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Trial WF : $\Psi_T(\vec{R}, \vec{S}; \vec{\Theta})$

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

$$\vec{S} = \{\vec{S}_1, \vec{S}_2, \ldots \vec{S}_N\}$$

$$\vec{X} = \{\vec{R}, \vec{S}\}$$

N = # of particles

$$\hat{\Theta} = \{\hat{\Theta}_1, \hat{\Theta}_2, \ldots \hat{\Theta}_M\}$$

parameters

$$E[e] = \frac{\sum_{s} \int d\vec{R}\; \psi_T^*(\vec{R},\vec{s};\vec{\theta})\, \hat{H}(\vec{R},\vec{s})\, \psi_T(\vec{R},\vec{s};\vec{\theta})}{\sum_{s} \int d\vec{R}\; |\psi_T(\vec{R},\vec{s};\vec{\theta})|^2}$$

$$\sum_{\vec{s}} \int d\vec{R} \longrightarrow \int d\vec{x}$$

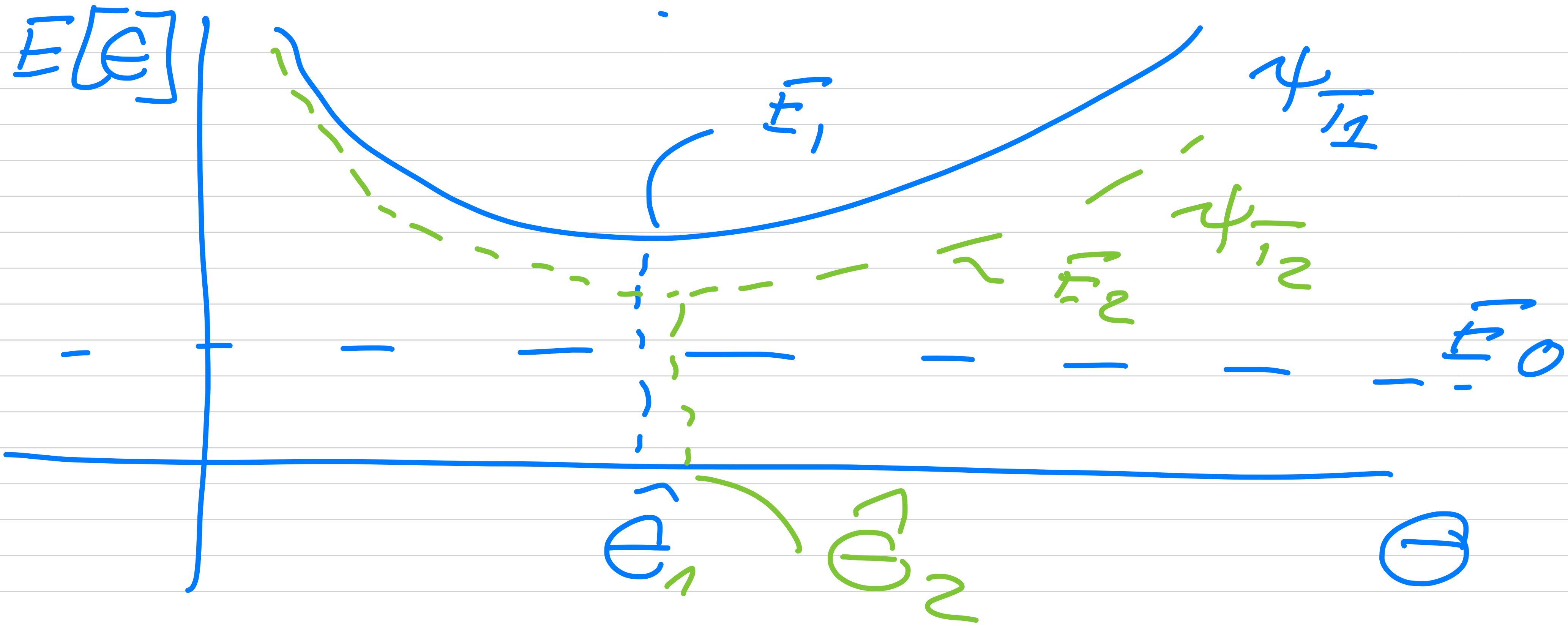
$$\int d\vec{R} = \int d\vec{r}_1 \int d\vec{r}_2 \cdots \int d\vec{r}_N$$

optimal parameters

$$\hat{\Theta} = \underset{\Theta \in \mathbb{C}^M}{\operatorname{argmin}} \; E[\Theta]$$

$$\Rightarrow \quad \vec{\nabla}_\Theta \, \mathbb{E}[\Theta] = 0$$

assume only one Θ



variational theorem

$$\hat{\Omega}\,|\psi_i\rangle = \lambda_i\,|\psi_i\rangle$$

$$\langle\psi_i|\psi_j\rangle = \delta_{ij}$$

$$|\varphi\rangle = \sum_i c_i |\psi_i\rangle$$

$$E[\varphi] = \frac{\langle\varphi|\hat{H}|\varphi\rangle}{\langle\varphi|\varphi\rangle}$$

$$= \frac{\sum_{i,j} c_i^* c_j \langle\psi_i|\underbrace{\hat{H}|\psi_j\rangle}_{\delta_{ij}\lambda_i}}{\sum_i |c_i|^2}$$

$$\sum_i |c_i|^2 = 1$$

$$E[\varphi] = \sum_i |c_i|^2 \lambda_i \geq E_0$$

unless all $|c_i|^2$ are zero except c_0, $\lambda_0 = E_0$

$$E_0 = \lambda_0 < \lambda_1 < \lambda_2 \ldots$$

To use MC-methods we would like to evaluate something which looks like

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

$$\left(\sum_i p(x_i)\, x_i^n \right)$$

mean value

$$\mu_x = \mathbb{E}[x] = \langle x \rangle$$

$$= \int p(x)\, x \, dx$$

$$\mathrm{var}[x] = \sigma_x^2 =$$

$$\int p(x)\,dx\,(x - \mu_x)^2$$

$$= \mathbb{E}[x^2] - \mu_x^2$$

$$= \langle x^2 \rangle - \langle x \rangle^2$$

$$\mathrm{STD} = \sigma_x$$

Define PDF:

$$P(\vec{x};\vec{e}) = \frac{|\psi_T(\vec{x};\vec{e})|^2}{\int d\vec{x}\, |\psi_T(\vec{x};\vec{e})|^2}$$

ψ_T / ψ_T

$$E[e] = \frac{\int dx\, \psi_T^* \hat{H} \psi_T}{\int dx\, |\psi_T|^2}$$

$$E_L(\vec{x};\vec{\theta}) = \frac{1}{\psi_T(\vec{x};\vec{\theta})} \mathcal{H}(\vec{x})\, \psi_T(\vec{x};\vec{\theta})$$

$$\Longrightarrow$$

$$E[\theta] = \int d\vec{x}\, P(\vec{x};\vec{\theta})\, E_L(\vec{x};\vec{\theta})$$

$$\simeq \frac{1}{M_{CS}} \sum_{i=1}^{M_{CS}} E_L(\vec{x}_i;\vec{\theta})$$

$$\mathrm{var}[\hat{H}] = \frac{\overbrace{\langle \psi_0 | \hat{H}^2 | \psi_0 \rangle}^{E_0^2}}{\underbrace{\langle \psi_0 | \psi_0 \rangle}_{=1}} - \left[\frac{\overbrace{\langle \psi_0 | \hat{H} | \psi_0 \rangle}^{E_0}}{\underbrace{\langle \psi_0 | \psi_0 \rangle}_{=1}} \right]^2 = 0$$

$$\hat{H} | \psi_0 \rangle = E_0 | \psi_0 \rangle$$

1-Dim HO

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x)+\frac{1}{2}kx^2\varphi(x)$$

$$=E\varphi(x)$$

$$\varphi_0(x)=N_0\,e^{-\frac{1}{2}\alpha^2x^2}$$

$(\theta \to \alpha)$ $\quad \hbar = \omega = m$

$$\therefore = \frac{1}{\quad}$$

$$E_n = (n+1/2) \leftarrow \hbar\omega$$

$$E_L(x;\alpha) = \frac{1}{\psi_T(x;\alpha)} \hat{H} \psi_T$$

$$\psi_T(x;\alpha) = e^{-\frac{1}{2}\alpha^2 x^2}$$

$$\frac{1}{\psi_T}\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right)\psi_T$$

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

$$E[\alpha] = \int dx\, P(x;\alpha)\, E_L(x;\alpha)$$

$$= \frac{1}{4}\left(\alpha^2 + \frac{1}{\alpha^2}\right) = E[\alpha]$$

$$\frac{d}{d\alpha} E[\alpha] = 0 \implies$$

$$\alpha = \underline{1}$$

$$E[\alpha]_{\alpha=1} = \frac{1}{2}$$

$$E_n = (n + 1/2)$$

$$n=0 \rightarrow E_0 = 1/2$$

$$\nabla^2_{E} = \frac{1}{4}\left(1 + (1-\alpha^4\right)\frac{3}{4\alpha}$$