Lecture January 14

$$\mathbb{E}[H] = \langle H \rangle = \frac{\int d\vec{R}\, \psi_T^*(\vec{R})\, \hat{H}\, \psi_T(\vec{R})}{\int d\vec{R}\, \psi_T^*(\vec{R})\, \psi_T(\vec{R})}$$

$$\vec{R} = (\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots \vec{r}_N)$$

$$d\vec{R} = d\vec{r}_1\, d\vec{r}_2 \ldots d\vec{r}_N$$

TRUE ground state E_0

variational principle

$$\hat{H}\, \psi_0(\vec{R}) = E_0\, \psi_0(\vec{R})$$

$$\psi_T(\vec{R}) \neq \psi_0(\vec{R})$$

$$H\, \psi_T(\vec{R}) \neq \text{const} \times \psi_T(\vec{R})$$

$$E_0 \leq \mathbb{E}[H]$$

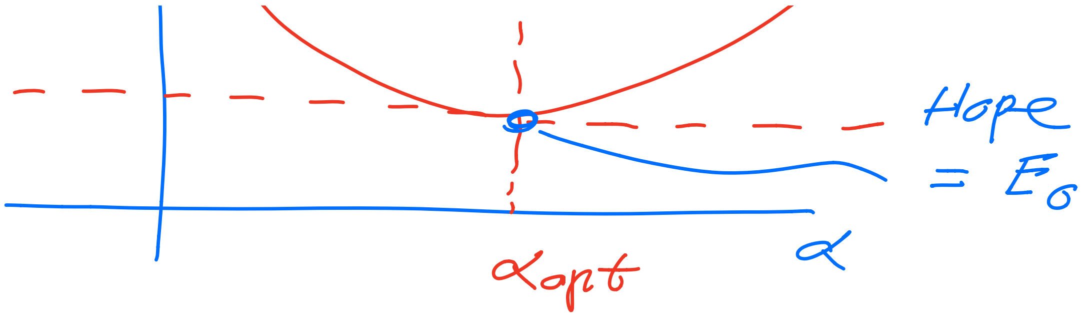
$$\psi_T(\vec{R}) \to \psi_T(\vec{R}; \vec{\alpha})$$

variational parameters

$$\mathbb{E}[H] = \mathbb{E}[H(\vec{\alpha})]$$

$$\vec{\alpha} = (\alpha_1, \alpha_2 \ldots \alpha_m)$$

$\mathbb{E}[H[\vec{\alpha}]]$



Want

$$\frac{d\,\mathbb{E}[H(\alpha)]}{d\alpha} = 0$$

$$\psi_T(\vec{R}) = \psi_T = \psi_{Exact}$$

$$\hat{H}\psi_{Exact} = E_0\,\psi_{Exact}$$

$$\mathbb{E}[H^2] = \int d\vec{R}\,\psi^*_{Exact}\,\underbrace{H^2\psi_{Exact}}_{E_0^2\psi_{Exact}}$$

$$\int d\vec{R}\,|\psi_{Exact}|^2 = \underline{1}$$

$$= E_0^2$$

$$\sigma_E = var[H] = \mathbb{E}[H^2] - (\mathbb{E}[H])^2$$

$$= E_0^2 - E_0^2 \equiv 0\,!$$

Expected values

$$\mathbb{E}[x^n] = \int dx\,\underline{p(x)}\,x^n$$

PDF

(Discrete version

$$\sum_i x_i^n p(x_i)$$)

Define

QM - PDF

$$P(\vec{R}) = \frac{|\Psi_T(\vec{R})|^2}{\int |\Psi_T(\vec{R})|^2 d\vec{R}}$$

$$E_L(\vec{R}) = \boxed{\frac{1}{\Psi_T(\vec{R})} \hat{H} \Psi_T(\vec{R})} = \frac{1}{\Psi_T} \hat{H} \Psi_T$$

$$E[H] = \frac{\int d\vec{R}\, \Psi_T^* \hat{H} \Psi_T}{\int d\vec{R}\, |\Psi_T|^2}$$

$$\frac{\Psi_T}{\Psi_T}$$

$$= \boxed{\int d\vec{R}\, P(\vec{R})\, E_L(\vec{R})}$$

$$E[H(\vec{\alpha})] = \int d\vec{R}\, P(\vec{R};\vec{\alpha})\, E_L(\vec{R};\vec{\alpha})$$

MCS

$$\simeq \underbrace{\frac{1}{MCS}}_{\text{Monte Carlo samples}} \sum_{i=1} E_L(R_i;\alpha)$$

$$E_L(\vec{R}) = \frac{1}{\psi_T(\vec{R})} \hat{H}\, \psi_T(\vec{R})$$

1-particle, 1-Dim

$$\vec{R} \Rightarrow x$$

$$E_L(x) = \frac{1}{\psi_T(x)}\left(-\frac{\hbar^2 \nabla^2}{2m} + V(x)\right)\psi_T(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\psi_T(x)}\frac{d^2}{dx^2}\psi_T(x)$$

$$V(x) = \frac{1}{2} k x^2$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\psi_T}\frac{d^2}{dx^2}\psi_T + \frac{1}{2} k x^2$$

HO ; $\psi_T \sim e^{-\alpha^2 x^2/2}$

$$E_0 = \hbar\omega \cdot \frac{1}{2}$$

$$\frac{d^2}{dx^2} u(x) \simeq \frac{u(x+h) + u(x-h) - 2u(x)}{h^2}$$