- čas závislost, ~~at~~ ρ, $\langle\rangle_{\text{eig}}$, $\langle\rangle_{\text{m-eig}}$ - rotátor explicitní nákgrál a pomocí lokrgie do el. skenu
- Lin. functions, pert. evolution? [or delay...] L_{00}
- LHO - ~~x~~$f(0) \to$ ~~x~~ $\sum c_i |i\rangle \to \psi(t)$, $\langle\rangle(t)$
- Ehrenfest explicitně

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V-1

Mějme ~~částici~~ rotátor - "volná částice" na $(0, 2\pi)$. $H = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2}$

$$\psi_n(\phi) = N e^{in\phi}, \quad n \in \mathbb{Z}$$

Normalizace - $N^2 \int_0^{2\pi} e^{-in\phi} e^{in\phi} d\phi = N^2 \int_0^{2\pi} 1\, d\phi = \frac{N^2}{2\pi} = 1$

$$\Rightarrow N = \frac{1}{\sqrt{2\pi}}$$

O.G. $\langle n|m\rangle = \delta_{nm}$

$$\int_0^{2\pi} \frac{1}{\sqrt{2\pi}} e^{-in\phi} \frac{1}{\sqrt{2\pi}} e^{im\phi} d\phi$$

$$= \frac{1}{2\pi}\int_0^{2\pi} e^{i(m-n)\phi} d\phi \underset{\uparrow}{=} \begin{cases} m \neq n: & \frac{1}{2\pi}\int_0^{2\pi} e^{im'\phi} d\phi = 0 \checkmark \\ m = n: & \frac{1}{2\pi}\int_0^{2\pi} \underbrace{e^0}_{=1} d\phi = 1 \checkmark \end{cases}$$

$\int$ přes celý interval

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

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

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

Normovaná? $\frac{1}{4\pi}\int_0^{2\pi} (1 + e^{-i\phi})(1 + e^{i\phi}) d\phi$

$$= \frac{1}{4\pi}\int_0^{2\pi} \left[1 + e^{-i\phi} + e^{i\phi} + 1\right] d\phi$$

$$= \frac{1}{4\pi}\int_0^{2\pi} 2\, d\phi = 1 \quad \underline{\text{OK}}$$

$$\frac{1}{\sqrt{2}}\left(\langle 0| + \langle 1|\right)\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) = \frac{1}{2}\left[\langle 0|0\rangle + \langle 0|1\rangle + \langle 1|0\rangle + \langle 1|1\rangle\right]$$

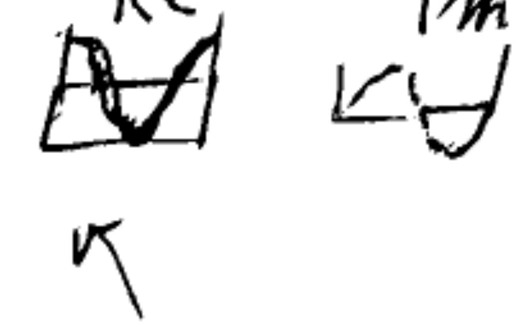
$$= \frac{1}{2}\left[\langle 0|0\rangle + \langle 1|1\rangle\right] = 1 \quad \underline{\text{OK}}$$

$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$

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

$\psi_n(t) = e^{in\phi} e^{-i\frac{\hbar t}{2I}n^2} = e^{i(n\phi - \frac{\hbar t n^2}{2I})}$

Re Im



- Jaká je $\psi(\phi, t)$?

$E_0 = 0$

$E_1 = \frac{\hbar^2}{2I} \longrightarrow \psi(\phi, t) = \frac{1}{2\sqrt{\pi}}\left(1 + e^{i\phi} e^{-\frac{i\hbar^2 t}{2I\hbar}}\right) = \frac{1}{2\sqrt{\pi}}\left[1 + e^{i(\phi - \frac{\hbar t}{2I})}\right]$

- Jaká je $\rho(\phi, t) = \psi^*(\phi, t)\,\psi(\phi, t)$?

$\rho = \frac{1}{4\pi}\left[1 + e^{-i(\phi - \frac{\hbar t}{2I})}\right]\left[1 + e^{i(\phi - \frac{\hbar t}{2I})}\right]$

$=1 \qquad =1$

$= \frac{1}{4\pi}\left[2 + e^{+i(\phi - \frac{\hbar t}{2I})} + e^{-i(\phi - \frac{\hbar t}{2I})}\right]$

$2\cos\left(\phi - \frac{\hbar t}{2I}\right)$

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

vlna

- Jaká je $\langle p\rangle$ $(-i\hbar\frac{d}{d\phi})$ pomocí stavů a explicitní integrací

vo stav $|n\rangle$

$-i\hbar\frac{\partial}{\partial\phi}\psi_n = -i\hbar\frac{\partial}{\partial\phi}\frac{1}{\sqrt{2\pi}}e^{in\phi}e^{-\frac{i\hbar t}{2I}} = -i\hbar\, in\frac{1}{\sqrt{2\pi}}e^{in\phi}e^{-\frac{i\hbar t}{2I}}$

$= n\hbar\,\psi_n(\phi, t)$ (keďže je vl. stav)

$\langle\psi|p|\psi\rangle = \frac{1}{\sqrt{2}}\left(\langle 0| + \langle 1|\right) p\, \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$

$= \frac{1}{2}\left[\langle 0| + \langle 1|\right]\left[0\cdot|0\rangle + \hbar|1\rangle\right]$

$= \frac{1}{2}\left[\langle 0|\hbar|1\rangle + \langle 1|\hbar|1\rangle\right] = \frac{\hbar}{2}$

čas sa pozrieme

čas

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

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V-3

- $\langle p \rangle$ explicitní integrací

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

$$\langle p \rangle = \frac{1}{4\pi}\int_0^{2\pi}\left[1 + e^{-i\left(\phi - \frac{\hbar t}{2I}\right)}\right](-i\hbar)\frac{\partial}{\partial\phi}\left[\cancel{1} + e^{+i\left(\phi - \frac{\hbar t}{2I}\right)}\right]d\phi$$

$$= \frac{1}{4\pi}\int_0^{2\pi}\left[\underbrace{1 + e^{-i\left(\phi - \frac{\hbar t}{2I}\right)}\right]\hbar\, e^{i\left(\phi - \frac{\hbar t}{2I}\right)}}_{\int = 0}\, d\phi \quad \to 1$$

$$= \frac{1}{4\pi}\int_0^{2\pi}\hbar\, d\phi = \frac{2\pi\hbar}{4\pi} = \frac{\hbar}{2} \quad \text{OK}$$

$\langle e^{i\phi}\rangle$ skrz integrace ? dospěje ka

$$\langle\psi| e^{i\phi}|\psi\rangle = \frac{1}{2}\left[\langle 0| + \langle 1|\right] e^{i\phi}\left[|0\rangle + |1\rangle\right]$$

$$= \frac{1}{2}\left[\langle 0|e^{i\phi}|0\rangle + \langle 0|e^{i\phi}|1\rangle + \langle 1|e^{i\phi}|0\rangle + \langle 1|e^{i\phi}|1\rangle\right]$$

$$\langle 0|e^{i\phi}|0\rangle = \frac{1}{2\pi}\int_0^{2\pi} 1\cdot e^{i\phi}\cdot 1\, d\phi = 0$$

$$\langle 1|e^{i\phi}|1\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-i\phi}e^{i\phi}e^{i\phi}\, d\phi = \frac{1}{2\pi}\int_0^{2\pi} e^{i\phi}d\phi = 0$$

$$\langle 0|e^{i\phi}|1\rangle = \frac{1}{2\pi}\int_0^{2\pi} 1\cdot e^{i\phi}\cdot e^{i\phi}d\phi = \frac{1}{2\pi}\int_0^{2\pi} e^{2i\phi}d\phi = 0$$

$$\langle 1|e^{i\phi}|0\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-i\phi}e^{i\phi}\, 1\, d\phi = \frac{1}{2\pi}\int_0^{2\pi} 1\, d\phi = 1$$

OK, trochu Hermiciity do toho...

$$V = A\left[e^{i\phi} + e^{-i\phi}\right]$$

$$\langle 0|A\left[e^{i\phi} + e^{-i\phi}\right]|0\rangle = \frac{1}{2\pi}A\int_0^{2\pi} 1\cdot\left[e^{i\phi} + e^{-i\phi}\right] 1\, d\phi = 0$$

$$\langle 1| \qquad |1\rangle = \frac{1}{2\pi}A\int_0^{2\pi} e^{-i\phi}\left[e^{i\phi} + e^{-i\phi}\right]e^{i\phi}d\phi = \frac{A}{2\pi}\int_0^{2\pi}\left(e^{i\phi} + e^{-i\phi}\right)d\phi = 0$$

$$\langle 0|A\left[e^{i\phi} + e^{-i\phi}\right]|1\rangle = \frac{A}{2\pi}\int_0^{2\pi} 1\left[e^{i\phi} + e^{-i\phi}\right]e^{i\phi}d\phi = \frac{A}{2\pi}\int_0^{2\pi}\left(\underset{\to 0}{e^{2i\phi}} + 1\right)d\phi = A$$

$$\langle 1|A\left[e^{i\phi} + e^{-i\phi}\right]|0\rangle = \frac{A}{2\pi}\int_0^{2\pi} e^{-i\phi}\left[e^{i\phi} + e^{-i\phi}\right] 1\, d\phi = \frac{A}{2\pi}\int_0^{2\pi}\left(1 + \underset{=0}{e^{-2i\phi}}\right)d\phi = A$$

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IV - 4

$\langle \psi | V | \psi \rangle =$

$= \frac{1}{2} \left(\langle 0| + \langle 1| \right) V \left(|0\rangle + |1\rangle \right)$

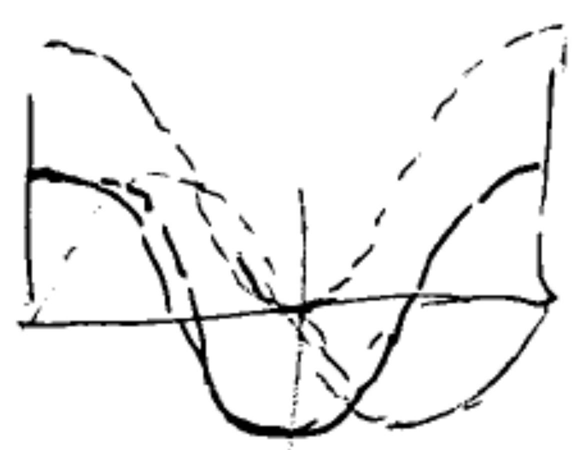
$= \frac{1}{2} \left[\langle 0|V|1\rangle + \langle 1|V|0\rangle \right] = \frac{1}{2} \left[A + A \right] = A$

včetně času:

$= \frac{1}{2} \left[\langle 0| + \langle 1| e^{-\frac{i\hbar t}{2I}} \right] V \left[|0\rangle + |1\rangle e^{\frac{i\hbar t}{2I}} \right]$

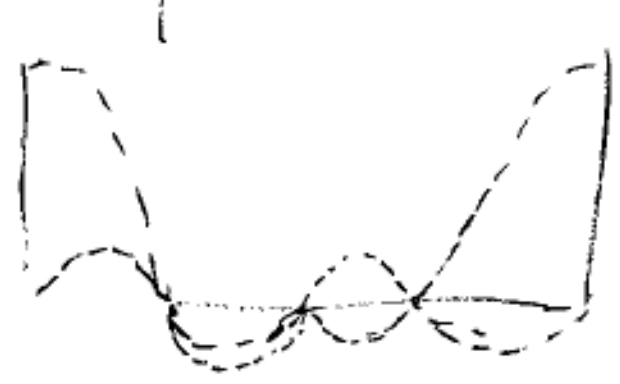
$= \frac{1}{2} \left[\langle 0|V|1\rangle e^{\frac{i\hbar t}{2I}} + \langle 1|V|0\rangle e^{-\frac{i\hbar t}{2I}} \right]$

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

$t = 0$ 

Im ← integrál se vyruší
Re ← integrál maximální

V · Im
V · Re



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V-5

$V = A[e^{i\phi} + e^{-i\phi}]$ v $\cos(n\phi), \sin(n\phi)$ bazi

$\psi_n = \cancel{\begin{cases} \cos(n\phi) & n \in N^0 \\ \sin(n\phi) & n \in N \end{cases}}$ $\qquad \int_0^{2\pi} \cos^2\phi \, d\phi = \int_0^{2\pi} \frac{1}{2} = \pi \rightarrow \frac{1}{\sqrt{\pi}} \cos(n\phi)$

$\langle cn | V | cn \rangle =$

$\langle \phi | cn \rangle = \frac{1}{\sqrt{2}} (\cancel{e^{i\phi}} |1\rangle + |-1\rangle) = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2\pi}} e^{i\phi} + \frac{1}{\sqrt{2\pi}} e^{-i\phi} \right)$

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

$\psi_n \begin{cases} 1 & n = 0 \\ \frac{1}{\sqrt{\pi}} \cos(n\phi) & n \in N \\ \frac{1}{\sqrt{\pi}} \sin(n\phi) & n \in N \end{cases}$

$\langle cn | V | cm \rangle = \frac{1}{\pi} \int_0^{2\pi} \cos(n\phi) V \cos(m\phi) d\phi$

$= \frac{1}{\pi} \int_0^{2\pi} \frac{1}{2} \left(e^{in\phi} + e^{-in\phi} \right) A [e^{i\phi} + e^{-i\phi}] \frac{1}{2} (e^{im\phi} + e^{-im\phi}) d\phi$

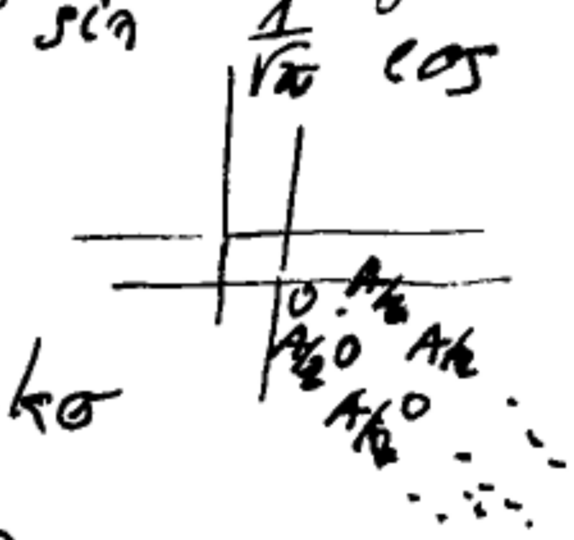
$= \frac{A}{4\pi} \int_0^{2\pi} \Big[e^{i(n+m+1)} + e^{i(n+m-1)} + e^{i(-n+m+1)} + e^{i(-n+m-1)}$

$+ e^{i(n-m+1)} + e^{i(n-m-1)} + e^{i(-n-m+1)} + e^{i(-n-m-1)} \Big] d\phi$

$= \frac{A}{4\pi} 4\pi = \frac{A}{4}$ pro $\left. \begin{matrix} n = -m+1 \\ n = -m+1 \end{matrix} \right\}$ odporuje $n \in N$

$n = m - 1$

$n = m + 1$



$\langle cn | V | sm \rangle = 0$ ← u členi se liší znaménko

$\langle cn | V | cm \rangle = \frac{1}{2} [\langle n | + \langle -n |] V [|m\rangle + |-m\rangle]$

$= \frac{1}{2} [\underbrace{\langle n | V | m \rangle}_{A\delta_{n,m\pm1}} + \underbrace{\langle n | V | -m \rangle}_{=0} + \underbrace{\langle -n | V | m \rangle}_{=0} + \underbrace{\langle -n | V | -m \rangle}_{A\delta_{n,m\pm1}}]$

$= A\delta_{n,m\pm1}$

$\langle sn | V | sm \rangle = \frac{1}{2} [\langle n | - \langle -n |] V [|m\rangle \mp |-m\rangle]$

$= \frac{1}{2} [\underbrace{\langle n | V | m \rangle}_{A\delta_{n,m\pm1}} - \underbrace{\langle -n | V | m \rangle}_{=0} - \underbrace{\langle -n | V | m \rangle}_{=0} + \underbrace{\langle -n | V | -m \rangle}_{=A\delta_{n,m\pm1}}]$

$= A\delta_{n,m\pm1}$

• operátor $V = A[e^{i\phi} + e^{-i\phi}]$

$$\mathbb{V} = \begin{pmatrix} \ddots & 0 & A & & & \\ & A & 0 & A & & 0 \\ & & A & 0 & A & \\ & 0 & & A & 0 & A \\ & & & & A & 0 & \ddots \end{pmatrix}$$

pro stavy $|0\rangle, |1\rangle, |-1\rangle$: $\begin{pmatrix} 0 & A & 0 \\ A & 0 & A \\ 0 & A & 0 \end{pmatrix}$

uvažujme transformaci báze

$0: \quad \frac{1}{\sqrt{2\pi}} \to \frac{1}{\sqrt{2\pi}} \qquad \to (0 \;\; 1 \;\; 0)$

$1: \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle) = \frac{1}{\sqrt{\pi}} \cos\phi \qquad \to \left(\frac{1}{\sqrt{2}} \;\; 0 \;\; \frac{1}{\sqrt{2}}\right)$

$-1: \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle) = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2\pi}} \frac{i}{i}(e^{i\phi} - e^{-i\phi}\right) = \frac{i}{\sqrt{\pi}} \sin\phi$

$\to -1: \; -\frac{i}{\sqrt{2}}(|1\rangle - |-1\rangle) = -\frac{i}{\sqrt{2}} \frac{1}{\sqrt{2\pi}} \frac{i}{i}(e^{i\phi} - e^{-i\phi}) = \frac{1}{\sqrt{\pi}} \sin\phi$

$\to \left(-\frac{i}{\sqrt{2}} \;\; 0 \;\; \mp\frac{i}{\sqrt{2}}\right)$

• Jaká je matice transformace:

$$U = \begin{pmatrix} -i/\sqrt{2} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ -i/\sqrt{2} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \qquad U^+ = \begin{pmatrix} -i/\sqrt{2} & 0 & \frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$|-1\rangle \quad |0\rangle \quad |1\rangle$

$$U^+U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{OK}$$

• Jak vypadá transformovaný $\mathbb{V}$

$U^+VU =$

$$\begin{pmatrix} -i/\sqrt{2} & 0 & i/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 & A & 0 \\ A & 0 & A \\ 0 & A & 0 \end{pmatrix} \begin{pmatrix} i/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \\ -i/\sqrt{2} & 0 & 1/\sqrt{2} \end{pmatrix} =$$

$$= (U^+) \begin{pmatrix} 0 & A & 0 \\ \frac{iA}{\sqrt{2}} - \frac{iA}{\sqrt{2}} = 0 & 0 & \sqrt{2}A \\ 0 & A & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sqrt{2}A \\ 0 & \sqrt{2}A & 0 \end{pmatrix}$$

Operátor $V = A[e^{i\phi} + e^{-i\phi}]$

- podívejme se na $e^{i\phi}$ a $e^{-i\phi}$
- Je operátor $e^{i\phi}$ Hermitovský? $\langle n|\hat{O}m\rangle \stackrel{?}{=} \langle \hat{O}n|m\rangle$?

$$\frac{1}{2\pi}\int_0^{2\pi} e^{-in\phi} e^{i\phi} e^{im\phi}\, d\phi \overset{?}{\neq} \frac{1}{2\pi}\int_0^{2\pi} e^{-i\phi} e^{-in\phi} e^{im\phi}\, d\phi$$

Evidentně ne

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

$$= \frac{\hbar m}{2\pi}\int_0^{2\pi} e^{-in\phi} e^{im\phi}\, d\phi = \frac{\hbar m}{2\pi}\delta_{nm} \ \checkmark$$

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

$$= \frac{\hbar n}{2\pi}\delta_{nm} \ \checkmark$$

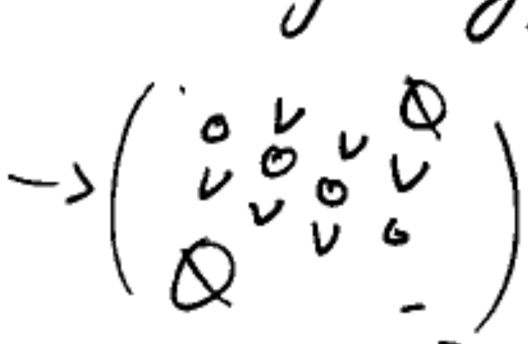
- co dělá operátor $e^{i\phi}$?

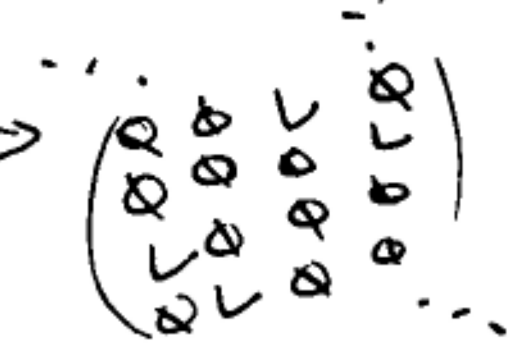
$$\frac{1}{2\pi}\int e^{-in\phi} e^{i\phi} e^{im\phi}\, d\phi = \frac{1}{2\pi}\int e^{i(m+1-n)}\, d\phi = \delta_{n,m+1}$$

- $e^{-i\phi} \to \delta_{n,m-1}$

$$\frac{1}{\sqrt{2\pi}} e^{i\phi} e^{im\phi} = \frac{1}{\sqrt{2\pi}} e^{i(m+1)\phi} = |m+1\rangle$$

"zvyšovací operátor" (zásadní pro LHO a molekul. systémy)

$\to V \approx (e^{i\phi} + e^{-i\phi}) \to$ kapluje stavy lišící se o 1 $\to$ 

$V \sim (e^{2i\phi} + e^{-2i\phi}) \to$ —//— 2 $\to$ 

⋮