FYS4411/9411 JANUARY 20, 2022

VMC calculations

essential elements

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

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

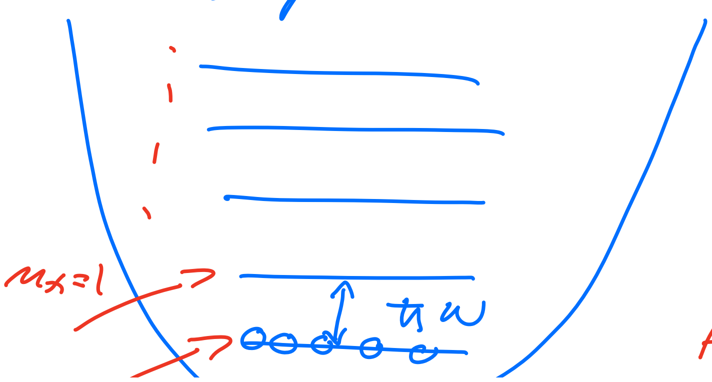
$$\vec{R}_i = \{r_{ix}, r_{iy}, r_{iz}\}$$

$$\vec{\alpha} = \{\alpha_1, \alpha_2, \ldots \alpha_M\}$$

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

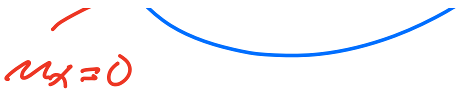
Harmonic oscillator

1-particle in 1 Dim



$$E_{n_x} = \hbar\omega(n_x + 1/2)$$

$$H(x) = -\frac{\hbar^2}{}\frac{d^2}{}$$



$2m\,\alpha x^2$

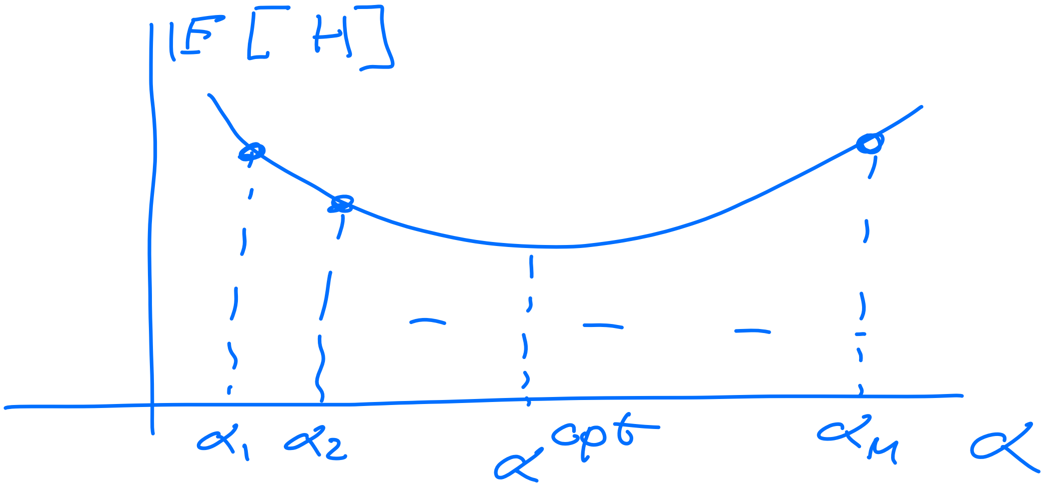
$+\frac{1}{2} m\omega^2 x^2$

$$\psi_{n_x=0} \sim e^{-\alpha x^2} \sim e^{-\frac{1}{2}\alpha^2 x^2}$$

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

Many Bosons in 1-Dim

$$\psi_T(x_1, x_2, \ldots x_N; \alpha)$$



$$\mathbb{E}[H(N)] = \sum_{i=1}^{N} \varepsilon_i$$

$$\varepsilon_i = \frac{1}{2}\hbar\omega$$

$N=20 \Rightarrow$ Exact $\mathbb{E}[H] =$

$10 \cdot \hbar\omega$

2-Dim ho, exact energy

$\varepsilon_i = \hbar\omega, \{n_x, n_y = 0\}$

$N=20 \Rightarrow$ Exact $\mathbb{E}[H] =$

$20\,\hbar\omega$

$\hbar\omega(n_x + n_y + 1)$

3-Dim ho

$\varepsilon_i = 3/2\,\hbar\omega$

$\varepsilon_i = \hbar\omega(n_x + n_y + n_z + 3/2)$

Trial wf in 1-Dim

$$\psi_T(x_1, x_2, \dots x_N; \alpha) =$$

$$e^{-\frac{1}{2}\alpha^2(x_1^2 + x_2^2 + \dots + x_N^2)}$$

$$\mathbb{E}[f(x)] = \int_{x\in\mathbb{D}} f(x)\,p(x)\,dx$$

$p(x)$ = probability

distribution function.

Quantum mech

$$\mathbb{E}[H] = \int_{x \in \mathbb{D}} dx \, \frac{\psi^*(x) H(x) \psi(x)}{\int dx \, |\underbrace{\psi(x)}_{\psi^* \psi}|^2}$$

MC - calculation

$$\int_{x \in \mathbb{D}} p(x) f(x) \, dx \simeq \frac{1}{M} \sum_{i=1}^{M} f(x_i)$$

Random configuration

ideally $M \Rightarrow \infty$

In QM, the PDF is –

$$P_T(x; \alpha) = \frac{|\psi_T(x; \alpha)|^2}{\int_{x \in D} dx \, |\psi_T(x; \alpha)|^2}$$

Local energy

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

$$\mathbb{E}[H] = \mathbb{E}[E_L(x;\alpha)]$$

$$= \int_{x\in\mathbb{D}} dx \; P_T(x;\alpha)\, E_L(x;\alpha)$$

$$\simeq \frac{1}{M} \sum_{i=1}^{M} E_L(x_i;\alpha)$$

1- Boson in 1-Dim

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

warm-up :

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

$$\times\, \psi_T$$