VARIAČNÍ METODA

Ritzův variační princip:

$$E_{var} = \frac{\langle \psi_t | H | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle}$$

$$E_{var} - E_0 = \frac{\langle \psi_t | H | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} - E_0 \frac{\langle \psi_t | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} =$$

$$= \frac{\langle \psi_t | (H - E_0) | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} =$$

spektrální rozklad H

$$= \frac{\langle \psi_t |}{\langle \psi_t | \psi_t \rangle} \left(\sum_j E_j |\psi_j\rangle\langle\psi_j| - E_0 \right) |\psi_t\rangle =$$

$$= \frac{\langle \psi_t |}{\langle \psi_t | \psi_t \rangle} \left[\sum_j (E_j - E_0) |\psi_j\rangle\langle\psi_j| \right] |\psi_t\rangle =$$

$$= \sum_j \underbrace{(E_j - E_0)}_{\geq 0} \underbrace{|\langle \psi_t | \psi_j \rangle|^2}_{\geq 0} \underbrace{\frac{1}{\langle \psi_t | \psi_t \rangle}}_{> 0} \geq 0$$

nelineární parametrizace

= vhodně přidáme parametr a optimalizujeme ho

př. $\quad H = \frac{p^2}{2} + \frac{x^2}{2} + \delta x^2$

$$|\psi_{LHO}\rangle = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{x^2}{2}} \Rightarrow |\psi_t\rangle = \frac{1}{\sqrt[4]{\pi}} e^{-\alpha \frac{x^2}{2}}$$

$\rightarrow$ potřebujeme $\langle \psi_t | H | \psi_t \rangle$ a $\langle \psi_t | \psi_t \rangle$

$$\rightarrow E_{var} = \frac{\langle \psi_t | H | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle}$$

$$\langle \psi_t | H | \psi_t \rangle = \int_{-\infty}^{} dx \, \frac{1}{\sqrt{\sqrt{\pi}}} e^{-\frac{\alpha x^2}{2}} \left[\frac{-1}{2} \frac{d^2}{dx^2} + \frac{x^2}{2} + \delta x^2 \right] \frac{1}{\sqrt{\sqrt{\pi}}} e^{-\frac{\alpha x^2}{2}} =$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dx \, \frac{-1}{2} e^{-\frac{\alpha x^2}{2}} \underbrace{\left(e^{-\frac{\alpha x^2}{2}} (-\alpha x)^2 - \alpha e^{-\frac{\alpha x^2}{2}} \right)}_{= \left(e^{-\frac{\alpha x^2}{2}}\right)''} +$$

$$+ \frac{1}{\sqrt{\pi}} \left(\frac{1}{2} + \delta\right) \int_{-\infty}^{+\infty} dx \, e^{-\alpha x^2} = \ldots$$

$$= \frac{\sqrt{\alpha}}{4} + \frac{1}{4\sqrt{\alpha^3}} + \delta \frac{1}{2\sqrt{\alpha^3}}$$

nápověda:

$$\int_{-\infty}^{+\infty} dx \, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

$$\int_{-\infty}^{+\infty} x^{2k+1} e^{-\alpha x^2} dx = 0 \text{ pro } k \in \mathbb{N}_0$$

$$\int_{-\infty}^{+\infty} x^{2k} e^{-\alpha x^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2^k} \sqrt{\frac{\pi}{\alpha^{2k+1}}}$$

$$\langle \psi_t | \psi_t \rangle = \int_{-\infty}^{+\infty} dx \, e^{-\alpha x^2} \frac{1}{\sqrt{\pi}} = \frac{1}{\sqrt{\alpha}}$$

$$E_{var}^{(\alpha)} = \frac{\alpha}{4} + \frac{1}{4\alpha} + \delta \frac{1}{2\alpha}$$

$$\frac{\partial E_{var}}{\partial \alpha} = -\frac{1}{4} \alpha^{-2} + \delta \left(-\frac{1}{2} \alpha^{-2}\right) + \frac{1}{4} \overset{!}{=} 0$$

$$\left(\frac{1}{4} + \frac{1}{2}\delta\right) \alpha^{-2} = \frac{1}{4}$$

$$\underline{\underline{\alpha^2 = 1 + 2\delta}}$$

$$\sqrt{1+x} \overset{x \to 0}{=} 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16} \pm \cdots$$

$$|\alpha| \approx 1 + \delta$$

$$E_{var}^{opt} = \frac{1+\delta}{4} + \frac{1}{4(1+\delta)} + \delta\frac{1}{2(1+\delta)} \approx$$

Lineární parametrizace

→ rozvedeme do báze: $|\psi_t\rangle = \sum_n c_n|n\rangle$

$$E_{var} = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_i\sum_j c_i c_j \langle i|H|j\rangle}{\sum_i\sum_j c_i c_j \langle i|j\rangle} = \frac{\sum_i\sum_j c_i c_j H_{ij}}{\sum_i\sum_j c_i c_j S_{ij}}$$

a optimalizujeme:

$$\left(\frac{f}{g}\right)' = \frac{f'}{g} - \underbrace{\frac{f}{g}}_{E_{var}}\frac{g'}{g} = \frac{f'}{g} - E_{var}\frac{g'}{g}$$

$$f = c_i c_j H_{ij} \Rightarrow f' \quad 2c_j H_{kj} \qquad \frac{\partial c_i}{\partial c_k} = \delta_{ik}$$

$$g = c_i c_j S_{ij} \Rightarrow g' = 2c_j S_{kj}$$

$$\frac{\partial E_{var}}{\partial c_k} = \frac{1}{\sum_{ij} S_{ij} c_i c_j}\left(\sum_j 2c_j H_{kj} - E_{var}\sum_j 2c_j S_{kj}\right) \overset{!}{=} 0$$

$$\sum_j (H_{kj} - E_{var} S_{kj}) c_j = 0$$

$$\boxed{(\mathbb{H} - E_{var}\mathbb{S})\vec{c} = 0}$$

př. $H = \frac{p^2}{2} + \frac{x^2}{2} + \delta x^2$

$\{|0\rangle\} \Rightarrow \langle 0|H|0\rangle = \frac{1}{2} + \delta\frac{1}{2} = E_{var}$

$\{|0\rangle, |1\rangle\} \Rightarrow \langle 0|H|1\rangle = \langle 1|H|0\rangle = 0$

$\langle 1|H|1\rangle = \frac{3}{2} + \frac{3}{2}\delta$

$$\Rightarrow \begin{pmatrix} \frac{1}{2}(1+\delta) & 0 \\ 0 & \frac{3}{2}(1+\delta) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

stavy spolu neinteragují
(sudý × lichý)

$$\Rightarrow E_{var} = \frac{1}{2}(1+\delta)$$

$$\{ |0\rangle, |1\rangle, |2\rangle \} \Rightarrow \langle 0|H|2\rangle = \langle 2|H|0\rangle = \frac{1}{2}\sqrt{2}\,\delta$$

$$\langle 2|H|2\rangle = \frac{5}{2}(1+\delta)$$

$$\begin{pmatrix} \frac{1}{2}(1+\delta) & \frac{1}{\sqrt{2}}\delta & 0 \\ \frac{1}{\sqrt{2}}\delta & \frac{5}{2}(1+\delta) & 0 \\ 0 & 0 & \frac{3}{2}(1+\delta) \end{pmatrix} \Rightarrow E_{var} = \ldots\ldots$$