- vlny, PBC,
- E_{kin} vs p vl. stavy -> jáma, + sin φ pert + $e^{i(\ldots)\phi}$ ↘ čas. vývoj, $\langle p \rangle$
- $E_{pot} + E_{kin}$ – LHO (DÚ) -> různé ω – variace
- 2D/3D – excit E pro e^- v f-centr
- excit e^- v lin. polyens

—.—.—.—

- částice letící prostorem $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}$ (v 1D)
- periodické okrajové podmínky $\psi_n(x) = N e^{ik_n x}$ (v 1D)
  - částice se pohybuje v omezeném prostoru $(0, L)$ s opakováním
  - musí platit $\psi(x+L) = \psi(x)$ $(\forall x)$ $-L$ 0 L $2L$ $3L$

$$N e^{ik_n(x+L)} = N e^{ik_n x}$$

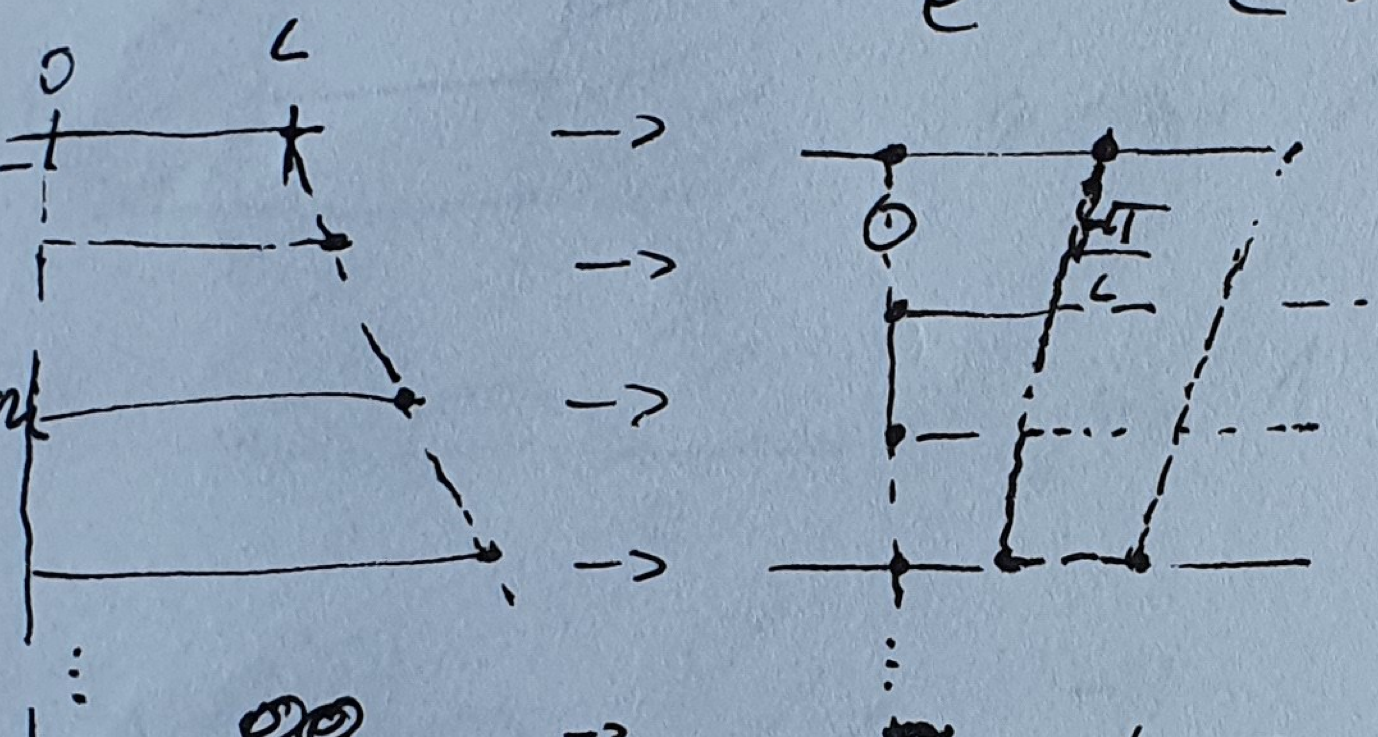
$$N e^{ik_n x} e^{ik_n L} = N e^{ik_n x}$$

$$e^{ik_n L} = 1 \Rightarrow k_n L = 2\pi n$$

$$k_n = \frac{2\pi n}{L} \; ; n \in \mathbb{Z}$$

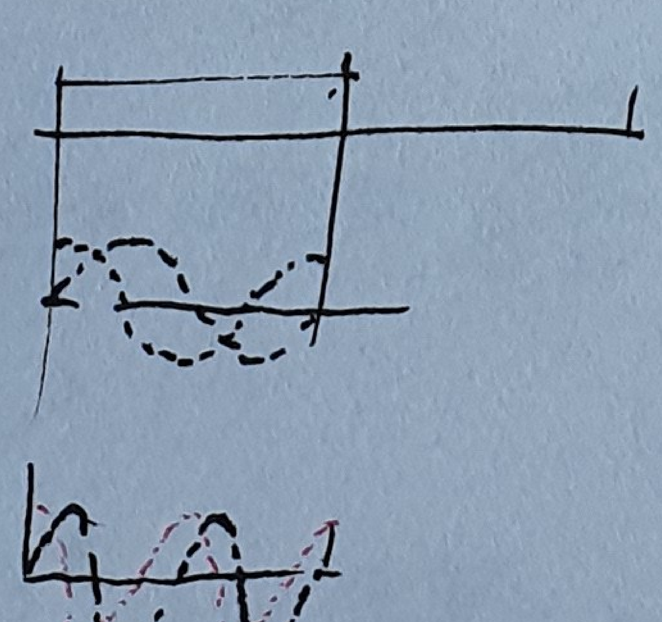
s: $0, \pm 1, \pm 2, \ldots$

zvětšuje-li jednotkovou buňku až do nekonečna



=> ~~přidá~~ vzdálenost mezi povolenými hodnotami k se snižuje, až do 0

povolená k:



0 konstanta

±1 1 celá vlna

±2 2 celé vlny

$f(x)$ ← nějaká periodická funkce, spojitá [na $(0,L)$]

$\to \frac{1}{\sqrt{L}} \sum_{n \in \mathbb{Z}} c_n e^{i\frac{2\pi n}{L}}$ ← rozložení do báze rovinných vln

≡ Fourierova transformace (diskrétní)

normování

$$N^2 \int_0^L \psi^*(x)\psi(x)\,dx = N^2 \int_0^L e^{-ikx} e^{ikx}\,dx = N^2 \int_0^L 1\,dx = N^2 L = 1$$

$$\Rightarrow N = \frac{1}{\sqrt{L}}$$

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$\boxed{V}$-2

• Mějme stav $\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$; $k_n = \frac{2\pi n}{L}$
n libovolné

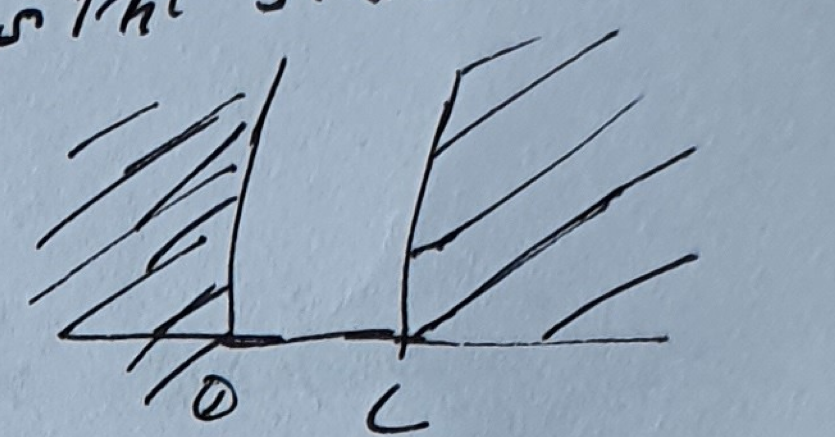
• je vlastní stav p?

$\hat{p}|n\rangle = -i\hbar \frac{\partial}{\partial x} \frac{1}{\sqrt{L}} e^{ik_n x} = -i\hbar (ik_n) \frac{1}{\sqrt{L}} e^{ik_n x} = \underbrace{\hbar k_n}_{p} \psi(x)$, je vlastní stav

• je vlastní stav $\hat{T}$? $= \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$\frac{p^2}{2m}\psi_n(x) = \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\frac{1}{\sqrt{L}} e^{ik_n x} = \frac{\hbar^2 k^2}{2m}\psi(x) = \frac{\hbar^2 4\pi^2 n^2}{2mL^2}$
← T, je vlastní stav

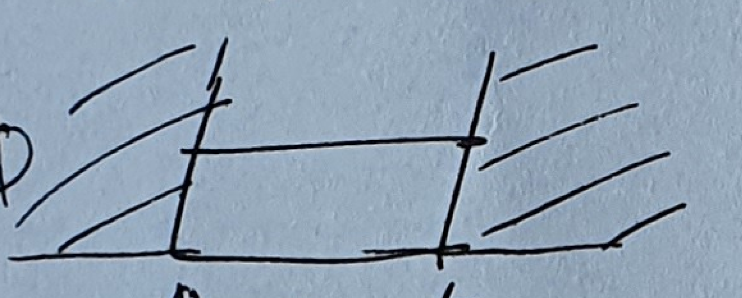
Nekonečná jáma – ~~ne~~ $V(x) \begin{cases} 0 & \text{~~mezi~~ na } (0, L) \\ \infty & \text{mimo } (0, L) \end{cases}$



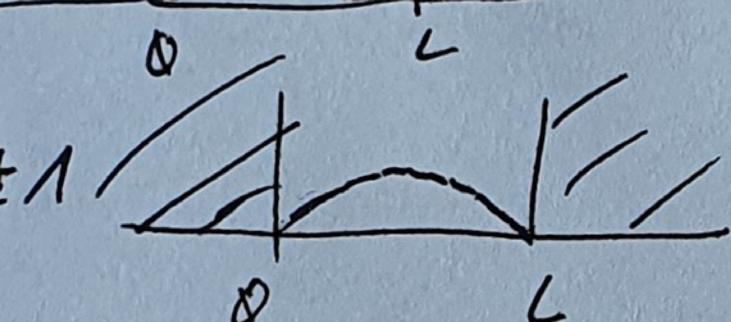
~~$\psi_n(x)$~~

$\hat{H} = \hat{T} \rightarrow \frac{1}{\sqrt{L}} e^{ik_n x}$ stále vlastní stavy

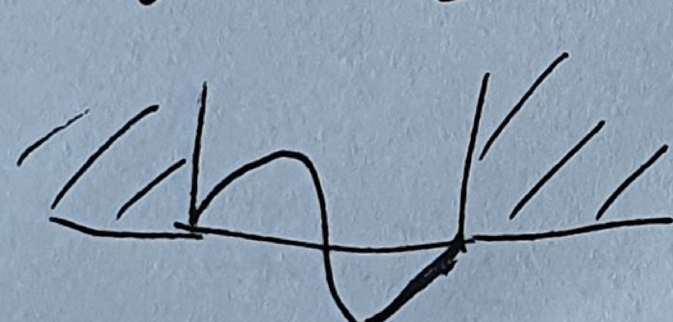
Ale $\psi_n(x) = 0$ pro $x = 0$ a $x = L$ (nová podmínka)

$n = 0$ 

není možné

$n = \pm 1$ 

jen 1 stav možný $\sin\frac{\pi x}{L}$

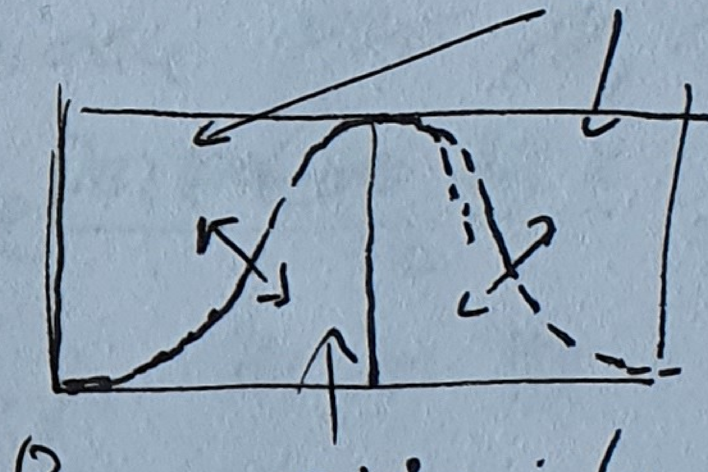
$n = 2$ 

-11- $\sin\frac{2\pi x}{L}$

⋮

• Normování: $N^2 \int_0^L \sin^2\left[\frac{n\pi x}{L}\right] dx$

$= \ldots = N^2 \frac{L}{2} \Rightarrow N = \sqrt{\frac{2}{L}}$

cos²x


sin²x

části stejné → každá 1/2 plochy
plocha 1 · L → $\frac{L}{2}$

• Vlastní stav p?

$\hat{p}|n\rangle = -i\hbar\frac{\partial}{\partial x}\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} = -i\hbar \frac{n\pi}{L}\sqrt{\frac{2}{L}} \cos\frac{n\pi x}{L}$ ~~$= -i\hbar\frac{n\pi}{L}$~~ $\neq \lambda \psi_n$

→ není vlastní stav p

• Vlastní stav $\frac{p^2}{2m}$?

$\frac{p^2}{2m}|n\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} =$

$= \frac{\hbar^2 n^2 \pi^2}{2mL^2}\psi_n(x) = E_n \psi_n(x)$

→ je vlastní stav

• závislost na L?

• závislost na n?

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IV - 7

· Mějme částici v PBC, s potenciálem $V(x) = 0$, interval $(0, L)$

→ stavy $\phi_n = \frac{1}{\sqrt{L}} \, \cancel{e^{2\pi i n}} \, e^{2\pi i \frac{x}{L} n}$

$$E = \frac{\hbar^2 \pi^2 n^2 4}{2mL^2} = \frac{\hbar^2 k_n^2}{2m} \quad ; \; k_n = \frac{2\pi n}{L}$$

· Uvažujme maticovou reprezentaci p, $H = \frac{p^2}{2m}$

→ diagonální $\begin{array}{c|c} & -1 \;\; 0 \;\; 1 \\ \hline \begin{array}{c} -1 \\ 0 \\ 1 \end{array} & \begin{bmatrix} \ddots & & & \\ & \bullet & & \\ & & \bullet & \\ & & & \ddots \end{bmatrix} \end{array}$ v obou případech.

· Uvažujme operátor $V' = A \sin\left(\frac{2\pi x}{L}\right)$, jak vypadá maticová repre.?

$$\langle m | V' | n \rangle = \int_0^L \frac{1}{\sqrt{L}} e^{-\frac{2\pi i m x}{L}} A \sin\left(\frac{2\pi x}{L}\right) \frac{1}{\sqrt{L}} e^{+\frac{2\pi i n x}{L}} dx$$

$$= \frac{1}{L} \int_0^L e^{\frac{2\pi i (n-m)x}{L}} A \sin\left(\frac{2\pi x}{L}\right) dx$$

$$= \frac{1}{L} \int_0^L e^{\frac{2\pi i (n-m)x}{L}} A \frac{1}{2i} \left(e^{\frac{2\pi i x}{L}} - e^{-\frac{2\pi i x}{L}}\right) dx$$

$$= \frac{A}{L} \frac{1}{2i} \int_0^L e^{\frac{2\pi i (n-m+1)x}{L}} - e^{\frac{2\pi i (n-m-1)x}{L}} dx$$

? ? ? ? ? ?

$\hbar m$ · integrál přes celou periodu pro n, m libovolná

· $\neq 0$ jen pro případ $e^{\frac{2\pi i \cancel{(n-m)} M x}{L}} = 1$

t.j. $M = 0$??

→ $\frac{A}{L} \frac{1}{2i} \int_0^L 1 \, dx$ | pro $n = m - 1$

$- \frac{A}{L} \frac{1}{2i} \int_0^L 1 \, dx$ | a pro $n = m + 1$

$= \frac{A}{2i}$

$n = 0 \quad m = 1$

$$\langle m | V' | n \rangle \doteq \begin{array}{c|c} & \begin{array}{ccc} -1 & 0 & 1 \end{array} \\ \hline \begin{array}{c} -1 \\ 0 \\ 1 \end{array} & \begin{bmatrix} 0 & & & & \\ \frac{A}{2i} & 0 & -\frac{A}{2i} & & 0 \\ & \frac{A}{2i} & 0 & -\frac{A}{2i} & \\ 0 & & \frac{A}{2i} & 0 & \\ & & & \frac{A}{2i} & 0 \; \ddots \\ & & & & \ddots \end{bmatrix} \end{array}$$

jáma s čísly

- Uvažujme e^- v jámě o šíři L
- Jaká je energie základního stavu a první excitační energie?
- Pro jakou šíři L deexcitaci uvidíme?

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2 m L^2}$$

můžeme uvažovat atomové jednotky $\hbar = m_e = e = 1$

- délka $a_B \doteq 0.529$ Å $\doteq 0.0529$ nm (klasický poloměr vodíku)

$\rightarrow$ energie $1\,\mathrm{Ha} = 2\,R_y \doteq 27.2\,\mathrm{eV}$

Rydberg - energie základního stavu vodíku

$$E_1 = \frac{\pi^2}{2L^2}$$

$$E_2 = \frac{\pi^2 4}{2L^2}$$

$$\Delta E = E_2 - E_1 = \frac{\pi^2}{2L^2}(4-1) = \frac{3\pi^2}{2L^2}$$

$\rightarrow$ s šíří jámy klesá excitační energie

$$E_p = \frac{hc}{\lambda}$$

v a.u.: $h = 2\pi\hbar = 2\pi$

$c \doteq 137$

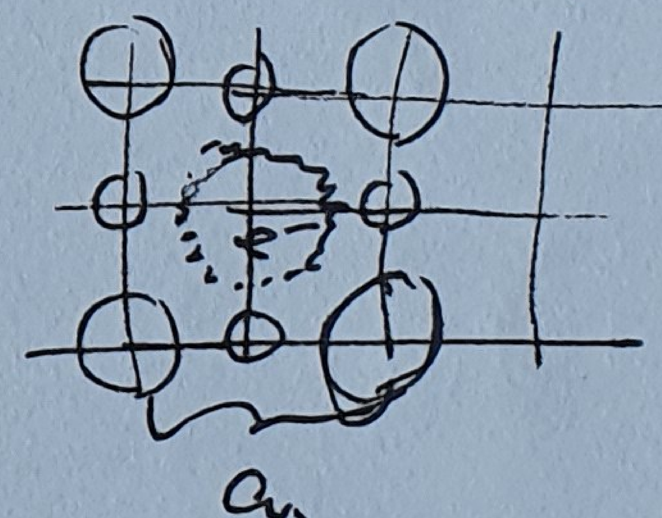
380 nm

$1[\mathrm{nm}] = 18.9\,[a_B]$

$$E_p = \frac{2\pi \cdot 137}{380 \cdot 18.9} = 0.120\,\mathrm{Ha}$$

$$\rightarrow 0.120 = \frac{3 \cdot \pi^2}{2L^2}$$

$$L = \sqrt{123} \doteq 5\,a_B \doteq 2.5\,\text{Å}$$



NaCl $a_0 \doteq 5.7$ Å

MgO $a_0 \doteq 4.$[illegible]

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IV . 8

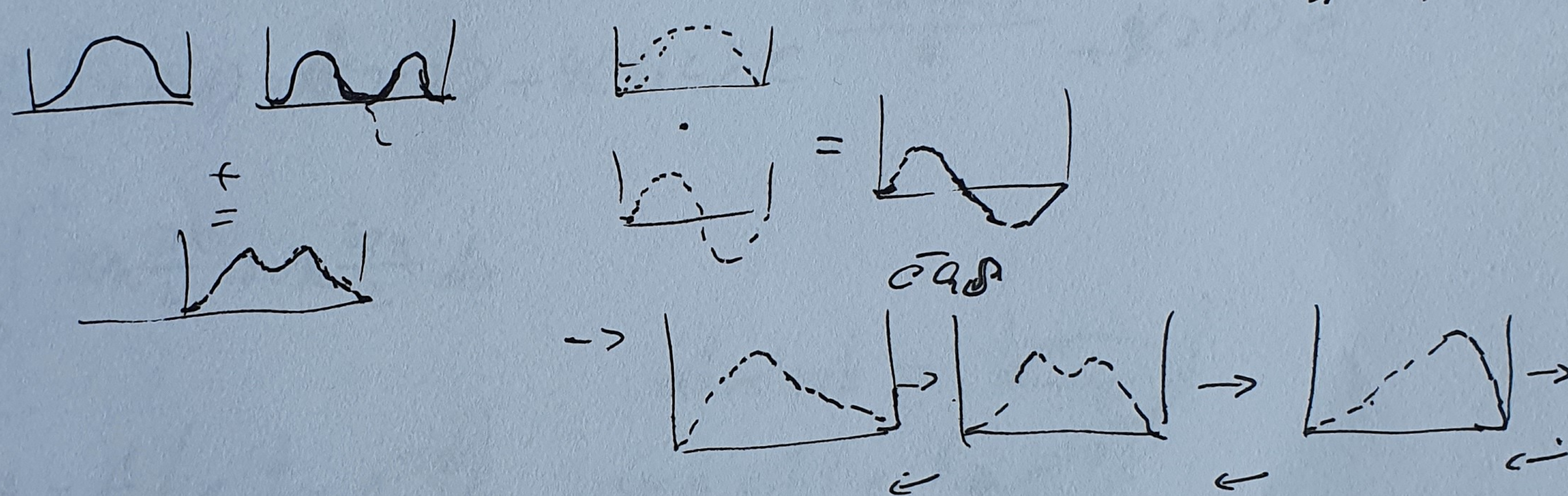
$$\psi(x,t) = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)e^{-\frac{iE_1 t}{\hbar}} + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)e^{-\frac{iE_2 t}{\hbar}}\right]$$

$$\rho(x,t) = \psi^* \psi$$

$$= \frac{1}{2}\left\{\frac{2}{L}\left[\sin\left(\frac{\pi x}{L}\right)e^{\frac{iE_1 t}{\hbar}} + \sin\left(\frac{2\pi x}{L}\right)e^{\frac{iE_2 t}{\hbar}}\right]\right.$$
$$\left.\left[\sin\left(\frac{\pi x}{L}\right)e^{-\frac{iE_1 t}{\hbar}} + \sin\left(\frac{2\pi x}{L}\right)e^{-\frac{iE_2 t}{\hbar}}\right]\right.$$

$$= \frac{1}{L}\left[\sin^2\left(\frac{\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right) + \right.$$
$$\left. + \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\left[e^{i(E_1-E_2)t/\hbar} + e^{-i(E_1-E_2)t/\hbar}\right]\right]$$

$$= \frac{1}{L}\left[\sin^2\left(\frac{\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right) + 2\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\cos\left[\frac{(E_1-E_2)t}{\hbar}\right]\right]$$



• Mějme jámu s částicí ve stavu

$\psi(x, t=0) = \frac{1}{\sqrt{2}}\left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}\right)\sqrt{\frac{2}{L}} \quad \rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |1\rangle)$

• Jaký je časový vývoj E, p, x?

$\psi(t) = \sum_n c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$

$\downarrow$

$\psi(x,t) = \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)e^{-\frac{iE_1 t}{\hbar}} + \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)e^{-\frac{iE_2 t}{\hbar}}$

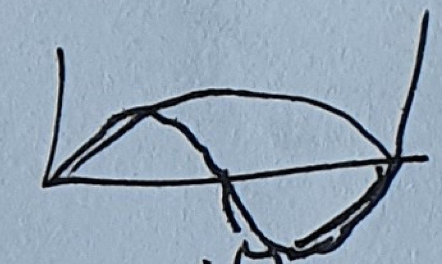
$\hat{E} = \hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

→ po aplikaci vypadne $\frac{\pi^2 n^2}{L^2}$, $(-)$ z $\sin \rightarrow -\cos \rightarrow \sin$

$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{2}}\left(\langle 1| e^{\frac{iE_1 t}{\hbar}} + \langle 2| e^{\frac{iE_2 t}{\hbar}}\right)\frac{1}{\sqrt{2}}\left(-\frac{\pi^2}{L^2}|1\rangle e^{-\frac{iE_1 t}{\hbar}} - \frac{\pi^2 4}{L^2}|2\rangle e^{-\frac{iE_2 t}{\hbar}}\right)$

$\rightarrow \frac{\hbar^2\pi^2}{2mL^2}\cdot\frac{1}{2}\left[\langle 1|1\rangle + 4\langle 2|2\rangle + 4\langle 1|2\rangle e^{\frac{i(E_1-E_2)t}{\hbar}} + \langle 2|1\rangle e^{-\frac{i(E_1-E_2)t}{\hbar}}\right]$

$\langle 1|2\rangle = \frac{2}{L}\int_0^L \sin\frac{\pi x}{L}\sin\frac{2\pi x}{L}\,dx$

součtová pravidla $= \dots$ obrázek = 

Euler: $\sin\phi = \frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right) \quad \cos\phi = \frac{1}{2}\left(e^{i\phi} + e^{-i\phi}\right)$

$= 0$

$\frac{\hbar^2\pi^2}{2mL^2}\cdot\frac{1}{2}\left[1 + 4\right] = \frac{5}{2}\cdot\frac{\hbar^2\pi^2}{2mL^2}$ ← průměr 2 hodnot (1 a 4)

⟺ nemění se v čase ⟺ vlastní stavy

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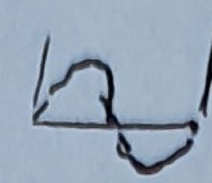
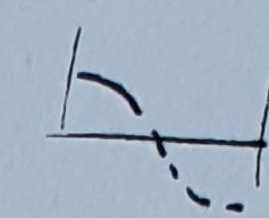
IV - 5

· $\langle p \rangle$ v čase pro $|\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$

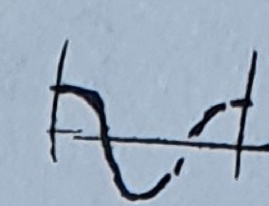
 

$$\langle p \rangle = \frac{1}{2}\left(\langle 1| e^{\frac{iE_1 t}{\hbar}} + \langle 2| e^{\frac{iE_2 t}{\hbar}}\right)\left(-i\hbar \frac{\partial}{\partial x}\right)\left(|1\rangle e^{-\frac{iE_1 t}{\hbar}} + |2\rangle e^{-\frac{iE_2 t}{\hbar}}\right)$$

$$-i\hbar \frac{\partial}{\partial x}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L} = -i\hbar\sqrt{\frac{2}{L}}\frac{\pi}{L}\cos\frac{\pi x}{L}$$



$$-i\hbar \frac{\partial}{\partial x}\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L} = -i\hbar\sqrt{\frac{2}{L}}\frac{2\pi}{L}\cos\frac{2\pi x}{L}$$



$\langle 1|p|1\rangle = 0$ sudá - lichá

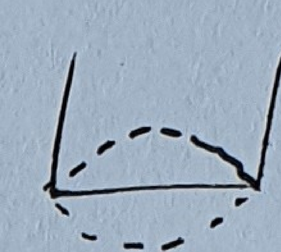
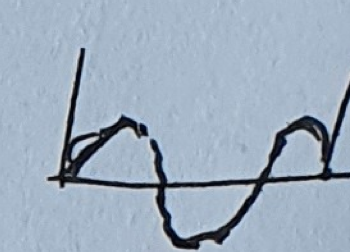
$\langle 1|p|2\rangle \dots \int_0^L \sin\frac{\pi x}{L}\cos\frac{2\pi x}{L}\,dx$ ← bez $(-i\hbar)$ & bez $\frac{2}{L}\frac{2\pi}{L}$

$\langle 2|p|2\rangle$ .. sudá - lichá $\Rightarrow 0$

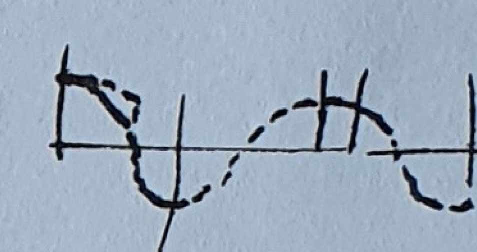
$$\int_0^L \frac{1}{2i}\left(e^{\frac{i\pi x}{L}} - e^{-\frac{i\pi x}{L}}\right)\frac{1}{2}\left(e^{\frac{i2\pi x}{L}} + e^{-i\frac{2\pi x}{L}}\right)dx$$

$$= \int_0^L \frac{1}{4i}\left[e^{i\frac{3\pi x}{L}} - e^{-i\frac{3\pi x}{L}} + e^{-i\frac{\pi x}{L}} - e^{\frac{i\pi x}{L}}\right]dx$$

$$= \int_0^L \frac{1}{2}\left[\sin\frac{3\pi x}{L} - \sin\frac{\pi x}{L}\right]dx$$

$$= -\frac{1}{2}\left[\frac{L}{3\pi}\cos\frac{3\pi x}{L}\Big|_0^L - \frac{L}{\pi}\cos\frac{\pi x}{L}\Big|_0^L\right]$$



$$= -\frac{1}{2}\left[\frac{L}{3\pi}[-1-1] - \frac{L}{\pi}[-1-1]\right]$$

$$= \frac{L}{\pi}\left(-\frac{1}{2}\right)\left[-\frac{2}{3}+2\right] = \frac{L}{\pi}\left(-\frac{2}{3}\right)$$

$$\Rightarrow \langle p \rangle = \frac{1}{2}\Big(\underbrace{\langle 1|p|1\rangle}_{\to 0} e^{\cdots} + \underbrace{\langle 2|p|2\rangle}_{\to 0} e^{\cdots} + \langle 1|p|2\rangle e^{i(E_1-E_2)t/\hbar}$$

$$+ \langle 2|p|1\rangle e^{i(E_2-E_1)t/\hbar}\Big)$$

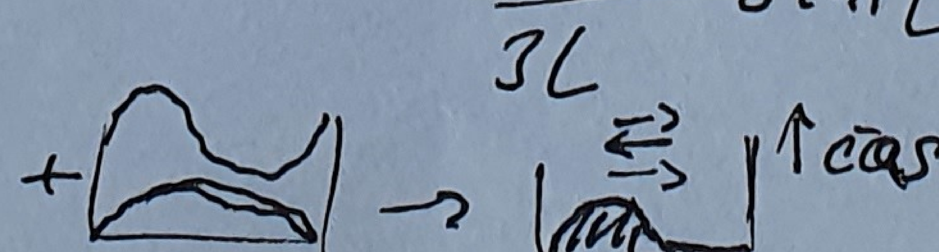
$$= \frac{1}{2}\Big[(-i\hbar)\sqrt{\frac{2}{L}}\sqrt{\frac{2}{L}}\frac{2\pi}{L}\frac{L}{\pi}\left(-\frac{2}{3}\right)e^{i(E_1-E_2)t/\hbar}$$

$$+ (-i\hbar)\sqrt{\frac{2}{L}}\sqrt{\frac{2}{L}}\frac{\pi}{L}\frac{L}{\pi}\left(\frac{4}{3}\right)e^{-i(E_1-E_2)t/\hbar}\Big]$$

$$= \frac{1}{2}\frac{2}{L}\frac{4}{3}\left[-i\hbar e^{i(E_1-E_2)t/\hbar} + i\hbar e^{-i(E_1-E_2)t/\hbar}\right]$$

$$= \frac{4\hbar}{3L}\left[i e^{i(E_2-E_1)t/\hbar} - i e^{-i(E_2-E_1)t/\hbar}\right]\cdot\frac{2i}{2i}$$

$$= \frac{4\hbar}{3L}\sin[(E_2-E_1)t/\hbar](-2) = \frac{8\hbar}{3L}\sin[(E_1-E_2)t/\hbar]$$



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IV - 6

$$\int_0^L \sin\frac{2\pi x}{L}\cos\frac{\pi x}{L}\,dx = \int_0^L \frac{1}{2i}\left(e^{\frac{i2\pi x}{L}} - e^{-\frac{2\pi i x}{L}}\right)\frac{1}{2}\left(e^{\frac{i\pi x}{L}} + e^{-\frac{i\pi x}{L}}\right)dx$$

$$= \int_0^L \frac{1}{4i}\left[e^{\frac{3\pi i x}{L}} + e^{\frac{i\pi x}{L}} - e^{-\frac{i\pi x}{L}} - e^{-\frac{3i\pi x}{L}}\right]dx$$

$$= \int_0^L \frac{1}{2}\left[\sin\left(\frac{3\pi x}{L}\right) + \sin\left(\frac{\pi x}{L}\right)\right]dx$$

$$= -\frac{1}{2}\left[\frac{L}{3\pi}\cos\left(\frac{3\pi x}{L}\right)\Big|_0^L + \frac{L}{\pi}\cos\left(\frac{\pi x}{L}\right)\Big|_0^L\right]$$

$$= -\frac{1}{2}\frac{L}{\pi}\left[\frac{1}{3}(-1-1) + (-1-1)\right]$$

$$= -\frac{1}{2}\frac{L}{\pi}\left[-\frac{2}{3} - 2\right] = \frac{L}{\pi}\frac{4}{3}$$