Outline

- **Chapter 4.1** Nearly-Free-Electron Model (近自由电子模型)
- **Chapter 4.2** Tight-Binding Model (紧束缚模型)
- **Chapter 4.3** Square-Potential-Well Model (方势阱模型)
- **Chapter 4.4** Conductors & Nonconductors (导体与非导体)

Objectives

- To learn the properties of **potential well** and **potential barrier.**
- To understand **the Kronig-Penney model.**

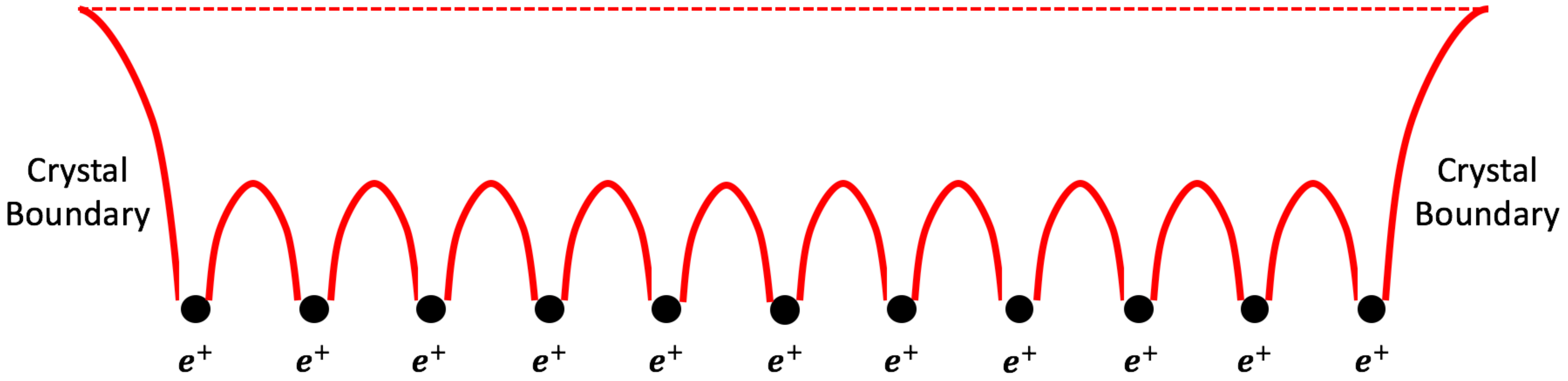
Potential Well and Potential Barrier (势阱与势垒)

Chapter 4.3: Square-Potential-Well Model (方势阱模型)

- **Periodic Potential (周期势)**

  - Periodic potential in crystal lattices:

$$\hat{V}\left(\vec{r}+\vec{R}_n\right)=\hat{V}(\vec{r})$$



➢ Periodic Potential (周期势)

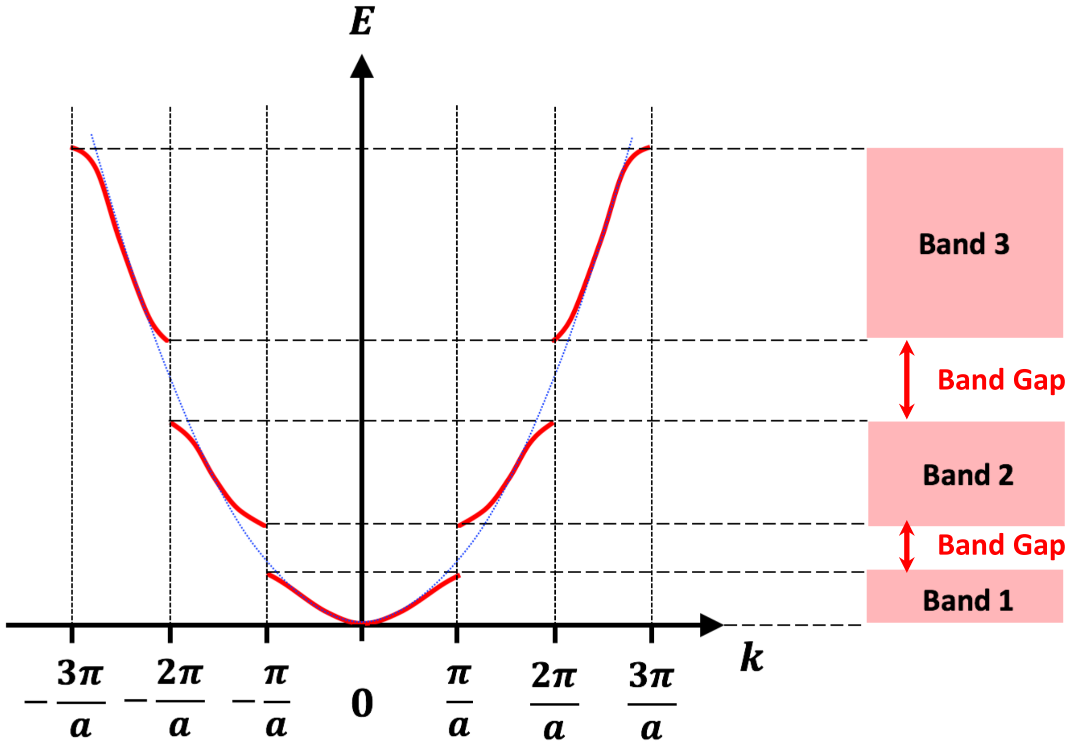
❖ The impacts of periodic potential:

$$E_{\text{gap}} = 2|V_n|$$

$$k = n\frac{\pi}{a} \quad (n = \pm 1, \pm 2, \cdots)$$

$$V_n = \frac{1}{a}\int_0^a e^{-i\frac{2\pi}{a}nx} V(x)dx$$

NFE Model in 1D



Chapter 4.3: Square-Potential-Well Model (方势阱模型)

➢ Periodic Potential (周期势)

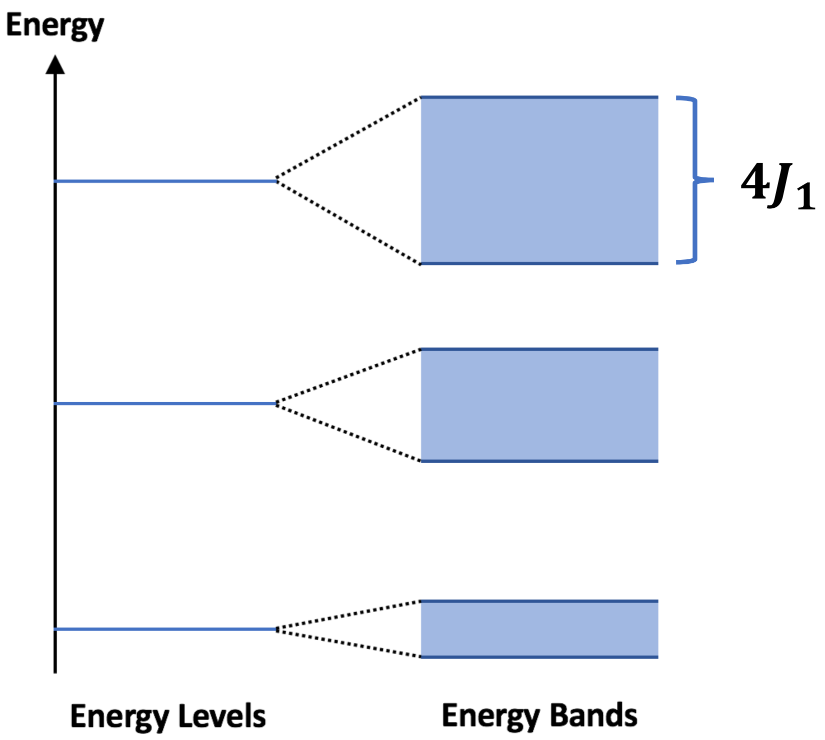
❖ The impacts of periodic potential:

$$W_{1D} = 4J_1$$

$$J_1 = -\int \varphi^*(\vec{\xi} - \vec{a})\hat{H}'(\vec{\xi})\varphi(\vec{\xi})\mathrm{d}\vec{\xi}$$

$$\hat{H}'(\vec{\xi}) = V(\vec{\xi}) - V_n(\vec{\xi})$$

TB Model in 1D



➢ Periodic Potential (周期势)

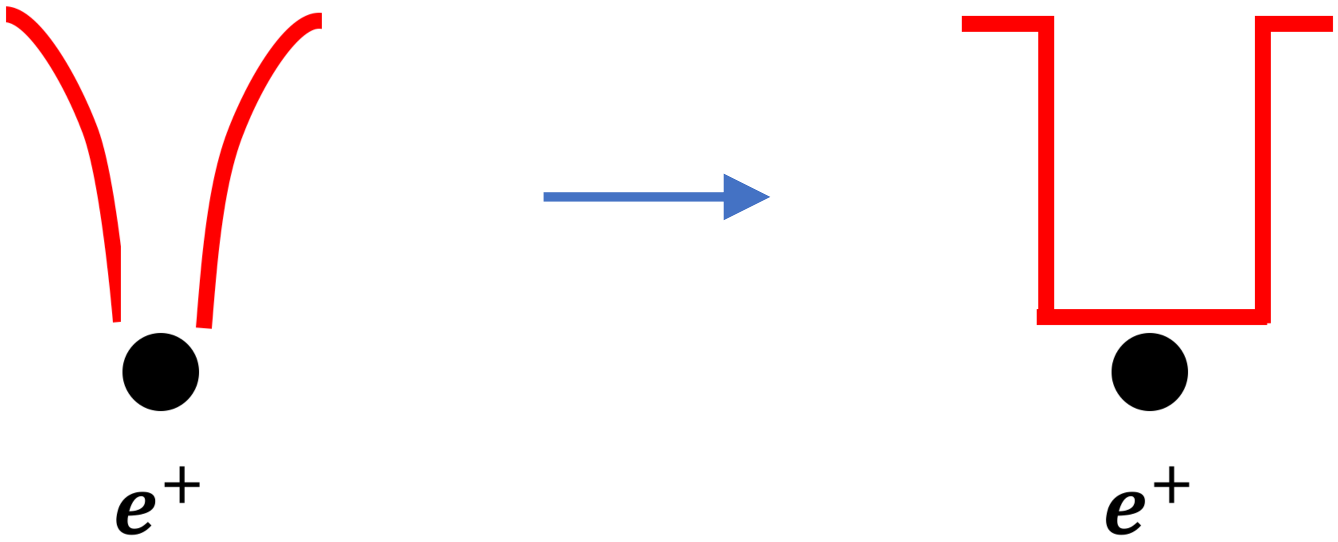
❖ In practice, to calculate the electronic structures of a specific crystal lattice, we have to know the **concrete form (具体形式)** of the periodic potential $\hat{V}(\vec{r})$.

$$\hat{V}(\vec{r}) = \ ?$$

Chapter 4.3: Square-Potential-Well Model (方势阱模型)

Potential Well (势阱)

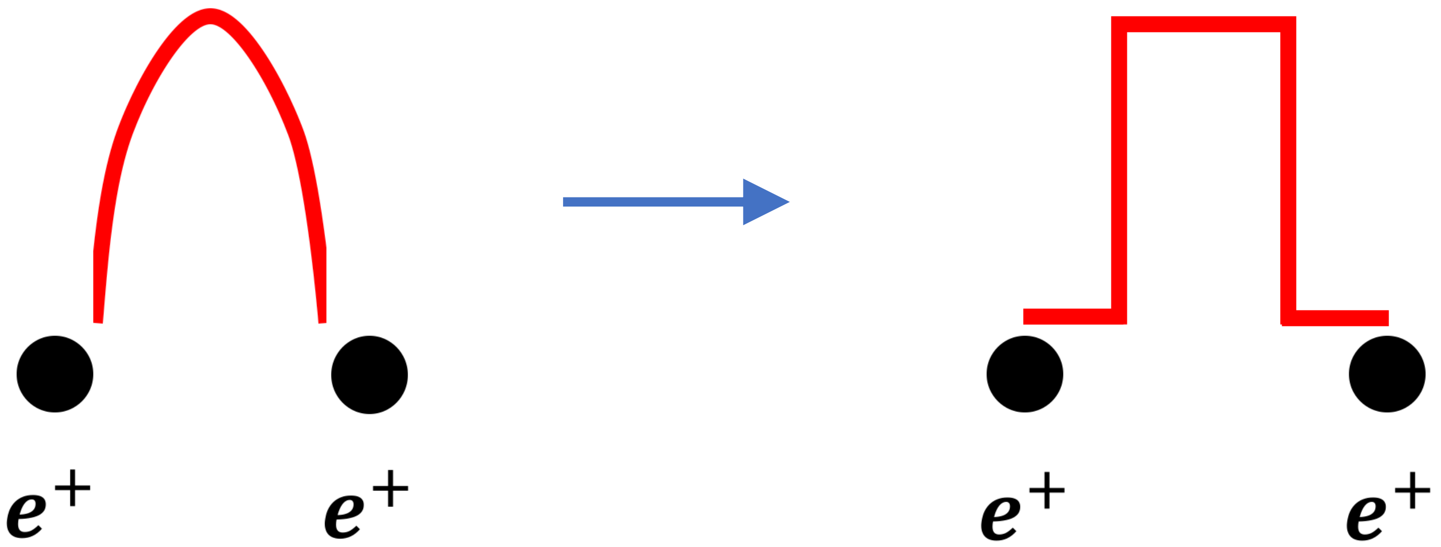
- In the case of 1D, the **potential near a lattice site** can be modeled by a **square potential well (方势阱):**



Chapter 4.3: Square-Potential-Well Model (方势阱模型)

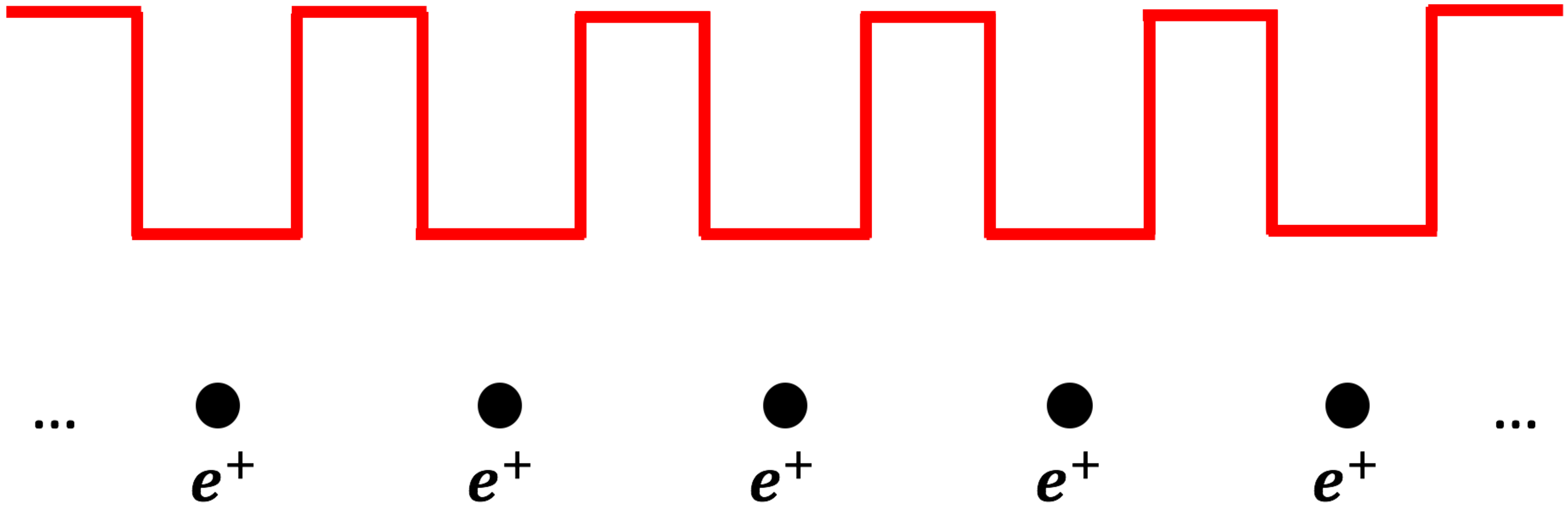
➢ Potential Barrier (势垒)

❖ In the case of 1D, the **potential between lattice sites** can be modeled by a **square potential barrier (方势垒):**



➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ **The Kronig-Penney model** represents the simplest 1D periodic-potential model consisting of an array of **alternating square potential wells and barriers:**



R. De. L. Kronig and W. G. Penney, **Proc. Roy. Soc. London** 130, 499 (1931).

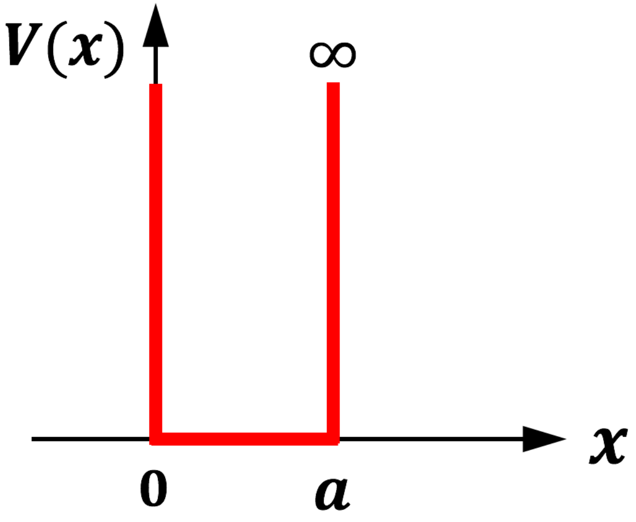
Infinite Potential Well
(无限深势阱)

➢ Infinite Potential Well (无限深势阱)

❖ An infinite potential well is a potential well with **an infinite depth (无限深度)**.

❖ The **infinite square potential well (无限深方势阱)** in 1D can be described as:

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & x \leq 0 \text{ and } x \geq a \end{cases}$$



Infinite Potential Well (无限深势阱)

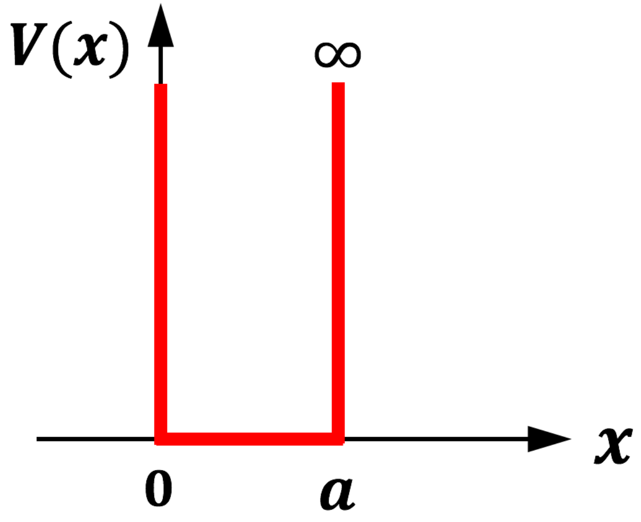
- The electronic Schrödinger equation:

  - Inside the well ($0 < x < a$):

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\psi = 0$$

  - Outside the well ($x \leq 0$ and $x \geq a$):

$$\psi = 0$$



➢ Infinite Potential Well (无限深势阱)

❖ Solutions to the Schrödinger equation:

$$\psi = Ae^{i\alpha x} + Be^{-i\alpha x}$$

$$\alpha = \sqrt{\frac{2m}{\hbar^2}E}$$

$$\begin{cases} x = 0 \rightarrow \psi = 0 \\ x = a \rightarrow \psi = 0 \end{cases} \xrightarrow{\text{Boundary Condition}} \begin{aligned} & A + B = 0 \\ & Ae^{i\alpha a} + Be^{-i\alpha a} = 0 \end{aligned}$$

➢ Infinite Potential Well (无限深势阱)

❖ Solutions to the Schrödinger equation:

$$\longrightarrow \quad 2Ai\sin(\alpha a) = 0 \quad \longrightarrow \quad \alpha a = n\pi \qquad (n = 0, 1, 2, 3, \cdots)$$

$$\longrightarrow \quad \int_{-\infty}^{+\infty} |\psi|^2 \mathrm{d}x = 1 \quad \longrightarrow \quad A = \sqrt{\frac{1}{2a}}$$

➢ Infinite Potential Well (无限深势阱)

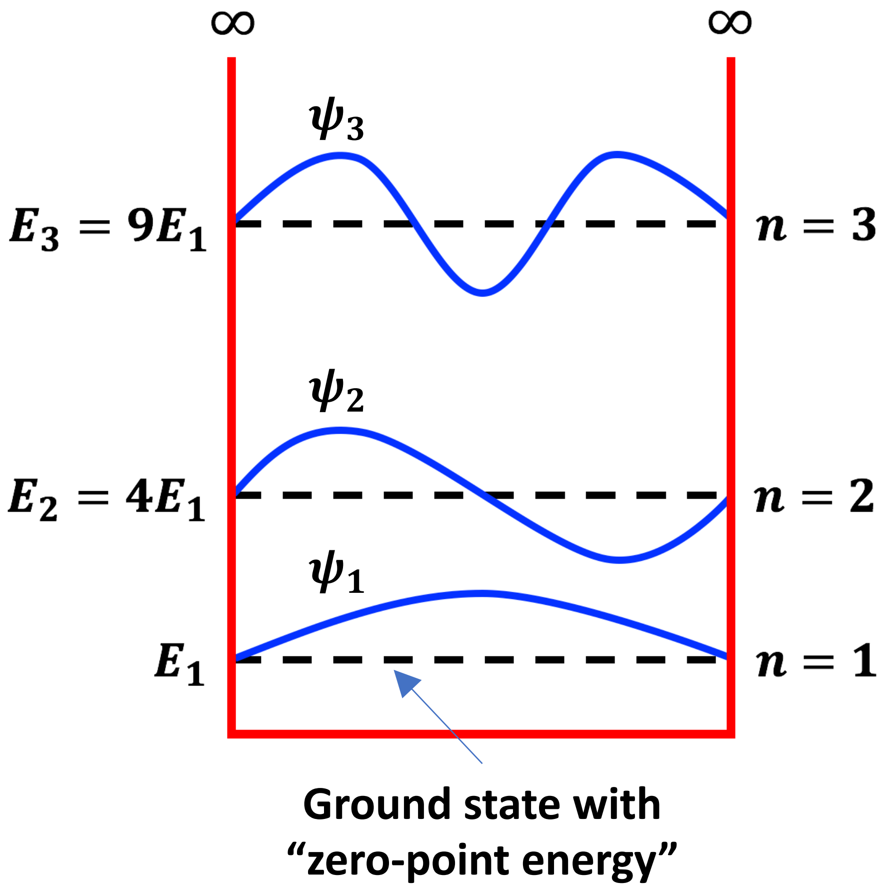
❖ Solutions to the Schrödinger equation:

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

$$\boxed{E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2}$$

$$(n = 1, 2, 3, \cdots)$$

*Note that it is meaningless for $n = 0$ because $\psi_0 \equiv 0$.

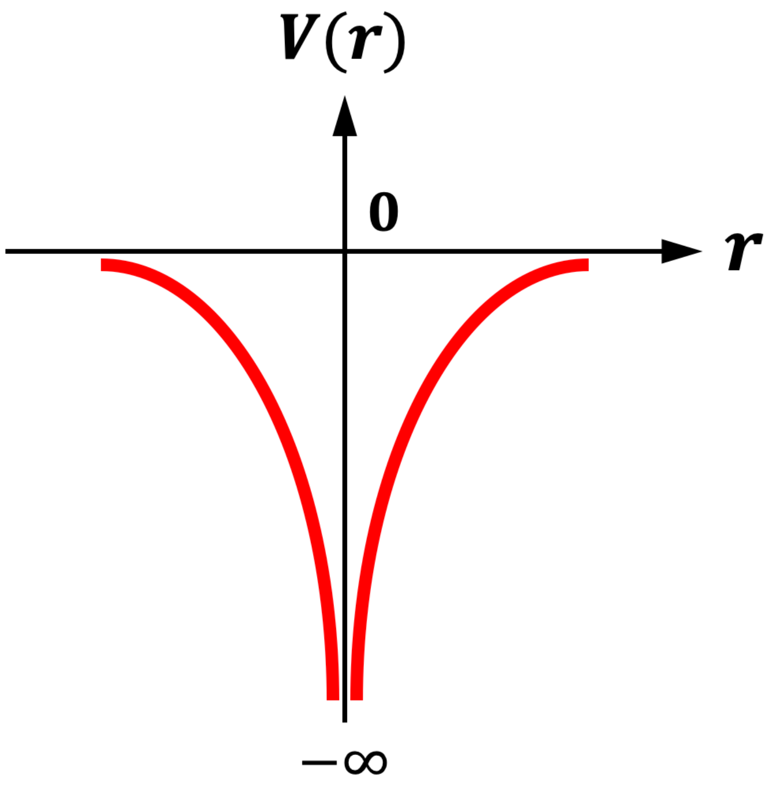


➤ Infinite Potential Well (无限深势阱)

❖ Comparison with the case of a **hydrogen atom**:

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$V(r) = \begin{cases} 0 & r \to +\infty \\ -\infty & r = 0 \end{cases}$$



➢ Infinite Potential Well (无限深势阱)

❖ Comparison with the case of a **hydrogen atom**:

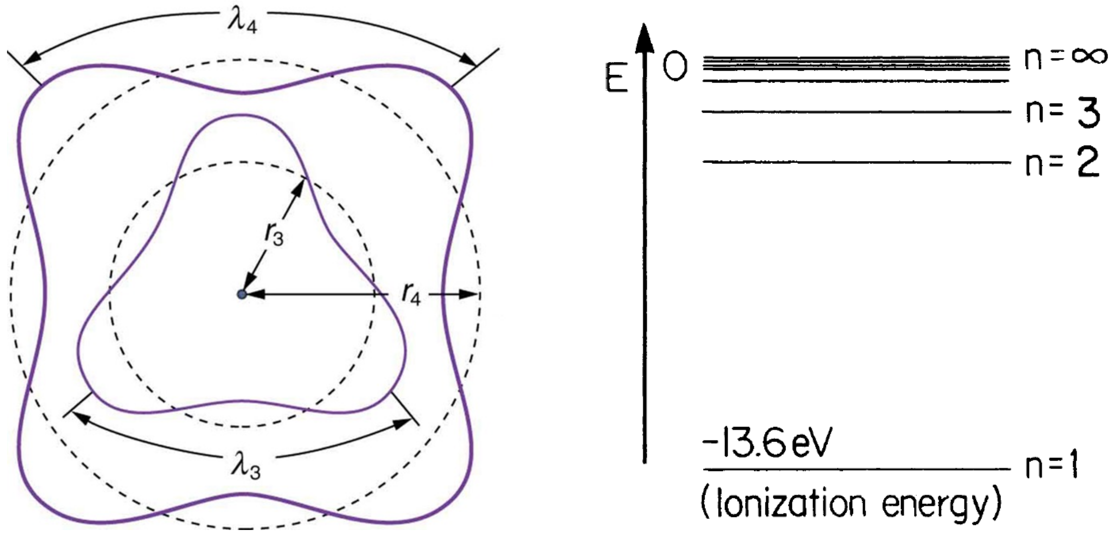
$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$E_n = -\frac{me^4}{2(4\pi\varepsilon_0\hbar)^2}\frac{1}{n^2}$$

$$= -13.6\frac{1}{n^2}\ \ (\mathrm{eV})$$

$$(n = 1, 2, 3, \cdots)$$

$$\boxed{2\pi r = n\lambda}$$



Schematic diagram of the allowed orbitals (left) and the energy levels (right) in a hydrogen atom.

Finite Potential Barrier
(有限高势垒)

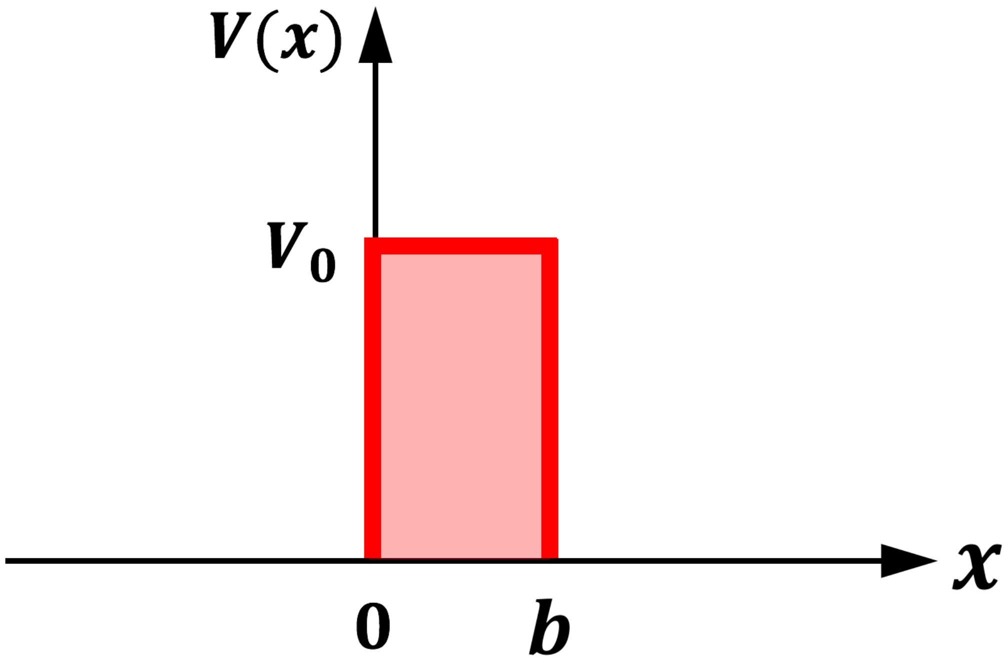
Chapter 4.3: Square-Potential-Well Model (方势阱模型)

➢ Finite Potential Barrier (有限高势垒)

❖ A finite potential barrier is a potential barrier with **a finite height (有限高度)**.

❖ The **finite square potential barrier (有限高方势垒)** in 1D can be described as:

$$V(x) = \begin{cases} 0 & x \le 0 \text{ and } x \ge b \\ V_0 & 0 < x < b \end{cases}$$



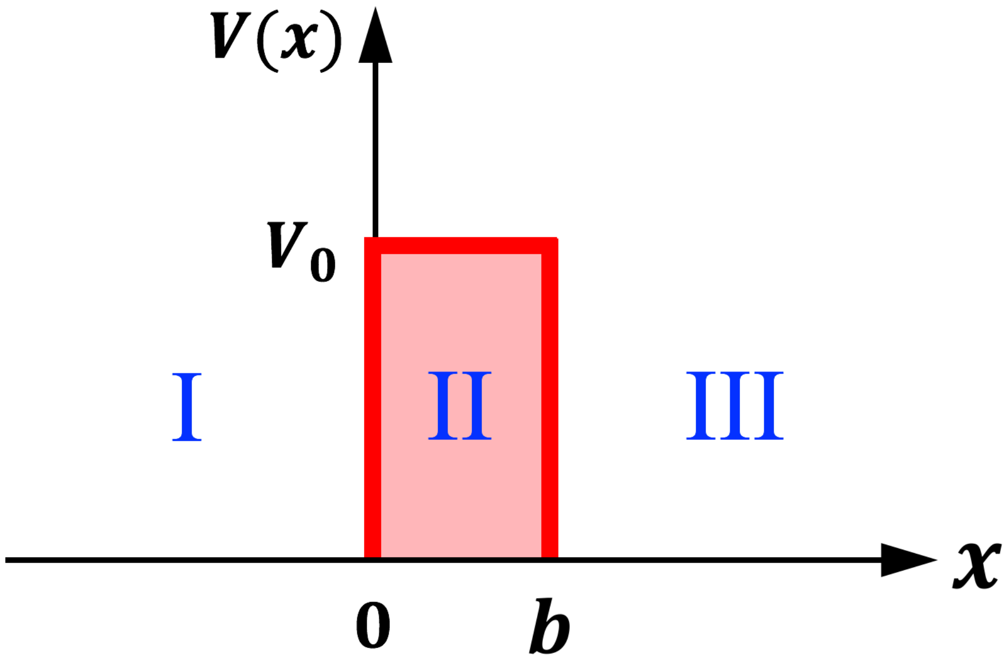
➢ Finite Potential Barrier (有限高势垒)

❖ For a free electron traveling from left to right, there is a probability that the electron can **tunnel (隧穿)** through the 1D finite square potential barrier.

❖ The electronic Schrödinger equation:

- Regions I and III ($x \leq 0$ and $x \geq b$):

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\psi = 0$$

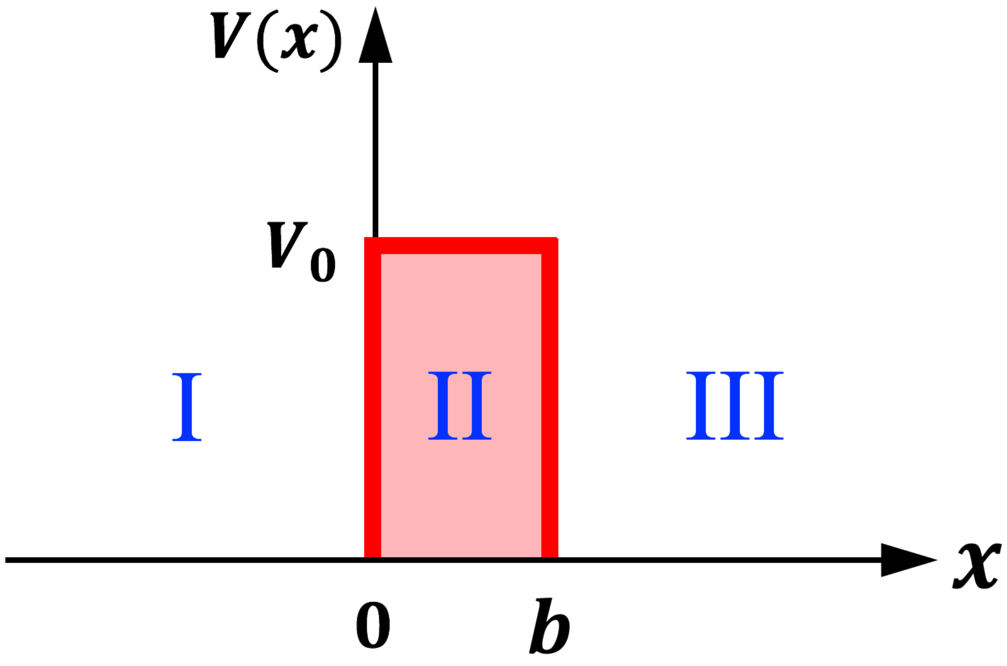


Finite Potential Barrier (有限高势垒)

- For a free electron traveling from left to right, there is a probability that the electron can **tunnel (隧穿)** through the 1D finite square potential barrier.

- The electronic Schrödinger equation:
  - Region II ($0 < x < b$):

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$



➢ Finite Potential Barrier (有限高势垒)

❖ Solutions to the Schrödinger equation:

- Region I ($x \leq 0$):

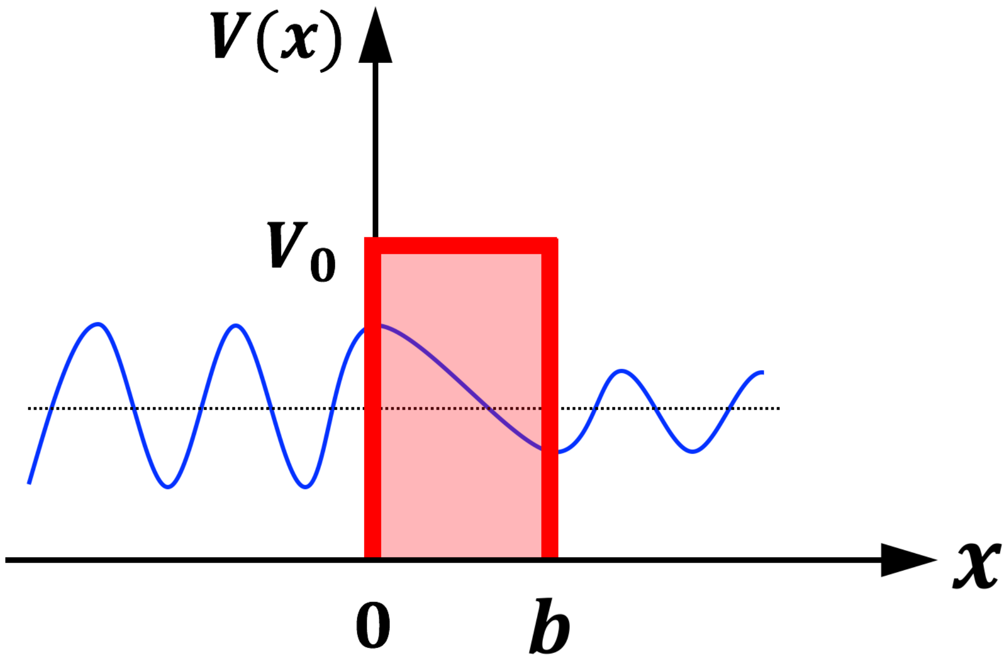
$$\psi_{\mathrm{I}} = \mathrm{e}^{i\alpha x} + R\mathrm{e}^{-i\alpha x} \qquad \alpha = \sqrt{\frac{2m}{\hbar^2}E}$$

- Region II ($0 < x < b$):

$$\psi_{\mathrm{II}} = A\mathrm{e}^{\gamma x} + B\mathrm{e}^{-\gamma x} \qquad \gamma = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

- Region III ($x \geq b$):

$$\psi_{\mathrm{III}} = T\mathrm{e}^{i\alpha x}$$



➢ Finite Potential Barrier (有限高势垒)

❖ The **boundary conditions** require the **continuity (连续) of both ψ and ψ'** at the boundary:

- At $x = 0$:

$$\mathbf{1} + \boldsymbol{R} = \boldsymbol{A} + \boldsymbol{B}$$

$$\frac{\boldsymbol{i\alpha}}{\boldsymbol{\gamma}}(\mathbf{1} - \boldsymbol{R}) = \boldsymbol{A} - \boldsymbol{B}$$

$\longrightarrow$

$$\boldsymbol{A} = \frac{\mathbf{1}}{\mathbf{2}}\left[\left(\mathbf{1} + \frac{\boldsymbol{i\alpha}}{\boldsymbol{\gamma}}\right) + \boldsymbol{R}\left(\mathbf{1} - \frac{\boldsymbol{i\alpha}}{\boldsymbol{\gamma}}\right)\right]$$

$$\boldsymbol{B} = \frac{\mathbf{1}}{\mathbf{2}}\left[\left(\mathbf{1} - \frac{\boldsymbol{i\alpha}}{\boldsymbol{\gamma}}\right) + \boldsymbol{R}\left(\mathbf{1} + \frac{\boldsymbol{i\alpha}}{\boldsymbol{\gamma}}\right)\right]$$

➢ Finite Potential Barrier (有限高势垒)

❖ The **boundary conditions** require the **continuity (连续) of both ψ and ψ'** at the boundary:

- At $x = b$:

$$Ae^{\gamma b} + Be^{-\gamma b} = Te^{i\alpha b}$$

$$Ae^{\gamma b} - Be^{-\gamma b} = \frac{i\alpha}{\gamma} Te^{i\alpha b}$$

$\rightarrow$

$$A = \frac{T}{2}\left(1 + \frac{i\alpha}{\gamma}\right) e^{i(\alpha-\gamma)b}$$

$$B = \frac{T}{2}\left(1 - \frac{i\alpha}{\gamma}\right) e^{i(\alpha+\gamma)b}$$

Chapter 4.3: Square-Potential-Well Model (方势阱模型)

➢ Finite Potential Barrier (有限高势垒)

❖ The **transmission coefficient (透射系数)**:

$$\longrightarrow \quad |\boldsymbol{T}|^2 = \left[\mathbf{1} + \frac{\mathbf{1}}{\frac{\boldsymbol{E}}{\boldsymbol{V}_0}\left(\mathbf{1} - \frac{\boldsymbol{E}}{\boldsymbol{V}_0}\right)} \mathbf{sinh}^2(\boldsymbol{\gamma b})\right]^{-1}$$

$$\sinh(x) = \frac{\mathbf{e}^{x} - \mathbf{e}^{-x}}{\mathbf{2}}$$

➢ Finite Potential Barrier (有限高势垒)

❖ The **reflection coefficient (反射系数)**:

$$\to \quad |\boldsymbol{R}|^2 = \frac{\left(\alpha^2+\gamma^2\right)^2 \sinh^2(\gamma b)}{(\alpha^2+\gamma^2)^2 \sinh^2(\gamma b) + 4\alpha^2\gamma^2}$$

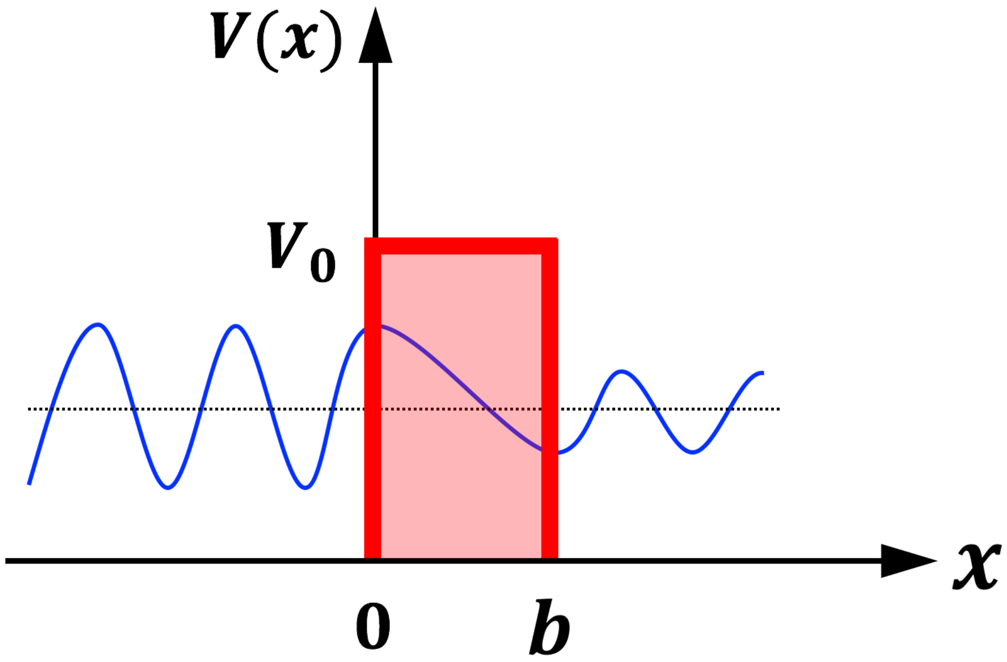
$$\sinh(x) = \frac{\mathrm{e}^x - \mathrm{e}^{-x}}{2}$$

- **Finite Potential Barrier (有限高势垒)**

  - The **conservation of probability (概率守恒)**:

$$\boxed{|T|^2 + |R|^2 = 1}$$

Quantum Tunneling Effect (量子隧道效应)!



➢ Finite Potential Barrier (有限高势垒)

❖ The limiting case of **infinite width ($b \to \infty$):**

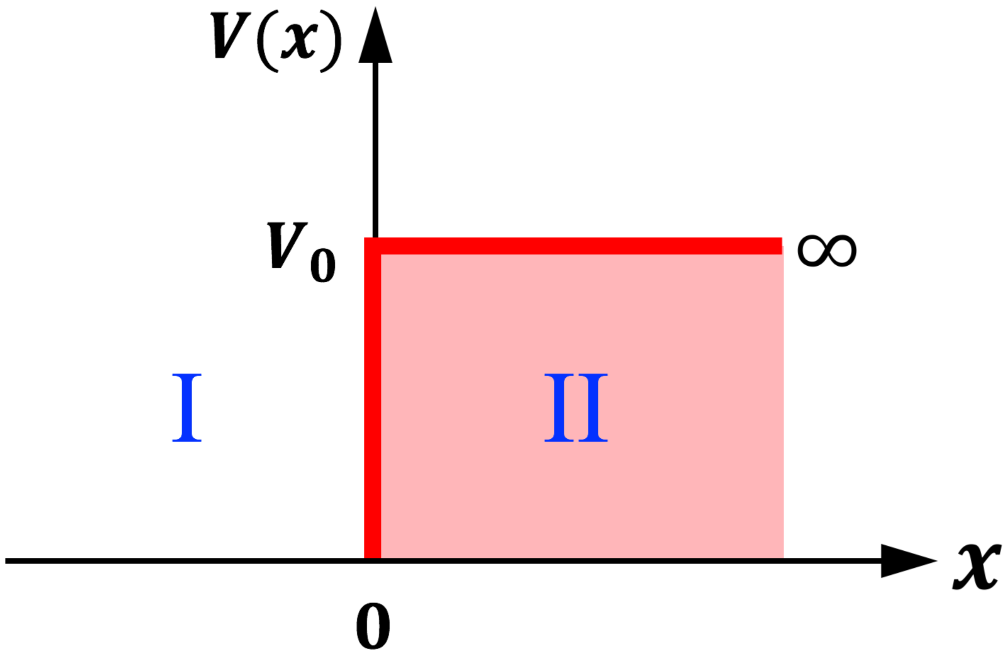
The electronic Schrödinger equation:

- Region I ($x \le 0$):

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$$

- Region II ($x > 0$):

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V_0)\psi = 0$$



➢ Finite Potential Barrier (有限高势垒)

❖ The limiting case of **infinite width ($b \to \infty$):**

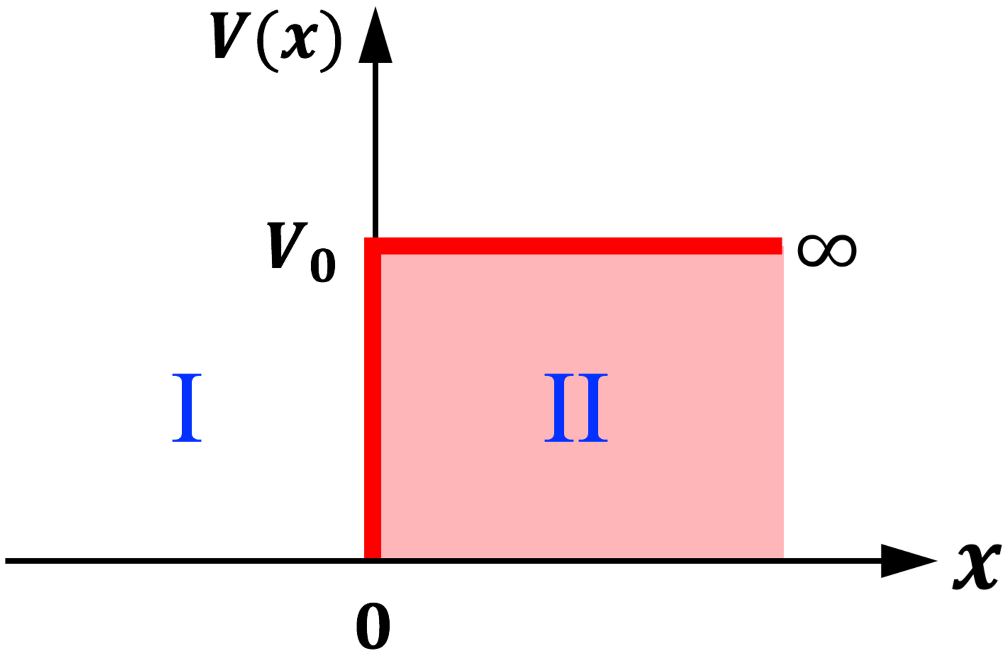
Solutions to the Schrödinger equation:

- Region I ($x \leq 0$):

$$\psi_{\mathrm{I}} = \mathrm{e}^{i\alpha x} + R\mathrm{e}^{-i\alpha x} \qquad \alpha = \sqrt{\frac{2m}{\hbar^2}E}$$

- Region II ($x > 0$):

$$\psi_{\mathrm{II}} = A\mathrm{e}^{\gamma x} + B\mathrm{e}^{-\gamma x} \qquad \gamma = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$



➢ Finite Potential Barrier (有限高势垒)

❖ The limiting case of **infinite width ($b \to \infty$):**

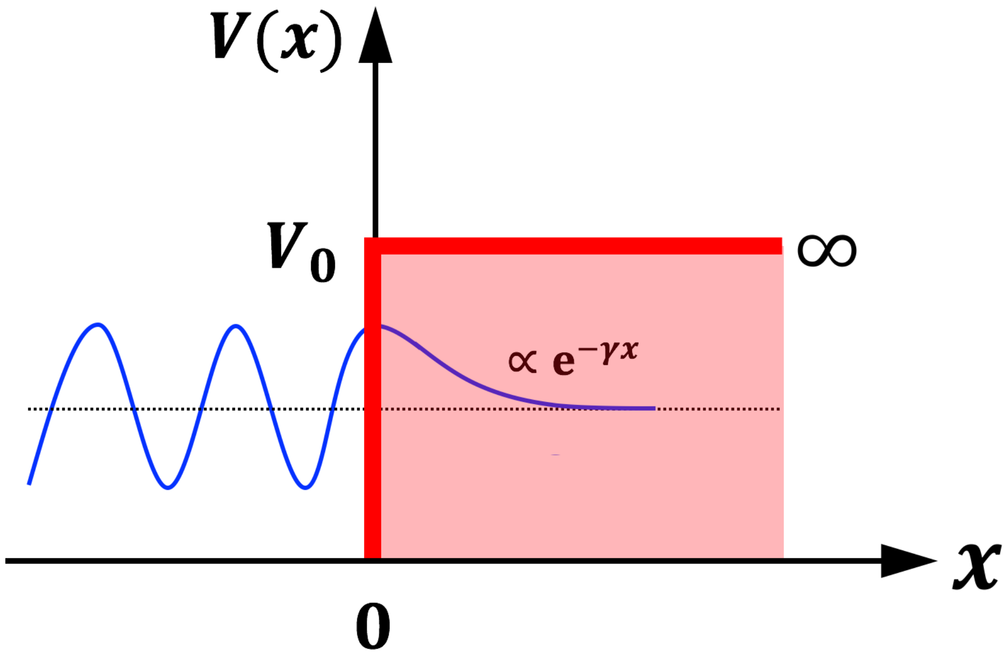
The **boundary conditions** of both ψ and ψ' require:

- At $x = 0$:

$$\mathbf{1 + R = A + B} \qquad \frac{\boldsymbol{i\alpha}}{\boldsymbol{\gamma}}(\mathbf{1 - R}) = \mathbf{A - B}$$

- At $x \to \infty$:

$$\boldsymbol{\psi}_{\mathbf{II}} = \mathbf{A \cdot \infty + B \cdot 0} \longrightarrow \boxed{\mathbf{A = 0}}$$



➢ Finite Potential Barrier (有限高势垒)

❖ The limiting case of **infinite width ($b \to \infty$):**

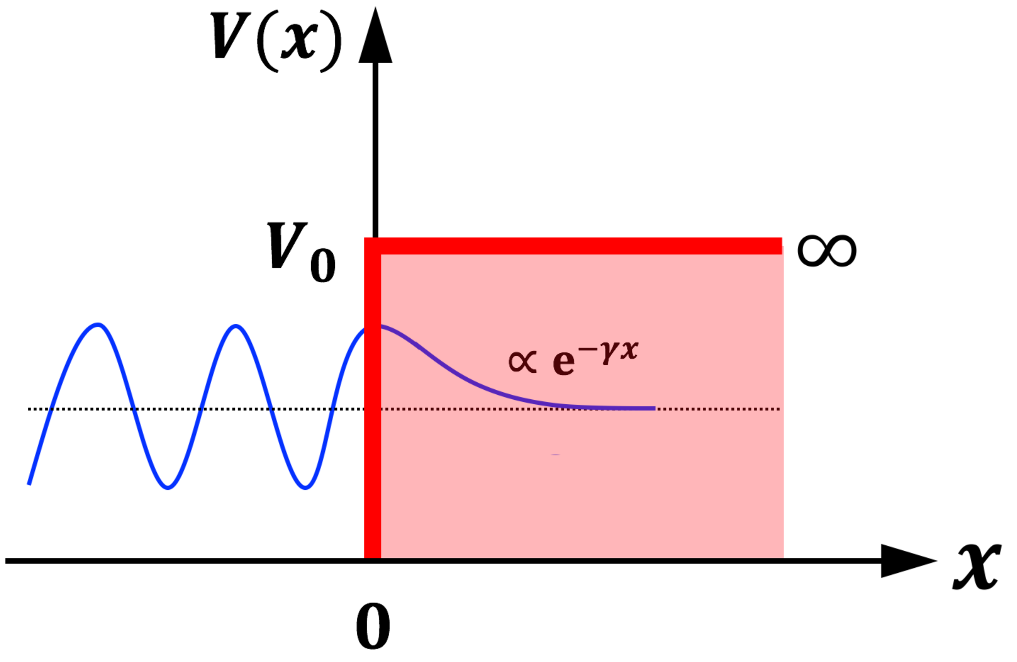
$$\boxed{\psi_{\mathrm{I}} = \mathrm{e}^{i\alpha x} + R\mathrm{e}^{-i\alpha x}}$$

$$\boxed{\psi_{\mathrm{II}} = B\mathrm{e}^{-\gamma x}}$$

$$\boxed{1 + R = B}$$

$$R = \frac{i\alpha + \gamma}{i\alpha - \gamma} \qquad B = \frac{2i\alpha}{i\alpha - \gamma}$$

The wave function of the tunneling electron **decay exponentially within the barrier**!



Finite Potential Barrier (有限高势垒)

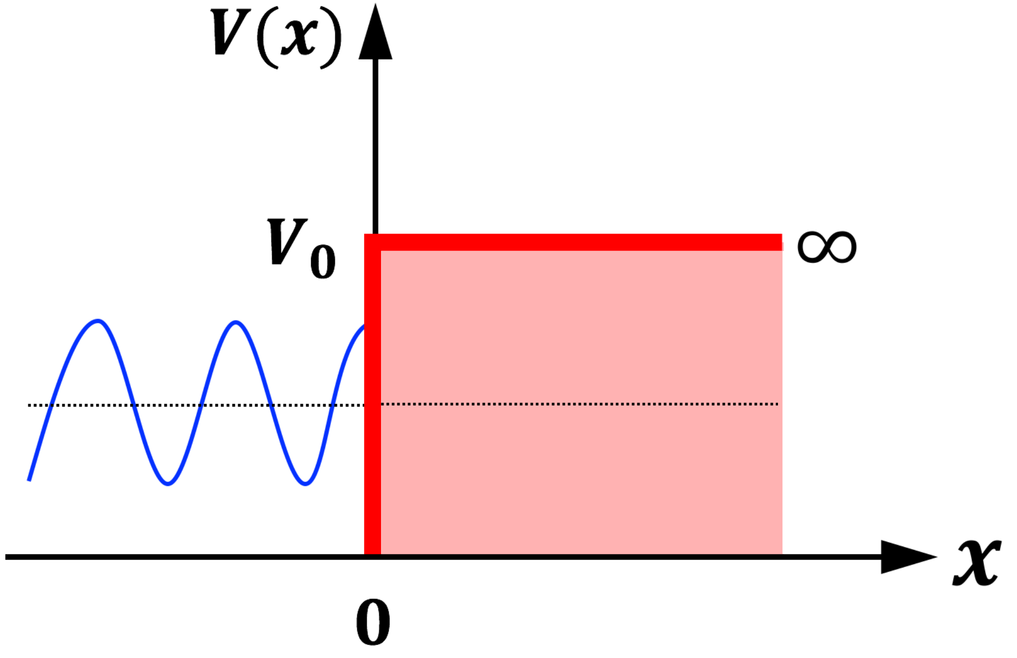
❖ The limiting case of **both infinite width and infinite height ($b \rightarrow \infty$ and $V_0 \rightarrow \infty$):**

When $V_0 \rightarrow \infty, \quad \gamma \rightarrow \infty$

$$\boxed{\psi_{\mathrm{II}} = Be^{-\gamma x} = 0}$$

$$\boxed{B = \frac{2i\alpha}{i\alpha - \gamma} = 0}$$

$$\boxed{R = -1}$$



The electron is **completely reflected** by the potential barrier **when** $V_0 \rightarrow \infty$!

Finite Potential Well
(有限深势阱)

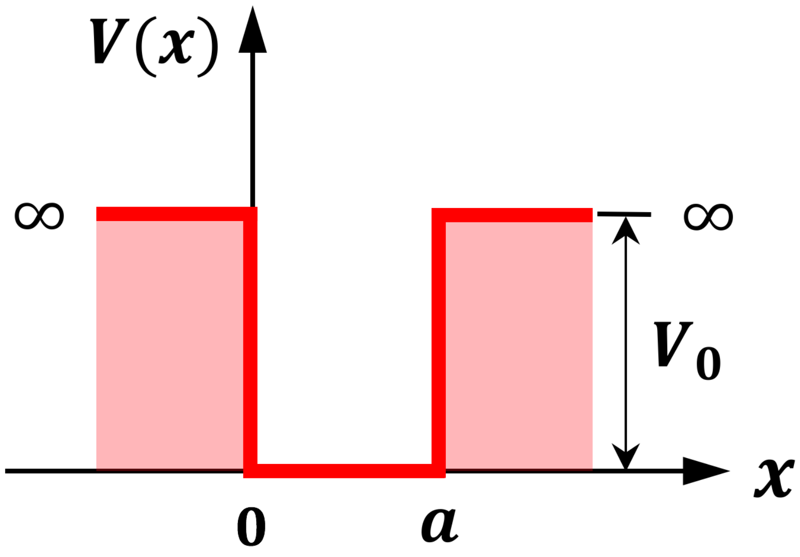
Chapter 4.3: Square-Potential-Well Model (方势阱模型)

➢ Finite Potential Well (有限深势阱)

❖ A finite potential well is a potential well with **a finite depth (有限深度)**.

❖ The **symmetric finite square potential well (对称有限深方势阱)** in 1D can be described as:

$$V(x) = \begin{cases} 0 & 0 < x < a \\ V_0 & x \le 0 \text{ and } x \ge a \end{cases}$$



Finite Potential Well (有限深势阱)

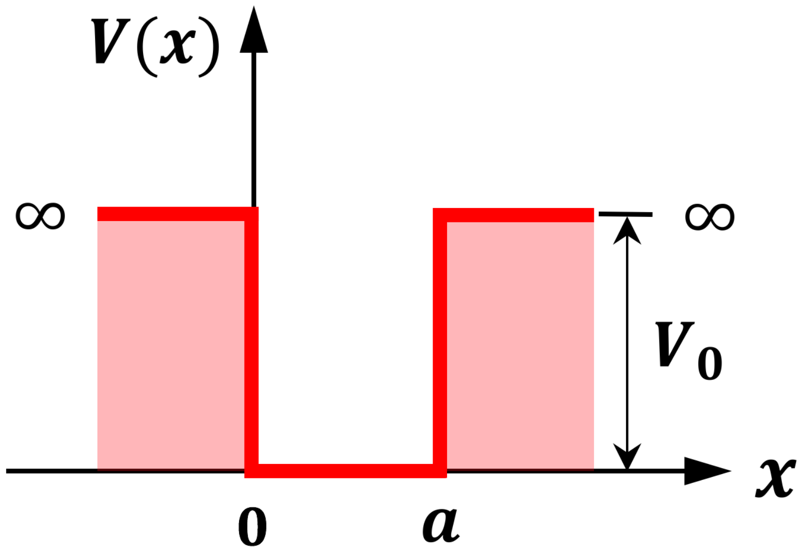
- The electronic Schrödinger equation:

  - Inside the well ($0 < x < a$):

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\psi = 0$$

  - Outside the well ($x \leq 0$ and $x \geq a$):

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$



Chapter 4.3: Square-Potential-Well Model (方势阱模型)

➢ Finite Potential Well (有限深势阱)

❖ Solutions to the Schrödinger equation:

- Inside the well ($0 < x < a$):

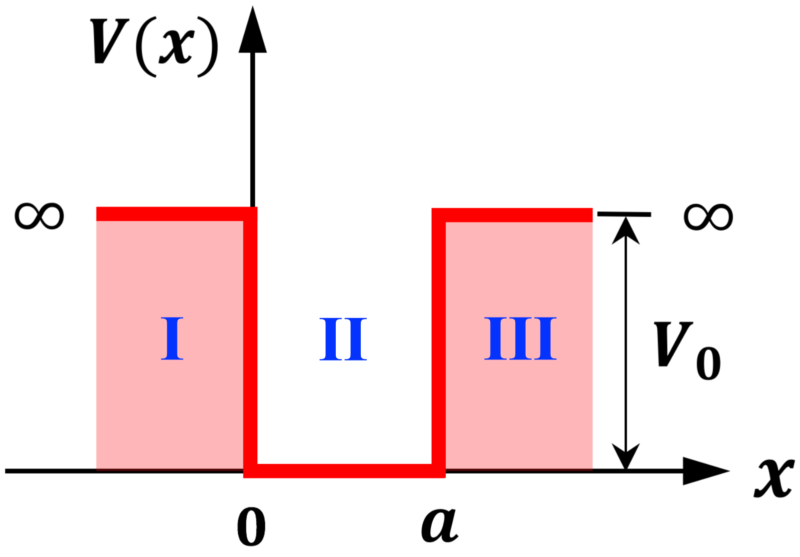
$$\psi_{\mathrm{II}} = A e^{i\alpha x} + B e^{-i\alpha x} \qquad \alpha = \sqrt{\frac{2m}{\hbar^2}E}$$

- Outside the well ($x \leq 0$ and $x \geq a$):

$$\psi_{\mathrm{I}} = C e^{\gamma x}$$

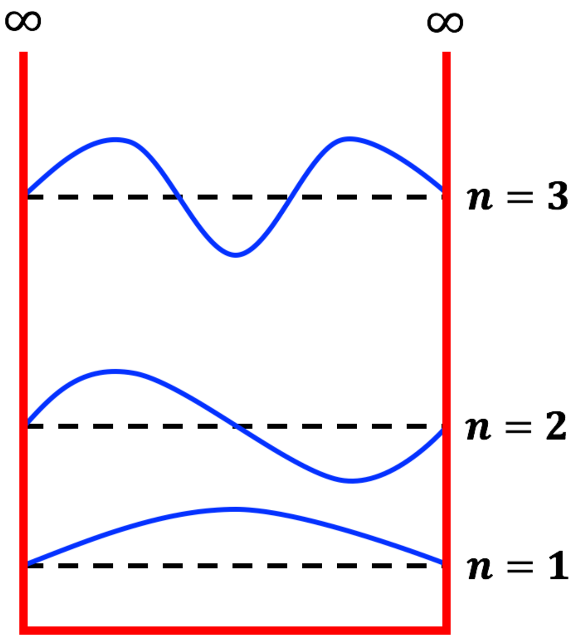
$$\gamma = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$\psi_{\mathrm{III}} = D e^{-\gamma x}$$

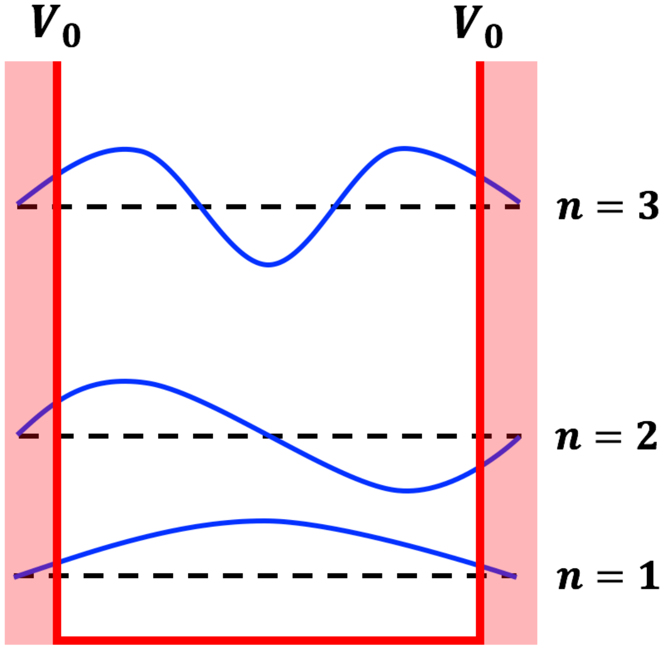


➢ Finite Potential Well (有限深势阱)

❖ Characteristics of the wavefunctions:



Infinite potential well

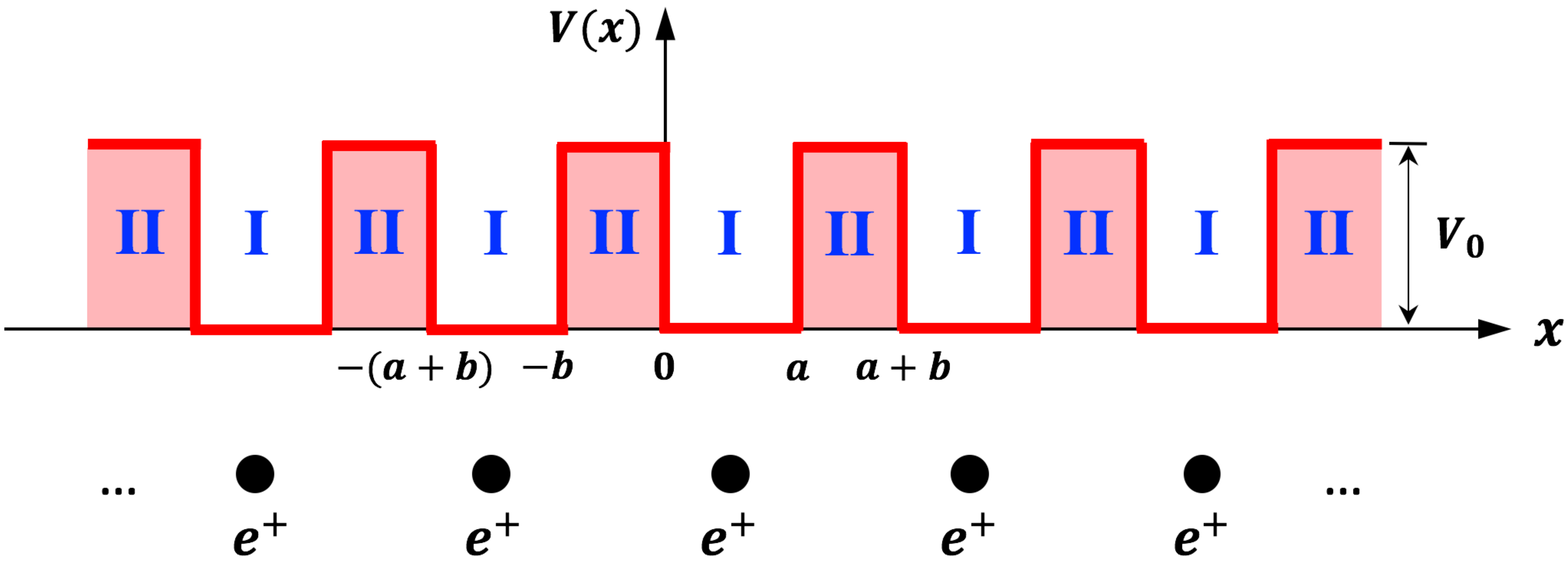


Finite potential well

The Kronig-Penney Model
(克勒尼希-彭尼模型)

➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ The Kronig-Penney model for a 1D monoatomic lattice:



➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ The periodic potential:

$$V(x) = \begin{cases} \mathbf{0} & \text{Regions } \mathbf{I} \\ V_0 & \text{Regions } \mathbf{II} \end{cases}$$

The Kronig-Penney Model (克勒尼希-彭尼模型)

- The electronic Schrödinger equation:

  - Regions I:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\psi = 0$$

  - Regions II:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ Solutions to the Schrödinger equation:

- Regions I:

$$\boldsymbol{\psi_{\mathrm{I}} = A\mathrm{e}^{i\alpha x} + B\mathrm{e}^{-i\alpha x}} \qquad \boldsymbol{\alpha = \sqrt{\frac{2m}{\hbar^2}E}}$$

- Regions II:

$$\boldsymbol{\psi_{\mathrm{II}} = C\mathrm{e}^{\gamma x} + D\mathrm{e}^{-\gamma x}} \qquad \boldsymbol{\gamma = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}}$$

➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ Solutions to the Schrödinger equation:

According to the **Bloch theorem**, the wavefunction must satisfy:

$$\psi(x+a+b) = \mathrm{e}^{ik(a+b)}\psi(x)$$

➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ Solutions to the Schrödinger equation:

The boundary conditions:

- At $x = 0$:

$$\boldsymbol{A + B = C + D}$$

$$\boldsymbol{i\alpha(A - B) = \gamma(C - D)}$$

- At $x = a$:

$$\boldsymbol{A\mathrm{e}^{i\alpha a} + B\mathrm{e}^{-i\alpha a} = \left(C\mathrm{e}^{-\gamma b} + D\mathrm{e}^{\gamma b}\right)e^{ik(a+b)}}$$

$$\boldsymbol{i\alpha\left(A\mathrm{e}^{i\alpha a} - B\mathrm{e}^{-i\alpha a}\right) = \gamma\left(C\mathrm{e}^{-\gamma b} - D\mathrm{e}^{\gamma b}\right)e^{ik(a+b)}}$$

It is required that **the determinant of the coefficients of $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$, and $\boldsymbol{D}$ is zero**.

➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ Solutions to the Schrödinger equation:

The energy dispersion:

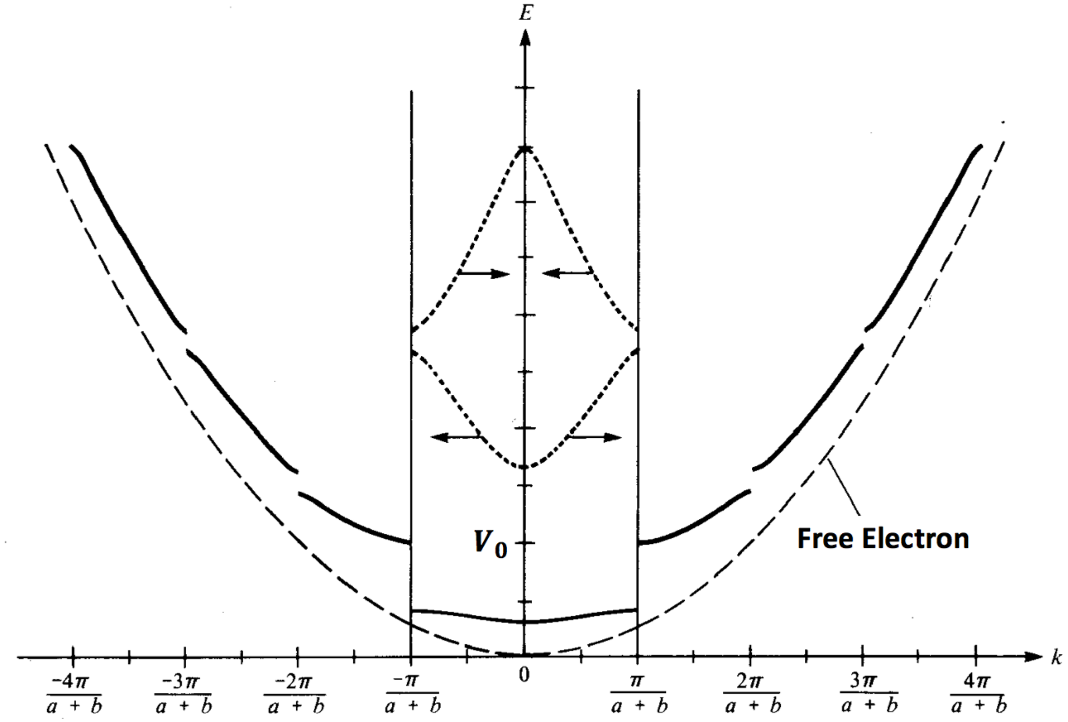
$$\boxed{\frac{\gamma^2-\alpha^2}{2\gamma\alpha}\sinh(\gamma b)\sin(\alpha a)+\cosh(\gamma b)\cos(\alpha a)=\cos[k(a+b)]}$$

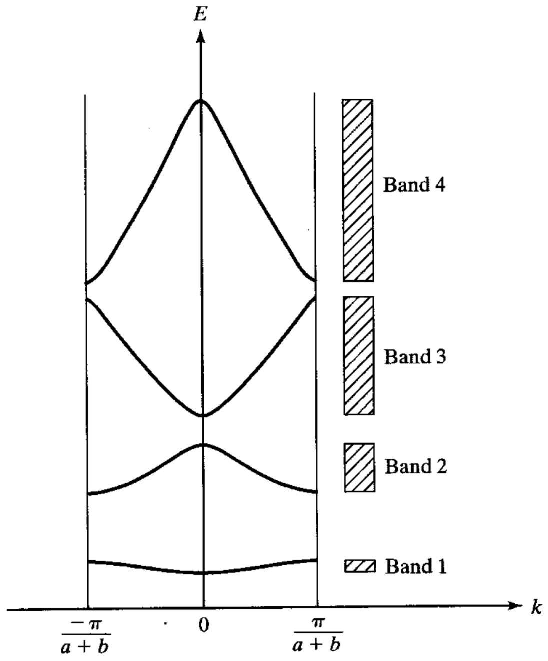
$$\alpha=\sqrt{\frac{2m}{\hbar^2}E}\qquad \gamma=\sqrt{\frac{2m}{\hbar^2}(V_0-E)}$$

$$\sinh(x)=\frac{e^x-e^{-x}}{2}\qquad \cosh(x)=\frac{e^x+e^{-x}}{2}$$

➢ **The Kronig-Penney Model (克勒尼希-彭尼模型)**

❖ **The band structures:**

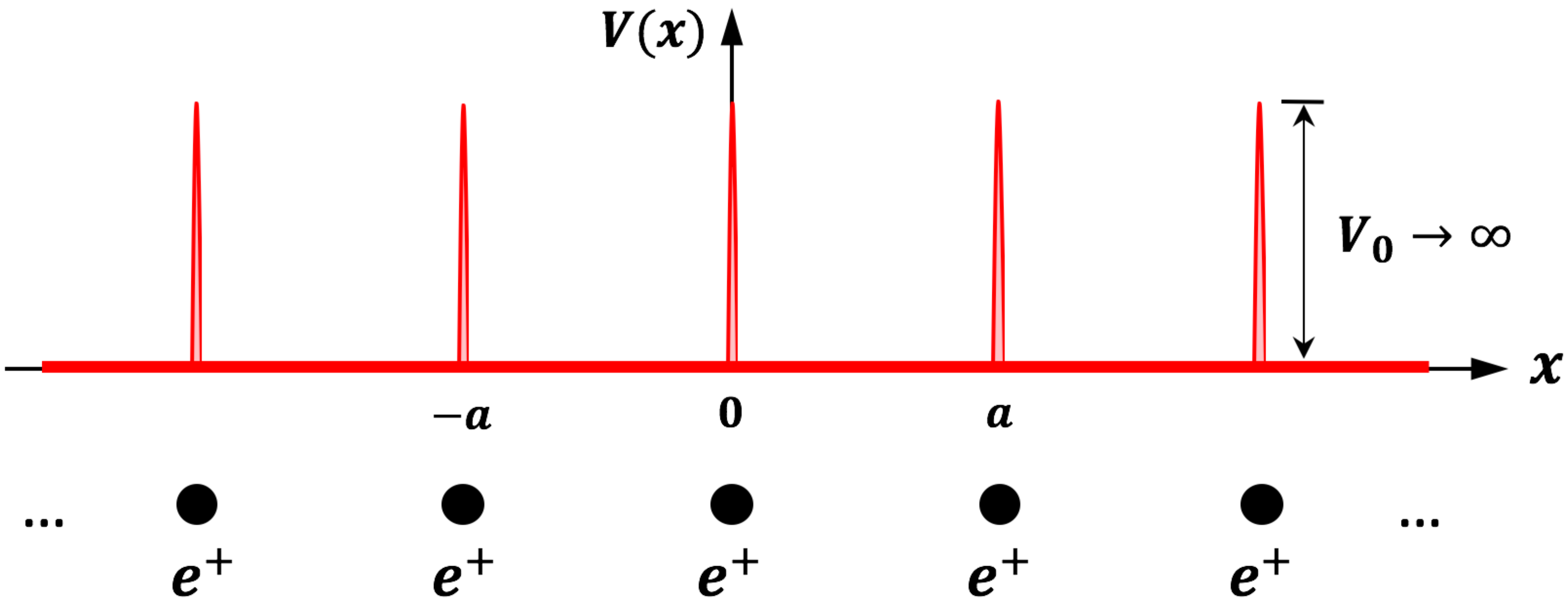




- **The Kronig-Penney Model (克勒尼希-彭尼模型)**

  - The limiting case of $\boldsymbol{\delta}$ **potential**:

$$\boxed{b \to 0, V_0 \to \infty}$$



➢ The Kronig-Penney Model (克勒尼希-彭尼模型)

❖ The limiting case of δ **potential**:

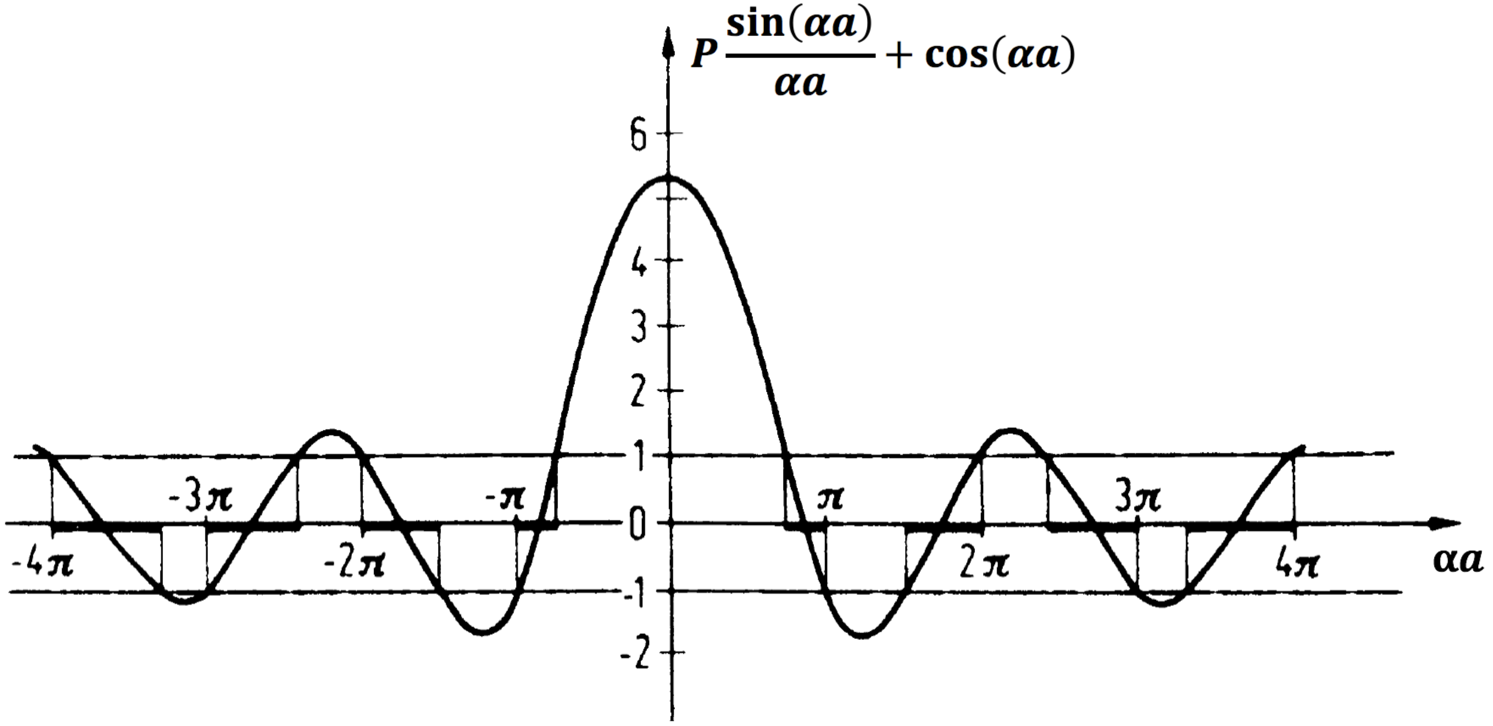
The energy dispersion:

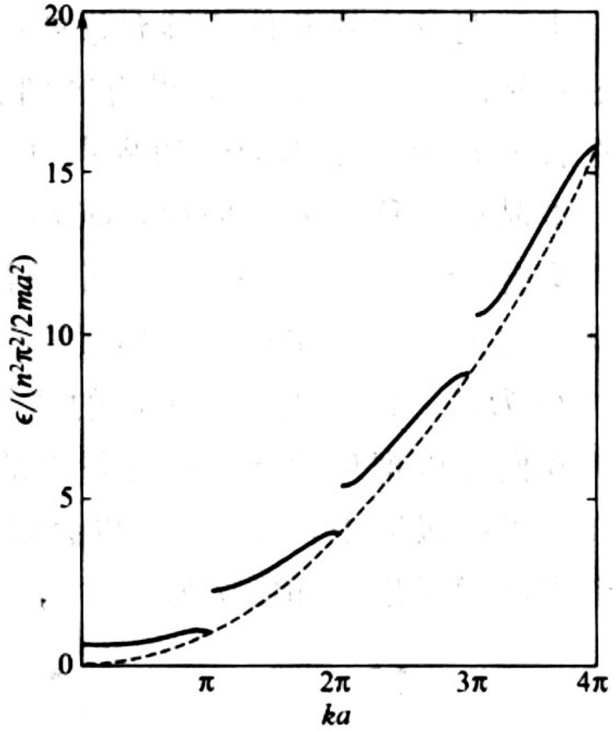
$$\boxed{P\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)=\cos(ka)}$$

$$P=\frac{ab}{2}\gamma^2 \qquad \alpha=\sqrt{\frac{2m}{\hbar^2}E} \qquad \gamma=\sqrt{\frac{2m}{\hbar^2}(V_0-E)}$$

➢ **The Kronig-Penney Model (克勒尼希-彭尼模型)**

❖ The limiting case of $\boldsymbol{\delta}$ **potential**:





Schematic diagram of $\boldsymbol{P}\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$ as a function of $\boldsymbol{\alpha a}$ (left) and the band structures (right).

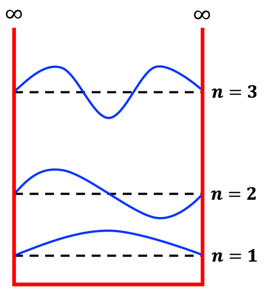
Summary (总结)

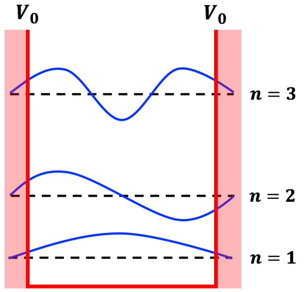
➢ Summary

❖ Potential Well:

1D **infinite** potential well

1D **finite** potential well

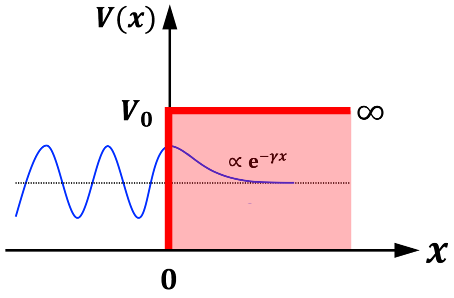




❖ Potential Barrier:

1D finite potential well

Quantum tunneling effect



❖ The Kronig-Penney model: