

## PŘIBLIŽNÉ METODY: PORUCHOVÁ

### A) NEDEGENEROVANÉ HLADINY

$$H = H_0 + \delta H_1$$

$$E_n = E_n^{(0)} + \delta E_n^{(1)} + \delta^2 E_n^{(2)} + \dots$$

$$|\Psi_n\rangle = |\psi_n^{(0)}\rangle + \delta |\psi_n^{(1)}\rangle + \delta^2 |\psi_n^{(2)}\rangle + \dots$$

právna Schrödingerova rovnice  $H|\Psi\rangle = E_n|\Psi\rangle$

$$\Rightarrow (H_0 + \delta H_1)(|\psi_n^{(0)}\rangle + \delta |\psi_n^{(1)}\rangle + \delta^2 |\psi_n^{(2)}\rangle) = (E_n^{(0)} + \delta E_n^{(1)} + \delta^2 E_n^{(2)} + \dots)(|\psi_n^{(0)}\rangle + \delta |\psi_n^{(1)}\rangle + \delta^2 |\psi_n^{(2)}\rangle + \dots)$$

$$\delta^0: H_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle \Rightarrow zdrojné / určitné$$

$$\delta^1: (H_0 - E_n^{(0)})|\psi_n^{(1)}\rangle + (f_{H_1} - E_n^{(0)})|\psi_n^{(0)}\rangle = 0$$

$$\delta^2: (H_0 - E_n^{(0)})|\psi_n^{(2)}\rangle + (H_1 - E_n^{(1)})|\psi_n^{(1)}\rangle - E_n^{(1)}|\psi_n^{(0)}\rangle = 0$$

etd.

$$\Rightarrow \langle \psi_n^{(0)} | (H_0 - E_n^{(0)})|\psi_n^{(1)}\rangle + \langle \psi_n^{(0)} | (H_1 - E_n^{(1)})|\psi_n^{(0)}\rangle = 0$$

$$\Rightarrow \boxed{E_n^{(1)} = \langle \psi_n^{(0)} | H_1 | \psi_n^{(0)} \rangle}$$

$$\Rightarrow \langle \psi_n^{(0)} | (H_0 - E_n^{(0)})|\psi_n^{(2)}\rangle + \langle \psi_n^{(0)} | (H_1 - E_n^{(1)})|\psi_n^{(1)}\rangle - E_n^{(1)} \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle = 0$$

normalizace:  $\langle \Psi | \Psi \rangle = 1$  }  $\Rightarrow \langle \psi_n^{(1)} | \psi_n^{(1)} \rangle = 0$   
 nebo  $\langle \psi_n^{(0)} | \Psi \rangle = 1$

$$\Rightarrow E_n^{(2)} = \langle n^{(0)} | H_1 | n^{(1)} \rangle$$

ale (zehn) rechnen...

$$|n^{(1)}\rangle = \sum_i c_i^{(1)} |i^{(0)}\rangle \quad \text{Koeffizienten der Basiszustände} \\ \{ |n^{(0)}\rangle \}$$

z. B. für pro  $\delta$ : pro  $\langle m^{(0)} | \neq \langle n^{(0)} | :$

$$\underbrace{\langle m^{(0)} | (H_0 - E_m^{(0)}) | n^{(1)} \rangle}_{\langle m^{(0)} | E_m^{(0)} } + \langle m^{(0)} | (H_1 - E_n^{(1)}) | n^{(0)} \rangle = 0$$

$$(E_m^{(0)} - E_n^{(0)}) \underbrace{\langle m^{(0)} | n^{(1)} \rangle}_{\delta_{mn}} + \langle m^{(0)} | H_1 | n^{(0)} \rangle - \underbrace{- E_n^{(1)} \underbrace{\langle m^{(0)} | n^{(0)} \rangle}_{\delta_{mn}}}_{\delta_{mn} = 0} = 0$$

$$\langle m^{(0)} | \sum_i c_i^{(1)} | i^{(0)} \rangle =$$

$$= \sum_i c_i^{(1)} \underbrace{\langle m^{(0)} | i^{(0)} \rangle}_{\delta_{mi}} = c_m^{(1)}$$

$$(E_m^{(0)} - E_n^{(0)}) c_m^{(1)} + \langle m^{(0)} | H_1 | n^{(0)} \rangle = 0$$

$$\Rightarrow c_m^{(1)} = - \frac{\langle m^{(0)} | H_1 | n^{(0)} \rangle}{E_m^{(0)} - E_n^{(0)}} \quad m \neq n$$

$$\Rightarrow |n^{(1)}\rangle = \sum_i c_i |i\rangle = \sum_i - \frac{\langle i^{(0)} | H_1 | n^{(0)} \rangle}{E_i^{(0)} - E_n^{(0)}} |i\rangle$$

$$\Rightarrow E_n^{(2)} = \langle n^{(0)} | H_1 | n^{(1)} \rangle$$

$$\boxed{E_n^{(2)} = \sum_i \frac{\langle n^{(0)} | H_1 | i^{(0)} \rangle \times \langle i^{(0)} | H_1 | n^{(0)} \rangle}{E_i^{(0)} - E_n^{(0)}}}$$

z.B.  $\text{LiO}$  s. vorheriger:

$$H = \underbrace{\frac{p^2}{2} + \frac{x^2}{2}}_{H_0} + \underbrace{S_x}_{H_1}$$

$$H_b|n\rangle = (n + \frac{1}{2})|n\rangle$$

$$\begin{aligned} a &= \frac{1}{\sqrt{2}}(x + i p) \\ a^\dagger &= \frac{1}{\sqrt{2}}(x - i p) \end{aligned} \quad \Rightarrow \quad x = \frac{1}{\sqrt{2}}(a + a^\dagger)$$

$$\begin{aligned} a|n\rangle &= \sqrt{n}|n-1\rangle \\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \end{aligned}$$

$$\begin{aligned} E_0^{(1)} &= \langle 0 | x | 10 \rangle = \langle 0 | \frac{1}{\sqrt{2}}(a + a^\dagger) | 10 \rangle = 0 \\ &= \int_{-\infty}^{+\infty} \sqrt{\frac{1}{\pi}} e^{-\frac{x^2}{2}} \times \sqrt{\frac{1}{\pi}} e^{-\frac{x^2}{2}} dx = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{\pi}} e^{-x^2} dx = 0 \\ &\quad \text{se da} \cdot \text{ lieber} = 0 \end{aligned}$$

$$\underline{\underline{E_0^{(2)}}} = \sum_{k \neq 0} \frac{\langle 0 | x | k \rangle \langle k | x | 10 \rangle}{\frac{1}{2} - (k + \frac{1}{2})} = \sum_{k \neq 0} \frac{1 \langle 0 | x | k \rangle^2}{-k} =$$

$$\begin{aligned} \langle 0 | x | k \rangle &= \frac{1}{\sqrt{2}} \langle 0 | (a + a^\dagger) | k \rangle = \\ &= \frac{1}{\sqrt{2}} \left( \sqrt{k} \langle 0 | k-1 \rangle + \sqrt{k+1} \langle 0 | k+1 \rangle \right) \end{aligned}$$

→ pro spez. parte  $k=1$

$$= \frac{|\frac{1}{\sqrt{2}}|^2}{-1} = \underline{\underline{-\frac{1}{2}}}$$

$$\Rightarrow \text{Energie } E_0 \approx E_0^{(0)} + \delta E_0^{(1)} + \delta^2 E_0^{(2)}$$

$$\frac{1}{2} + \delta \cdot 0 + \delta^2 \cdot (-\frac{1}{2}) = \underline{\underline{\frac{1}{2} - \frac{1}{2}\delta^2}}$$

$$\Rightarrow \text{für } \delta = 0,1 : E_0 \approx 0,495$$

$$\delta = 901 : \underline{E_0 \approx 0,49995}$$

## B) DEGENEROVANÉ HLADINY

vše hladiny se stejnou energií  $E_n \rightarrow \sum_{l=1}^N l$

$\Rightarrow$  řešení v. problém

$$\begin{pmatrix} W_{11} - E_n^{(1)} & W_{12} & \dots \\ W_{21} & W_{22} - E_n^{(1)} & \\ W_{31} & W_{32} & \dots \\ & \vdots & \\ & W_{NN} - E_n & \end{pmatrix} \begin{pmatrix} d_1 \\ \vdots \\ d_N \end{pmatrix} = 0$$

principy  
jednotlivých staveb

pr. správane oscilatory:

$$H = \underbrace{\frac{P_x^2}{2} + \frac{x^2}{2}}_{H_0} + \underbrace{\frac{P_y^2}{2} + \frac{y^2}{2}}_{H_0} + \delta \underbrace{x^2 y^2}_{H_1}$$

$$v.l.-stavy |i\rangle_x \otimes |j\rangle_y = |ij\rangle$$

$$H|ij\rangle = (H_x|i\rangle)|j\rangle + |i\rangle(H_y|j\rangle) =$$

$$= (i + \frac{1}{2})|ij\rangle + (j + \frac{1}{2})|ij\rangle$$

$$= \underbrace{(i+j+1)}_{E_{ij}} |ij\rangle$$

$$E_{ij} = E_{i+j}$$

$$\Rightarrow E_0 = 1 \text{ 100\% nedeg.}$$

$$E_1 = 2 \text{ 110\%, 101\% deg.}$$

$$E_2 = 3 \text{ 120\%, 111\%, 102\% deg.}$$

:

→ pro první exc. stav:

$$\begin{pmatrix} \langle 10|H_n|10\rangle - E_1^{(1)} & \langle 10|H_n|01\rangle \\ \langle 01|H_n|10\rangle & \langle 01|H_n|01\rangle - E_1^{(1)} \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = 0$$

$$\begin{aligned} \langle 10|H_n|10\rangle &= \langle 10|x^2y^2|10\rangle = \\ &= \langle 10|x^2|10\rangle \langle 01|y^2|0\rangle = \\ &= \langle 10| \frac{1}{2}(aa + ata + aat + atat) |10\rangle \times \\ &\quad \times \langle 01| \frac{1}{2}(bb + btb + bbt + btb^*) |0\rangle = \\ &= \frac{1}{4} \underbrace{\langle 10(aaa + aat) |10\rangle}_{1+2} \underbrace{\langle 01(bbb + bbt) |0\rangle}_{=1} = \\ &\approx \frac{3}{4} \end{aligned}$$

$$\langle 01|H_n|01\rangle = \dots = \frac{3}{4}$$

$$\langle 01|H_n|10\rangle = (\langle 10|H_n|01\rangle)^* = 0$$

$$\Rightarrow \begin{pmatrix} \frac{3}{4} - E_1^{(1)} & 0 \\ 0 & \frac{3}{4} - E_1^{(1)} \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = 0$$

$$\Rightarrow \det \begin{pmatrix} \frac{3}{4} - E_1^{(1)} & 0 \\ 0 & \frac{3}{4} - E_1^{(1)} \end{pmatrix} = 0$$

$$(\frac{3}{4} - E_1^{(1)})^2 = 0$$

$E_1^{(1)} = \frac{3}{4}$  → neložit k sejméni degenerace,

bloking je jen paráha

$$\Rightarrow \underline{\underline{E_1}} \approx E_1^{(0)} + \delta E_1^{(1)} = \underline{\underline{2 + \delta \frac{3}{4}}}$$

pro  $\delta = 0,1 \approx 2,075$

## WSD LHU v Moqr. poti

$$H = H_1 + H_2 = \frac{1}{2}(P_x^2 + x^2) + \frac{1}{2}(P_y^2 + y^2) + \frac{1}{2}(P_z^2 + z^2)$$

$$a = \frac{i}{\hbar} (x + i p)$$

$$a^\dagger = \frac{i}{\hbar} (x - i p)$$

$$[a, a^\dagger] = 1$$

$$H = a_x^\dagger a_x + \frac{1}{2} + a_y^\dagger a_y + \frac{1}{2} + a_z^\dagger a_z + \frac{1}{2}$$

$$H = a_x^\dagger a_x + a_y^\dagger a_y + a_z^\dagger a_z + \frac{3}{2}$$

$$L_i = \sum_{j,k} x_j P_k$$

$$L_x = y P_z - z P_y$$

$$y = \frac{i}{\hbar} (a_y + a_y^\dagger) \quad P_y = \frac{i}{\hbar} (a_y^\dagger - a_y)$$

$$z = \frac{i}{\hbar} (a_z + a_z^\dagger) \quad P_z = \frac{i}{\hbar} (a_z^\dagger - a_z)$$

$$\begin{aligned} L_x &= \frac{i}{2} (a_y + a_y^\dagger)(a_z^\dagger - a_z) - \\ &\quad - \frac{i}{2} (a_z + a_z^\dagger)(a_y^\dagger - a_y) = \\ &= \frac{i}{2} \left[ \cancel{a_y a_z^\dagger} + \cancel{a_y^\dagger a_z^\dagger} - \cancel{a_y a_z} - \cancel{a_y^\dagger a_z} - \right. \\ &\quad \left. - \text{const} \right], \end{aligned}$$

$$\begin{aligned} & -\omega_{xy} - \alpha_2 \cancel{\alpha_y} + \cancel{\alpha_2 \alpha_y} + \cancel{\alpha_2^+ \alpha_y} = \\ & = \underline{i(\alpha_y \alpha_2^+ - \alpha_y^+ \alpha_2)} \end{aligned}$$

energie reprezentace 3D LHO:

$$E_n = h_x + h_y + h_z + \frac{3}{2}$$

$\Rightarrow$  první excitovaný stav:

$$E_1 = \frac{5}{2} \quad \{|100\rangle, |010\rangle, |001\rangle\}$$

PM pro degenerované hladiny

$$\begin{aligned} & \langle n'_x n'_y n'_z | \alpha_y \alpha_2^+ | n_x n_y n_z \rangle = \\ & = \underbrace{\langle n'_x | n_x \rangle}_{\delta n'_x | n_x \rangle} \underbrace{\langle n'_y | n_y - 1 \rangle}_{\delta n'_y | n_y - 1 \rangle} \underbrace{\langle n'_z | n_z + 1 \rangle}_{\delta n'_z | n_z + 1 \rangle} \sqrt{n_y(n_z + 1)} \end{aligned}$$

$$\begin{aligned} & \langle n'_x n'_y n'_z | \alpha_2 \alpha_y^+ | n_x n_y n_z \rangle = \\ & = \underbrace{\langle n'_x | n_x \rangle}_{\delta n'_x | n_x \rangle} \underbrace{\langle n'_y | n_y + 1 \rangle}_{\delta n'_y | n_y + 1 \rangle} \underbrace{\langle n'_z | n_z - 1 \rangle}_{\delta n'_z | n_z - 1 \rangle} (n_y + 1) n_z \end{aligned}$$

$\Rightarrow$  dostaneme matici

$$\begin{matrix} & |100\rangle & |010\rangle & |001\rangle \\ \langle 100| & \left( \begin{array}{ccc} 0 & 0 & 0 \end{array} \right) & & \\ \langle 010| & & \left( \begin{array}{ccc} 0 & 0 & 1 \end{array} \right) & \end{matrix}$$

$$\langle 001 | \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$$

$$\Rightarrow \det \begin{vmatrix} -\lambda & 0 & 0 \\ 0 & \lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} = -\lambda \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} =$$

$$= -\lambda \cdot (\lambda^2 - 1) = 0$$

$$\Rightarrow \lambda = 0, \pm 1$$

$$\Rightarrow \underbrace{E_1^{(n)} = 0, \pm \frac{qB}{2m}}$$