FYS4411/9411, lecture March 21

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Total mean of m - experiments

$$\overline{X} = \frac{1}{m} \sum_{i=1}^{m} \overline{x_i}$$

$$\overline{x_i} = \frac{1}{n} \sum_{j=1}^{n} x_{ij}$$

Total variance (sample)

$$\sigma_m^2 = \frac{1}{m} \sum_{i=1}^{m} \underbrace{(\overline{x_i} - \overline{X})}^{2}$$

$$\overline{x_i} - \overline{X} = \frac{1}{n} \sum_{j=1}^{n} x_{ij} - \overline{X} = \tilde{x}_{ij}$$

$$\underline{\sigma_m^2} = \frac{1}{m} \sum_{i=1}^{m} \left[\frac{1}{n} \sum_{j=1}^{n} x_{ij}^{\sim} \right]^2$$

$$= \frac{1}{m} \frac{1}{n^2} \sum_{i=1}^{m} \sum_{j=1}^{n} x_{ij}^{\sim 2}$$

$$\frac{1}{n^2} \sum_{j} \sum_{k} \tilde{x}_{ij} \times \tilde{x}_{ik}$$

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

Total sample

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

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

$$d = |j-k|$$

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

$$d = 0$$

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

$$= \sigma^2$$

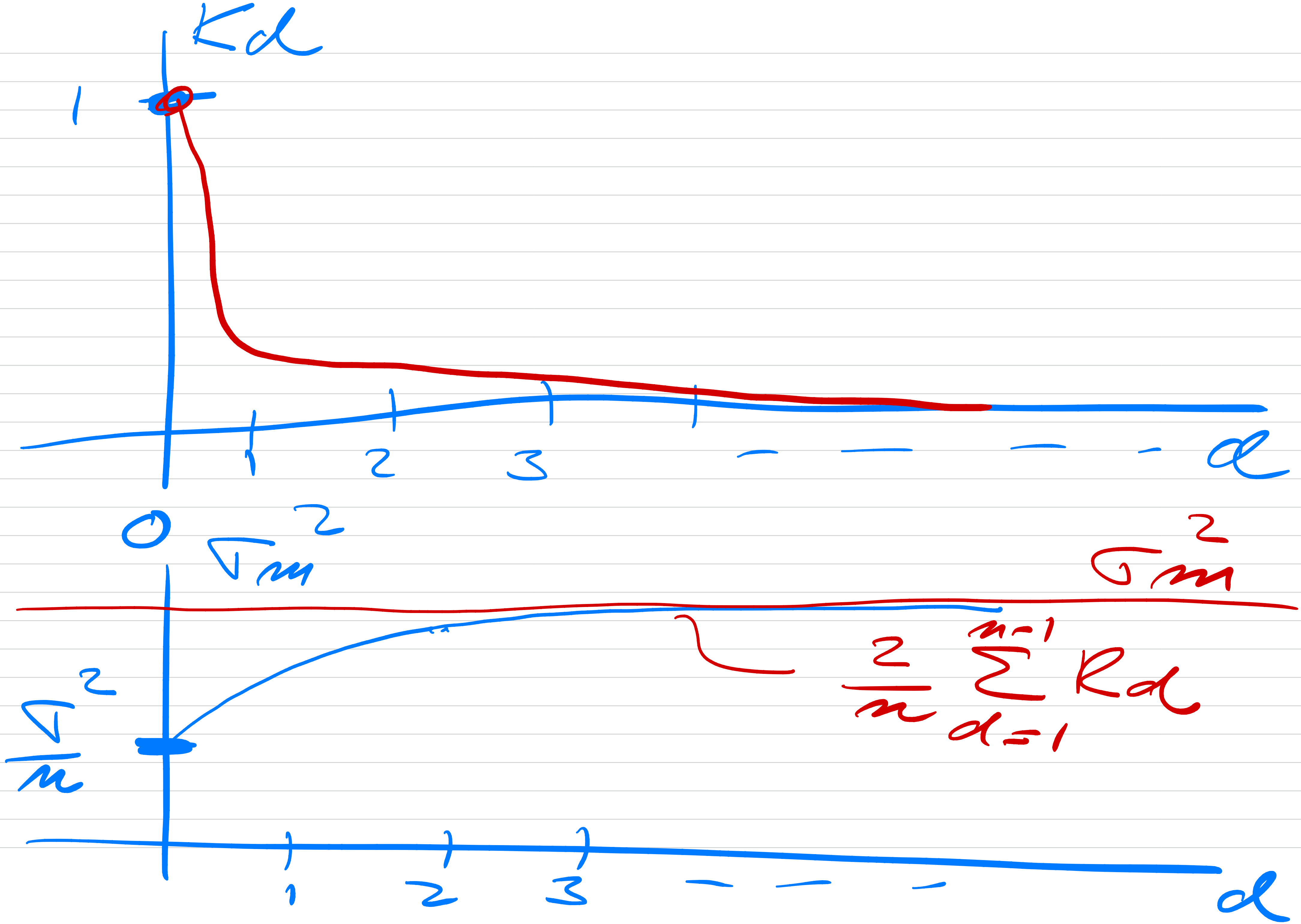
$$\sigma_m^2 = \frac{\sigma^2}{n} + \underbrace{\frac{2}{n} \sum_{d=1}^{n-1} \gamma_d}_{\text{autocovariance}}$$

correlation function

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

$$\gamma_0 / \sigma^2 = 1 = R_0$$

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



K_d
1
0
1
2
3
d
σ_m^2
σ_m^2
$\frac{\sigma^2}{n}$
$\frac{2}{n}\sum_{d=1}^{n-1} R_d$
1
2
3
d

Blocking of statistics: STD (standard deviation)

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

Iterated splitting into blocks of half the size,

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

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

Monte Carlo samples 2^P

$$X = \{1, 2, 3, 4, 5, 6\}$$

$$\mu = \frac{1}{6} \sum_{i=1}^{6} x_i = 7/2$$

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

$$X' = \left\{ \frac{x_1 + x_2}{2}, \frac{x_3 + x_4}{2}, \frac{x_5 + x_6}{2} \right\}$$

$$\mu' = \frac{1}{3} \sum_{i=1}^{3} x_i' = 7/2$$

$$\sigma^2(\mu) = \frac{1}{6}\sum_{i=1}^{6}(x_i - \mu)^2 = 8/3$$

$$\sigma^{2\,\prime}(\mu') = \frac{1}{3}\sum_{i=1}^{3}\left(\frac{x_{2i-1} + x_{2i}}{2}\right)^2 - \mu'^2$$

$$= 8/3$$

$$\mu^{(0)} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\mu^{(i)} = \frac{1}{n^{(i)}}\sum_{j=1}^{n^{(i)}} x_j^{(i)} \qquad n^{(i)} = \frac{n}{2^i}$$

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

$\mu^{(0)} = \mu^{(i)}$ invariant.

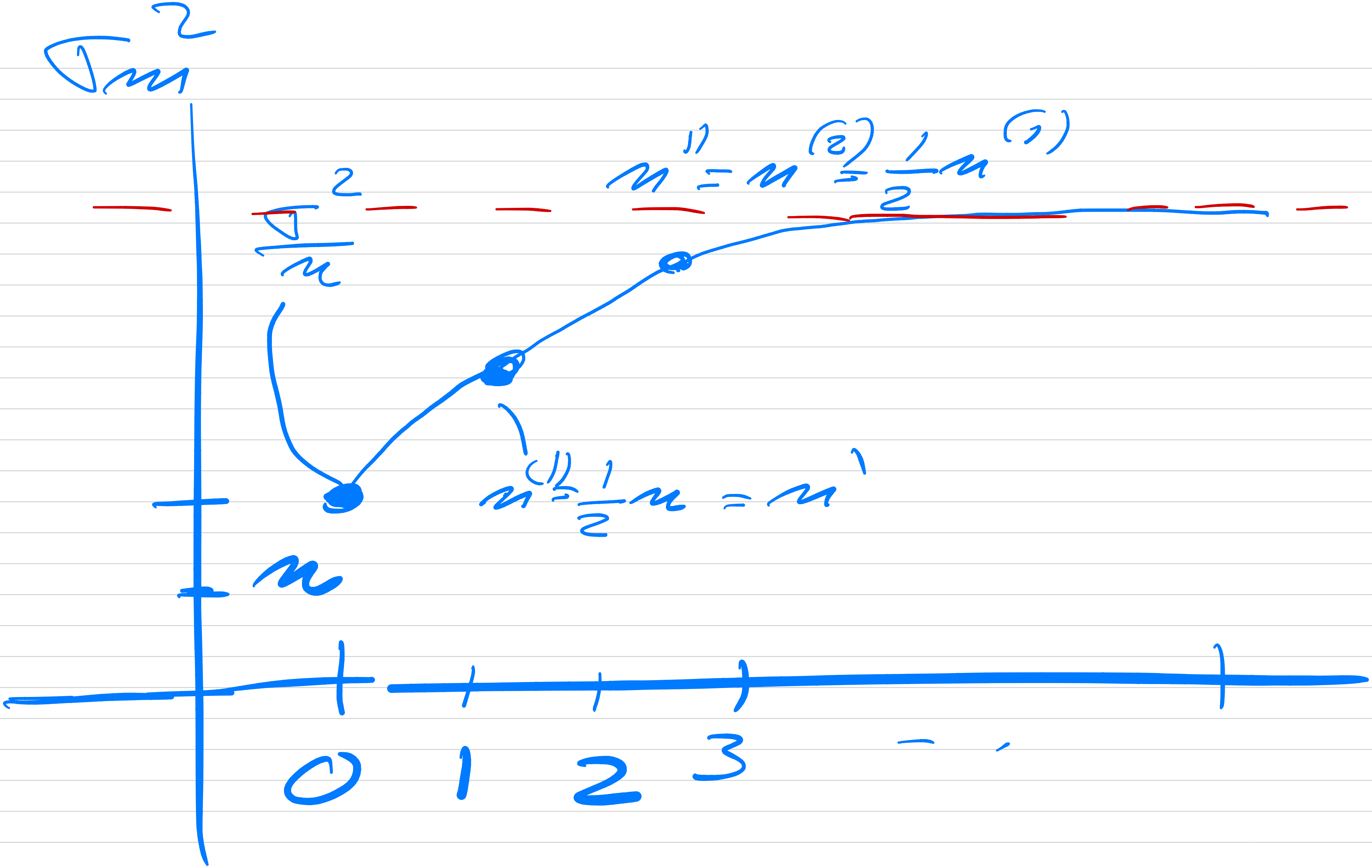
Flyvberg & Petersen 1989

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

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

$$h = |i-j|$$

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



σ_m^2
$\frac{\sigma^2}{n}$
$m'' = m^{(2)} = \frac{1}{2} m^{(1)}$
$m^{(1)} = \frac{1}{2} n = m'$
n
0
1
2
3

Onebody density
(after optimization and
VMC calculation)
we have then $\Psi_T(\vec{R};\hat{\alpha})$

one body density

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

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

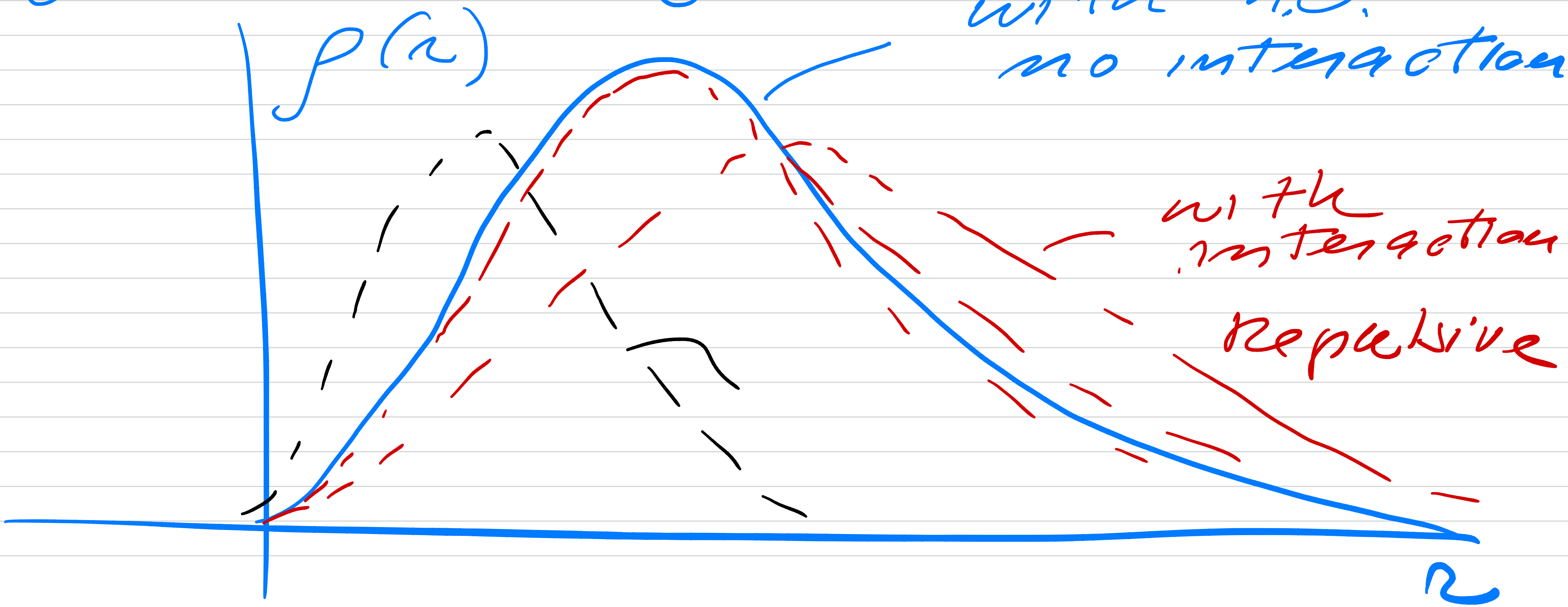
2-dim $\quad \vec{r}_i = x_i \vec{e}_x + y_i \vec{e}_y$

$$\rho(\vec{r}_1) = \rho(\vec{r}) = \rho(x, y)$$

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

assume ground is isotropic

$$\rho(x, y) \longrightarrow \rho(r)$$



non-interacting case

$\varphi(\vec{r}) \propto e^{-\hat{\alpha} r^2} \qquad \hat{\alpha} = 1/2$

with two particles

$\int d\vec{r}_2 \, e^{-\hat{\alpha}(r_1^2 + r_2^2)2}$

$= 2\pi \int_0^\infty dr_2 \, r_2 \, e^{-2\alpha(r_1^2 + r_2^2)}$