- čas sch. eq.
- bariéra
- δ jáma
- čas matice!

2022 - UKM - T4. 1

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \quad , \text{ vlastní stav } n: \ \psi(t) = \psi_n(\phi) e^{-iE_n t/\hbar}$$

$$\Rightarrow \ i\hbar \frac{\partial \psi_n}{\partial t} = \mathcal{E}_n \psi_n$$

$$\frac{\partial \psi_n}{\partial t} = -\frac{i\mathcal{E}_n}{\hbar}\psi_n \ \to \text{ čas } e^{-\frac{i\mathcal{E}_n}{\hbar}t}$$

kombinace stavů $\psi = \sum_n c_n \psi_n$

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \ \to \ i\hbar \sum_n c_n \frac{\partial \psi_n}{\partial t} = \sum_n \mathcal{E}_n c_n \psi_n$$

c_n nezávislé $\to$?(enough?) $\frac{\partial \psi_n}{\partial t} = -\frac{i\mathcal{E}_n}{\hbar}\psi_n \ \to \ \psi_n(t) = \psi_n(\phi) e^{-\frac{i\mathcal{E}_n t}{\hbar}}$

$$\psi(t) = \sum_n c_n \psi_n(\phi) e^{-\frac{i\mathcal{E}_n t}{\hbar}}$$

$$\psi(0) = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2\pi}} + \frac{e^{i\phi}}{\sqrt{2\pi}}\right) \Rightarrow \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$H = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial \phi^2} \qquad \hat{H}|0\rangle = 0 \qquad \hat{H}|1\rangle = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial \phi^2}\frac{1}{\sqrt{2\pi}}e^{i\phi} = \underbrace{\frac{\hbar^2}{2I}}_{\mathcal{E}_1}\underbrace{\frac{1}{\sqrt{2\pi}}e^{i\phi}}_{|1\rangle}$$

$$\psi(t) = \frac{1}{\sqrt{2}}\left(|0\rangle e^{0} + |1\rangle e^{-\frac{i\hbar^2 t}{2I\hbar}}\right) = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle e^{-\frac{i\hbar t}{2I}}\right)$$

$$= \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2\pi}} + \frac{1}{\sqrt{2\pi}}e^{i\phi - \frac{i\hbar}{2I}t}\right)$$

$$\rho = \psi^*(t)\psi(t) = \frac{1}{2}\left(\frac{1}{\sqrt{2\pi}} + \frac{1}{\sqrt{2\pi}}e^{-i\phi + \frac{i\hbar}{2I}t}\right)\left(\frac{1}{\sqrt{2\pi}} + \frac{1}{\sqrt{2\pi}}e^{i\phi - \frac{i\hbar}{2I}t}\right)$$

$$= \frac{1}{2}\left(\frac{1}{2\pi} + \frac{1}{2\pi} + \frac{1}{2\pi}\left[e^{-i\phi + \frac{i\hbar}{2I}t} + e^{i\phi - \frac{i\hbar}{2I}t}\right]\right)$$

$$= \frac{1}{2}\left[\frac{1}{\pi} + \frac{1}{\pi}\cos\left(\phi - \frac{\hbar}{2I}t\right)\right] = \frac{1}{2\pi} + \frac{1}{2\pi}\cos\left(\phi - \frac{\hbar t}{2I}\right)$$

$$\int_0^{2\pi}\rho\, d\phi = \int_0^{2\pi}\left[\frac{1}{2\pi} + \underbrace{\frac{1}{2\pi}\cos\left(\phi - \frac{\hbar t}{2I}\right)}_{0}\right]d\phi = \underline{1} \quad \text{OK}$$

$$\to i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \ \to \ \psi(t) = \sum_n c_n \psi_n(\phi) e^{-\frac{i\mathcal{E}_n t}{\hbar}}$$

$$t \to -i\tau \qquad i\hbar \frac{\partial \psi_n}{-i\,\partial \tau} = \hat{H}\psi_n \ \to \ -\hbar \frac{\partial \psi_n}{\partial \tau} = \mathcal{E}_n \psi_n$$

$$\frac{\partial \psi_n}{\partial \tau} = -\frac{\mathcal{E}_n}{\hbar}\psi_n \Rightarrow \psi_n(t) = \psi_n(\phi) e^{-\frac{\mathcal{E}_n t}{\hbar}}$$

why! $\psi(t) = \sum_n c_n \psi_n$

$$\to \ \psi(t) = \sum_n c_n \psi_n(\phi) e^{-\frac{\mathcal{E}_n t}{\hbar}}$$

$$\frac{1}{\sqrt{2}}\left[|0\rangle + |1\rangle e^{-\frac{i\hbar}{2I}(-i\tau)}\right]$$

$$= \frac{1}{\sqrt{2}}\left[|0\rangle + |1\rangle e^{-\frac{\hbar\tau}{2I}}\right]$$

volná částice, bariéra,
δ-potenciál, čas. závislost stavu

• $\left(\frac{p^2}{2m}+V(x)\right)\psi(x)=E\,\psi(x)$ (x-repre.., $p=-i\hbar\frac{\partial}{\partial x}$)

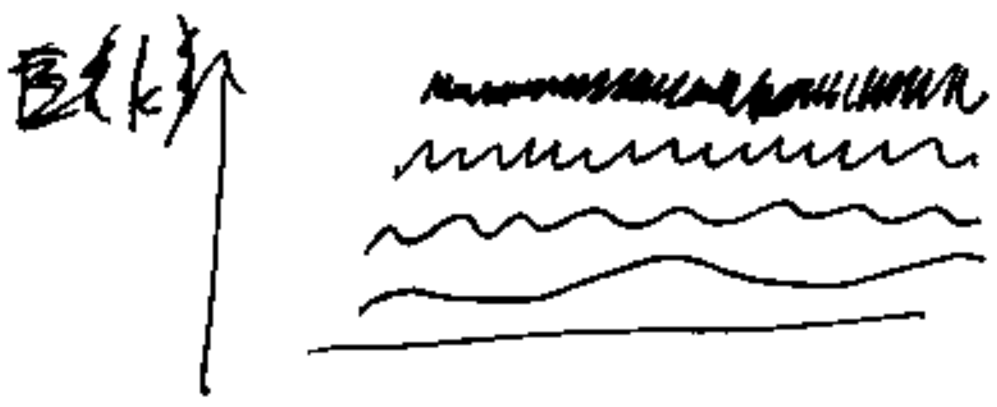
• volná částice $V(x)=\text{const}$, BÚNO: $V(x)=0$
tedy ψ se nezmění

úplně volná částice → E je vlastní parametr

→ $\frac{p^2}{2m}\psi(x)=E\,\psi(x)$

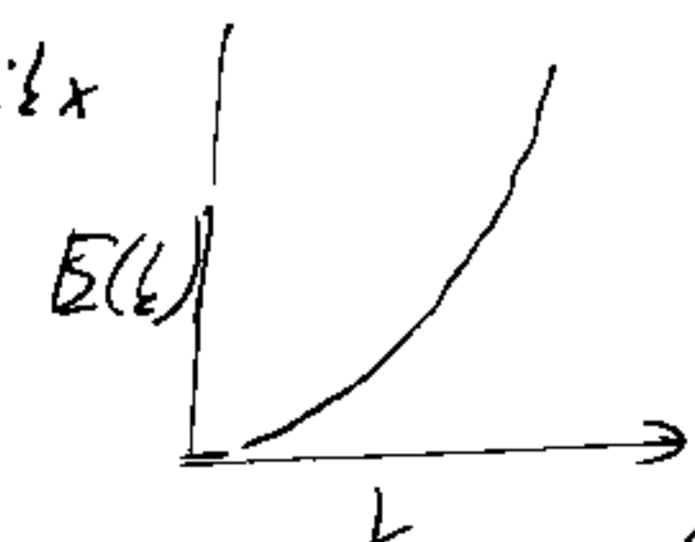
⇒ $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}=E\,\psi(x)$

uhodneme e^{ikx} → $-\frac{\hbar^2}{2m}\frac{\partial^2 e^{ikx}}{\partial x^2}=E\,e^{ikx}$

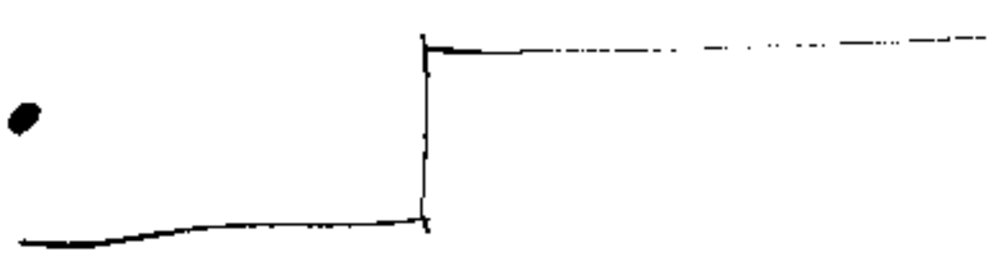


$\frac{\hbar^2k^2}{2m}e^{ikx}=E\,e^{ikx}$

⇒ $E=\frac{\hbar^2k^2}{2m}$

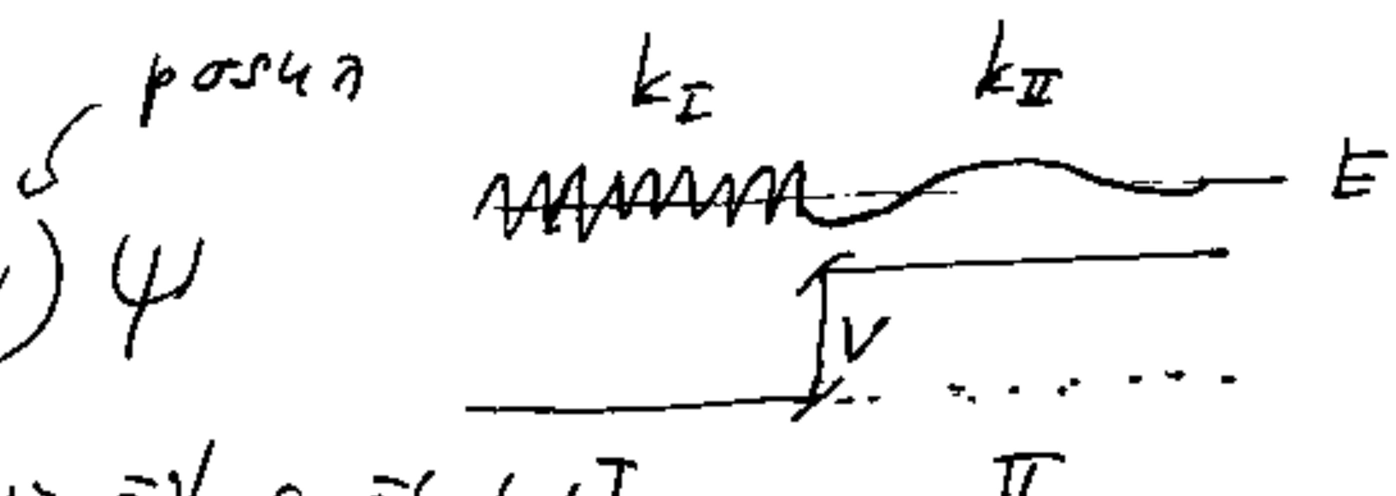


"disperzní relace"
(viďte Fyz IV)

• 

$\frac{p^2}{2m}\psi+V\{\psi\}=E\psi$

$\frac{p^2}{2m}\psi\cancel{+(V-E)\psi=0}=(E-V)\psi$



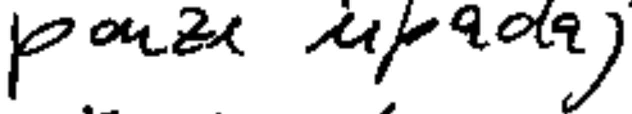
$E>V$ ⇒ změna k → je třeba řešit sešívání


→ ups, co teď? $\frac{p^2}{2m}\psi=(E-V)\psi$
$<0\to-\varepsilon$

$\frac{p^2}{2m}\psi=-\varepsilon\psi$

$-\frac{\hbar^2\partial^2\psi}{2m\,\partial x^2}=-\varepsilon\psi$

$\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=\varepsilon\,\psi$

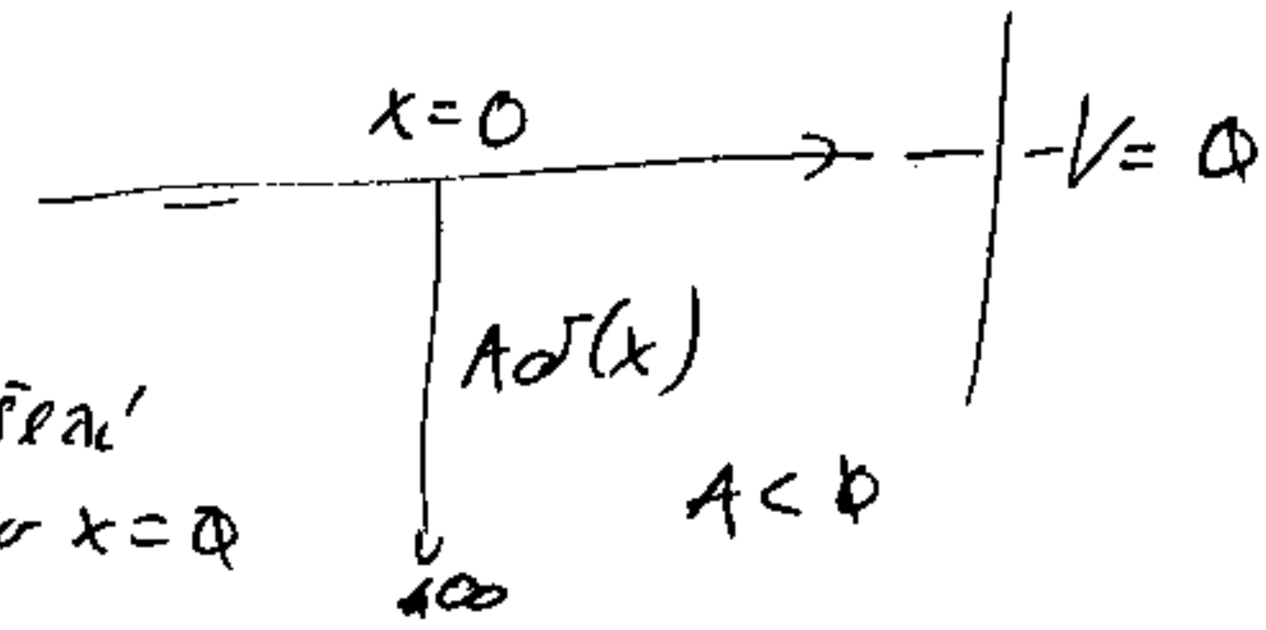
→ $e^{\pm kx}$; pokud je bariéra  pouze ubývající řešení


ubývající a rostoucí

UKM 2021
VI - 2

δ(x) potenciál, vázaný stav

$$\left(\frac{p^2}{2m} + A\delta(x)\right)\psi(x) = E\,\psi(x)$$

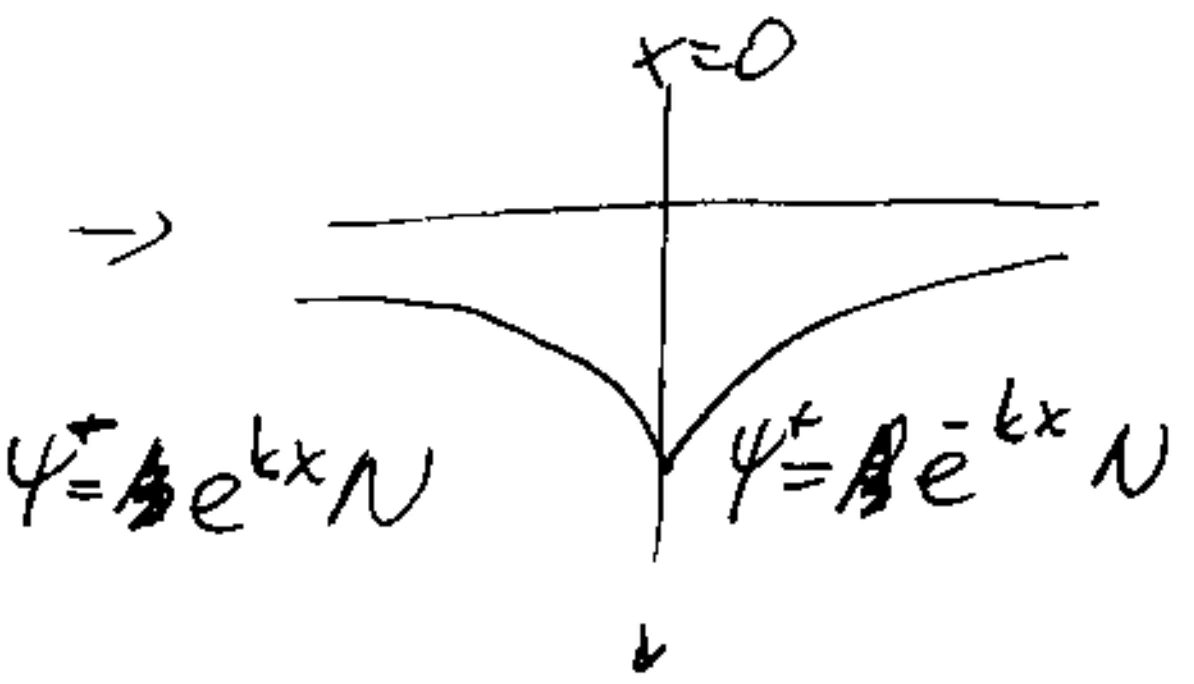


• vázaný stav → $E < 0$ → $e^{\pm kx}$ řešení mimo $x=0$

• v $x=0$ $\quad \frac{p^2}{2m}\psi = -A\delta(x)\psi(x)$

$$+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = +A\delta(x)\psi(x)$$

– nekonečná 2. derivace
– skok v 1. derivaci
ψ stále musí být spojitá



$$\rightarrow \psi^-(0) = \psi^+(0)$$

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

„δ(x) má smysl při integraci"

$$-\int_{-\varepsilon}^{\varepsilon}\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \int_{-\varepsilon}^{\varepsilon}A\delta(x)\psi(x) = \int_{-\varepsilon}^{\varepsilon}E\,\psi(x) \qquad \varepsilon \to 0$$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial\psi}{\partial x}\right]_{-\varepsilon}^{\varepsilon} + A\psi(0) \qquad \underset{\varepsilon E\psi(0)}{\rightarrow 0}$$

$$\rightarrow \frac{\hbar^2}{2m}\left[\psi_+^{(\prime)}(0) - \psi_-^{\prime}(0)\right] = A\psi(0)$$

$$\frac{\hbar^2}{2m}\left[N(-k)e^{-kx} - Nk\,e^{kx}\right] = AN\,e^{0} \qquad A<0$$

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

$$\rightarrow k = -\frac{Am}{\hbar^2} = \frac{|A|m}{\hbar^2}$$

Normalizace

$$N^2\int_0^\infty e^{-\frac{2|A|m}{\hbar^2}x} = \frac{N^2\hbar^2}{2|A|m}\left[e^{-\frac{2|A|m}{\hbar^2}x}\right]_{0\to 1}^{\infty\to 0} = \frac{N^2\hbar^2}{2|A|m} = \frac{1}{2}$$

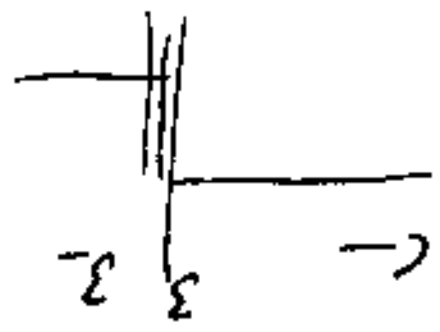
jedna polovina intervalu

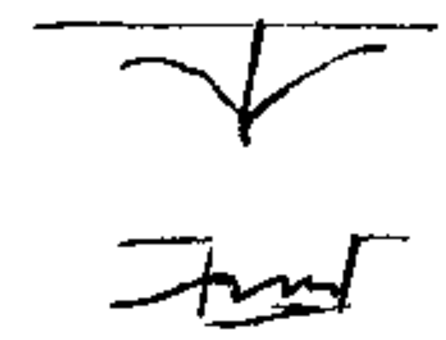
$$\Rightarrow N = \frac{\sqrt{|A|m}}{\hbar}$$

$$\rightarrow \psi = \frac{\sqrt{|A|m}}{\hbar}\,e^{-k|x|} \qquad k = \frac{|A|m}{\hbar^2}$$

• větší hmotnost → užší ψ ✓
• menší |A| → širší ψ ⟺ malé masy ✓

$$-\int_{-\varepsilon}^{+\varepsilon}\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\int_{-\varepsilon}^{\varepsilon}V(x)\psi(x)=\int_{-\varepsilon}^{\varepsilon}E\,\psi(x) \quad \hookrightarrow 0$$





$\to \varepsilon V^+\psi + \varepsilon V^-\psi$
$\to 0$ pro $\varepsilon \to 0$ → hladká $\psi(x)$

$\delta(\phi - \pi)$ potenciál pro periodickou částici / rotor

$\psi_n = \frac{1}{\sqrt{2\pi}}e^{in\phi}$, $n \in \mathbb{Z}$, $\phi \in (0, 2\pi)$

maticové elementy pro $V = A\,\delta(\phi - \pi)$?

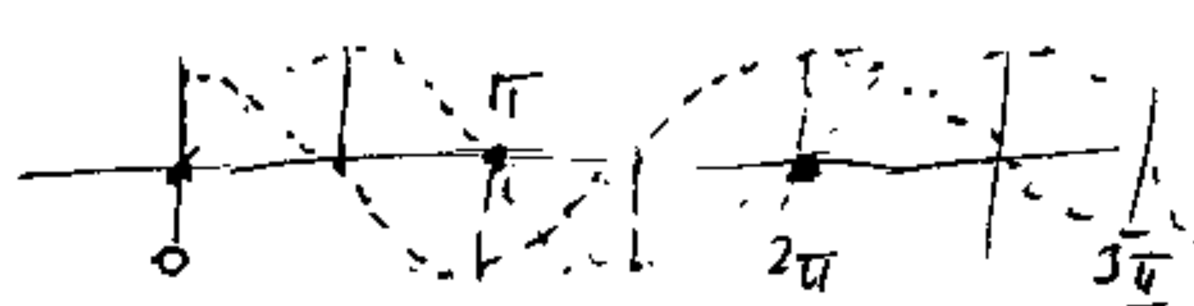
$$\langle n|V|m\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-in\phi} A\,\delta(\phi-\pi)\,e^{im\phi}\,d\phi$$

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

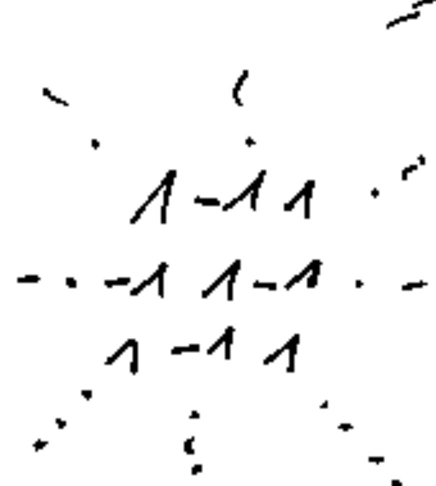
$$= \frac{A}{2\pi}\int_0^{2\pi}\delta(\phi-\pi)\left[\cos[(m-n)\phi] + i\sin[(m-n)\phi]\right]d\phi$$

$$= \frac{A}{2\pi}\left[\cos((m-n)\pi) + i\sin[(m-n)\pi]\right]$$

$= 0$

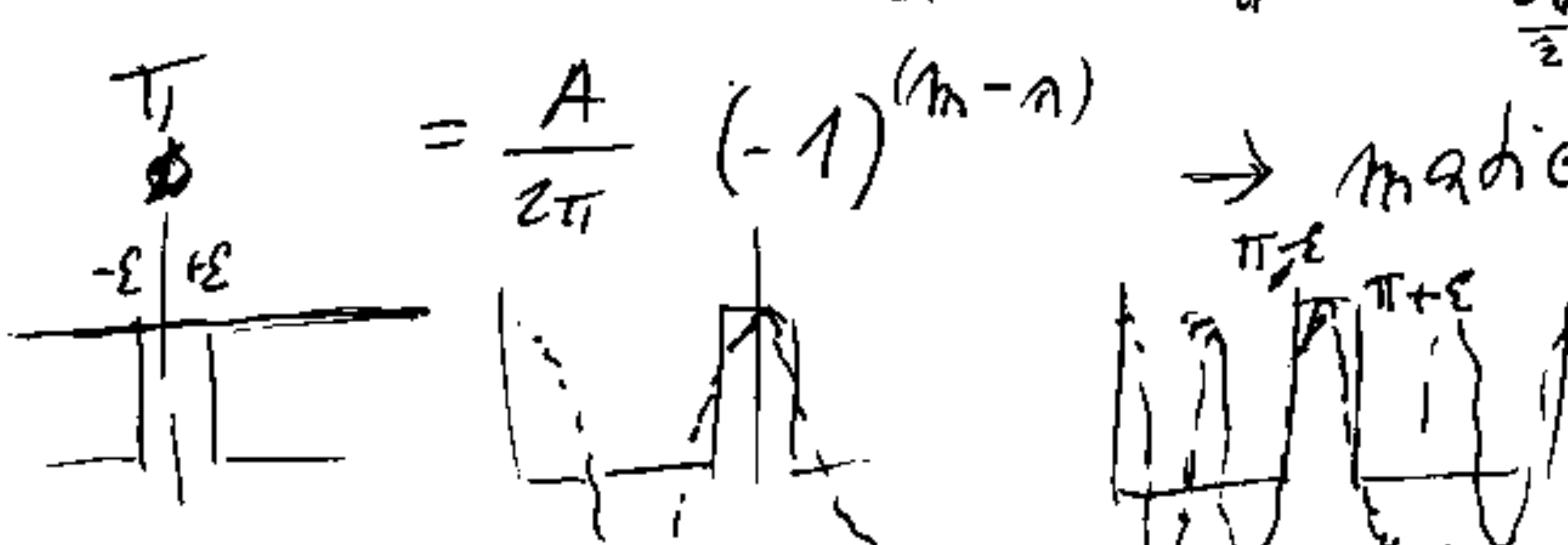


$$= \frac{A}{2\pi}(-1)^{(m-n)} \to \text{matice plná}$$

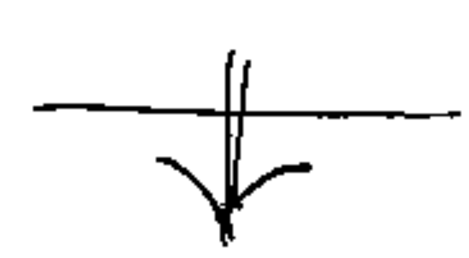


→ přispívají všechny ϕ_n k ψ_0, ψ_0 má cusp

c.f.



$m-n=0$ $\quad$ $m-n=2$ $\quad$ $m-n=4$



$$\int_{\pi-\varepsilon}^{\pi+\varepsilon}\cos[(m-n)\phi]\,d\phi = -\frac{\sin[(m-n)\phi]}{(m-n)}\Bigg|_{\pi-\varepsilon}^{\pi+\varepsilon}$$

$m \neq n$

→ maticové elementy se snižují pro $|(m-n)|$ rostoucí

→ není cusp

~~cosφ~~ $\hat{B} = \sin\phi$ - matrix form?

$\Rightarrow$ simpler $|n\rangle = \frac{1}{\sqrt{2\pi}} e^{in\phi}$ $\phi \in (0, 2\pi)$

$\hat{B} = \sin\phi = \frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right)$, $\langle n|\hat{B}|n\rangle = \int_0^{2\pi} e^{-in\phi} \underbrace{\frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right) e^{in\phi}}_{=1} d\phi = 0$

$$\langle m|\hat{B}|n\rangle = \int_0^{2\pi} \frac{1}{2\pi} e^{-im\phi} \frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right) e^{in\phi}\, d\phi$$

$$= \frac{1}{4\pi i} \int_0^{2\pi} \Big[\underbrace{e^{i(n-m+1)\phi}}_{n-m+1=0} - \underbrace{e^{i(n-m-1)\phi}}_{n-m-1=0}\Big] d\phi$$

$\cancel{= \frac{n}{4\pi i} \int_0^{2\pi}}$ $n = m-1$ $n = m+1$ $\to \int_0^{2\pi} e^{i0\phi} d\phi = 2\pi$

$$= \frac{1}{2i}\left[\delta_{n,m-1} - \delta_{n,m+1}\right]$$

m \ n	-2	-1	0	1	2
-2	0	$-\frac{1}{2i}$			
-1	$\frac{1}{2i}$	0	$-\frac{1}{2i}$		
0		$\frac{1}{2i}$	0	$-\frac{1}{2i}$	
1			$\frac{1}{2i}$	0	$-\frac{1}{2i}$
2				$\frac{1}{2i}$	0

$H\Psi_n = $

Hamiltonian: $-\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2} \overbrace{\frac{1}{\sqrt{2\pi}} e^{in\phi}}^{\Psi_n} =$

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

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

$= E_n \Psi$

$$\mathbb{H} = \begin{pmatrix} \frac{4\hbar^2}{2I} & & & & \\ & \frac{\hbar^2}{2I} & & & \\ & & 0 & & \\ & & & \frac{\hbar^2}{2I} & \\ & & & & \frac{4\hbar^2}{2I} \end{pmatrix}$$

- solution?