FYS4411/9411, APRIL 13, 2023

(i) Extension of P1, but now with fermions

a) reuse everything from P1

b) change $\Psi_T(\vec{r}_1, \dots \vec{r}_N; \vec{\alpha})$ from Boson system to an antisymmetrized Ψ_T

Define a so-called Slater-determinant

$$\Psi_T(\vec{r}_1, \dots \vec{r}_N; \vec{\alpha}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(\vec{r}_1) & \varphi_1(\vec{r}_2) & \cdots & \varphi_1(\vec{r}_N) \\ \varphi_2(\vec{r}_1) & \varphi_2(\vec{r}_2) & \cdots & \\ \vdots & \vdots & & \\ \varphi_N(\vec{r}_1) & \varphi_N(\vec{r}_2) & \cdots & \varphi_N(\vec{r}_N) \end{vmatrix}$$

system: 2-dim quantum dots (harmonic oscillator)

$$H = H_0 + H_I$$

$$H_0 = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} k r_i^2 \right)$$

$$r_i^2 = x_i^2 + y_i^2$$

$$H_I = \sum_{i<j}^{N} \frac{k e^2}{|\vec{r}_i - \vec{r}_j|}$$

$$|\vec{r}_i - \vec{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

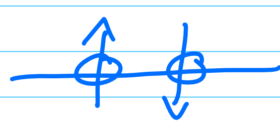
$$H_0 = \sum_{i=1}^{N} h_0(\vec{r}_i)$$

$$h_0 \varphi_\alpha(\vec{r}_i) = \varepsilon_\alpha \varphi_\alpha(r_i)$$

harmonic oscillator

$$\varepsilon_\alpha = \hbar\omega(n_{x\alpha} + n_{y\alpha} + 1)$$

$$n_x, n_y = 0, 1, 2, \ldots$$

 $n_x = n_y = 0$

$N = 2$

$$\Psi_T = \frac{1}{\sqrt{2!}} \begin{vmatrix} \varphi_{00\uparrow}(\vec{r}_1) & \varphi_{00\uparrow}(\vec{r}_2) \\ \varphi_{00\downarrow}(\vec{r}_1) & \varphi_{00\downarrow}(\vec{r}_2) \end{vmatrix}$$

$$\varphi_{00\uparrow} = \psi_{00}(\vec{r}_1)\, \chi_{\frac{1}{2}\frac{1}{2}}$$

$$S = 1/2 \qquad m_s = \pm 1/2$$

$$\chi_{\frac{1}{2}\frac{1}{2}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \chi_\uparrow$$

$$\chi_{\frac{1}{2}-\frac{1}{2}} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \chi_\downarrow$$

$$\Psi_T = \frac{1}{\sqrt{2!}} \psi_{00}(\vec{r}_1)\, \psi_{00}(\vec{r}_2) \times \left[\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\uparrow(2)\chi_\downarrow(1)\right]$$

$= \Psi_{SD}$

add a correlation term

$\Rightarrow$

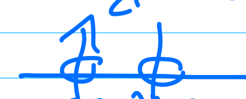
$$\Psi_T = \Psi_{SD}\, \Psi_C$$

single-particle variational parameters: α

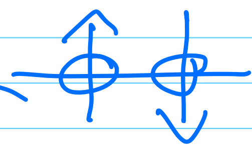
$$\psi_{n_x n_y}(\vec{r}) = H_{n_x}(x,y)\, H_{n_y}(x,y) \times e^{-r^2\alpha^2/2}$$

$N = 6$

$H_1(x)\, H_0(y)\, e^{-r^2\alpha^2/2}$ $\qquad$ $H_0(x)\, H_1(y)$

$n_x = 1 \;\; n_y = 0$ $\qquad$ $n_x = 0 \;\; n_y = 1$



$n_x = 0 = n_y$

$H_0(x)\, H_0(y) \times e^{-r^2\alpha^2/2}$ $\qquad$ $\mathcal{E} = \hbar\omega(n_x + n_y + 1)$

$n_x, n_y = 0, 1, 2, \ldots$

$\Rightarrow$ 6×6 SD (Slater determinant)

(applies to TDHF + coupled cluster)

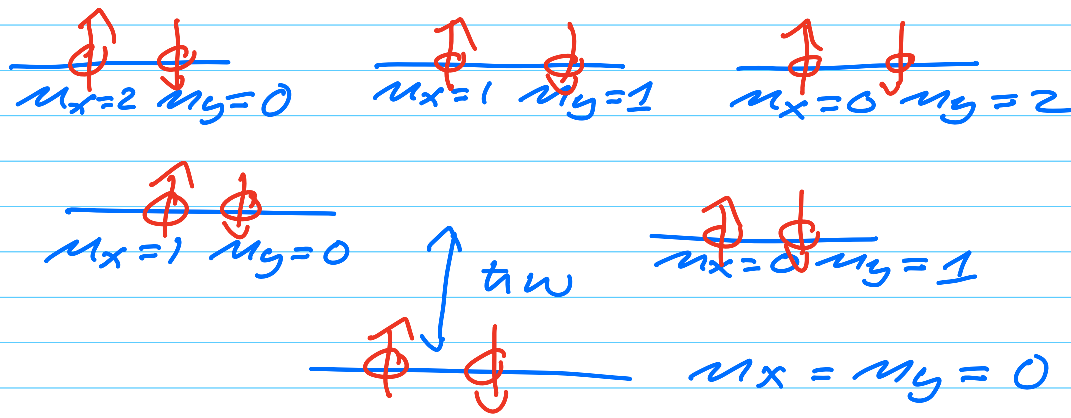
in general we have

$$\#\,SD = \binom{n}{N} = \frac{n!}{(n-N)!\,N!}$$

n = # sp states

$m \geq N$

$N = 12$



$\Rightarrow \quad 12 \times 12$ SD.

$\left(SD \rightarrow \begin{array}{l} 6\times6 \uparrow \text{ Block} \\ 6\times6 \downarrow \text{ Block} \end{array} \right)$