Optimalizace lineárních parametrů

$$H|\Psi\rangle = E|\Psi\rangle \qquad ; \quad |\Psi\rangle = \sum_n a_n |\Psi_n\rangle$$

obecně: $S_{nm} = \langle \Psi_n | \Psi_m \rangle$

$$\langle \Psi|H|\Psi\rangle = E\langle\Psi|\Psi\rangle$$

$$E = \frac{\langle \Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum_{nm} a_n a_m \overbrace{\langle \Psi_n|H|\Psi_m\rangle}^{H_{nm}}}{\sum_{nm} a_n a_m S_{nm}}$$

$$\frac{\partial}{\partial a_k} E = \frac{\sum_{nm}\left(\frac{\partial a_n}{\partial a_k} a_m + a_n \frac{\partial a_m}{\partial a_k}\right) H_{nm}}{\sum_{nm} a_n a_m S_{nm}} - \frac{\overbrace{\left(\sum_{nm} a_n a_m H_{nm}\right)}^{\langle\Psi|H|\Psi\rangle} \sum_{nm}\left(\frac{\partial a_n}{\partial a_k} a_m + a_n \frac{\partial a_m}{\partial a_k}\right) S_{nm}}{\underbrace{\left(\sum_{nm} a_n a_m S_{nm}\right)}_{\langle\Psi|\Psi\rangle}^2} = 0$$

$$\frac{\partial a_n}{\partial a_k} = \delta_{nk}$$

$$\Rightarrow \sum_{nm}\left(a_m \delta_{nk} + a_n \delta_{mk}\right) H_{nm} - E \sum_{nm}\left(a_m \delta_{nk} + a_n \delta_{mk}\right) S_{nm} = 0$$

$$\sum_m a_m H_{km} + \sum_n H_{nk} a_n - E\left(\sum_m a_m S_{km} + \sum_n a_n S_{nk}\right) = 0$$

$$\boxed{\sum_m H_{km} a_m = E \sum_m S_{km} a_m}$$

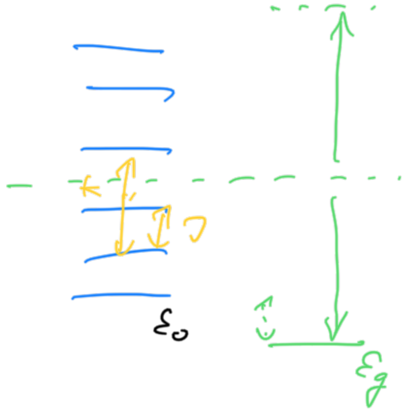
$$H\vec{a} = E S \vec{a}$$ ← zobecněný vlastní problém

$S_{kl} = \delta_{kl}$ ← požadavek orthonormality báze

$$\boxed{H\vec{a} = E\vec{a}}$$

Důsledky

$$H = \begin{pmatrix} \varepsilon_0 & & J & & K \\ & \varepsilon_1 & & & \\ & J & \ddots & & \\ & & & \ddots & \\ K & & & & \varepsilon_N \end{pmatrix}$$



$$H' = U^{-1} H U$$

$$\mathrm{Tr}\{H'\} = \mathrm{Tr}\{U^{-1}HU\} = \mathrm{Tr}\{HUU^{-1}\} = \mathrm{Tr}\{H\}$$

$$= \sum_n \varepsilon_n$$

$$\bar{E} = \frac{\sum_n \varepsilon_n}{N}$$ ← také zachovávána při diagonalizaci