Lecture FYS4411/9411, April 19, 2024

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$$\Psi_T = \Psi_{SD} \cdot \Psi_J$$

anti sym

symmetric

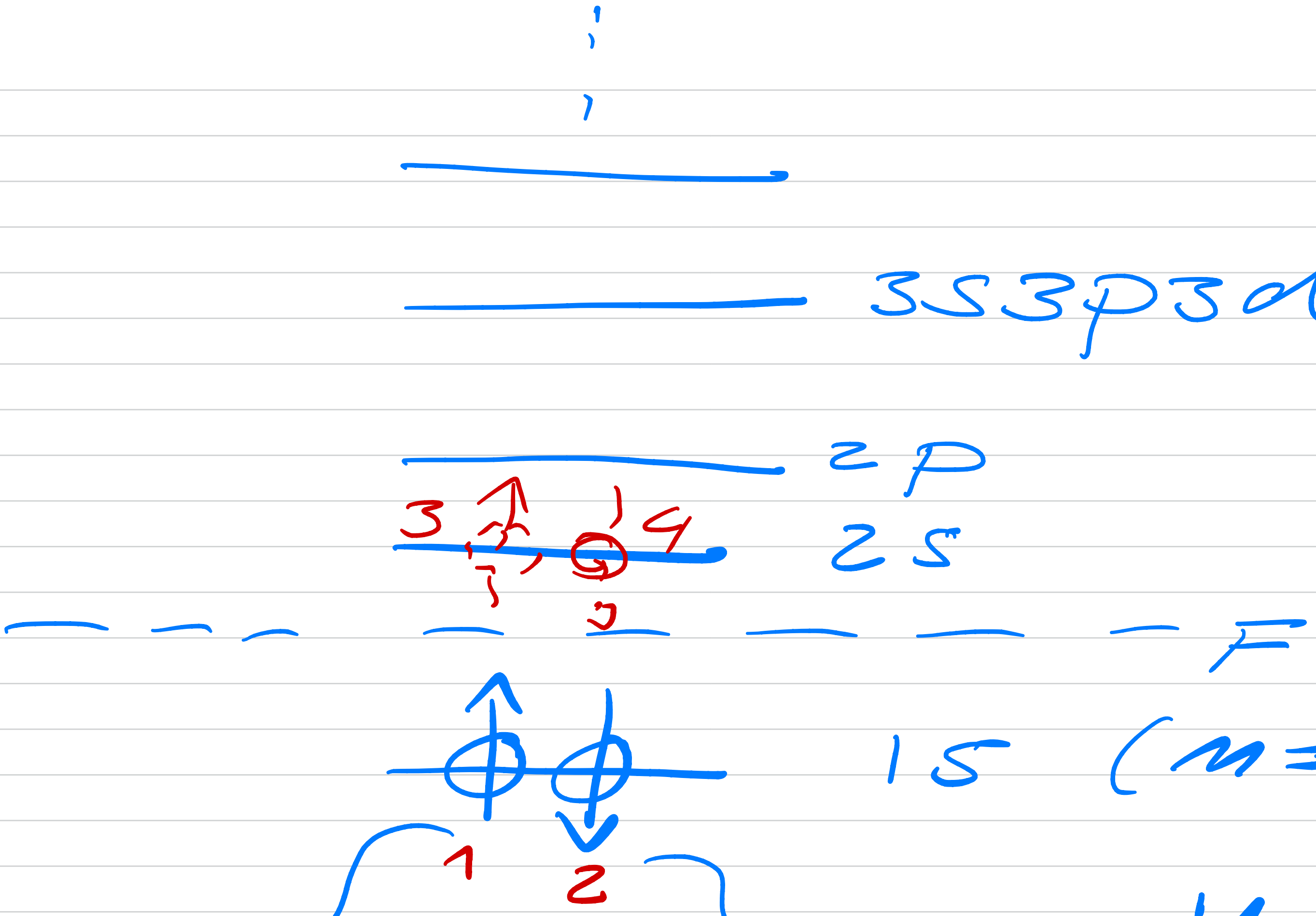
Defined as determinant in terms of single-particle wave functions. Viable if a mean-field is a good approximation.

$$\Psi_{SD}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \underbrace{\gamma_1, \gamma_2, \ldots \gamma_N}_{\text{single-particle quantum numbers}}; \vec{\alpha})$$

$\vec{\alpha}$: variational params

Example: $N = 2$, He

Model based on Hydrogen-like single-particle states



$(n=0,\ l=0,\ m_l=0)$

$\phi_{1s\uparrow}$ $\qquad$ $\phi_{1s\downarrow}$

$$M_S = m_{s_1} + m_{s_2} = 0$$

$$\phi_{1s\uparrow} \longrightarrow \varphi_{\gamma_i}\,\chi_{s m_s}(i)$$

$$\chi_{1/2\,\pm 1/2}$$

$$\chi_{1/2\, \pm 1/2} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \wedge \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$m_s = +1/2 \qquad m_s = -1/2$$

$$\uparrow$$

$$\phi_{1s\uparrow}(\vec{r}_1) = \varphi_{1s}(\vec{r}_1) \otimes \chi_{1/2\, m_s}(i)$$

$$= |1s\uparrow\rangle$$

ansatz :

$$\Psi_{SD} = \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_{1s\uparrow}(\vec{r}_1) & \phi_{1s\downarrow}(\vec{r}_1) \\ \phi_{1s\uparrow}(\vec{r}_2) & \phi_{1s\downarrow}(\vec{r}_2) \end{vmatrix}$$

rows : particle in $\vec{r}_i$

columns : sp-state γ_i

$$|D| = \frac{1}{\sqrt{N!}} \begin{vmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ \vdots & & & \\ d_{N1} & \cdots & & d_{NN} \end{vmatrix}$$

$$d_{ij} = \phi_j(x_i)$$

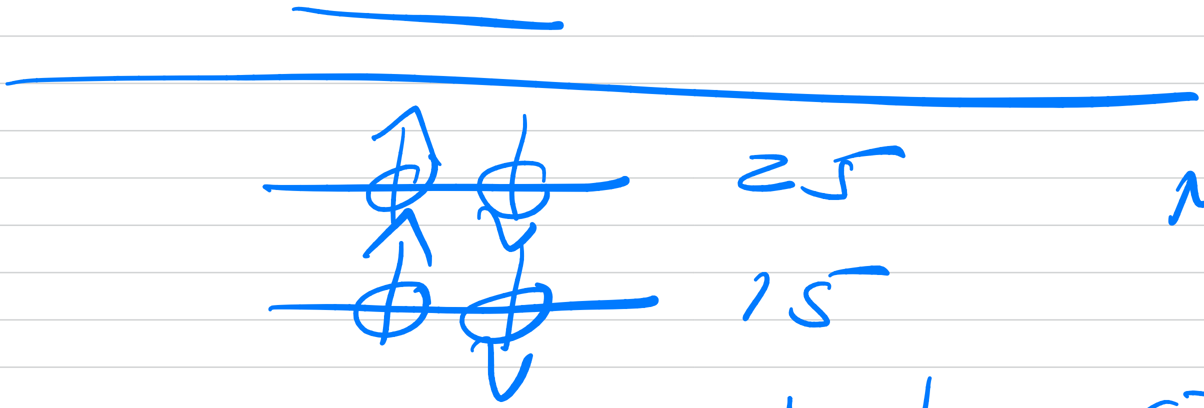
rows are positions

columns are specific quantum states

(n, l, ml, s, ms

$N = 4$, Beryllium

$\vdots$



$$M_S = m_{s_1} + m_{s_2} + m_{s_3} + m_{s_4} = 0$$

$$\Psi_{SD} = \frac{1}{\sqrt{4!}} \begin{vmatrix} \phi_{1s\uparrow}(\vec{r}_1) & \phi_{1s\downarrow}(\vec{r}_1) & \phi_{2s\uparrow} & \phi_{2s\downarrow} \\ \phi_{1s\uparrow}(\vec{r}_2) & - & - & , \\ \vdots & & & \\ \phi_{1s\uparrow}(\vec{r}_4) & - & - & , \end{vmatrix}$$

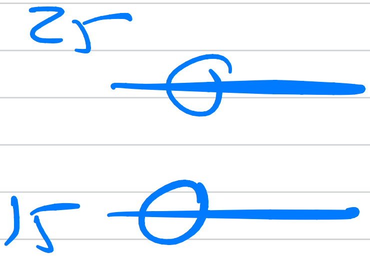
$$\Psi_{SD}(\ldots \vec{r}_i \ldots \vec{r}_j, \ldots) = -\Psi_S(\ldots \vec{r}_j, \ldots \vec{r}_i \ldots)$$

N=2 (Helium case)

For the ground state:

$$\Psi_{SD}(N=2) = \varphi_{1s}(\vec{r}_1)\,\varphi_{1s}(\vec{r}_2)\,\frac{1}{\sqrt{2}}$$

$$\times \Big(\underbrace{\chi_\uparrow(1)\,\chi_\downarrow(2) - \chi_\uparrow(2)\,\chi_\downarrow(1)}_{\text{antisymm in spin}}\Big)$$



Total spin = 0

$$\frac{1}{\sqrt{2}}\,\chi_\uparrow(1)\,\chi_\uparrow(2)\Big[\varphi_{1s}(\vec{r}_1)\,\varphi_{1s}(\vec{r}_2) - \varphi_{1s}(\vec{r}_2)\,\varphi_{1s}(\vec{r}_1)\Big]$$

$$= 0$$

System: 2dim, quantum dot system, electrons confined in 2-dim harmonic oscillator-like traps

$$H = H_0 + H_I$$

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

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

$$D_1^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2}$$

$$H_I = \sum_{i<j}^{N} v(|\vec{r}_{ij}|)$$

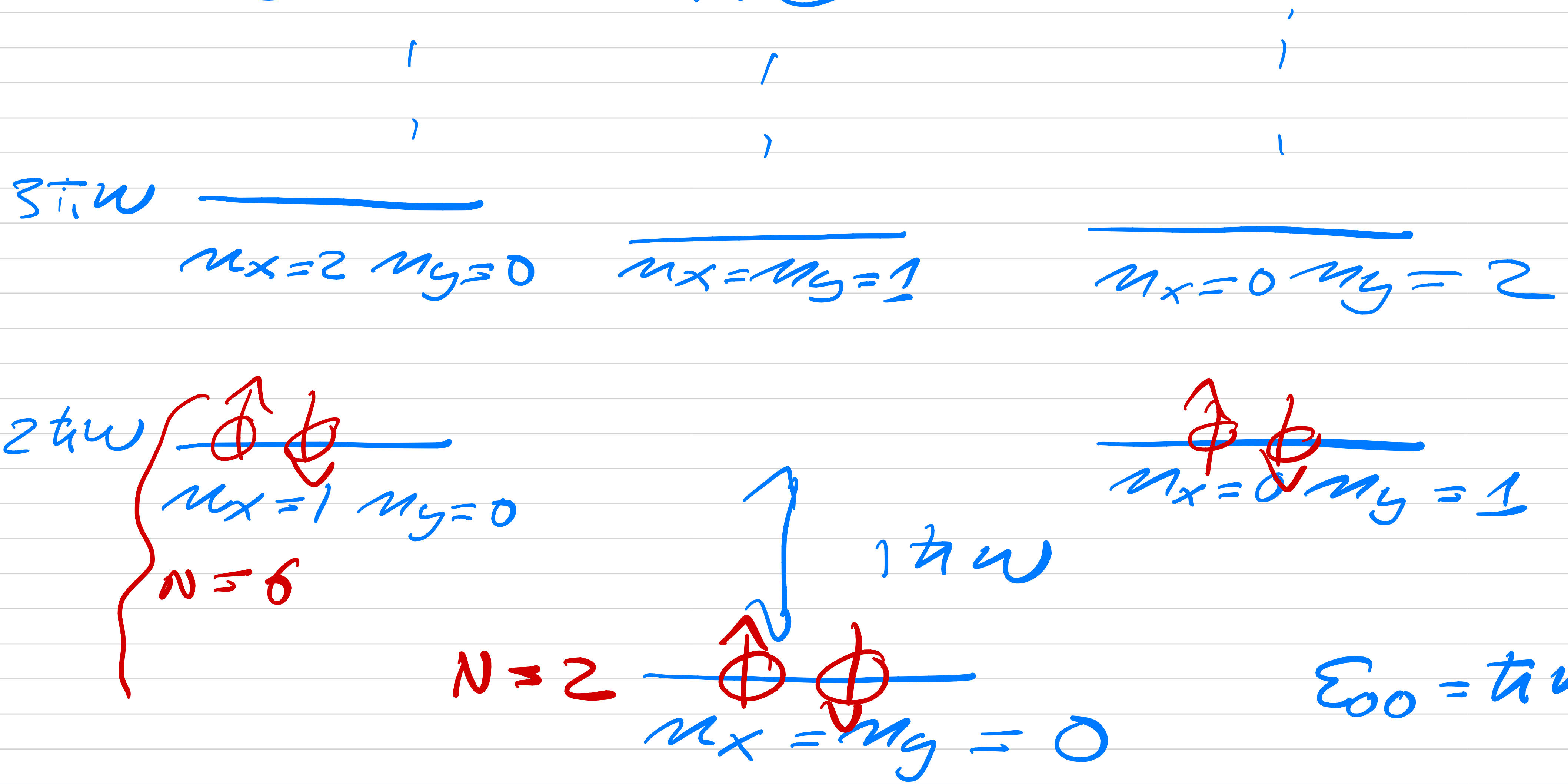
$$|\vec{r}_{ij}| = \sqrt{(x_i-x_j)^2+(y_i-y_j)^2}$$

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

$$H_0 = \sum_i h_0(\vec{r}_i)$$

$$h_0(\vec{r}_i)\,\varphi_\alpha(\vec{r}_i) = \hbar\omega\,(n_{x_\alpha}+n_{y_\alpha}+1)$$

2D m HO



$E_{00}=\hbar\omega$

2, 6, 12, 20, 30, 42, 56, 72,

4 6 8

Trial wave functions (SP)

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

$$r^2 = x^2 + y^2$$

Hermite polynomial

$$H_{n_{x,y}=0}(x) = 1$$

$$H_{n=1}(x) = x$$

$$H_{n=2}(x) = x^2 - 1$$

$$H_{n=3}(x) = x^3 - 3x$$

$$\phi_{n_x=1\, n_y=0}(x,y) = x\, e^{-(x^2+y^2)\alpha^2/2}$$

variational parameter.

$N=2$ $(2\times 2$ SD$)$

$N=6$ $(6\times 6$ SD$)$

$N=12$ $(12\times 12$ SD$)$

Non-int energy

$E_2 = 2\hbar\omega$

$E_6 = 10\hbar\omega$

$E_{12} = 28\hbar\omega$

To calculate a determinant requires $O(n^3)$ FLOPS

Efficient calculation of the SD

$$|D| = \begin{vmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ \vdots & & & \\ d_{N1} & \cdots & \cdots & d_{NN} \end{vmatrix}$$

$$d_{ij} = \phi_j(x_i)$$

$$R = \frac{|D(R_{new})|}{|D(R_{old})|}$$

Need intermediate step

$$d_{ij}^{-1} = \frac{C_{ji}}{|D|} \longleftarrow \text{cofactors}$$

$N = 3$

$$|D| = \begin{vmatrix} d_{11} & d_{12} & d_{13} \\ d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \end{vmatrix}$$

$$d_{11} \underbrace{\begin{vmatrix} d_{22} & d_{23} \\ d_{32} & d_{33} \end{vmatrix}}_{C_{11}} - d_{12} C_{12} + d_{13} C_{13}$$

ith row

$$|D| = \sum_{j=1}^{N} d_{ij} C_{ij}$$

if D is invertible, $D^{-1} D = \mathbb{1}$

which translates into

$$\sum_{k=1}^{N} d_{ik} d^{-1}_{kj} = \delta_{ij}$$

How can we use this to calculate the Metropolis Ratio?

$$R = \frac{\sum_{j=1}^{N} d_{ij}'(r_{new})\, C_{ij}'(r_{new})}{\sum_{j=1}^{N} d_{ij}'(r_{old})\, C_{ij}(r_{old})}$$

Suppose we move only one particle at the time, then

$C_{ij}(r_{new}) = C_{ij}(r_{old})$ for all $j = \{1, 2, \ldots, N\}$

$$R = \frac{\sum_{j=1}^{N} d_{ij}(r^{new})\, d_{ji}^{-1}(r^{old})}{\underbrace{\sum_{j=1}^{N} d_{ij}(r^{old})\, d_{ji}^{-1}(r^{old})}_{=\delta_{ii}}}$$

$$= \sum_{j=1}^{N} d_{ij}(r^{new})\, d_{ji}^{-1}(r^{old})$$

$$= \sum_{j=1}^{N} \phi_j(r_i^{new})\, d_{ji}^{-1}(r_i^{old})$$

$$\frac{\nabla_i |D|}{|D|} = \sum_{j=1}^{N} \left(\nabla_i \phi_j (\vec{r}_i) \right) d_{ji}^{-1}(r_i)$$

$$\frac{\nabla_i^2 |D|}{|D|} = \sum_{j=1}^{N} \left(\nabla_i^2 \phi_j (\vec{r}_i) \right) d_{ji}^{-1}(r_i)$$