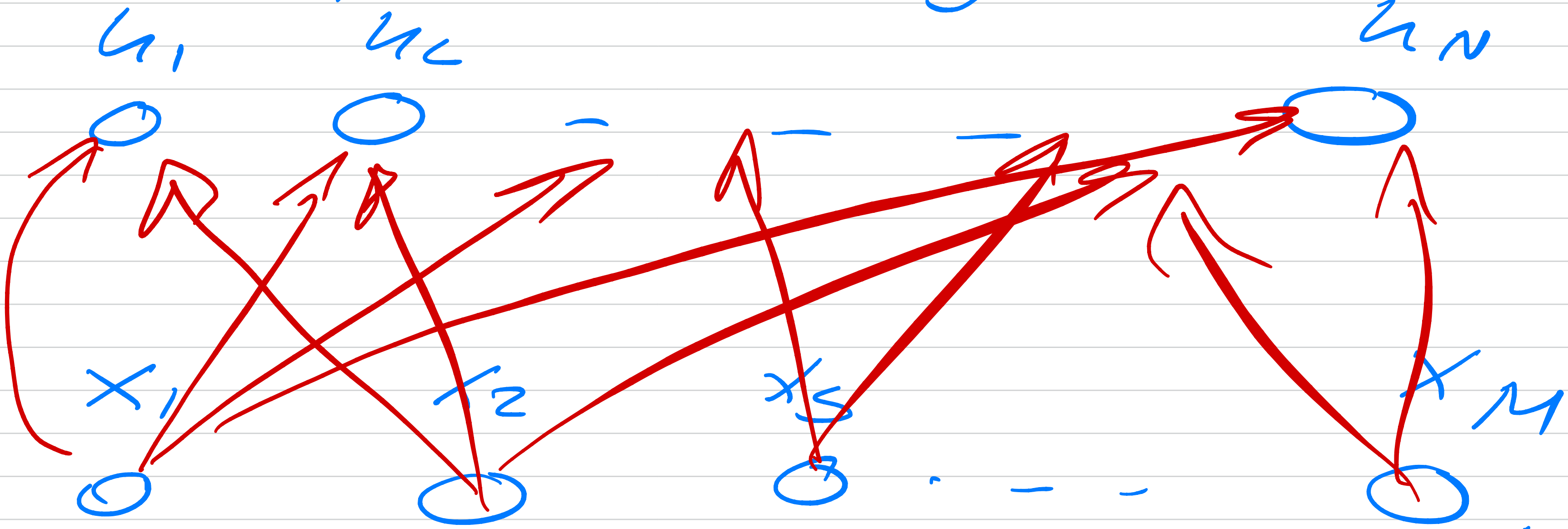
FYS5411/9411 APRIL 11

Restricted BM (RBM)

Hidden layers



visible layer/
input layer

$$|\psi(x;\theta)|^2 = \frac{1}{Z(\theta)} e^{-E(x;\theta)}$$

$$= \frac{1}{Z(\theta)} \sum_{\{h\}} e^{-E(x,h;\theta)}$$

$$\sum_{\{h\}} = \sum_{h_1=\{0,1\}} \sum_{h_2=\{0,1\}} \cdots \sum_{h_N=\{0,1\}}$$

Gaussian – Binary

$$E(x,h;\theta) = \sum_{i=1}^{M} \frac{(x_i-a_i)^2}{2\sigma^2} + \sum_{j=1}^{N} b_j h_j + \sum_{ij}^{MN} x_i w_{ij} h_j$$

$$\sigma^2 = 1$$

$$Z(\theta) = \sum_{\{x\}\{h\}} e^{-E(x, h; \theta)}$$

$$\theta = \{ a, b, W \}$$

$$h_j = \{0, 1\} \qquad x \in (-\infty, \infty)$$

$$P(x; \theta) = \frac{1}{Z(\theta)} e^{-\sum_{i=1}^{M} (x_i - a_i)^2 / 2}$$

$$\times \prod_{j=1}^{N} \left(1 + e^{-(b_j + \sum_{i=1}^{M} x_i w_{ij})} \right)$$

$$E_L = \frac{1}{\psi} H \psi \qquad \left(\psi(x;\theta) = \sqrt{P(x;\theta)} \right)$$

$$\nabla_\theta \langle E_L \rangle =$$

$$2\left[\left\langle E_L \frac{1}{\psi} \frac{\partial \psi}{\partial \theta} \right\rangle - \langle E_L \rangle \left\langle \frac{1}{\psi} \frac{\partial \psi}{\partial \theta} \right\rangle \right]$$

$$\frac{1}{\psi} \frac{\partial \psi}{\partial \theta} = \frac{\partial \ln \psi}{\partial \theta}$$

$$\ln \psi = - \ln Z - \sum_{i=1}^{M} \frac{(x_i - a_i)^2}{2} - \sum_{j=1}^{N} \ln\left(1 + e^{-(b_j + \sum_{i=1}^{M} x_i w_{ij})}\right)$$

$$\frac{\partial \ln \psi}{\partial a_i} = (x_i - a_i)$$

$$\frac{\partial \ln \psi}{\partial b_j} = - \frac{1}{1 + e^{-(b_j + \sum_{i=1}^{M} x_i w_{ij})}}$$

$$\frac{\partial \ln \psi}{\partial w_{ij}} = -\frac{x_i}{1+e^{-(b_j+\sum_{i=1}^{M} x_i w_{ij})}}$$

$$E_L = \frac{1}{\psi} \hat{H} \psi$$

P = # particles

$$\hat{H} = \sum_{p=1}^{P} \left(-\frac{1}{2} \nabla_p^2 + \frac{1}{2} \omega^2 r_p^2 \right)$$

$$+ \sum_{p<q} v(r_{pq})$$

$$r_{pq} = |\vec{r}_p - \vec{r}_q|$$

$$\hbar = c = e = m = 1$$

$$E_c = -\frac{1}{2}\frac{1}{4}\left(\sum_{p=1}^{P} \nabla_p^2\right)\psi$$

$$+\ \frac{1}{2}\sum_{p=1}^{P} \omega^2 r_p^2 +$$

$$\sum_{p<q} v(r_{pq})$$

1 particle in ~~one~~ one dim

$$\nabla_p^2 \psi \rightarrow \boxed{\frac{d^2}{dx^2}\psi} =$$

$$\frac{1}{\psi}\frac{d^2}{dx^2}\psi = \left(\frac{d}{dx}\ln\psi\right)^2 + \frac{d^2}{dx^2}\ln\psi$$

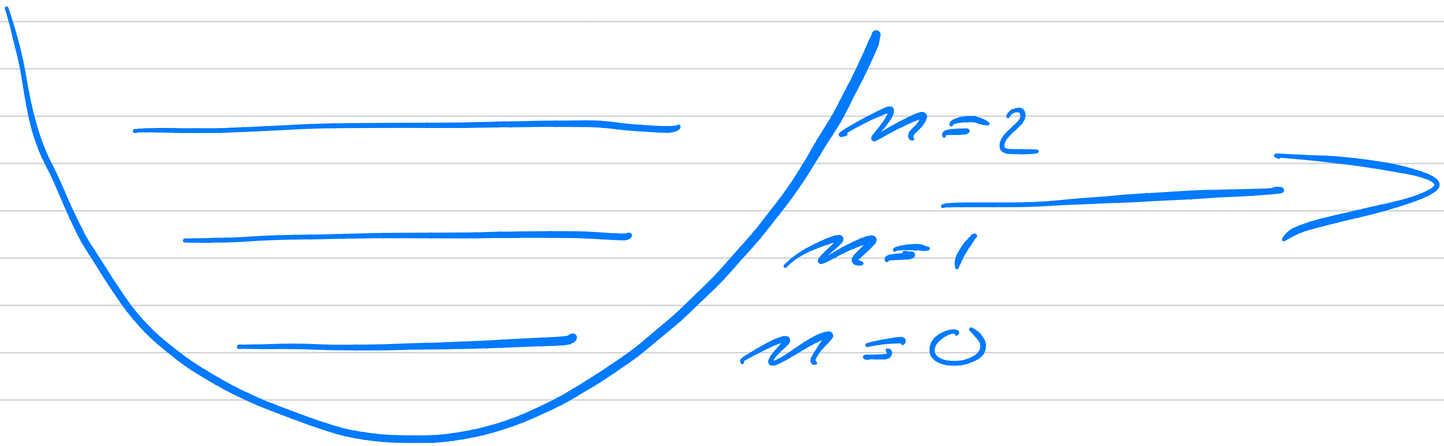
$$\ln\psi = -\frac{(x_i' - a_i')^2}{2} - \sum_{j=1}^{N}\ln\left(1 + e^{-(b_j' + \sum_{i=1}^{M} x_i' w_{ij}')}\right)$$

System of 2 electrons in a 2-dim HO trap.

$\hbar = c = e = m = 1$

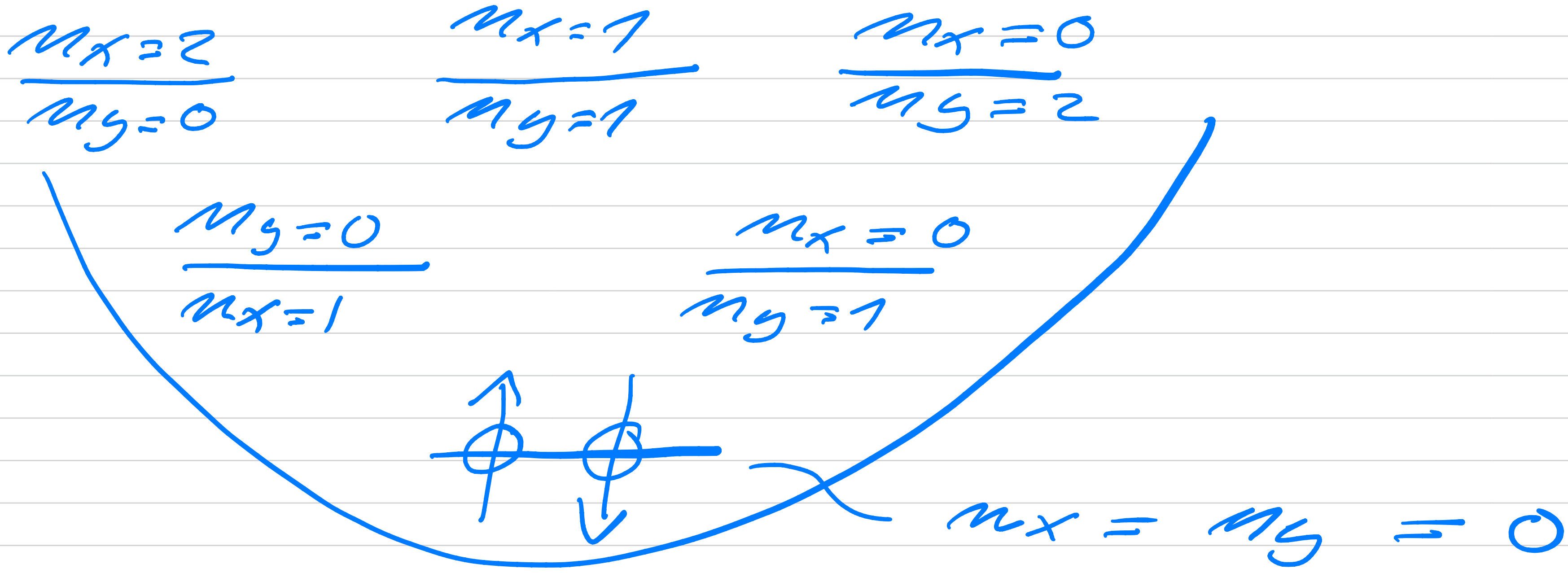
oscillator frequency $\omega = 1$

1 dim



$$E_n = \hbar\omega(n + 1/2)$$

2 dim (Fermions)



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

$$\psi(x,y) \to \psi_{n_x n_y}(x,y) = \; ?$$

no interaction

Exact ground state

$$\psi_0(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_0(\vec{r}_1)\xi_\uparrow & \varphi_0(\vec{r}_2)\xi_\uparrow \\ \varphi_0(\vec{r}_1)\xi_\downarrow & \varphi_0(\vec{r}_2)\xi_\downarrow \end{vmatrix}$$

$$= \frac{1}{\sqrt{2}} \underbrace{\varphi_0(\vec{r}_1)\varphi_0(\vec{r}_2)}_{\text{spatial part}} \underbrace{\left(\xi_\uparrow(1)\xi_\downarrow(2) - \xi_\downarrow(1)\xi_\uparrow(2)\right)}_{\text{spin part}}$$

symmetric

antisym

$S = 0$

$M_S = 0$

$$\varphi_0(\vec{r}_\perp) = H_{n_x=0}(x_\perp) H_{n_y=0}(y_\perp) \times e^{-\alpha r_\perp^2} \times \text{const}$$

$H_n(x)$ = Hermite polynomial

$$H_{n=0}(x) = \underline{1}$$

$$\varphi_0(\vec{r}_\perp) \propto e^{-\alpha r_\perp^2}$$

$$r_\perp^2 = x_\perp^2 + y_\perp^2 \qquad \alpha \propto \sqrt{\omega}$$

$$E_{n_x=0\, n_y=0} = \hbar\omega = 1$$

$$\hbar = \omega = 1$$

Two particles (non interacting)

$$E_0 = 2\hbar\omega = \underline{\underline{2}} \; \text{a.u.}$$

(label above: E_0)

interaction $v(r_{ij}) = \dfrac{1}{|\vec{r}_i - \vec{r}_j|}$

can be solved analytically

$$E = 3 \text{ a.u.}$$