Bariéra 1

21.3.

ŠR: $\hat H \psi = E \psi$ $\hat H = \hat T + \hat V$

$\hat T \psi = E \psi$ ↳ $\hat V = 0$

$$\hat T = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

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

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2Em}{\hbar^2}\psi(x)$$

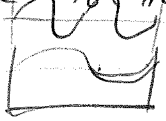
$$\psi(x) = c\, e^{\pm i\frac{\sqrt{2Em}}{\hbar}x}$$

set $E = \frac{\hbar^2 k^2}{2m} \to \frac{\sqrt{2Em}}{\hbar} = \frac{\sqrt{2\frac{\hbar^2k^2}{2m}m}}{\hbar} = k$

$\to \psi(x) = c\, e^{\pm ikx}$

disperzní relace pro volnou částici

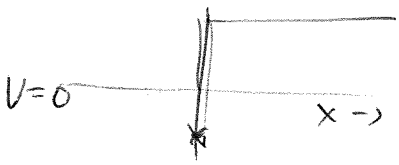
k - vlnový vektor



← ~~k = 2k_1~~ $k = 2k_1$

← $k = k_1$

← $k = 0$



$$(\hat T + \hat V_+)\psi(x) = E\psi(x)$$

pro $x>0$: $\hat T\psi(x) = (E - V_+)\psi(x)$

$(E - V_+) \geq 0$

↓

$\psi(x) = c\, e^{\pm ik'x}$

$$k' = \frac{\sqrt{2(E-V_+)m}}{\hbar}$$

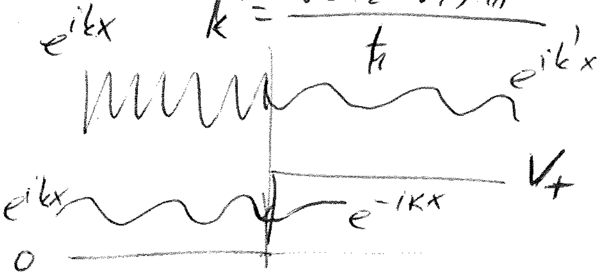
$(E - V_+) < 0$

↓

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

$$\psi(x) = c\, e^{\pm \kappa x}$$

$$\kappa = \frac{\sqrt{2|E-V_+|m}}{\hbar}$$

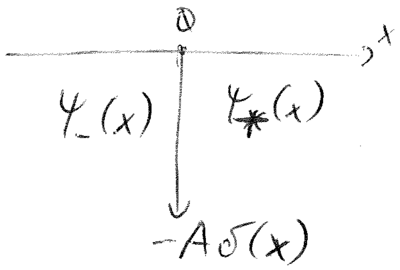


- sešívací podmínky – fce musí být hladká při konečné změně potenciálu

$$\psi_+(0) = \psi_-(0)$$

$$\psi'_+(0) = \psi'_-(0)$$

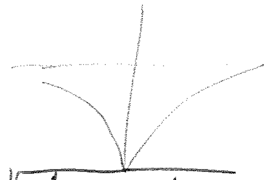
1D δ potenciál



• E částice nižší než 0:

$$\psi_+ = N e^{-kx}$$

$\boxed{2.1}$ $$\psi_- = N e^{kx}$$



$$k = \frac{\sqrt{2|E - V_+|m}}{\hbar}$$

$$V_+ = 0 \Rightarrow \frac{\sqrt{-2Em}}{\hbar} = k$$

$\boxed{2.2}$ integrace Šr.

$$T\psi + V\psi = E\psi$$

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

$$\int_{-\varepsilon}^{+\varepsilon} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)\,dx - A\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)\,dx = E\int_{-\varepsilon}^{\varepsilon}\psi(x)\,dx$$

$$-\frac{\hbar^2}{2m}\left[\frac{d}{dx}\psi(\varepsilon) - \frac{d}{dx}\psi(-\varepsilon)\right] - A\psi(0) = 0$$

$$\frac{d\psi_+(\varepsilon)}{dx} - \frac{d\psi(-\varepsilon)}{dx} = -\frac{2mA}{\hbar^2}\psi(0)$$

$$-\frac{\sqrt{-2Em}}{\hbar}\psi(\varepsilon) - \frac{\sqrt{-2Em}}{\hbar}\psi(\varepsilon) = -\frac{2mA}{\hbar^2}\psi(0)$$

$$\sqrt{-2Em} = \frac{mA}{\hbar}$$

$$-2Em = \frac{m^2A^2}{\hbar^2}$$

$$E = -\frac{mA^2}{2\hbar^2} \quad \text{OK} \quad \to \psi = N e^{-|x|\frac{\sqrt{-2\left(-\frac{mA^2}{2\hbar^2}\right)m}}{\hbar}} = N e^{-|x|\frac{mA}{\hbar^2}}$$

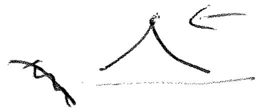
Normalizace

$$\frac{1}{2} = \int_0^\infty N^2 e^{-2kx}\,dx = N^2\frac{1}{-2k}\left[e^{-2kx}\right]_0^\infty = \frac{N^2}{2k} = \frac{1}{2} \Rightarrow N = \sqrt{k}$$

$$\Rightarrow \psi = \sqrt{k}\, e^{-|x|k} = \frac{\sqrt{mA}}{\hbar} e^{-|x|\frac{mA}{\hbar^2}}$$

$$k = \frac{\sqrt{-2Em}}{\hbar} = \cancel{\sqrt{-2(}}\ \frac{mA}{\hbar^2}$$

$A \uparrow\downarrow$?

 ← cusp, změna potenciálu nekonečná!

3. Rotátor $+A\cos(\phi)$

UKM-2013-T

str. 3

$\boxed{3.1}$ $\langle n|H|n\rangle$

$$= \int_0^{2\pi} \frac{1}{\sqrt{2\pi}} e^{-in\phi} \left(-\frac{\hbar^2}{2I}\right) \frac{d^2}{d\phi^2} \frac{1}{\sqrt{2\pi}} e^{in\phi} d\phi$$

$$= -\frac{\hbar^2}{2I} \frac{1}{2\pi} \int_0^{2\pi} e^{-in\phi} (in)^2 e^{in\phi} d\phi$$

$$= +\frac{\hbar^2}{2I} \frac{1}{2\pi} (+n^2)\, 2\pi$$

$$= \frac{\hbar^2 n^2}{2I}$$

$$\hat{H}\psi_n(\phi) = E_n \psi_n(\phi): \quad -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2}\frac{1}{\sqrt{2\pi}} e^{in\phi} = -\frac{\hbar^2}{2I}(in)^2 \frac{1}{\sqrt{2\pi}} e^{in\phi}$$

$$= \frac{\hbar^2 n^2}{2I} \frac{1}{\sqrt{2\pi}} e^{in\phi} = \frac{\hbar^2 n^2}{2I} \psi_n(\phi)$$

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2} + A\cos(\phi)$$

$\boxed{3.2}$

$$\hat{H}\psi_n(\phi) = \left[-\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2} + A\cos(\phi)\right]\frac{1}{\sqrt{2\pi}} e^{in\phi} =$$

$$= \frac{\hbar^2 n^2}{2I}\frac{1}{\sqrt{2\pi}} e^{in\phi} + A\cos(\phi)\frac{1}{\sqrt{2\pi}} e^{in\phi} \neq \lambda \frac{1}{\sqrt{2\pi}} e^{in\phi}$$

$\boxed{3.3}$ $V = A\cos(\phi) = \frac{A}{2}\left[e^{i\phi} + e^{-i\phi}\right]$

$$H = \begin{array}{c} -2 \\ -1 \\ 0 \\ 1 \\ 2 \end{array} \begin{pmatrix} \frac{2\hbar^2}{I} & & & & \\ & \frac{\hbar^2}{2I} & & 0 & \\ & & 0 & & \\ & 0 & & \frac{\hbar^2}{2I} & \\ & & & & \frac{2\hbar^2}{I} \end{pmatrix} + \begin{pmatrix} 0 & A/2 & 0 & & \\ A/2 & 0 & A/2 & 0 & \\ & A/2 & 0 & A/2 & 0 \\ & & A/2 & 0 & A/2 \\ & & & A/2 & 0 \end{pmatrix} = \begin{pmatrix} \frac{2\hbar^2}{I} & A/2 & & 0 & \\ A/2 & \frac{\hbar^2}{2I} & A/2 & & \\ & A/2 & 0 & A/2 & \\ 0 & & A/2 & \frac{\hbar^2}{2I} & \\ & & & & \end{pmatrix}$$

$$H_{3\times3} = \begin{pmatrix} \frac{\hbar^2}{2I} & A/2 & 0 \\ A/2 & 0 & A/2 \\ 0 & A/2 & \frac{\hbar^2}{2I} \end{pmatrix} \rightsquigarrow \begin{pmatrix} B-\lambda & A/2 & 0 \\ A/2 & -\lambda & A/2 \\ 0 & A/2 & B-\lambda \end{pmatrix}$$

$$|\;\;| = -\lambda(B-\lambda)^2 - 2(B-\lambda)\frac{A^2}{4} = -(B-\lambda)\left[\lambda(B-\lambda) + \frac{A^2}{2}\right]$$

$$+\lambda^2 - B\lambda - A^2/2 \quad : \quad D = B^2 + 2A^2$$

$$\lambda_{1,2} = \frac{+B \pm \sqrt{B^2 + 2A^2}}{2} \overset{A \ll B}{\approx} \frac{B \pm B\sqrt{1 + \frac{2A^2}{B^2}}}{2} \approx \frac{B \pm B\left(1 + \frac{A^2}{B^2} - \frac{A^4}{2B^4}\right)}{2}$$

$$= \frac{B \pm \left[B + A^2/B - A^4/2B^3\right]}{2} \quad \begin{array}{l} B + A^2 \ldots \\ -A^2/2B + \ldots \end{array} \leftarrow \text{základní stav snižuje energii}$$

$\boxed{4}$ δ pro rotor

$\boxed{4.1}$ $\quad V = -A\delta(\phi - \pi)$

$$\langle m|V|n\rangle = \int_0^{2\pi} \frac{1}{2\pi} e^{-im\phi} \left[-A\delta(\phi-\pi)\right] e^{in\phi}\, d\phi$$

$$= \int_0^{2\pi} \frac{1}{2\pi} e^{i(n-m)\phi} (-A)\delta(\phi-\pi)\, d\phi$$

$$= -\frac{A}{2\pi} e^{i(n-m)\pi}$$

$n-m$ sudé $\to -\frac{A}{2\pi}$

liché $\to \frac{A}{2\pi}$

$\to$ nekonečná matice (OK, v pořádku)

$\boxed{4.2}$ $\quad \int_{-\varepsilon}^{\varepsilon} \frac{1}{2\pi} e^{i(n-m)\phi} (-A)\, d\phi$

$e^{i(n-m)\phi} = \cos[(n-m)\phi] + i\sin[(n-m)\phi]$

$\uparrow$ sudá, $\uparrow$ lichá

$$\int_{-\varepsilon}^{\varepsilon} \frac{1}{2\pi} \cos[(n-m)\phi](-A)\, d\phi$$

$n \neq m$ $\quad = -\frac{A}{2\pi}\frac{1}{(n-m)}\left[\sin[(n-m)\phi]\right]_{-\varepsilon}^{\varepsilon}$ $\qquad \sin(x) \approx x$

$$\approx -\frac{A}{2\pi}\frac{1}{n-m}\left[(n-m)\varepsilon - [(n-m)(-\varepsilon)]\right]$$

$= -\frac{A}{2\pi} 2\varepsilon + \text{H.O.T.}$ $\quad \leftarrow$ měly by i klesat pro $|n-m|$ rostoucí...

$n = m \to -\frac{2\varepsilon A}{2\pi}$ $\quad$ ~~potenciál~~ nulicové pravý není než $u\delta(\phi)$