# QMII-cv01 Stacionární poruchová teorie

**ÚLOHA 1** – Lineární harmonický potenciál v konst. poli

$$\hat H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \qquad H_1 = \lambda X \qquad \lambda \in \mathbb{R}$$

**ÚKOL:** • přesné řešení • poruchové $E^{(1)}$, $|\psi^{(1)}\rangle$, $E^{(2)}$

**ŘEŠENÍ:**

$$\boxed{H_0|n\rangle = \epsilon_n|n\rangle \qquad \epsilon_n = \hbar\omega\left(n+\tfrac{1}{2}\right)}$$

• přesné řešení: $H = \dfrac{p^2}{2m} + \underbrace{\dfrac{1}{2} m\omega^2 x^2 + \lambda x + 0}_{\frac{1}{2} m\omega^2 (x+\bar x)^2 + \bar\epsilon}$

$$\frac{1}{2} m\omega^2 (x+\bar x)^2 + \bar\epsilon$$

$$= \frac{1}{2} m\omega^2 x^2 + m\omega^2 x\bar x + \underbrace{\frac{1}{2} m\omega^2 \bar x^2 + \bar\epsilon}_{0}$$

$$\lambda = m\omega^2 \bar x \qquad \boxed{\bar x = \frac{\lambda}{m\omega^2}}$$

$$\bar\epsilon = -\frac{1}{2} m\omega^2 \bar x^2$$

$$\boxed{\bar\epsilon = -\frac{1}{2}\frac{\lambda^2}{m\omega^2}} \leftarrow$$

porušené přesné energie $E_n = \bar\epsilon + \hbar\omega\left(n+\frac{1}{2}\right)$

$$x = x_0 \frac{\hat a + \hat a^+}{\sqrt 2} = \sqrt{\frac{\hbar}{2m\omega}}\,(a+a^+)$$

• poruchové řešení:

$$E_n^{(1)} = \langle n|H_1|n\rangle = \langle n|X|n\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|\hat a + \hat a^+|n\rangle = 0$$

$$E_n = \epsilon_n + \lambda E_n^{(1)} + \dots$$

$$\langle n|\psi_n^{(1)}\rangle = 0$$

$$\langle n'|\psi_n^{(1)}\rangle = \frac{\langle n'|H_1|n\rangle}{\epsilon_n - \epsilon_{n'}}$$

$$\langle n'|H_1|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle n'|\left(\sqrt n\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)$$

$$= \underbrace{\sqrt{\frac{\hbar}{2m\omega}}}_{A}\left\{\sqrt n\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right\}$$

$$|\psi_n\rangle = |n\rangle + \sum_{m\neq n}|m\rangle A \frac{\left\{\sqrt n\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right\}}{\epsilon_n - \epsilon_m}$$

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

$$= |n\rangle + A\left\{\frac{\sqrt n\,|n-1\rangle}{\underbrace{\epsilon_n - \epsilon_{n-1}}_{\hbar\omega}} + \frac{\sqrt{n+1}\,|n+1\rangle}{\underbrace{\epsilon_n - \epsilon_{n+1}}_{-\hbar\omega}}\right\}$$

$$|\psi_n\rangle = |n\rangle + \frac{A}{\hbar\omega}\left\{\sqrt{n}\,|n-1\rangle - \sqrt{n+1}\,|n+1\rangle\right\} + O(\lambda^2)$$

$$H_1 = A(a+a^\dagger)$$

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

$$= \frac{A^2}{\hbar\omega}\langle n|(a+a^\dagger)\left\{\sqrt{n}\,|n-1\rangle - \sqrt{n+1}\,|n+1\rangle\right\} \qquad \sqrt{n}\sqrt{n}\,|n\rangle$$

$$= \frac{A^2}{\hbar\omega}\Big(n - \underbrace{\sqrt{n+1}\cdot\sqrt{n+1}}_{n+1}\Big) = -\frac{A^2}{\hbar\omega} = -\frac{\hbar}{2m\omega}\,\frac{1}{\hbar\omega}$$

$$-\frac{1}{2}\,\frac{\lambda^2}{m\omega^2}$$

$$E_n = E_n^{(0)} + \lambda \underset{0}{\underset{\shortparallel}{E_n^{(1)}}} + \lambda^2 E_n^{(2)}$$

$$E_n = \hbar\omega\left(\frac{1}{2}+n\right) - \frac{1}{2}\frac{\lambda^2}{m\omega^2} + \underbrace{O(\lambda^3)}_{=0}$$

## ÚLOHA 2: $\mathcal{H} = \mathbb{C}^2 \qquad H_0 = \begin{pmatrix}\epsilon_1 & 0\\ 0 & \epsilon_2\end{pmatrix} \qquad H_1 = \begin{pmatrix}0 & v\\ v^* & 0\end{pmatrix}$

### a) přesné řešení

$|1\rangle \quad |2\rangle$ -- $H_0|n\rangle = \epsilon_n|n\rangle$

vl. č. $H = H_0 + H_1 = \begin{pmatrix}\epsilon_1 & v\\ v_* & \epsilon_2\end{pmatrix}$ $\qquad (\epsilon_1-\lambda)(\epsilon_2-\lambda) - |v|^2 = 0$

$$\Rightarrow \lambda^2 - (\epsilon_1+\epsilon_2)\lambda + \epsilon_1\epsilon_2 - |v|^2 = 0$$

$$\lambda_{1,2} = \frac{\epsilon_1+\epsilon_2}{2} \pm \sqrt{\left(\frac{\epsilon_1-\epsilon_2}{2}\right)^2 + |v|^2}$$

$\epsilon_2 > \epsilon_1$

### b) RS poruch. teorie:

$$E_1^{(1)} = \langle 1|H_1|1\rangle = 0$$

$$E_1 = \epsilon_1 + E_1^{(1)} + E_1^{(2)} + \dots = \epsilon_1 + \frac{|v|^2}{\epsilon_1-\epsilon_2}$$

$$\underbrace{E_1^{(2)} = \frac{|\langle 2|H_1|1\rangle|^2}{\epsilon_1-\epsilon_2}} \sim |v|^2$$

$$\lambda_1 = \frac{\epsilon_1+\epsilon_2}{2} - \sqrt{\left(\frac{\epsilon_2-\epsilon_1}{2}\right)^2} \left[1 + \underbrace{\frac{4|v|^2}{(\epsilon_2-\epsilon_1)^2}}\right]^{\hat{\frac{1}{2}}}$$

$$(1+\varepsilon)^{\alpha} \doteq 1 + \alpha\varepsilon$$

$$\lambda_1 = \underbrace{\frac{\epsilon_1+\epsilon_2}{2} - \frac{\epsilon_2-\epsilon_1}{\cancel{2}}}\left(1 + \frac{\cancel{2}|v|^2}{(\epsilon_2-\epsilon_1)^2} + \dots\right)$$

$$= \epsilon_1 - \frac{|v^2|}{\epsilon_2-\epsilon_1} \quad \checkmark$$

použiteľné pokiaľ $\boxed{|v| \leq \epsilon_2 - \epsilon_1}$

$\forall m \neq n \quad \underline{|\langle m|H_1|n\rangle| \leq |\epsilon_m - \epsilon_n|}$

nedegenerovaná teória

$\dots \ \epsilon_1 \neq \epsilon_2$

$\boxed{\text{degenerovaná teória}}$ ? $\dots \quad \epsilon_1 = \epsilon_2$

$$\underline{H_0 = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_1 \end{pmatrix}} \qquad H_1 = \begin{pmatrix} 0 & v \\ v^* & 0 \end{pmatrix} \qquad H_0 = \epsilon_0 \hat{I}$$

primárnej báze $\underset{m=1}{|1,1\rangle_0}, \underset{r=1,2}{|1,2\rangle_0}$ $\longrightarrow$ $|1,t\rangle$ adaptovaná báze

matica $\langle 1r|H_1|1r'\rangle \longrightarrow \underline{\begin{pmatrix} 0 & v \\ v^* & 0 \end{pmatrix}} \dots$

adaptovaná báze $\to$ presné riešenie

B-W poruchová teória

$$E_1 = \epsilon_1 + \underset{\overset{\parallel}{0}}{\langle 1|H_1|1\rangle} + \frac{|\langle 2|H_1|1\rangle|^2}{E_1 - \epsilon_2} \sim |v|^2$$

$2 = m \neq n$ !

$$E_1(E_1-\epsilon_2) = \epsilon_1(E_1-\epsilon_2) + |v^2|$$

$$\boxed{(E_1-\epsilon_2)(E_1-\epsilon_1) - |v|^2 = 0}$$

$\lambda = E_1$ $\qquad\qquad$ $E_1 = \lambda_1, \lambda_2$