Poruchová teorie

Schrödingerova rovnice $(\hat{H} - E)|\Psi\rangle = 0 \Rightarrow E_\xi , |\Psi_\xi\rangle$

$$\hat{H}|\Psi_\xi\rangle = E_\xi|\Psi_\xi\rangle$$

$$\hat{H} = \hat{H}_0 + \lambda\hat{H}' + \lambda^2\hat{H}'' + \dots$$

neporušený problém $\lambda = 0$

$\hat{H}_0|\Psi_\xi^0\rangle = E_\xi^0|\Psi_\xi^0\rangle$ hledáme $\boxed{|\Psi_\xi\rangle = |\Psi_\xi^0\rangle + \lambda|\Psi_\xi'\rangle + \lambda^2|\Psi_\xi''\rangle + \dots}$

nemá degeneraci

$$\boxed{E_\xi = E_\xi^0 + \lambda E_\xi' + \lambda^2 E_\xi'' + \dots}$$

$\hat{H}|\Psi_\xi\rangle = E_\xi|\Psi_\xi\rangle \Rightarrow$

$$(\hat{H}_0 + \lambda\hat{H}' + \lambda^2\hat{H}'' + \dots)(|\Psi_\xi^0\rangle + \lambda|\Psi_\xi'\rangle + \lambda^2|\Psi_\xi''\rangle + \dots) =$$

$$= (E_\xi^0 + \lambda E_\xi' + \lambda^2 E_\xi'' + \dots)(|\Psi_\xi^0\rangle + \lambda|\Psi_\xi'\rangle + \lambda^2|\Psi_\xi''\rangle + \dots)$$

λ^0 $\qquad = 0 \qquad\qquad \lambda^1$

$$(\hat{H}_0|\Psi_\xi^0\rangle - E_\xi^0|\Psi_\xi^0\rangle) + \lambda(\hat{H}'|\Psi_\xi^0\rangle + \hat{H}_0|\Psi_\xi'\rangle - E_\xi^0|\Psi_\xi'\rangle - E_\xi'|\Psi_\xi^0\rangle)$$

$$+ \lambda^2(\hat{H}''|\Psi_\xi^0\rangle + \hat{H}_0|\Psi_\xi''\rangle + \hat{H}'|\Psi_\xi'\rangle - E_\xi^0|\Psi_\xi''\rangle - E_\xi'|\Psi_\xi'\rangle - E_\xi''|\Psi_\xi^0\rangle) + \dots$$

$$= 0$$

$$\sum_{n=0}^{\infty} x^n a_n = 0$$

$a_0 = 0$

$\longrightarrow$ každý člen zvlášť musí být roven nule

λ^1:

$$\hat{H}'|\psi_\varepsilon^0\rangle + \hat{H}_0|\psi_\varepsilon^1\rangle - E_\varepsilon^0|\psi_\varepsilon^1\rangle - E_\varepsilon^1|\psi_\varepsilon^0\rangle = 0$$

$$|\psi_\varepsilon^1\rangle = \sum_\ell a_\ell^\varepsilon |\psi_\ell^0\rangle$$

$\langle\psi_\varepsilon^0|$

$$\Rightarrow \langle\psi_\varepsilon^0|\hat{H}'|\psi_\varepsilon^0\rangle + \cancel{E_\varepsilon^0 a_\varepsilon^\varepsilon} - \cancel{E_\varepsilon^0 a_\varepsilon^\varepsilon} - E_\varepsilon^1 = 0$$

$$\boxed{E_\varepsilon^1 = \langle\psi_\varepsilon^0|H'|\psi_\varepsilon^0\rangle}$$

$\langle\psi_\ell^0|$ $\ell \neq \varepsilon$

$$\Rightarrow \langle\psi_\ell^0|H'|\psi_\varepsilon^0\rangle + E_\ell^0 a_\ell^\varepsilon - E_\varepsilon^0 a_\ell^\varepsilon = 0$$

$$\boxed{a_\ell^\varepsilon = \frac{\langle\psi_\ell^0|H'|\psi_\varepsilon^0\rangle}{E_\varepsilon^0 - E_\ell^0}}$$

$$\boxed{|\psi_\varepsilon^1\rangle = \sum_{\ell\neq\varepsilon} \frac{\langle\psi_\ell^0|H'|\psi_\varepsilon\rangle}{E_\varepsilon^0 - E_\ell^0}}$$

Opravy druhého řádu

λ^2:

$$\hat{H}''|\psi_\varepsilon^0\rangle + H_0|\psi_\varepsilon''\rangle + H'|\psi_\varepsilon'\rangle - E_\varepsilon^0|\psi_\varepsilon''\rangle - E_\varepsilon'|\psi_\varepsilon'\rangle - E_\varepsilon''|\psi_\varepsilon^0\rangle = 0$$

$$|\psi_\varepsilon''\rangle = \sum_\ell b_\ell^\varepsilon |\psi_\varepsilon^0\rangle$$

$\langle\psi_\varepsilon^0| \Rightarrow$

$$\langle\psi_\varepsilon^0|H''|\psi_\varepsilon^0\rangle + \cancel{E_\varepsilon^0 b_\varepsilon^\varepsilon} + \langle\psi_\varepsilon^0|H'|\psi_\varepsilon'\rangle - \cancel{E_\varepsilon^0 b_\varepsilon^\varepsilon} - \overbrace{E_\varepsilon' a_\varepsilon^\varepsilon}^{=0} - E_\varepsilon'' = 0$$

$$\boxed{E_\varepsilon'' = \sum_{\ell\neq\varepsilon} \frac{\langle\psi_\varepsilon^0|H'|\psi_\ell^0\rangle\langle\psi_\ell^0|H'|\psi_\varepsilon^0\rangle}{E_\varepsilon^0 - E_\ell^0} + \langle\psi_\varepsilon^0|H''|\psi_\varepsilon''\rangle}$$

$\langle\psi_\ell^0| \Rightarrow$

$$\langle\psi_\ell^0|\hat{H}''|\psi_\varepsilon^0\rangle + E_\ell^0 b_\ell^\varepsilon + \sum_m \langle\psi_\ell^0|H'|\psi_m^0\rangle a_m^\varepsilon - E_\varepsilon^0 b_\ell^\varepsilon - E_\varepsilon' a_\ell^\varepsilon = 0$$

$$(E_\ell^0 - E_\varepsilon^0) b_\ell^\varepsilon = \langle\psi_\ell^0|\hat{H}''|\psi_\varepsilon^0\rangle + \sum_m \langle\psi_\ell^0|H'|\psi_\varepsilon'\rangle a_m^\varepsilon - E_\varepsilon' a_\ell^\varepsilon$$

$$b_\ell^\varepsilon = \dots$$