

1D vremenski neovisna Schrödingerova jednadžba

Slobodna čestica

$$V(x) = 0 \quad \frac{d^2\psi}{dx^2} = -k^2\psi, \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \dots \text{ravni val}$$

$$\Psi(x, t) = \psi(x)e^{-i\omega t} = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}, \quad \omega = \frac{E}{\hbar}$$

$Ae^{i(kx-\omega t)}$ val iz $x = -\infty$ u $x = +\infty$
 $Be^{-i(kx+\omega t)}$ val iz $x = +\infty$ u $x = -\infty$

Beskonačno duboka potencijalna jama

Primjer 1:

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

izvan jame: $\psi(x) = 0$

unutar jame: $\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k^2 = \frac{2mE}{\hbar^2}$, rubni uvjeti \Rightarrow kvantizacija energije

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, \quad n = 1, 2, 3, \dots$$

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2, \quad n = 1, 2, 3, \dots$$

Primjer 2:

$$V(x) = \begin{cases} 0 & \text{za } -\frac{L}{2} < x < \frac{L}{2} \\ \infty & \text{drugdje} \end{cases}$$

izvan jame: $\psi(x) = 0$

unutar jame:

parna rješenja (sa svojstvom $\psi(-x) = \psi(x)$):

$$\psi_n(x) = \sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L}, \quad n = 1, 3, 5, \dots$$

neparna rješenja (sa svojstvom $\psi(-x) = -\psi(x)$)

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, \quad n = 2, 4, 6, \dots$$

E_n ista kao u primjeru 1

Raspršenje na potencijalnim barijerama - koeficijenti refleksije i transmisije

Jednadžba kontinuiteta: $\frac{\partial P}{\partial t} + \frac{\partial j_x}{\partial x} = 0$ gdje je $P = \Psi^* \Psi$ i

$$j_x = \frac{\hbar}{2mi} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)$$

za rješenje vremenski neovisne Sch. jednadžbe $\frac{\partial P}{\partial t} = 0 \Rightarrow \frac{\partial j_x}{\partial x} = 0$.

Specijalni slučajevi:

- za $\Psi = A e^{i(kx-\omega t)}$ $\Rightarrow j_x = \frac{\hbar}{m} k |A|^2$
- za $\Psi = B e^{-i(kx+\omega t)}$ $\Rightarrow j_x = -\frac{\hbar}{m} k |B|^2$
- za $\Psi = C e^{-\kappa x} e^{-i\omega t}$ $\Rightarrow j_x = 0$

j_{in} ... val iz $x = -\infty$ u $x = +\infty$

j_{refl} ... reflektirani val u $x = -\infty$

j_{trans} ... transmitirani val u $x = +\infty$

Koeficijent (vjerojatnost) refleksije R :

$$R = \left| \frac{j_{refl}}{j_{in}} \right|$$

Koeficijent (vjerojatnost) transmisije T :

$$T = \left| \frac{j_{trans}}{j_{in}} \right|$$

Za vremenski neovisne probleme vrijedi

$$T + R = 1.$$

Step potencijal

$$V(x) = \begin{cases} 0 & \text{za } x < 0 \quad (\text{područje 1}) \\ V_0 & \text{za } x > 0 \quad (\text{područje 2}) \end{cases}$$

a) $E < V_0$

$$\begin{aligned} \text{područje 1: } \frac{d^2\psi}{dx^2} &= -k^2\psi, & k^2 &= \frac{2mE}{\hbar^2} \\ \text{područje 2: } \frac{d^2\psi}{dx^2} &= \kappa^2\psi, & \kappa^2 &= \frac{2m(V_0 - E)}{\hbar^2}, \quad k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2} \\ \psi_1(x) &= A \left(e^{ikx} - \frac{\kappa + ik}{\kappa - ik} e^{-ikx} \right) & x < 0 \\ \psi_2(x) &= -A \frac{2ik}{\kappa - ik} e^{-\kappa x} & x > 0 \end{aligned}$$

$$R = 1, \quad T = 0$$

b) $E > V_0$

$$\begin{aligned} \text{područje 1: } \frac{d^2\psi}{dx^2} &= -k^2\psi, & k^2 &= \frac{2mE}{\hbar^2} \\ \text{područje 2: } \frac{d^2\psi}{dx^2} &= -\kappa^2\psi, & \kappa^2 &= \frac{2m(E - V_0)}{\hbar^2}, \quad k^2 - \kappa^2 = \frac{2mV_0}{\hbar^2} \\ \psi_1(x) &= A \left(e^{ikx} + \frac{k - \kappa}{k + \kappa} e^{-ikx} \right) & x < 0 \\ \psi_2(x) &= A \frac{2k}{k + \kappa} e^{i\kappa x} & x > 0 \end{aligned}$$

$$R = \left(\frac{1 - \frac{\kappa}{k}}{1 + \frac{\kappa}{k}} \right)^2, \quad T = 1 - R = \frac{4 \frac{\kappa}{k}}{\left(1 + \frac{\kappa}{k} \right)^2} \quad \frac{\kappa}{k} = \sqrt{1 - \frac{V_0}{E}}$$

Pravokutna barijera

$$V(x) = \begin{cases} 0 & \text{za } x < 0 \quad (\text{područje 1}) \\ V_0 & \text{za } 0 < x < L \quad (\text{područje 2}) \\ 0 & \text{za } x > L \quad (\text{područje 3}) \end{cases}$$

a) $E < V_0$

područje 1 i 3: $\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k^2 = \frac{2mE}{\hbar^2}$

područje 2: $\frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}, \quad k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}, \quad x < 0$$

$$\psi_2(x) = Ce^{\kappa x} + De^{-\kappa x}, \quad 0 < x < L$$

$$\psi_3(x) = Fe^{ikx}, \quad x > L$$

$$\frac{1}{T} = 1 + \frac{1}{4} \frac{V_0^2}{E(V_0 - E)} \sinh^2(\kappa L), \quad R = 1 - T$$

b) $E > V_0$

područje 1 i 3: $\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k^2 = \frac{2mE}{\hbar^2}$

područje 2: $\frac{d^2\psi}{dx^2} = -\kappa^2\psi, \quad \kappa^2 = \frac{2m(E - V_0)}{\hbar^2}, \quad k^2 - \kappa^2 = \frac{2mV_0}{\hbar^2}$

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}, \quad x < 0$$

$$\psi_2(x) = Ce^{i\kappa x} + De^{-i\kappa x}, \quad 0 < x < L$$

$$\psi_3(x) = Fe^{ikx}, \quad x > L$$

$$\frac{1}{T} = 1 + \frac{1}{4} \frac{V_0^2}{E(E - V_0)} \sin^2(\kappa L), \quad R = 1 - T$$

Pravokutna jama tj. konačna potencijalna jama

Primjer 1:

$$V(x) = \begin{cases} V_0 & \text{za } x < 0 \quad (\text{područje 1}) \\ 0 & \text{za } 0 < x < L \quad (\text{područje 2}) \\ V_0 & \text{za } x > L \quad (\text{područje 3}) \end{cases}$$

a) $E < V_0$

područje 1 i 3: $\frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \boxed{\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}}$

područje 2: $\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \boxed{k^2 = \frac{2mE}{\hbar^2}}, \quad k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$

$$\psi_1(x) = Ae^{\kappa x}, \quad x < 0$$

$$\psi_2(x) = Ce^{ikx} + De^{-ikx}, \quad 0 < x < L$$

$$\psi_3(x) = Ge^{-\kappa x}, \quad x > L$$

vezana stanja, uvjet kvantizacije energije: $\tan kL = \frac{2k\kappa}{k^2 - \kappa^2}$

b) $E > V_0$

područje 1 i 3: $\frac{d^2\psi}{dx^2} = -\kappa^2\psi, \quad \boxed{\kappa^2 = \frac{2m(E - V_0)}{\hbar^2}}$

područje 2: $\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \boxed{k^2 = \frac{2mE}{\hbar^2}}, \quad k^2 - \kappa^2 = \frac{2mV_0}{\hbar^2}$

$$\psi_1(x) = Ae^{i\kappa x} + Be^{-i\kappa x}, \quad x < 0$$

$$\psi_2(x) = Ce^{ikx} + De^{-ikx}, \quad 0 < x < L$$

$$\psi_3(x) = Fe^{-i\kappa x}, \quad x > L$$

$$\boxed{\frac{1}{T} = 1 + \frac{1}{4} \frac{V_0^2}{E(E - V_0)} \sin^2(kL), \quad R = 1 - T}$$

Primjer 2:

$$V(x) = \begin{cases} 0 & \text{za } x < 0 \text{ (područje 1)} \\ -V_0 & \text{za } 0 < x < L \text{ (područje 2)} \\ 0 & \text{za } x > L \text{ (područje 3)} \end{cases}$$

a) $E < 0$

isto kao u primjeru 1 uz zamjenu $E \rightarrow V_0 - E$

b) $E > 0$

isto kao u primjeru 1 uz zamjenu $E \rightarrow E + V_0$

Primjer 3:

$$V(x) = \begin{cases} 0 & \text{za } x < -L/2 \text{ (područje 1)} \\ -V_0 & \text{za } -L/2 < x < L/2 \text{ (područje 2)} \\ 0 & \text{za } x > L/2 \text{ (područje 3)} \end{cases}$$

a) $E < 0$

slično primjeru 1 uz zamjenu $E \rightarrow V_0 - E$, a analogno kao u slučaju bekonačne potencijalne jame postoji parna i neparna rješenja

$$\psi_1(x) = Ae^{\kappa x} \quad x < -L/2$$

$$\psi_2(x) = \begin{cases} C_+ \cos kx & -L/2 < x < L/2 \\ C_- \sin kx & \end{cases}$$

$$\psi_3(x) = Ge^{-\kappa x} \quad x > L/2$$

uvjeti kvantizacije:

$$\tan(\kappa L/2) = \frac{k}{\kappa} \quad \text{parna rješenja}$$

$$\cot(\kappa L/2) = -\frac{k}{\kappa} \quad \text{neparna rješenja}$$

Harmonički oscilator

$$V(x) = \frac{Kx^2}{2}, \quad K = m\omega_O^2$$

vezana stanja:

$$\psi_n(x) = A_n H_n(\xi) e^{-\frac{\xi^2}{2}}, \quad \xi = \sqrt{\frac{m\omega_O}{\hbar}} x, \quad n = 0, 1, 2, \dots$$

$$A_n = \sqrt{\sqrt{\frac{m\omega_O}{\hbar\pi}} \frac{1}{2^n n!}}$$

kvantizirana energija

$$E_n = \hbar\omega_O \left(n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots$$

$H_n \dots$ n-ti Hermiteov polinom

- relacije ortonormiranosti

$$\int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) e^{-\xi^2} d\xi = \delta_{nm} \sqrt{\pi} 2^n n!$$

- rekurzione formule

$$\begin{aligned} H_{n+1}(\xi) &= 2\xi H_n(\xi) - 2n H_{n-1}(\xi), \quad n \geq 1 \\ H'_n(\xi) &= 2n H_{n-1}(\xi), \quad n \geq 1 \end{aligned}$$

- nekoliko prvih Hermiteovih polinoma

$$\begin{aligned} H_0 &= 1 \\ H_1 &= 2\xi \\ H_2 &= 4\xi^2 - 2 \\ H_3 &= 8\xi^3 - 12\xi \\ &\dots \end{aligned}$$