FYS4411 MARCH 18

VMC and have optimal variational parameters

$$\vec{\alpha}^{opt} = \{\alpha_0\ \alpha_1, \dots \alpha_{p-1}\}$$

$$\Psi_T(\vec{R}; \vec{\alpha}^{opt})$$

$$\rho(\vec{r}_1) = \int d\vec{r}_2\, d\vec{r}_3 \dots d\vec{r}_N \left|\Psi_T(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N; \vec{\alpha}^{opt})\right|^2$$

$$\vec{r}_1 \Rightarrow \vec{r}$$

$$\rho(\vec{r}) = \int d\vec{r}_2\, d\vec{r}_3 \dots d\vec{r}_N \left|\Psi(\vec{r}, \vec{r}_2, \dots r_N; \vec{\alpha}^{opt})\right|^2$$

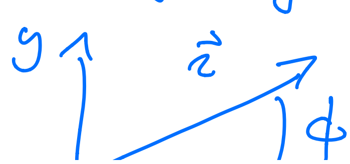
— perform an MC integration

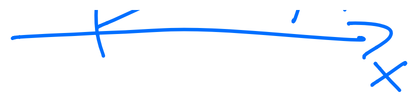
2-Dim: set up a grid of

x an $y \in [a, b]$

$$r = \sqrt{x^2+y^2}$$

$\rho(x, y)$

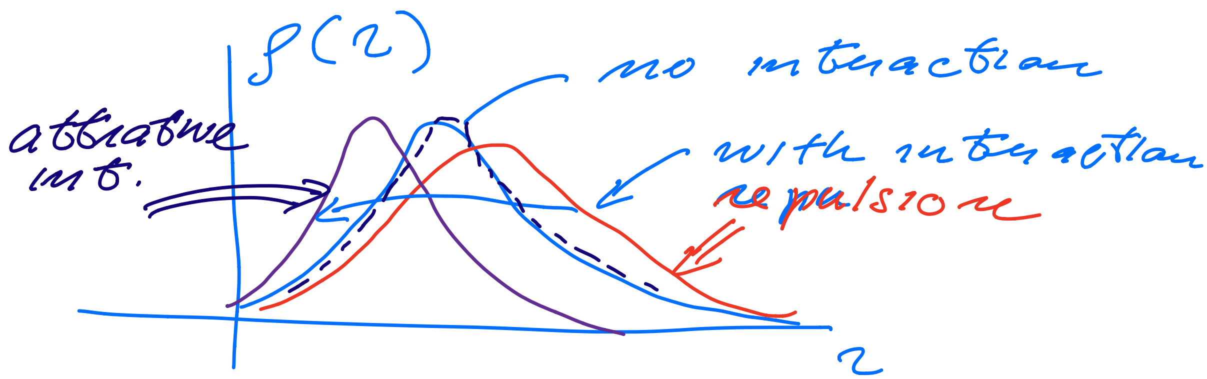




$r \in [0, \infty)$

$\phi \in [0, 2\pi]$

(zero spin, no dependence on ϕ)



(i) check: non-interacting case

$$\psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N; \vec{\alpha}^{opt}) \propto e^{-\alpha^{opt} r_1^2} e^{-\alpha^{opt} r_2^2} \ldots e^{-\alpha^{opt} r_N^2}$$

$$\rho(r) \propto e^{-\alpha^{opt} r^2}$$

(ii) with interacting case

$E_0, E_1, \ldots E_M$

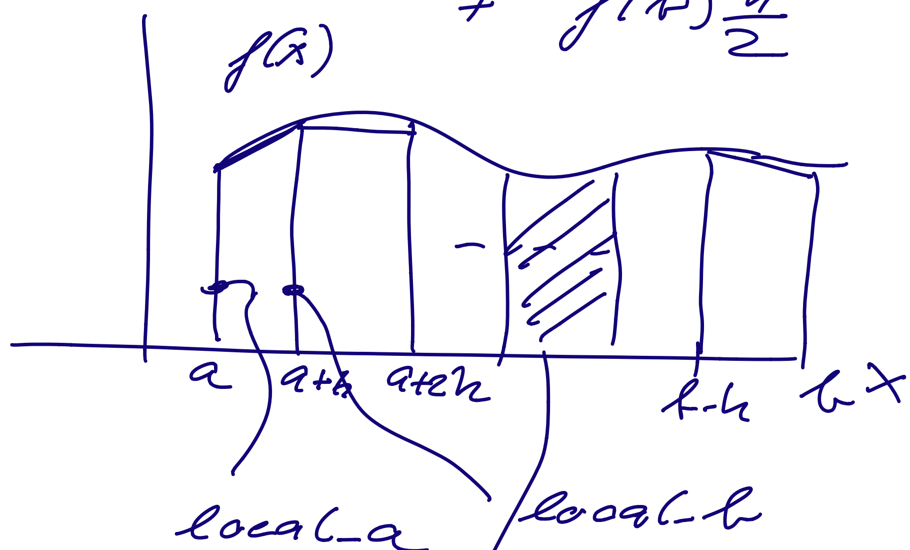
$$\underline{var(E)} = \frac{1}{M} \sum_{i=1}^{M} (E_i - \mu_E)^2$$

$$\mu_E = \frac{1}{M} \sum_{i=1}^{N} E_i$$

$$\underline{cov(E)} = \frac{2}{M} \sum_{k<l} (E_k - \mu_E)(E_l - \mu_E)$$

— MPI integration —

$$I = \int_a^b f(x)\,dx \simeq f(a)\frac{h}{2} + f(a+h)h + f(a+2h)\cdot h + \dots f(b-h)h + f(b)\frac{h}{2}$$



$$I \simeq h \sum_{i=1}^{n-1} f(a+i\cdot h) + \frac{h}{2} f(a) + \frac{h}{2} f(b)$$

local_n

local_h

n = 1000

p = 100 processes

$$\int_{local\_a}^{local\_b} f(x)\,dx \qquad local\_n = n/p$$

- each process calculates its own $\int_{local\_a}^{local\_b}$
- One process (master) collects data from all the processes (slaves)

$\Rightarrow$ Need a communication function

$$local\_a = a + \underbrace{rank}_{0,1,2,\,\dots\, p-1} \times local\_n * h$$

$$local\_b = local\_a + local\_n * h$$