FYS4411/9411 APRIL 8

Room 1

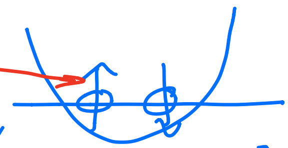
Fermionic VMC : quantum dots

HO

2 Dim

$n_x = n_y = 0$

$E = \hbar\omega$



$\uparrow$

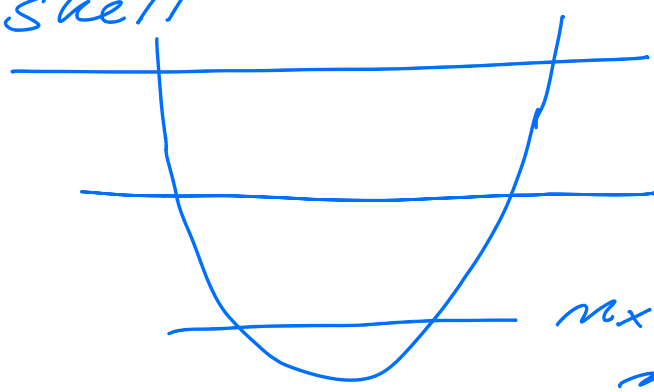
$s = 1/2$

$m_s = 1/2$

$\downarrow \quad m_s = -1/2$

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i=1}^{N} \frac{1}{2} k r_i^2 + \sum_{i<j}^{N} V(r_{ij})$$

$N=2$, $\boxed{N=6}$, $N=12$, closed shell



$n_x=2 \quad n_y=0$

$n_x=1 \quad n_y=1$

$n_x=0 \quad n_y=2$

$n_x=1 \wedge n_y=0$

$n_x=0 \quad n_y=1$

$n_x = n_y = 0$

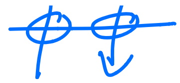
$n_x, n_y \geq 0$

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

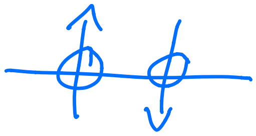
3 4

5 6

~~$n_x=1,\ n_y=0$~~



$n_x=0 \quad n_y=1$



$n_x=n_y=0$

$1 \quad 2 \longrightarrow$ $m_s=-1/2 \quad S=1/2$
$n_x=n_y=0$

ansatz for ground state
(without Jastrow factor)

$$\phi_0(\vec{r}_1 \vec{r}_2 \ldots \vec{r}_6;\ 1,2,\ldots 6) = \frac{1}{\sqrt{6!}} \begin{vmatrix} \varphi_1(\vec{r}_1) & \varphi_1(\vec{r}_2) & \ldots & \varphi_1(\vec{r}_6) \\ \varphi_2(\vec{r}_1) & \varphi_2(\vec{r}_2) & & \\ \vdots & \vdots & & \\ \varphi_6(\vec{r}_1) & \varphi_6(\vec{r}_2) & \ldots & \varphi_6(\vec{r}_6) \end{vmatrix}$$

$\boxed{\text{slater determinant}}$

$$\psi_T(\vec{r}_1, \ldots \vec{r}_6;\ 1\,2 \ldots 6) =$$

$$\phi_0 \, J$$

$$J(\vec{r}_1 \vec{r}_2, \ldots \vec{r}_6) = \prod_{i<j} f(r_{ij})$$

$$f(r_{ij}) = e^{\frac{a r_{ij}}{1+\beta r_{ij}}}$$

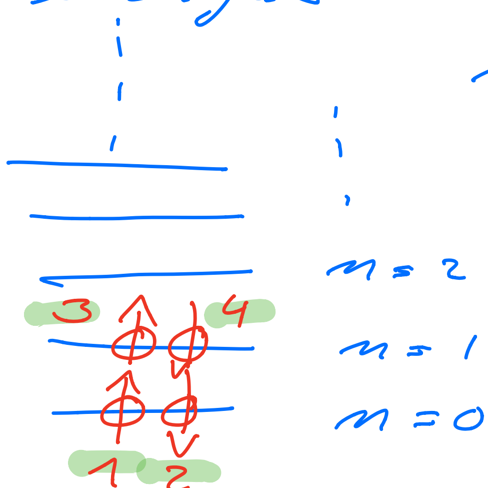
β = variational parameter,

Room 2 TDHF

1-Dim QD system.

SP energies : $\varepsilon_i = \hbar\omega(n_i + 1/2)$

$n_i = 0, 1, 2, \ldots$



$$\hat{h}_0 \varphi_i = \varepsilon_i \varphi_i$$

$$\varphi_i = H_{n_i}(x_i)\, e^{-\alpha x_i^2}$$

$N = 4$ ansatz Φ_0

$$= \frac{1}{\sqrt{4!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \cdots & \varphi_1(x_4) \\ \varphi_2(x_1) & \varphi_2(x_2) & & \vdots \\ \varphi_3(x_1) & \varphi_3(x_2) & & \vdots \\ \varphi_4(x_1) & \varphi_4(x_2) & & \varphi_4(x_4) \end{vmatrix}$$

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx_i^2} + \frac{1}{2} k x_i^2 \right)$$

$$+ \sum_{i<j} V(x_{ij})$$

$$x_{ij} = |x_i - x_j|$$

$$V(x_{ij}) = \frac{\lambda}{x_{ij} + \delta}$$

1-dim for the two-fermion case, there is no $\frac{1}{x_{ij}}$ in the kinetic

Room 3

Deep learning variant of project 1

Room 4

QML

Room 5-8 P1