
- ❖ Hoặc (tổng quát): $\vec{i}_m \cdot \vec{i}_n = \delta_{mn} = \begin{cases} 0\ if\ m \neq n \\ 1\ if\ m = n \end{cases}$
- ❖ δ_{mn} được gọi là delta Kronecker

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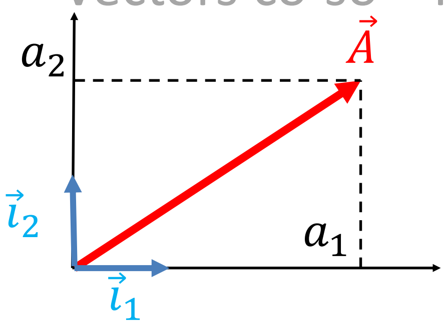
Vectors cơ sở - Trực chuẩn, đầy đủ



❖ Vector $\vec{A}$ bất kỳ đều có thể được biểu diễn qua hai vectors cơ sở $\vec{i}_1$ và $\vec{i}_2$.

❖ $\vec{A} = a_1\vec{i}_1 + a_2\vec{i}_2 = \sum a_n\,\vec{i}_n$

❖ $a_1 = \vec{i}_1 \cdot \vec{A}$ (hình chiếu của $\vec{A}$ lên $\vec{i}_1$)
và $a_2 = \vec{i}_2 \cdot \vec{A}$ (hình chiếu của $\vec{A}$ lên $\vec{i}_2$)

Vectors cơ sở - trực chuẩn, đầy đủ

Không gian vector thông thường	→	Không gian Hilbert (nơi hàm sóng "sống")
Vector	→	Hàm riêng, vector riêng, trạng thái riêng
$\vec{i}_n$	→	$\psi_n(x)$
$\vec{i}_m \cdot \vec{i}_n = \delta_{mn}$ Tích vô hướng	→	$\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x) = \delta_{mn}$ Tích trong

Some properties of $\psi_n(x)$

3. The eigenstates $\psi_n(x)$ are orthonormal

$$\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x) = \delta_{mn} \qquad [2.30]$$

$$\delta_{mn} = \begin{cases} 0 \; if \; m \neq n \\ 1 \; if \; m = n \end{cases} \qquad [2.31]$$

δ_{mn}: Kronecker delta.

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Some properties of $\psi_n(x)$

4. They are complete: Any other function, , can be expressed as a linear combination of them:

[Chúng đầy đủ: một vector bất kỳ (trạng thái bất kỳ hoặc hàm bất kỳ) đều có thể được biểu diễn qua hệ cơ sở này]:

- ❖ $f(x) = \sum_n c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_n c_n sin(\frac{n\pi}{a} x)$ [2.32]
- ❖ This is the Fourier series for $f(x)$
  [Đây cũng chính là chuỗi (phép biến đổi) Fourier của hàm $f(x)$].

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The coefficients c_n

- $f(x) = \sum_n c_n\psi_n(x) = \sqrt{\frac{2}{a}}\sum_n c_n sin(\frac{n\pi}{a}x)$ [2.32]
- Multiply both sides of 2.32 by $\psi_m^*(x)$ and integrate:

$$\int \psi_m^*(x)f(x)\,dx = \sum_n c_n \int \psi_m^*(x)\psi_n(x)dx$$

$$= \sum_n c_n\,\delta_{mn} = c_m \quad [2.33]$$

$$c_n = \int \psi_n^*(x)f(x)\,dx \quad [2.34]$$

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Vectors cơ sở - trực chuẩn, đầy đủ

Không gian vector thông thường	→	Không gian Hilbert (nơi hàm sóng "sống")
Vector	→	Hàm riêng, vector riêng, trạng thái riêng
$\vec{\imath}_n$	→	$\psi_n(x)$
$\vec{\imath}_m \cdot \vec{\imath}_n = \delta_{mn}$	→	$\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x) = \delta_{mn}$
$\vec{A} = \sum a_n\,\vec{\imath}_n$	→	$\psi(x) = \sum_{n=1}^{\infty} c_n\psi_n(x)$
$a_1 = \vec{\imath}_1 \cdot \vec{A}$ $a_n = \vec{\imath}_n \cdot \vec{A}$	→	$c_n = \int \psi_n^*(x)f(x)\,dx$

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States $\Psi_n(x,t)$ và $\Psi(x,t)$

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

$$= \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t} \qquad [2.35]$$

❖ The general solution: $\Psi(x,t) = \sum_n c_n \Psi_n(x,t) =$

$$= \sum_n c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t} \qquad [2.36]$$

$$\Psi(x,0) = \sum_n c_n \psi_n(x)$$

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A common problem

Given the initial wave function: $\Psi(x,0)$
Find $\Psi(x,t)$.
[Similarly, in classical mechanics: Given the initial condition: $x_0 = x(t=0)$. Find $x(t)$.]

❖ $\Psi(x,0) = \sum_n c_n \psi_n(x)$ [Given/Known]

❖ $c_n = \int \psi_n^*(x) \Psi(x,0)\, dx$ [Calculate the coefficients]

$$= \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0)\, dx \qquad [2.37]$$

❖ → $\Psi(x,t) = \sum_n c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$

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Example

A particle in the infinite square well has the initial wave function: $\Psi(x,0) = Ax(a-x), 0 \le x \le a$

Find: $\Psi(x,t)$.

- [Firstly, we have determine A in $\Psi(x,0)$]
- $1 = \int_0^a |\Psi(x,0)|^2\,dx = |A|^2 \int_0^a x^2(a-x)^2\,dx$
- $1 = |A|^2 \frac{a^5}{30} \;\rightarrow A = \sqrt{\frac{30}{a^5}}$
- $c_n = \int \psi_n^*(x)\Psi(x,0)\,dx$

$$= \sqrt{\frac{30}{a^5}}\sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)x(a-x)dx$$

- $c_n = \int \psi_n^*(x)\Psi(x,0)\,dx$

$$= \sqrt{\frac{30}{a^5}}\sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)x(a-x)dx$$

- $c_n = \begin{cases} 0, & \text{n even,} \\ \frac{8\sqrt{15}}{(n\pi)^3}, & \text{n odd.} \end{cases}$
- → $\Psi(x,t) =$

$$\sqrt{\frac{30}{a}}\left(\frac{2}{\pi}\right)^3 \sum_{n=1,3,5\ldots} \frac{1}{n^3}\sin\left(\frac{n\pi}{a}x\right)e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

A common problem

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Energy E_n

- ❖ $\Psi(x,0) = \sum_n c_n \psi_n(x)$
- ❖ c_n tells us the amount of $\psi_n(x)$ that is contained in Ψ.
- ❖ $|c_n|^2$ is the probability that a measurement of the energy would return a value E_n .
- ❖ The sum of these probabilities should be 1: [CM!]

$$\sum_n |c_n|^2 = 1 \qquad [2.38]$$

- ❖ And the expectation value of the energy [CM!]

$$\langle H \rangle = \sum_n |c_n|^2 E_n \qquad [2.39]$$

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BT

1. Hạt khối lượng m chuyển động tự do trong giếng thế vô hạn ($0 \leq x \leq a$) có hàm sóng ban đầu:

$$\psi(x,0) = \frac{A}{\sqrt{a}}\sin\left(\frac{\pi x}{a}\right) + 2\sqrt{\frac{1}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{i}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right),$$

với A là số thực.

a) Tìm A .

b) Nếu thực hiện phép đo năng lượng thì có thể tìm được những giá trị năng lượng nào và với xác suất tương ứng bao nhiêu? Tính năng lượng trung bình.

c) Tìm hàm sóng tại thời điểm $t > 0$.

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