FYS4411/9411, January 24, 2025

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VMC: $\Psi_T \Rightarrow \Psi_T(\vec{R};\Theta)$

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

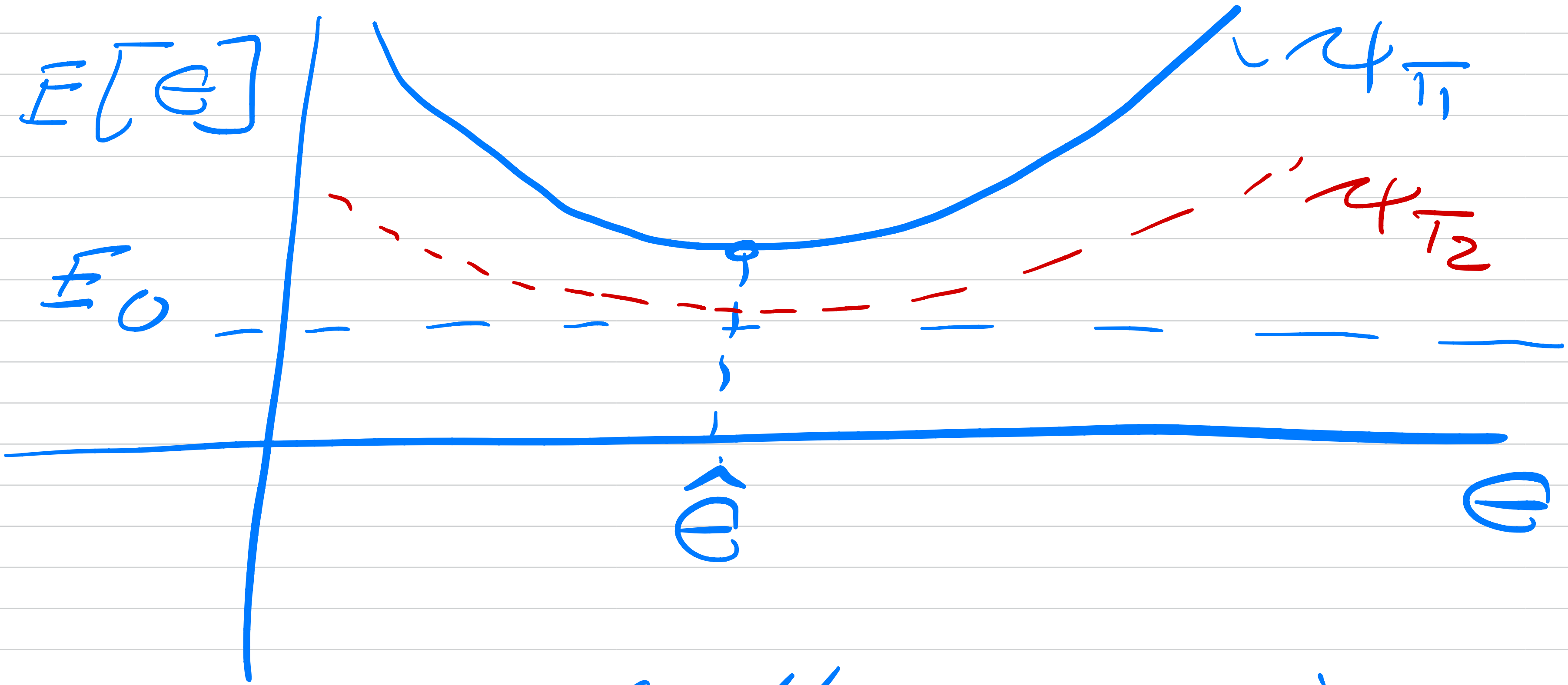
n' = # of particles

$$\underbrace{\Theta = \{\theta_1, \theta_2, \dots, \theta_M\}}_{\text{parameters of } \Psi_T}$$

$$\Rightarrow \quad E[\Theta] = \frac{\int d\vec{R}\, \Psi_T^*(\vec{R};\Theta)\hat{H}\Psi_T(\vec{R};\Theta)}{\int d\vec{R}\, |\Psi_T|^2}$$

$$\frac{dE[\epsilon]}{d\epsilon} = 0$$

assume one ϵ



Variational theorem:

$\hat{H}\psi_i = \lambda_i \psi_i$ $\quad$ ψ_i is an ONB

$$\varphi = \sum_{i=0}^{\infty} c_i \psi_i$$

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

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

$$= \frac{\sum_i E_i |c_i|^2}{\sum_i |c_i|^2} = \sum_i E_i |c_i|^2$$

$$\varphi \equiv \psi_0 \Rightarrow \langle \varphi | \hat{H} | \varphi \rangle = E_0$$

$$\underline{|c_i|^2 = 1}$$ if not $\Rightarrow$

$$E_0 \le \sum_i |c_i'|^2 E_i'$$

$$\frac{\psi_i}{\psi_T}$$

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

Define $PDF = \underbrace{\dfrac{|\psi_T(\vec{R};\theta)|^2}{\int d\vec{R}\, |\psi_T|^2}}_{= P(\vec{R};\theta)}$

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

Local energy

$$E[\theta] = \boxed{\int_{\vec{R}\in D} d\vec{R}\, P(\vec{R};\theta)\, E_L(\vec{R};\theta)}$$

Expectation values in stat

$$\mathbb{E}[x^n] = \langle x^n \rangle = \int_{x\in D} dx\, p(x)\, x^n$$

$$\simeq \boxed{\frac{1}{M}\sum_{i=1}^{M} E_L(\vec{R}_i;\theta)}$$

M = # Monte Carlo cycles

variance

$$\mathrm{var}[x] = \int dx\, p(x)\,(x - \mathbb{E}[x])^2$$

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

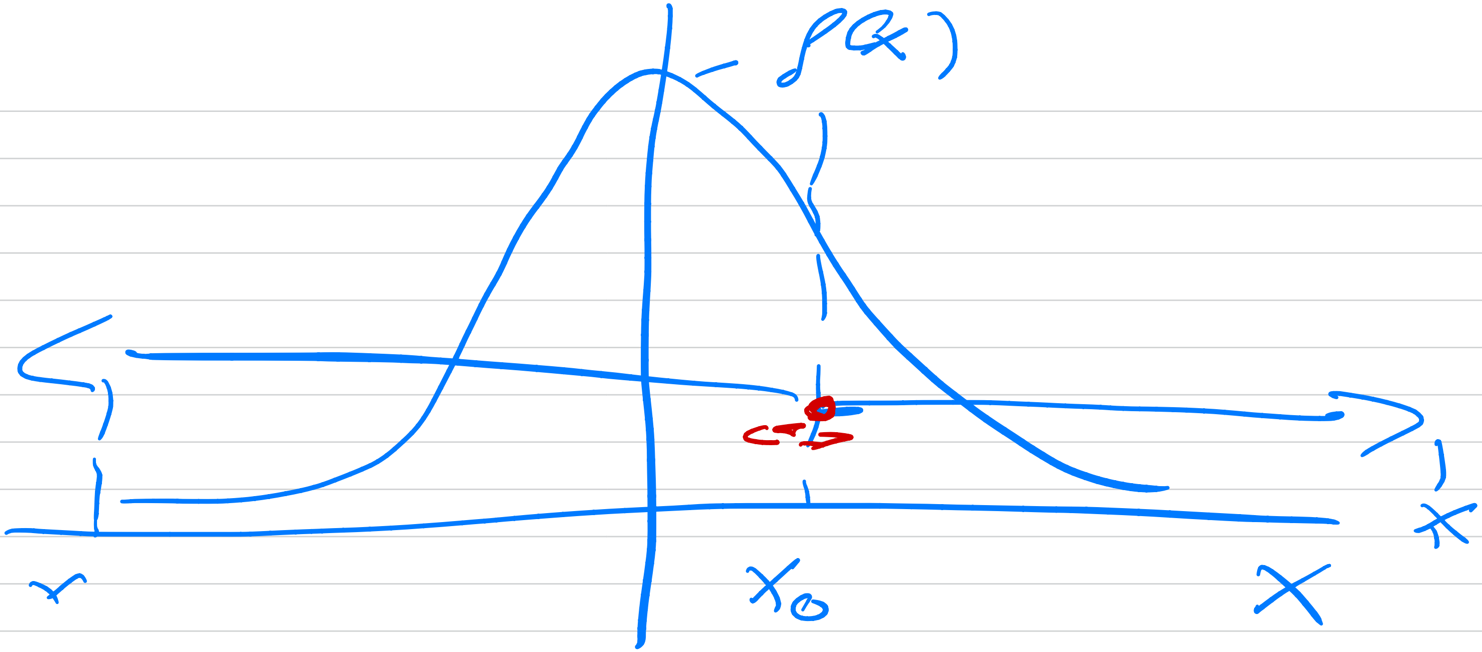
mean value squared.

$H\psi = E\psi$

QM

$$\frac{\int dx\, \psi^*(x)\, H^2 \psi(x)}{\int dx\, |\psi|^2} - \left[\frac{\int dx\, \psi^* H \psi}{\int dx\, |\psi|^2}\right]^2$$

$= 0$



$$\int f(x)\,p(x)\,dx \;\simeq\; \frac{1}{M}\sum_i f(x_i)$$