I

pro 1D (zcela obecně): (pro x_2 zcela analogicky)

$$\frac{\partial \psi(x_T,x_R)}{\partial x_1} = \frac{\partial \psi}{\partial x_T}\frac{\partial x_T}{\partial x_1} + \frac{\partial \psi}{\partial x_R}\frac{\partial x_R}{\partial x_1}$$ ← derivace složené funkce

$$\frac{\partial^2 \psi(x_T,x_R)}{\partial x_1^2} = \frac{\partial}{\partial x_1}\left(\frac{\partial \psi}{\partial x_T}\frac{\partial x_T}{\partial x_1} + \frac{\partial \psi}{\partial x_R}\frac{\partial x_R}{\partial x_1}\right) =$$ derivace součinu funkcí

$$= \frac{\partial^2 \psi}{\partial x_T^2}\left(\frac{\partial x_T}{\partial x_1}\right)^2 + \frac{\partial^2 \psi}{\partial x_T \partial x_R}\left(\frac{\partial x_R}{\partial x_1}\right)\left(\frac{\partial x_T}{\partial x_1}\right) + \frac{\partial \psi}{\partial x_T}\underbrace{\frac{\partial^2 x_T}{\partial x_1^2}}_{=0} +$$

$=0$ protože transformace je lineární

$$+ \frac{\partial^2 \psi}{\partial x_R^2}\left(\frac{\partial x_R}{\partial x_1}\right)^2 + \frac{\partial^2 \psi}{\partial x_T \partial x_R}\left(\frac{\partial x_R}{\partial x_1}\right)\left(\frac{\partial x_T}{\partial x_1}\right) + \frac{\partial \psi}{\partial x_R}\underbrace{\frac{\partial^2 x_R}{\partial x_1^2}}_{=0}$$

pro nás: $x_R = x_1 - x_2 \Rightarrow \frac{\partial x_R}{\partial x_1} = 1 \quad \frac{\partial x_R}{\partial x_2} = -1$

$$x_T = \frac{m_1 x_1 + m_2 x_2}{m_1+m_2} \Rightarrow \frac{\partial x_T}{\partial x_1} = \frac{m_1}{m_1+m_2} \equiv \frac{m_1}{M}$$

$$\frac{\partial x_T}{\partial x_2} = \frac{m_2}{m_1+m_2} = \frac{m_2}{M}$$

⇒ dosadíme:

$$\frac{\partial^2}{\partial x_1^2} = \left(\frac{m_1}{M}\right)^2\frac{\partial^2}{\partial x_T^2} + 2\frac{m_1}{M}\frac{\partial^2}{\partial x_T \partial x_R} + \frac{\partial^2}{\partial x_R^2}$$

$$\frac{\partial^2}{\partial x_2^2} = \left(\frac{m_2}{M}\right)^2\frac{\partial^2}{\partial x_T^2} - 2\frac{m_2}{M}\frac{\partial^2}{\partial x_T \partial x_R} + \frac{\partial^2}{\partial x_R^2}$$

⇒ hamiltonián: $$\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} =$$

$$= -\frac{\hbar^2}{2}\left(\frac{m_1}{M^2}\right)\frac{\partial^2}{\partial x_T^2} - \frac{\hbar^2}{M}\frac{\partial^2}{\partial x_T \partial x_R} - \frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_R^2} +$$

$$- \frac{\hbar^2}{2}\left(\frac{m_2}{M^2}\right)\frac{\partial^2}{\partial x_T^2} + \frac{\hbar^2}{M}\frac{\partial^2}{\partial x_T \partial x_R} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_R^2}$$

$$= -\frac{\hbar^2}{2}\left(\frac{m_1+m_2}{M^2}\right)\frac{\partial^2}{\partial x_T^2} - \left(\frac{\hbar^2}{2m_1} + \frac{\hbar^2}{2m_2}\right)\frac{\partial^2}{\partial x_R^2}$$

$$= \frac{p_T^2}{2M} + \frac{p_R^2}{2\mu}$$

II

$$H_0 = \frac{p_R^2}{2\mu} + U(|\vec{r}_R|)$$

↳ položíme $=0$ (jen konstanta, protože $|\vec{r}_R| = r_0$ konst.)

$$= -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{(\nabla^n)^2}{r^2}\right) = -\frac{\hbar^2}{2\underbrace{\mu r_0}_{=I}}(\nabla^n)^2 = \frac{L^2}{2I}$$

už druhá přednáška

→ vypadnou ($=0$) protože $r = r_0 = $ konst.

(III)

$$H_0 = \frac{L^2}{2I} \Rightarrow \quad H_0 |l,m\rangle = \frac{L^2}{2I}|l,m\rangle = \frac{\hbar^2 l(l+1)}{2I}|l,m\rangle$$

$\Rightarrow$ vlastními stavy jsou kulové funkce $|l,m\rangle$

s energiemi $E_l = \dfrac{\hbar^2 l(l+1)}{2I}$ $\qquad E_0 = 0\,eV,\ E_1 = 1{,}3\cdot 10^{-3}\,eV,$
$E_2 = 7{,}8\cdot 10^{-3}\,eV$

$\hookrightarrow$ pro daní l existuje $-m,\dots,+m = 2l+1$ hodnot m

$\Rightarrow$ každá hladina je $(2l+1)$-krát degenerovaná

(IV)

$$\underline{[H, L_z]} = [\frac{L^2}{2I} + |\vec{D}||\vec{\mathcal{E}}|\cos\theta, L_z] =$$

$$= \frac{1}{2I}\underbrace{[L^2, L_z]}_{=0} + D\mathcal{E}\underbrace{[\cos\theta, L_z]}_{=0} = \underline{\underline{0}}$$

(V)

$$E^{(1)}_{l,m} = \langle l m|H_1|l,m\rangle = D\mathcal{E}\,\langle l,m|\cos\theta|l,m\rangle = \dots = \underline{\underline{0}}$$

protože:

(a) $\int$ lichá fce $= 0$

(b) působení $\cos\theta|l,m\rangle = a_{l+1}|l+1,m\rangle + a_l|l-1,m\rangle$

a dále orthogonalita $\langle l,m|l',m'\rangle = \delta_{ll'}\delta_{mm'} \rightarrow = 0$

(VI)

$$E^{(2)}_{lm} = \sum_{\substack{l',m' \\ \neq l,m}} \frac{|\langle l m|H_1|l',m'\rangle|^2}{E^{(0)}_{l,m} - E^{(0)}_{l',m'}} = \sum_{l',m' \neq l,m} \frac{|\langle l,m|\,D\mathcal{E}\cos\theta\,|l',m'\rangle|^2}{E^{(0)}_l - E^{(0)}_{l'}} =$$

$$= D^2\mathcal{E}^2 \sum_{l'} \frac{\left|\langle l,m|\left(\sqrt{\frac{(l'+m+1)(l'-m+1)}{(2l'+1)(2l'+3)}}\,|l'+1,m\rangle + \sqrt{\frac{(l'+m)(l'-m)}{(2l'-1)(2l'+1)}}\,|l'-1,m\rangle\right)\right|^2}{\frac{\hbar^2}{2I}l(l+1) - \frac{\hbar^2}{2I}l'(l'+1)}$$

$\leftarrow$ přispívají pouze členy $l' = l\pm 1$

$$= \frac{2D^2\mathcal{E}^2 I^2}{\hbar^2}\left\{ \underbrace{\frac{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}}{l(l+1)-(l+1)(l+2)}}_{l'=l+1} + \underbrace{\frac{\frac{(l+m)(l-m)}{(2l-1)(2l+1)}}{l(l+1)-(l-1)l}}_{l'=l-1} \right\}$$

$$= \dots = \underline{\underline{D^2\mathcal{E}^2\frac{I}{\hbar^2}\frac{l(l+1)-3m^2}{l(l+1)(2l-1)(2l+3)}}}$$