Lecture FYS4411, March 15, 2024

Total mean of m experiments

$$\bar{X} = \frac{1}{m} \sum_{i=1}^{m} \bar{x}_i$$

$$\bar{x}_i = \frac{1}{n} \sum_{j=1}^{n} x_{ij}$$

$$\sigma_m^2 = \frac{1}{m} \sum_{i=1}^{m} \left(\bar{x}_i - \bar{X}\right)^2$$

$$\underbrace{\bar{x}_i - \bar{X}} = \underbrace{\frac{1}{n} \sum_{j=1}^{n} x_{ij}}_{\bar{x}_i} - \bar{X}$$

$$= \tilde{x}_{ij}$$

Total sample variance

$$\sigma^2 = \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} (\underbrace{x_{ij} - \bar{X}}_{\tilde{x}_{ij}})$$

$$\sigma_m^2 = \frac{1}{m} \sum_{i=1}^{m} \left[\frac{1}{n} \sum_{j=1}^{n} \tilde{x}_{ij} \right]^2$$

$$= \frac{1}{mn^2} \sum_{i=1}^{m} \sum_{j=1}^{n} \tilde{x}_{ij}^2$$

$$+ \frac{2}{mn^2} \sum_{i=1}^{m} \sum_{j<k}^{n} \tilde{x}_{ij} \tilde{x}_{ik}$$

$$= \frac{\sigma^2}{n} + \frac{2}{mn^2} \sum_{i=1}^{m} \sum_{j<k} \tilde{x}_{ij} \tilde{x}_{ik}$$

$$d = |j-k|$$

$$\rho_d = \frac{1}{m} \frac{1}{n} \sum_{i=1}^{m} \sum_{k=1}^{n-d} \tilde{x}_{ik} \tilde{x}_{i(k+d)}$$

$$d = 0$$

$$\rho_0 = \frac{1}{m} \frac{1}{n} \sum_{i=1}^{m} \sum_{k=1}^{n} \tilde{x}_{ik}^2 = \sigma^2$$

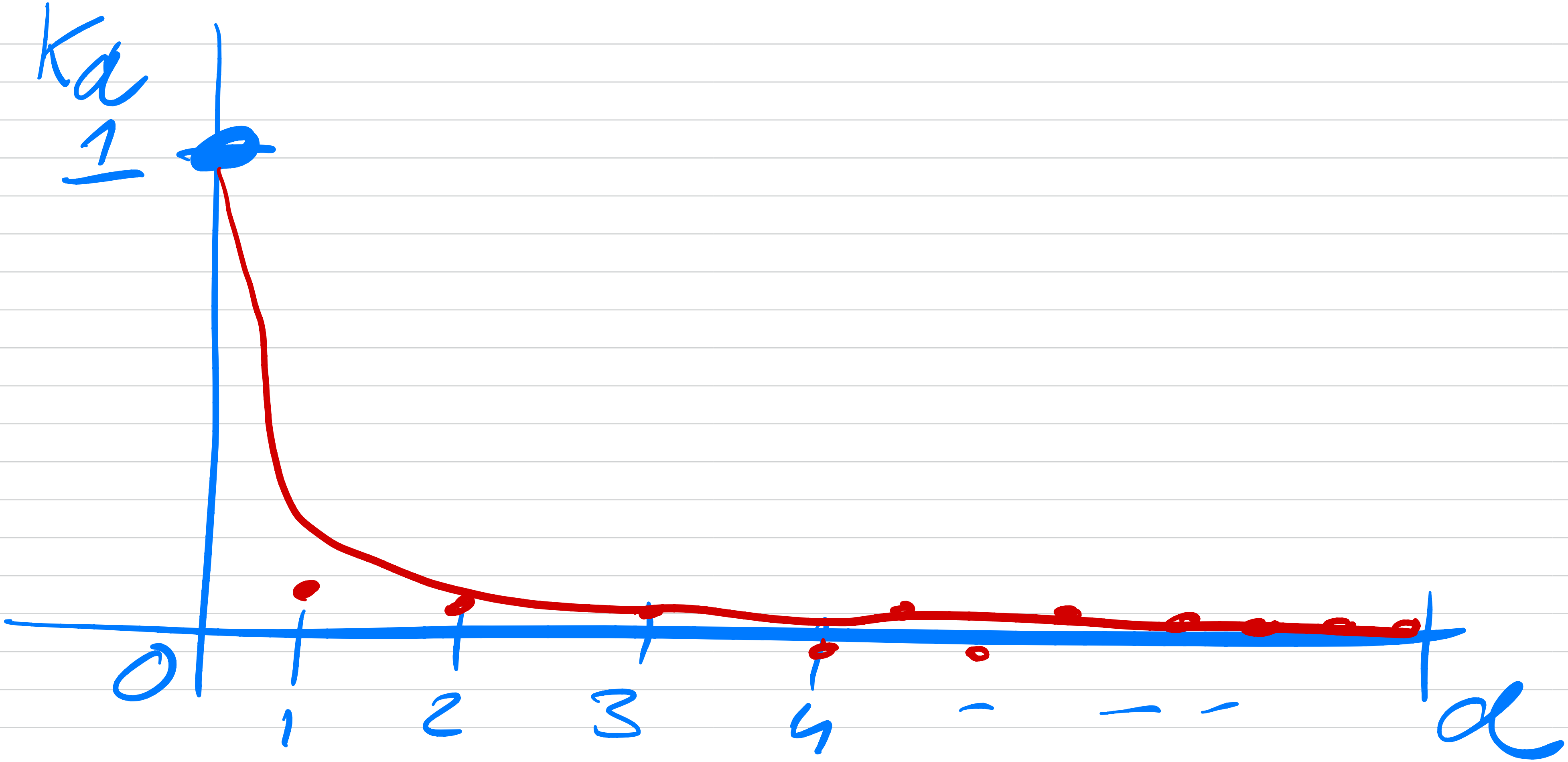
$$\sigma_m^2 = \frac{\sigma^2}{n} + \underbrace{\frac{2}{n} \sum_{d=1}^{n-1} \rho_d}_{\text{autocovariance}}$$

$$R_d = \rho_d / \sigma^2$$

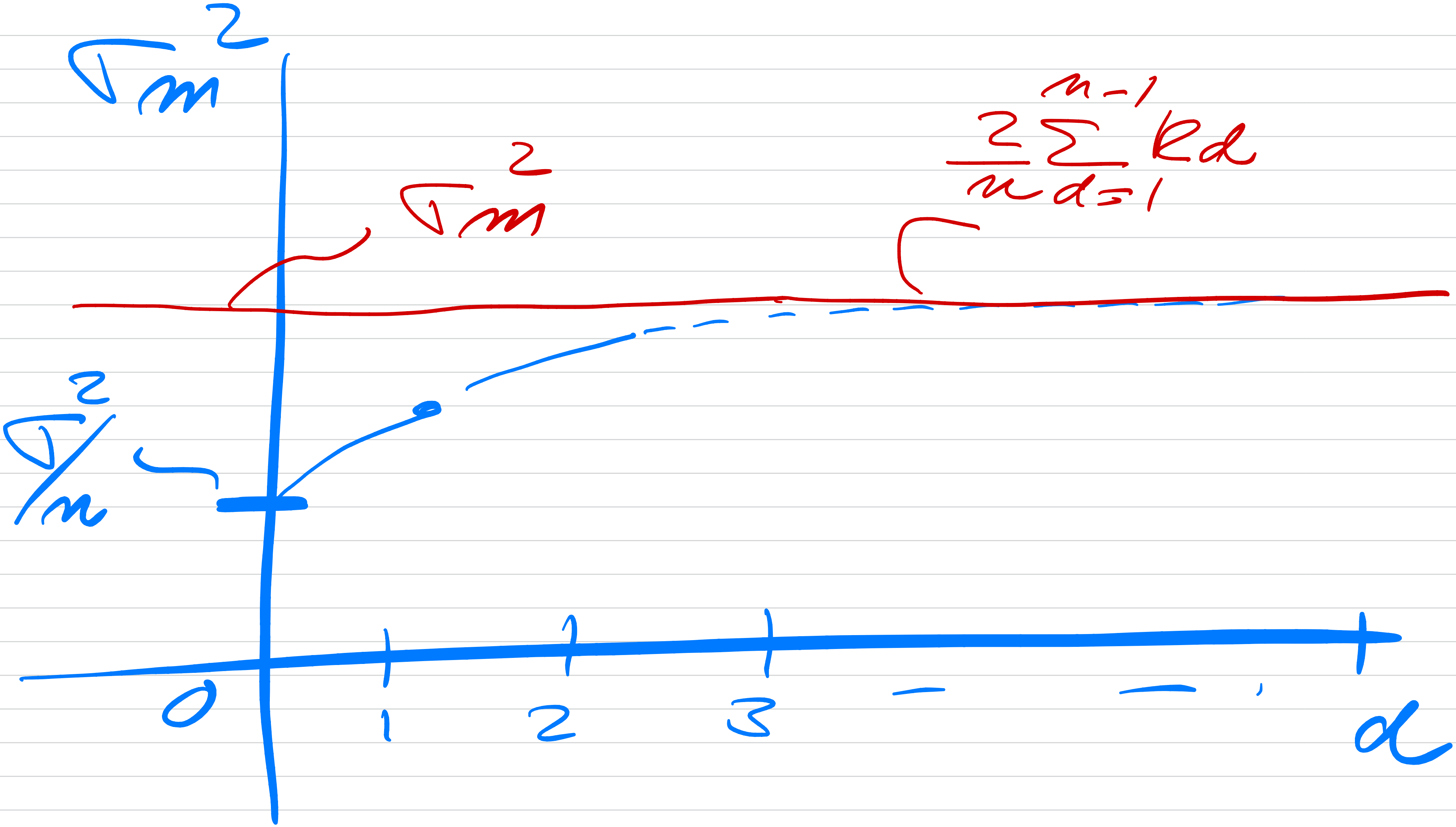
correlation function

$$\rho_0 / \sigma^2 = \frac{1}{} = K_0$$

$$\sigma_m^2 = \frac{\sigma^2}{n}\left[\overline{1} + \underbrace{2 \sum_{d=1}^{n-1} R_d}_{\text{error or contribution from correlation}}\right]$$



K_α
1
0
1
2
3
4
α



σm²
σm²
2/n Σ_{d=1}^{n-1} Rd
σ²/n
0
1
2
3
d

Blocking method

$$X = \{ x_0, x_1 \dots x_{n-1} \}$$

X' has $n' = \frac{1}{2} n$

$$x_0' = \frac{x_0 + x_1}{2}, \quad x_1' = \frac{x_2 + x_3}{2}, \dots$$

Monte Carlo samples 2^P

Example

$$\{ x_0, x_1 \dots x_{15} \} = \{ x_0^{(0)}, x_1^{(0)} \dots \}$$

Divide by 2 ($n/2$)

$$x_0' = x_0^{(1)}, \; x_1^{(1)}, \; \ldots$$

$$x_k^{(i+1)} = \qquad 1 \le i \le d-1$$

$$= \frac{1}{2}\left[x_{2k-1}^{(i)} + x_{2k}^{(i)} \right]$$

$$\mu^{(0)} = \frac{1}{n} \sum x_i \;=\; \mu^{(i)} = \frac{1}{n^{(i)}} \times \sum_{j=1}^{n^{(i)}} x_j^{(i)}$$

$$n^{(i)} = \frac{n}{2^i}$$

$$\sigma_m^2(\mu^{(0)}) = \sigma_m^2(\mu^{(i)})$$

invariant

$$\sigma^2(\mu) = \frac{\sigma^2_{(k)}}{n^{(k)}} + \frac{2}{n^{(k)}} \sum_{h=1}^{n^{(k)}-1} \left(1 - \frac{h}{n^{(k)}}\right)$$

$$\times \gamma^{(k)}(h)$$

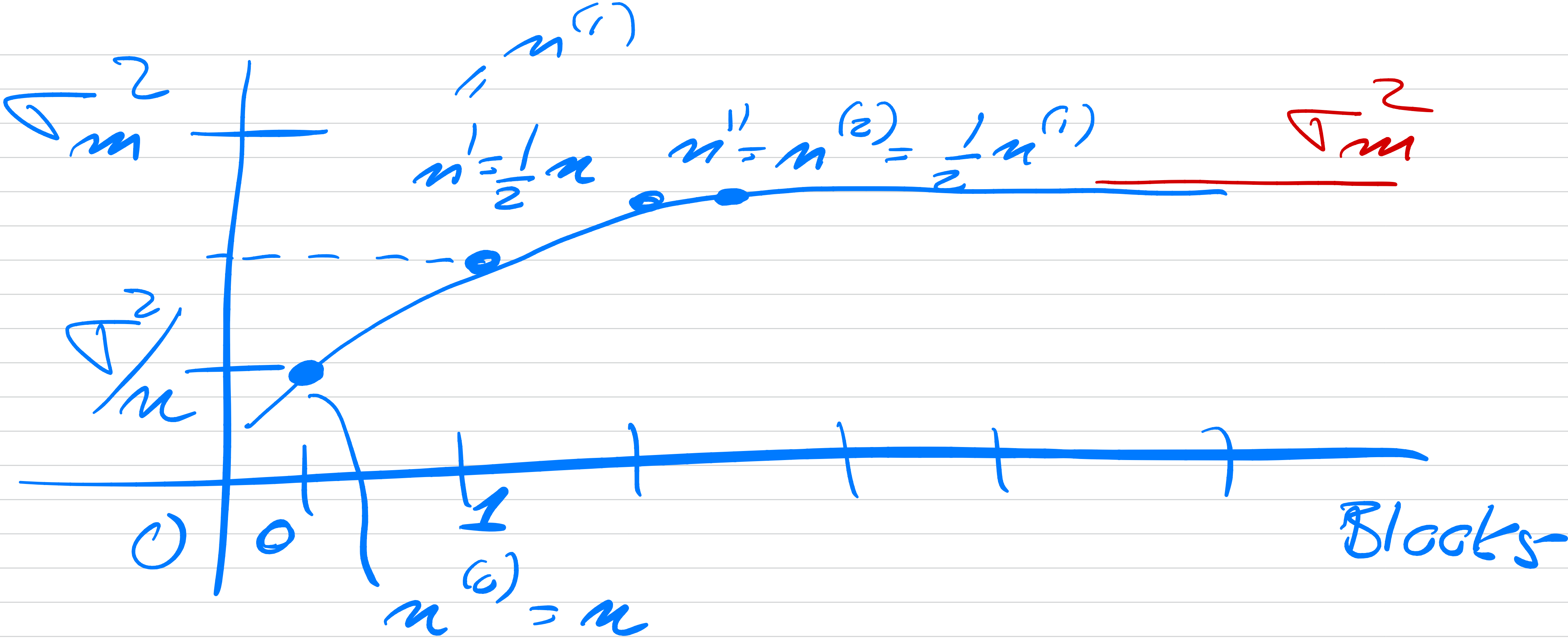
$$\gamma^{(k)}(h) = \mathrm{cov}\left(x_i^{(k)}, x_{j+h}^{(k)}\right)$$

$$h = |i - j|$$

Flyvbjerg and Petersen

$$\gamma^{(k+1)}(h) = \begin{cases} \frac{1}{2}\gamma^{(k)}(2h) + \frac{1}{2}\gamma^{(k)}(2h+1) & h = 0 \\ \frac{1}{4}\gamma^{(k)}(2h-1) + \frac{1}{2}\gamma^{(k)}(2h) \\ \quad + \frac{1}{4}\gamma^{(k)}(2h+1) & \text{else} \end{cases}$$

$$\sigma^2(\mu) = \frac{\sigma^{2(k)}}{n^{(k)}} + \frac{2}{n^{(k)}} \sum_{h=1}^{n^{(k)}-1} \left(1 - \frac{h}{n^{(k)}}\right) \times \gamma^{(k)}(h)$$



σ_m^2
σ^2/n
$n^{(1)}$
$n' = \frac{1}{2} n$
$n'' = n^{(2)} = \frac{1}{2} n^{(1)}$
σ_m^2
0
0
1
$n^{(0)} = n$
Blocks

One body (after optimization)

$$\rho(\vec{r}_1) = \int d\vec{r}_2 d\vec{r}_3 \cdots \int d\vec{r}_N$$

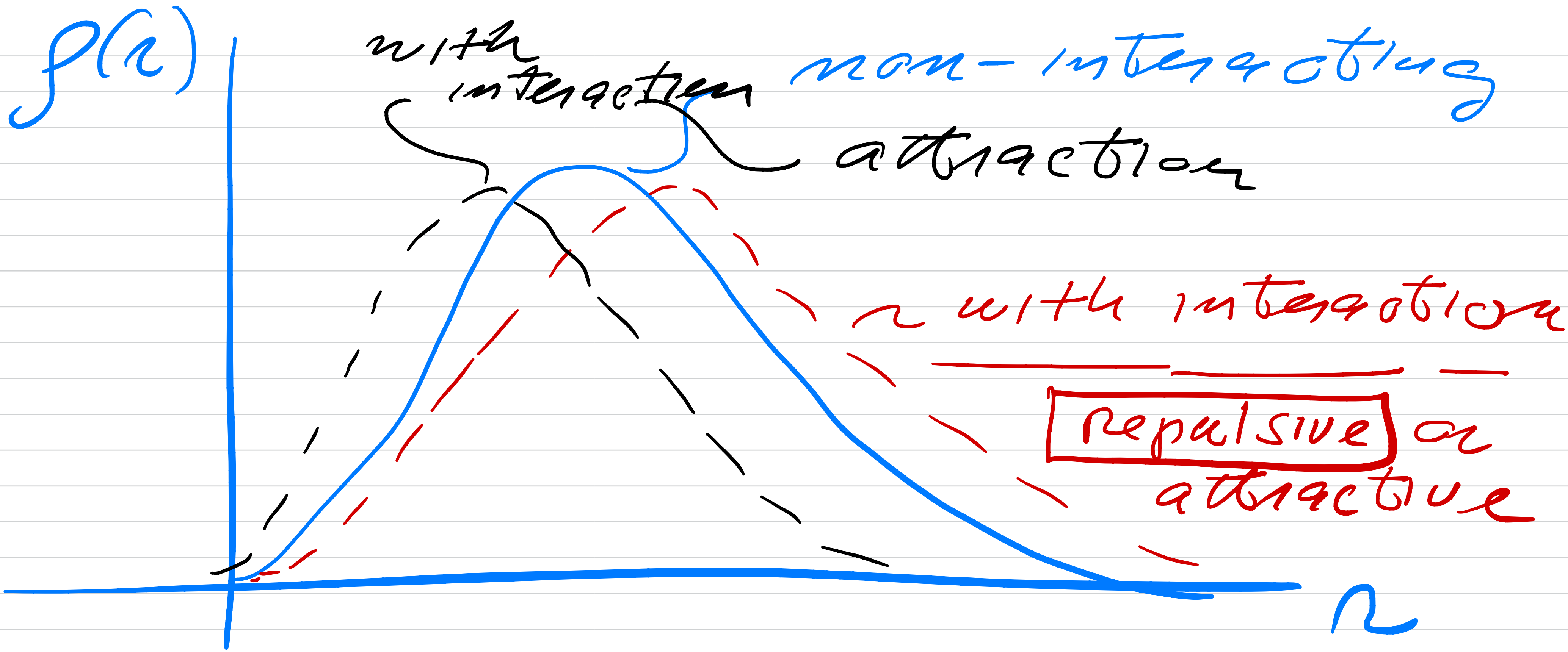
$$\times \left| \Psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N ; \hat{\Theta}) \right|^2$$

2-dim $\quad \vec{r}_1 = x\vec{e}_x + y\vec{e}_y$

$\rho(x,y) \longrightarrow \rho(r) \qquad r = \sqrt{x^2+y^2}$

(assume that ρ is isotropic)

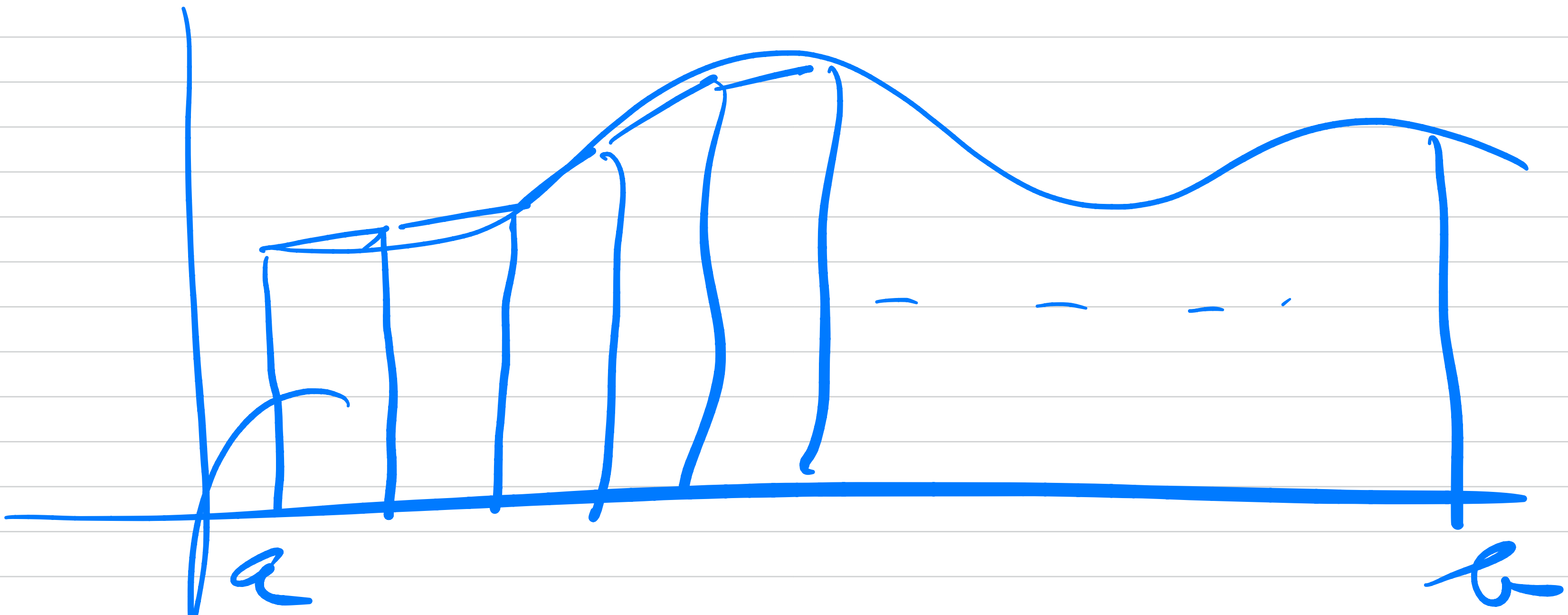
Table of x and y



(1) non-interacting case, harmonic oscillator,

$$\psi_{exact} \sim e^{-\alpha^2 r^2}$$

Parallelization strategies



n - points between a and b

$n_e = n / \text{processes}$

Full run for each process

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For i=1, MCS
    do something
    ⋮
END FOR
RETURN <E>, <E^2> etc to main process
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