LHO

T6.1

LHO/1

- amplituda kmitů - základní stav

$$\psi_0(x) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}} e^{-x^2/2\alpha^2} \qquad \alpha = \sqrt{\frac{\hbar}{m\omega}}$$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

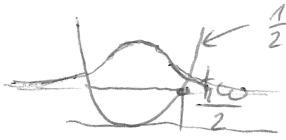
$$H\psi_0 = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2} =$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}\frac{d}{dx}\left(-\frac{2x}{2\alpha^2}e^{-x^2/2\alpha^2}\right) + \frac{1}{2}m\omega^2x^2\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}\frac{1}{\alpha^2}\left[-e^{-x^2/2\alpha^2} + \frac{x^2}{\alpha^2}e^{-x^2/2\alpha^2}\right] + \frac{1}{2}m\omega^2x^2\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2}$$

$$= \underbrace{\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\left[e^{-x^2/2\alpha^2} - x^2\frac{m\omega}{\hbar}e^{-x^2/2\alpha^2}\right]}_{\text{kin}} + \underbrace{\frac{1}{2}m\omega^2x^2\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2}}_{\text{pot.}}$$

stejné, jen opačné znaménko



$$E_{pot} = E_{tot}$$

$$\frac{1}{2}m\omega^2A^2 = \frac{\hbar\omega}{2} \qquad \text{nebo obecně } \hbar\omega(n+1/2)$$

$$A^2 = \frac{\hbar}{m\omega} \qquad A = \sqrt{\frac{\hbar}{m\omega}} \quad (=\alpha)$$

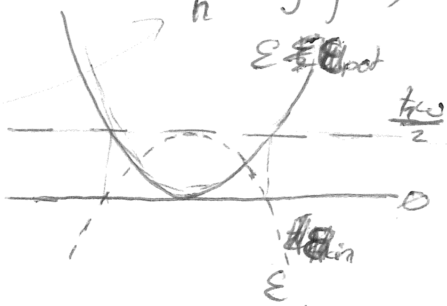
$$E_{kin}(x) = \psi \frac{p^2}{2m}\psi\Big|_{x=A} = \left[\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2}\right]\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\left[1-\frac{m\omega}{\hbar}x^2\right]\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2}$$

$$= \frac{\hbar\omega}{2}\left[1-\frac{m\omega}{\hbar}x^2\right]\underbrace{\frac{1}{\sqrt{\pi}}\frac{1}{\alpha}e^{-\frac{x^2}{\alpha^2}}}_{\rho(x)} = \frac{\hbar\omega}{2}\left[1-\frac{m\omega}{\hbar}x^2\right]\rho(x)$$

$$E_{pot}(x) = \frac{1}{2}m\omega^2x^2\rho(x)$$

$$E_{kin}(A) = \frac{\hbar\omega}{2}\left[1-\frac{m\omega}{\hbar}\frac{\hbar}{m\omega}\right]\rho(x) = 0$$

$\to$ amplituda $\sim A = \sqrt{\frac{\hbar}{m\omega}}$



hustota energie

$$\varepsilon(x) = \frac{\hat{E}|\psi\rangle}{|\psi\rangle}$$

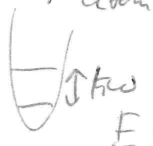
vodíková vazba ve vodě X energie O-H vibračních excitací T6.1b

$k \sim 3000\,\mathrm{cm}^{-1} \rightarrow \lambda = \frac{1\,\mathrm{cm}}{3000} = \frac{1\,\mathrm{mm}}{300} \doteq 3{,}3\,\mu\mathrm{m} = 3300\,\mathrm{nm} = 33000\,\text{Å}$

$\doteq 62400\,\mathrm{Bohr}$

$E = \hbar\omega = 2\pi\hbar\nu = 2\pi\hbar \frac{c}{\lambda}$

atomic units: $\hbar = m_e = e = \frac{1}{4\pi\varepsilon_0} = 1$



$c = 137$

$E = 2\pi \frac{137}{62400} = \frac{6.28}{62400} \cdot 137 \doteq 137 \cdot 10^{-4} = 0.0137\ \mathrm{Ha} \doteq \cancel{0.0137\,\mathrm{eV}}$ $\cancel{0.037\,\mathrm{eV}}$ $0.37\,\mathrm{eV}$

ħω in a.u. ... atomic units

$\rightarrow \frac{1}{2}\hbar\omega = 0.185\,\mathrm{eV}$

$A = \sqrt{\frac{\hbar}{m\omega}}$ $\qquad m_p \doteq 1836\, m_e$

$= \sqrt{\frac{1}{1836 \cdot 0.0137}} \doteq \sqrt{0.04} = 0.2\,\mathrm{Bohr}$ $\qquad$ vazebná energie $\sim 0.22\,\mathrm{eV}$

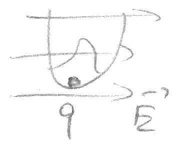
~ 0.1 Ångstrom - délka vazby je ~ 0.92 Ångstromů

Deuterium

$= \sqrt{\frac{1}{2 \cdot 1836 \cdot 0.0137}} = \frac{0.2\,\mathrm{Bohr}}{\sqrt{2}} \doteq 0.14\,\mathrm{Bohr} \sim 0.7$ Ångstrom

LHO/2 $\times$ $\odot$ T6.2

- LHO v el. poli $\vec{E}$



$H = H_0 \mp qEx$ $\quad$ ± ← orientace pole, náboj, ... $\quad E = -\frac{dU}{dx}$

$U = -Ex$

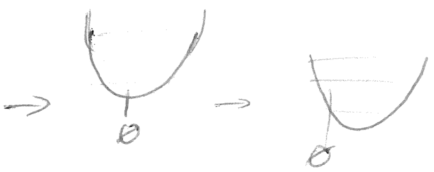
$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 - qEx$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 - \frac{2qE}{m\omega^2}x\right)$$

$$\frac{1}{2}m\omega^2\left(x^2 - \frac{2qE}{m\omega^2}x\right) = \frac{1}{2}m\omega^2\left(x - \frac{qE}{m\omega^2}\right)^2 - \frac{q^2E^2}{m^2\omega^4}\cdot\frac{1}{2}m\omega^2$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\underbrace{\left(x - \frac{qE}{m\omega^2}\right)^2}_{x' = x - \frac{qE}{m\omega^2}} - \underbrace{\frac{q^2E^2}{m^2\omega^4}\cdot\frac{1}{2}m\omega^2}_{\text{posun energie}} = \frac{q^2E^2}{2m\omega^2}$$

posun středu vlnové fce



$$E_n = \hbar\omega\left(\tfrac{1}{2} + n\right) - \cancel{\frac{q^2E^2}{m^2\omega^4}} - \frac{q^2E^2}{2m\omega^2}$$

LHO/3 ✕ T6.2b

- LHO ve stacionárním stavu s kv. číslem n.

určete $\langle x^2\rangle_n$ & $\langle V\rangle_n$

příklady - pomocí Hermiteových polynomů

$$\cancel{a = \frac{1}{\sqrt{2m\hbar\omega}}(p - i\omega m x)} \leftarrow \text{anihilační}$$

$$\cancel{a^+ = \frac{1}{\sqrt{2m\hbar\omega}}(p + i\omega m x)} \leftarrow \text{kreační}$$

! DT6.4 jinak

$$a|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle \qquad [a, a^+] = 1$$

$$a^+|\psi_n\rangle = \sqrt{n+1}|\psi_{n+1}\rangle \qquad a a^+ = 1 + a^+ a$$

$$a + a^+ = \frac{1}{\sqrt{2m\hbar\omega}}2p \rightarrow p = \sqrt{\frac{m\hbar\omega}{2}}(a + a^+)$$

$$a - a^+ = \frac{1 \cdot 2}{\sqrt{2m\hbar\omega}}(-i\omega m x)$$

! DT6.4 jinak

$$= \sqrt{\frac{2\omega m}{\hbar}}(-ix) \qquad x = i\sqrt{\frac{\hbar}{2\omega m}}(a - a^+)$$

$$x^2 = i \cdot i \frac{\hbar}{2\omega m}(a - a^+)^2 = -\frac{\hbar}{2\omega m}(a^2 - a a^+ - a^+ a + a^{+2}) =$$

$$= -\frac{\hbar}{2\omega m}(a^2 + a^{+2} - 1 - 2a^+ a)$$

$$= \frac{\hbar}{2m\omega}(2a^+ a + 1 - a^2 - a^{+2})$$

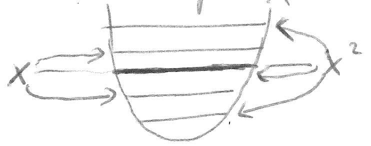
! pro LHO: $\langle n|x|n\rangle = c\langle n|a - a^+|n\rangle = c[\langle n|a|n\rangle - \langle n|a^+|n\rangle] =$

střední hodnota x pro vlastní stavy $= c'\langle n|n-1\rangle - c''\langle n|n+1\rangle = 0$ VŽDY

$$\langle n|x|m\rangle = c'\langle n|m-1\rangle - c''\langle n|m+1\rangle = c'\delta_{n\,m-1} - c''\delta_{n\,m+1}$$

- maticový element nenulový pouze pro sousední stavy !

- pro x^2 → ± 2 a ~~stav~~ původní stav



LHO/3 contn'd

X

$$x^2 = \frac{\hbar}{2m\omega}\left(2a^+a + 1 - a^2 - a^{+2}\right) = \frac{\hbar}{m\omega}\left(a^+a + \frac{1}{2} - a^2 - a^{+2}\right)$$

$$a^+a|n\rangle = a^+\sqrt{n}\,|n-1\rangle = n|n\rangle$$

$$x^2 = \frac{\hbar}{m\omega}\left(n + \frac{1}{2} - a^2 - a^{+2}\right)$$

$$\langle n|x^2|n\rangle = \frac{\hbar}{m\omega}\langle n|\left(n + \frac{1}{2} - a^2 - a^{+2}\right)|n\rangle$$

$$= \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)$$

$$\langle n|V|n\rangle = \langle n|\frac{1}{2}m\omega^2x^2|n\rangle = \frac{1}{2}m\omega^2\langle n|x^2|n\rangle = \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)$$

$$= \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) = \frac{1}{2}E_n$$

← druhá polovina připadá na kinetickou energii

e.g. pro základní stav

$x^4 \ldots \frac{3}{2B}\frac{1}{2B}\sqrt{\frac{\pi}{B}}$ $\quad \int_{-\infty}^{\infty} e^{-Bx^2} = \sqrt{\frac{\pi}{B}}$

$\int_{-\infty}^{\infty} x^2 e^{-Bx^2} = \frac{1}{2B}\sqrt{\frac{\pi}{B}}$

$$\psi_0 = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}e^{-x^2/2\alpha^2} \qquad \alpha = \sqrt{\frac{\hbar}{m\omega}}$$

$$\langle 0|x^2|0\rangle = \frac{1}{\sqrt{\pi}}\frac{1}{\alpha}\int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{\alpha^2}}dx = \frac{1}{\sqrt{\pi}}\frac{1}{\alpha}\frac{\alpha^2}{2}\alpha\sqrt{\pi} = \frac{\alpha^2}{2} = \frac{\hbar}{2m\omega} \qquad \text{OK}$$

$$\psi_1 = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}\sqrt{2}\,\frac{x}{\alpha}e^{-\frac{x^2}{2\alpha^2}} \qquad B = \frac{1}{\alpha^2}$$

$$\langle 1|x^2|1\rangle = \frac{1}{\sqrt{\pi}}\frac{2}{\alpha^3}\int_{-\infty}^{\infty} x^4 e^{-\frac{x^2}{\alpha^2}}dx = \frac{2}{\alpha\sqrt{\pi}}\frac{3\alpha^2}{\alpha^2 2}\cdot\frac{\alpha^2}{2}\cdot\alpha\sqrt{\pi} = \frac{3}{2}\alpha^2 = \frac{3\hbar}{2m\omega}$$

$$\psi_2 = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}\frac{1}{\sqrt{2}}\left(2\frac{x^2}{\alpha^2} - 1\right)e^{-\frac{x^2}{2\alpha^2}}$$

$$\langle 2|x^2|2\rangle = \frac{1}{\sqrt{\pi}}\frac{1}{2\alpha}\int_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2}}x^2\left(4\frac{x^4}{\alpha^4} - 4\frac{x^2}{\alpha^2} + 1\right) =$$

$$= \frac{1}{\sqrt{\pi}}\frac{1}{\alpha 2}\left[4\cdot\frac{5\alpha^2}{2}\cdot\frac{3\alpha^2}{2}\cdot\frac{\alpha^2}{2}\frac{\alpha\sqrt{\pi}}{\alpha^4} - 4\frac{3\alpha^2}{2}\cdot\frac{\alpha^2}{2}\frac{\alpha\sqrt{\pi}}{\alpha^2} + \frac{\alpha^2}{2}\alpha\sqrt{\pi}\right] =$$

$$= \frac{1}{2}\left[\frac{15\alpha^2}{2} - 3\alpha^2 + \frac{\alpha^2}{2}\right] = \frac{1}{2}5\alpha^2 = \frac{5}{2}\frac{\hbar}{m\omega}$$

vlastní fce

T 6.3b

$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$; $\cancel{a^+ = \frac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{d}{dx} + i\omega m x\right)}$

$\cancel{= \frac{-i}{\sqrt{2m\hbar\omega}}\left(\hbar\frac{d}{dx} \mp \omega m x\right)}$

$a^+_{wiki} = -i\, a^+_{skála}$

$\uparrow$ $e^{-i\pi/2}$ fáze

wiki $a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{i}{m\omega}p\right) =$

$= \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)$ — makes more sense...!

$= \boxed{\sqrt{\frac{1}{2\alpha^2}}\left(x - \alpha^2\frac{d}{dx}\right)\frac{1}{\sqrt2}\frac{1}{\alpha}}$

$\psi_0 = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt\alpha}e^{-x^2/2\alpha^2}$ $\qquad \alpha = \sqrt{\frac{\hbar}{m\omega}}$

$a^+\psi_0 = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt\alpha}\frac{1}{\sqrt2\,\alpha}\left(x - \alpha^2\frac{d}{dx}\right)e^{-x^2/2\alpha^2}$

$= \frac{1}{\pi^{1/4}}\frac{1}{\sqrt2}\frac{1}{\sqrt\alpha}\frac{1}{\alpha}\left[x - \alpha^2\cdot\frac{-2x}{2\alpha^2}\right]e^{-x^2/2\alpha^2} = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt\alpha}\cdot\frac{x}{\alpha}\cdot\frac{2}{\sqrt2}e^{-x^2/2\alpha^2}$

$= \frac{1}{\pi^{1/4}}\frac{\sqrt2}{\sqrt\alpha}\frac{x}{\alpha}e^{-x^2/2\alpha^2} = \psi_1 = \frac{1}{\pi^{1/4}}\sqrt{\frac{2}{\alpha}}\frac{x}{\alpha}e^{-x^2/2\alpha^2}$

$a^+\psi_0 = \sqrt1\,\psi_1$

$a^+\psi_1 = \sqrt2\,\psi_2$

$\psi_2 = \frac{a^+\psi_1}{\sqrt2}$

$\psi_2 = \frac{1}{\sqrt2}\underbrace{\frac{1}{\pi^{1/4}}\sqrt{\frac{2}{\alpha}}}_{c}\underbrace{\frac{1}{\alpha}\frac{1}{\sqrt2}\left(x - \alpha^2\frac{d}{dx}\right)}_{a^+}\frac{x}{\alpha}e^{-\frac{x^2}{2\alpha^2}}$ ← lichá...

$= \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2\alpha}}\frac{1}{\alpha}\left[\frac{x^2}{\alpha}e^{-\frac{x^2}{2\alpha^2}} - \alpha^2\frac{e^{-\frac{x^2}{2\alpha^2}}}{\alpha} + \frac{\alpha^2 x}{\alpha}\frac{2x}{2\alpha^2}e^{-\frac{x^2}{2\alpha^2}}\right]$

$= \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2\alpha}}\left[2\frac{x^2}{\alpha^2}e^{-\frac{x^2}{2\alpha^2}} - e^{-\frac{x^2}{2\alpha^2}}\right] = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2\alpha}}\left[2\frac{x^2}{\alpha^2} - 1\right]e^{-\frac{x^2}{2\alpha^2}}$

← sudá!

$\psi_3 = \frac{a^+\psi_2}{\sqrt3} = \frac{1}{\sqrt3}\frac{1}{\pi^{1/4}\sqrt{2\alpha}}\frac{1}{\sqrt2}\left(\frac{x}{\alpha} - \alpha\frac{d}{dx}\right)\left[\frac{2x^2}{\alpha^2} - 1\right]e^{-\frac{x^2}{2\alpha^2}}$

$= \frac{1}{\sqrt3}\frac{1}{\pi^{1/4}\sqrt{2\alpha}}\frac{1}{\sqrt2}\left[2\frac{x^3}{\alpha^3} - \frac{x}{\alpha} - \alpha\frac{d}{dx}\left(\frac{2x^2}{\alpha^2}\right) + \alpha\left(-\frac{x}{\alpha^2}\right)\right]e^{-\frac{x^2}{2\alpha^2}}$

$= \frac{1}{\sqrt3}\frac{1}{\pi^{1/4}}\frac{1}{2}\frac{1}{\sqrt\alpha}\left[2\frac{x^3}{\alpha^3} - \frac{2x}{\alpha} - \alpha\left(\frac{4x}{\alpha^2} + \frac{2x^2}{\alpha^2}\left(-\frac{x}{\alpha^2}\right)\right)\right]e^{-\frac{x^2}{2\alpha^2}}$

$= \frac{1}{\pi^{1/4}}\frac{1}{2\sqrt{3\alpha}}\left[4\frac{x^3}{\alpha^3} - \frac{6x}{\alpha}\right]e^{-\frac{x^2}{2\alpha^2}} = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{3\alpha}}\left[\frac{2x^3}{\alpha^3} - \frac{3x}{\alpha}\right]e^{-\frac{x^2}{2\alpha^2}}$ OK

← lichá...

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$$

~~podle wiki~~ ☺

$$a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

$a|n\rangle = \sqrt{n}\,|n-1\rangle$

$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$$a + a^+ = \sqrt{\frac{m\omega}{2\hbar}}(2x) \rightarrow x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^+)$$

← aspoň vyjde reálné

$$a - a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{2ip}{m\omega}\right) \rightarrow p = i\sqrt{\frac{m\omega\hbar}{2}}(a^+ - a)$$

$$= \sqrt{\frac{2}{m\omega\hbar}}\, ip$$

$[a, a^+] = 1$

$aa^+ = 1 + a^+a$

$$x^2 = \frac{\hbar}{2m\omega}(a + a^+)^2 = \frac{\hbar}{2m\omega}(a^2 + a^{+2} + aa^+ + a^+a)$$

$$= \frac{\hbar}{2m\omega}(a^2 + a^{+2} + 1 + 2a^+a) = \frac{\hbar}{m\omega}\left(a^+a + \tfrac{1}{2} + \frac{a^2 + a^{+2}}{2}\right)$$

$$\langle n|x|m\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle n|a|m\rangle + \langle n|a^+|m\rangle\right) = \text{☺}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{m}\,\langle n|m-1\rangle + \sqrt{m+1}\,\langle n|m+1\rangle\right) =$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{m}\,\delta_{n,m-1} + \sqrt{m+1}\,\delta_{n,m+1}\right)$$

$\langle n\vert x\vert m\rangle$	0	m 1	2	
0	0	1	0	0
1	1	0	$\sqrt{2}$	0
n 2	0	$\sqrt{2}$	0	$\sqrt{3}$
	0	0	$\sqrt{3}$	0

← z anihilačního op.

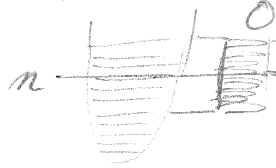
↑ z kreačního operátoru

LHO/11 $\times$ T6.5

$$\psi(x,t) = \frac{1}{\sqrt{2\nu+1}} \sum_{j=-\nu}^{\nu} \psi_{n+j}(x)\, e^{-i\omega(n+j+1/2)t}$$

vlnový balík

$0<\nu\leq n$



$$\langle\psi(0)|\psi(0)\rangle = \frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu} \langle n+j| \sum_{l=-\nu}^{\nu} |n+l\rangle$$

platí $\langle i|j\rangle = \delta_{ij}$

$$= \frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu} \langle n+j|n+l\rangle = \frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu}\delta_{n+j,n+l}$$

$$= \frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu} 1 = \frac{1}{2\nu+1}(2\nu+1) = 1 \quad \text{OK}$$

$$\langle\psi|x|\psi\rangle = \frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu}\langle n+j|x|\sum_{l=-\nu}^{\nu}|n+l\rangle e^{i\omega(n+j+1/2)t}\, e^{-i\omega(n+l+1/2)t}$$

$$= \frac{1}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu}\langle n+j|a+a^+|n+l\rangle e^{i\omega(j-l)t}$$

$$= \frac{1}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu}\left[\langle n+j|\sqrt{n+l}|n+l-1\rangle + \langle n+j|\sqrt{n+l+1}|n+l+1\rangle\right] e^{i\omega(j-l)t}$$

$$= \frac{1}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu}\Big[\sqrt{n+l}\,\underbrace{\delta_{n+j,n+l-1}}_{l=j+1} + \sqrt{n+l+1}\,\underbrace{\delta_{n+j,n+l+1}}_{l=j-1}\Big] e^{i\omega(j-l)t}$$

$$= \frac{1}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\left[\sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1}\,e^{-i\omega t} + \underbrace{\sum_{j=-\nu+1}^{\nu}}_{j\to j+1}\sqrt{n+j}\,e^{i\omega t}\right]$$

$$= \frac{1}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\left[\sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1}\,e^{-i\omega t} + \sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1}\,e^{i\omega t}\right]$$

$$= \frac{1}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\left\{\sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1}\left[e^{-i\omega t}+e^{i\omega t}\right]\right\}$$

$$\frac{1}{2}m\omega^2A^2 = \hbar\omega(n+\tfrac{1}{2})$$

$$= \frac{2}{2\nu+1}\sqrt{\frac{\hbar}{2m\omega}}\sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1}\,\cos(\omega t) \quad \text{OK}$$

$$A^2 = \frac{2\hbar}{m\omega}(n+1/2)$$

$$A = \sqrt{\frac{2\hbar}{m\omega}(n+1/2)}$$

$$= \sqrt{\frac{2\hbar}{m\omega}}\cos(\omega t)\cdot\frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1}$$

$$\frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu-1}\sqrt{n+j+1} \quad \xleftarrow{} 2\nu \text{ členů} \quad \times \quad \text{vs.} \quad \sqrt{n+1/2}$$ T6.5b

$$\frac{1}{2\nu+1}\sum_{j=-\nu+1/2}^{\nu-1/2}\sqrt{n+1/2+j}$$

pro $\frac{\nu}{j} \ll n$ vyruší se

$$= \frac{1}{2\nu+1}\sum_{j=-\nu+1/2}^{\nu-1/2}\sqrt{n+1/2}\sqrt{1+\frac{j}{n+1/2}} = \frac{1}{2\nu+1}\sum_{j=-\nu+1/2}^{\nu-1/2}\sqrt{n+1/2}\left(1+\frac{j}{2(n+1/2)}-\frac{j^2}{8(n+1/2)^2}\right)$$

malé

$$= \frac{1}{2\nu+1}\sum_{j=-\nu+1/2}^{\nu-\frac{1}{2}}\sqrt{n+1/2}\left[1-\frac{j^2}{8(n+1/2)^2}\right] =$$

$$= \frac{2\nu}{2\nu+1}\sqrt{n+1/2} \lesssim \sqrt{n+1/2}$$ ← amplituda s časem klesá

$n=2 \quad \nu=1$ "klasická" amplituda

$$\frac{1}{3}\sum_{j=1}^{0}\sqrt{2+j+1} = \frac{1}{3}(\sqrt{2}+\sqrt{3}) = 1{,}049 \qquad \sqrt{2+1/2} = 1{,}58$$

$n=20 \quad \nu=1$

$$\frac{1}{3}(\sqrt{20}+\sqrt{21}) = 3.0782 \qquad \frac{2\nu}{2\nu+1}\sqrt{n+1/2} = 3.0185 \qquad \sqrt{20+1/2} = 4{,}52$$

$n=20 \quad \nu=2$

$$\frac{1}{5}(\sqrt{18}\ \dots\ \sqrt{22}) = 3.6208$$

$$\frac{2\nu}{2\nu+1}\sqrt{n+1/2} = 3.6222$$

$n=20 \quad \nu=3$

$$\frac{1}{7}(\sqrt{17}\ \dots\ \sqrt{23}) = 3.8775$$

$$= 3.8809$$

$n=20 \quad \nu=4$

$$\frac{1}{9}(\sqrt{17}\ \dots\ \sqrt{24}) = 4.0783$$

$$= 4.0246$$

$$\langle x^2\rangle = \frac{1}{2\nu+1}\sum_{j=-\nu}^{\nu} \langle n+j|\, x^2 \,\Big|\sum_{l=-\nu}^{\nu} |n+l\rangle\, e^{i\omega(n+j+1/2)t}\, e^{-i\omega(n+l+1/2)t}$$

$$= \frac{1}{2\nu+1}\,\frac{\hbar}{2m\omega}\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu} \langle n+j|\, a^2 + a^{\dagger 2} + 1 + 2a^\dagger a \,|n+l\rangle\, e^{i\omega(j-l)t}$$

$$= \frac{1}{2\nu+1}\,\frac{\hbar}{2m\omega}\Big[\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu}\big(\langle n+j|a^2|n+l\rangle + \langle n+j|a^{\dagger 2}|n+l\rangle + \langle n+j|n+l\rangle + 2\langle n+j|a^\dagger a|n+l\rangle\big)\, e^{i\omega(j-l)t}$$

$$= \frac{1}{2\nu+1}\,\frac{\hbar}{2m\omega}\Big[\sum_{j=-\nu}^{\nu}\sum_{l=-\nu}^{\nu}\sqrt{n+l}\sqrt{n+l-1}\,\underbrace{\delta_{n+j,\,n+l-2}}_{l=j+2} + \sqrt{n+l+1}\sqrt{n+l+2}\,\underbrace{\delta_{n+j,\,n+l+2}}_{l=j-2}$$

$$+\,\delta_{n+j,\,n+l}\,\big(2(n+l)+1\big)\Big]\, e^{i\omega(j+l)t}$$

$$= \frac{1}{2\nu+1}\,\frac{\hbar}{2m\omega}\Big[\sum_{j=-\nu}^{\nu-2}\sqrt{n+j+2}\sqrt{n+j+1}\; e^{2i\omega t} + \sum_{j=-\nu+2}^{\nu}\sqrt{n+j-1}\sqrt{n+j}\; e^{-2i\omega t}$$

$$+\sum_{j=-\nu}^{\nu}\big[2(n+j)+1\big]\Big]$$

$$= \frac{1}{2\nu+1}\,\frac{\hbar}{2m\omega}\Big[\sum_{j=-\nu}^{\nu-2}\sqrt{n+j+2}\sqrt{n+j+1}\; e^{2i\omega t} + \sum_{j=-\nu+2}^{\nu}\sqrt{n+j-1}\sqrt{n+j}\; e^{-2i\omega t}$$

$$+\sum_{j=-\nu}^{\nu}\big[2(n+j)+1\big]\Big]$$

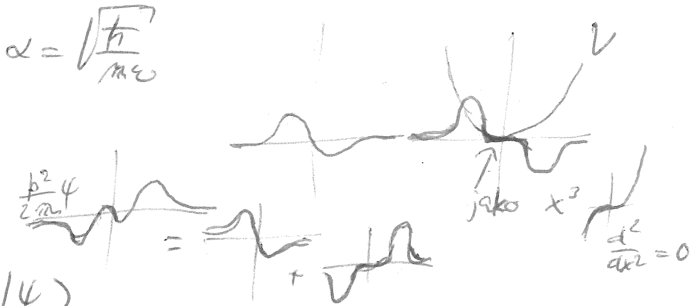
$$= \frac{1}{2\nu+1}\,\frac{\hbar}{2m\omega}\Big[\sum_{j=-\nu}^{\nu-2}\sqrt{n+j+2}\sqrt{n+j+1}\; e^{2i\omega t} + \sum_{j=-\nu}^{\nu-2}\sqrt{n+j+1}\sqrt{n+j+2}\; e^{-2i\omega t}$$

$$+\underbrace{\sum_{j=-\nu}^{\nu}\big[2(n+j)+1\big]}_{(2\nu+1)(2n+1)}\Big]$$

$$= \frac{\hbar}{2m\omega}(2n+1) + \frac{2}{2\nu+1}\,\frac{\hbar}{2m\omega}\sum_{j=-\nu}^{\nu-2}\sqrt{n+j+2}\sqrt{n+j+1}\,\cos(2\omega t)$$

$\mathcal{E}(x)$ pro $\psi_1(x)$

$$\psi_1 = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{\alpha}} \sqrt{2} \frac{x}{\alpha} e^{-\frac{x^2}{2\alpha^2}} \qquad \alpha = \sqrt{\frac{\hbar}{m\omega}}$$



$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2$$

$$V_{pot}|\psi_1\rangle = \frac{1}{2} m\omega^2 x^2 |\psi_1\rangle = \mathcal{E}_{pot}(x)|\psi_1\rangle$$

$$E_{kin}|\psi_1\rangle = \left(-\frac{\hbar^2}{2m}\frac{\sqrt{2}}{\pi^{1/4}\sqrt{\alpha}}\right)\frac{d^2}{dx^2}\frac{x}{\alpha}e^{-\frac{x^2}{2\alpha^2}} = \left(-\frac{\hbar^2}{2m}\frac{\sqrt{2}}{\pi^{1/4}\sqrt{\alpha}}\right)\frac{d}{dx}\left[\frac{1}{\alpha}e^{-\frac{x^2}{2\alpha^2}} - \frac{x^2}{\alpha^3}e^{-\frac{x^2}{2\alpha^2}}\right]$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\sqrt{2}}{\pi^{1/4}\sqrt{\alpha}}\right)\left[-\frac{x}{\alpha^3}e^{-\frac{x^2}{2\alpha^2}} - \frac{2x}{\alpha^3}e^{-\frac{x^2}{2\alpha^2}} + \frac{x^3}{\alpha^5}e^{-\frac{x^2}{2\alpha^2}}\right]$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\sqrt{2}}{\pi^{1/4}\sqrt{\alpha}}\right)\left(-\frac{3x}{\alpha^3}e^{-\frac{x^2}{2\alpha^2}} + \frac{x^3}{\alpha^5}e^{-\frac{x^2}{2\alpha^2}}\right)$$

$$= \left(-\frac{\hbar^2}{2m}\right)\left[-\frac{3}{\alpha^2} + \frac{x^2}{\alpha^4}\right]\underbrace{\frac{\sqrt{2}}{\pi^{1/4}\sqrt{\alpha}}\frac{x}{\alpha}e^{-\frac{x^2}{2\alpha^2}}}_{\psi_1}$$

$$= \left(+\frac{\hbar^2}{2m}\right)\left(3\frac{m\omega}{\hbar} - x^2\frac{m^2\omega^2}{\hbar^2}\right)|\psi_1\rangle$$

$$= \frac{3\hbar\omega}{2}|\psi_1\rangle - \frac{m\omega^2x^2}{2}|\psi_1\rangle = \mathcal{E}_{kin}(x)|\psi_1\rangle$$

$$= 0 \Rightarrow \frac{3\hbar\omega}{2} = \frac{m\omega^2x^2}{2}$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(a^+ - a)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|n\rangle = -\frac{\hbar^2}{2m} \qquad \frac{p^2}{2m}|n\rangle \qquad p^2 = -\frac{m\omega\hbar}{2}(a^+a^+ + aa - a^+a - aa^+)$$

$$= -\frac{m\omega\hbar}{2}(a^{+2} + a^2 - 2a^+a - 1)$$

$$\frac{p^2}{2m}|n\rangle = -\frac{m\omega\hbar}{4m}(a^{+2} + a^2 - 2a^+a - 1)|n\rangle =$$

$$= -\frac{\hbar\omega}{4}\left[\sqrt{n+1}\sqrt{n+2}|n+2\rangle + \sqrt{n}\sqrt{n-1}|n-2\rangle - 2(n+\tfrac{1}{2})|n\rangle\right]$$

$$= \frac{\hbar\omega}{2}(n+\tfrac{1}{2})|n\rangle - \frac{\hbar\omega}{4}\left[\sqrt{n+1}\sqrt{n+2}|n+2\rangle + \sqrt{n}\sqrt{n-1}|n-2\rangle\right]$$

$\langle n|$ → střední hodnota $E_n/2$

$$\frac{1}{2}m\omega^2x^2|n\rangle = \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}\left(a^+a + \frac{1}{2} + \frac{a^2 + a^{+2}}{2}\right)|n\rangle = \frac{1}{2}\hbar\omega(n+\tfrac{1}{2})|n\rangle +$$

$$+ \frac{1}{4}\hbar\omega\left[\sqrt{n}\sqrt{n-1}|n-2\rangle + \sqrt{n+1}\sqrt{n+2}|n+2\rangle\right]$$

$\langle n|$ → střední hodnota $E_n/2$

VIRIÁLOVÝ TEORÉM

LHO ve stavu $\psi_0 + \psi_1$, časový vývoj * T6.8

$$\psi_0 = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}} e^{-\frac{x^2}{2\alpha^2}}$$

$$\psi_1 = \frac{1}{\pi^{1/4}}\sqrt{\frac{2}{\alpha}}\frac{x}{\alpha} e^{-\frac{x^2}{2\alpha^2}} \qquad \alpha = \sqrt{\frac{\hbar}{m\omega}}$$

$$\psi(t=0) = \frac{1}{\sqrt{2}}(\psi_0+\psi_1) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\alpha}}\left(1+\sqrt{\frac{2}{\cancel{3}}}\frac{x}{\alpha}\right)e^{-\frac{x^2}{2\alpha^2}}$$

$$\langle\psi|\psi\rangle = \frac{1}{2\alpha\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2}}\left[1+\cancel{\sqrt{\frac{2}{3}}\frac{2x}{\alpha}}+\frac{2x^2}{\alpha^2}\right]dx$$

$$= \frac{1}{2\alpha\sqrt{\pi}}\int_{-\infty}^{\infty}\left[1+\frac{2x^2}{\alpha^2}\right]e^{-\frac{x^2}{\alpha^2}}dx \qquad \int_{-\infty}^{\infty} e^{-Ax^2}dx = \sqrt{\frac{\pi}{A}}$$

$$= \frac{1}{2\alpha\sqrt{\pi}}\left[\alpha\sqrt{\pi}+\frac{2}{\alpha^2}\cdot\frac{\alpha^2}{2}\alpha\sqrt{\pi}\right] = \qquad x^2 e^{-Ax^2} = \frac{1}{2A}\sqrt{\frac{\pi}{A}} \quad A=\frac{1}{\alpha^2}$$

$$= \frac{1}{2\alpha\sqrt{\pi}}\cdot 2\alpha\sqrt{\pi} = 1 \qquad \text{OK}$$

$$\psi(t) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\alpha}}\left(e^{-\frac{iE_0 t}{\hbar}}+\sqrt{2}\frac{x}{\alpha}e^{-\frac{iE_1 t}{\hbar}}\right)e^{-\frac{x^2}{2\alpha^2}}$$

$$= \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\alpha}}\left(e^{-\frac{i\omega t}{2}}+\sqrt{2}\frac{x}{\alpha}e^{-\frac{3i\omega t}{2}}\right)e^{-\frac{x^2}{2\alpha^2}}$$

$$\langle x\rangle(t) = \frac{1}{\sqrt{\pi}}\frac{1}{2\alpha}\int_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2}}\left(e^{\frac{i\omega t}{2}}+\sqrt{2}\frac{x}{\alpha}e^{\frac{3i\omega t}{2}}\right)x\left(e^{-\frac{i\omega t}{2}}+\sqrt{2}\frac{x}{\alpha}e^{-\frac{3i\omega t}{2}}\right)dx$$

$$= \frac{1}{\sqrt{\pi}}\frac{1}{2\alpha}\int_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2}}\left[e^{\frac{i\omega t}{2}}x\,\sqrt{2}\frac{x}{\alpha}e^{-\frac{3i\omega t}{2}}+\sqrt{2}\frac{x}{\alpha}e^{\frac{3i\omega t}{2}}x\,e^{-\frac{i\omega t}{2}}\right]dx$$

$$= \frac{1}{\sqrt{\pi}}\frac{1}{2\alpha}\int_{-\infty}^{\infty}\sqrt{2}\frac{x^2}{\alpha}e^{-\frac{x^2}{\alpha^2}}\left[e^{i\omega t}+e^{-i\omega t}\right] =$$

$$= \frac{1}{\sqrt{\pi}}\frac{1}{2\alpha}\frac{\sqrt{2}}{\alpha}2\cos(\omega t)\frac{\alpha^2}{2}\alpha\sqrt{\pi} =$$

$$= \frac{\alpha}{\sqrt{2}}\cos(\omega t)$$

$$\psi(0) = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\alpha}}\left(1+\frac{\sqrt{2}x}{\alpha}\right)e^{-\frac{x^2}{2\alpha^2}} \qquad x$$

$\to \psi_0$?
$\psi = \sum c_n \psi_n$?
$\psi(t)$?

$$\psi = \frac{1}{\sqrt{2}}(\psi_0 + \psi_1) = \frac{1}{\sqrt{2}}\left(\psi_0 e^{-\frac{i\omega t}{2}} + \psi_1 e^{-\frac{3i\omega t}{2}}\right)$$ $\left| e^{\frac{E_n t}{i\hbar}} \right.$ T6.8b

$e^{-i\omega t n}$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^+)$$

$$\langle\psi|x|\psi\rangle = \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}\left(\langle\psi_0| e^{\frac{i\omega t}{2}} + \langle\psi_1| e^{\frac{3i\omega t}{2}}\right)(a + a^+)\left(|\psi_0\rangle e^{-\frac{i\omega t}{2}} + |\psi_1\rangle e^{-\frac{3i\omega t}{2}}\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}\left[\langle\psi_0|a|\psi_1\rangle e^{-i\omega t} + \langle\psi_1|a^+|\psi_0\rangle e^{i\omega t}\right]$$

$$= \frac{\alpha}{\sqrt{2}}\frac{1}{2}\left[\sqrt{1}\langle\psi_0|\psi_0\rangle e^{-i\omega t} + \sqrt{1}\langle\psi_1|\psi_1\rangle e^{i\omega t}\right] =$$

$$= \frac{\alpha}{\sqrt{2}}\left[1\cos(\omega t)\right] = \frac{\alpha}{\sqrt{2}}\cos(\omega t)$$

pro ψ_n a ψ_{n+1}: $\psi = \frac{1}{\sqrt{2}}\left[\psi_n e^{-i\omega t(n+\frac{1}{2})} + \psi_{n+1} e^{-i\omega t(n+\frac{3}{2})}\right]$

$$= \frac{\alpha}{\sqrt{2}}\frac{1}{2}\left[\sqrt{n+1}\langle\psi_n|\psi_n\rangle e^{-i\omega t} + \sqrt{n+1}\langle\psi_{n+1}|\psi_{n+1}\rangle e^{i\omega t}\right]$$

$$= \frac{\alpha\sqrt{n+1}}{\sqrt{2}}\cos(\omega t) \doteq \frac{A_{average}}{2}\cos(\omega t)$$ OK

$$\frac{1}{2}m\omega^2 A^2 = \hbar\omega\left(n + \tfrac{1}{2}\right)$$

$$m\omega A^2 = 2\hbar\left(n + \tfrac{1}{2}\right)$$

$$A = \sqrt{\frac{2\hbar}{m\omega}\left(n + \tfrac{1}{2}\right)} = \alpha\sqrt{2\left(n + \tfrac{1}{2}\right)}$$

$$\rho(x) = \psi^*\psi = \frac{1}{2}\left[\psi_0^* e^{\frac{i\omega t}{2}} + \psi_1^* e^{+\frac{3i\omega t}{2}}\right]\left[\psi_0 e^{-\frac{i\omega t}{2}} + \psi_1 e^{-\frac{3i\omega t}{2}}\right]$$

$$= \frac{1}{2}\left[\psi_0^*\psi_0 + \psi_1^*\psi_1 + \psi_0^*\psi_1 e^{-i\omega t} + \psi_0\psi_1^* e^{i\omega t}\right]$$

ψ_n nedělá, je to jedno...

$$= \frac{1}{2}\left[\rho_0 + \rho_1\right] + \psi_0\psi_1\cos(\omega t)$$