Quantum dots

- electrons that are in trapped in 2-dim systems.
- Trapped in harmonic oscillator-like potentials.

- $N = 2, 6, 12, 20$

$$\hat{H} = \sum_{i=1}^{N} \underbrace{\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right)}_{\text{one-body operator}} + H_I$$

$$H_I = \sum_{\substack{i,j \\ i<j}}^{N} \frac{1}{|\vec{r}_i - \vec{r}_j|} = \sum_{i<j}^{N} \frac{1}{r_{ij}}$$

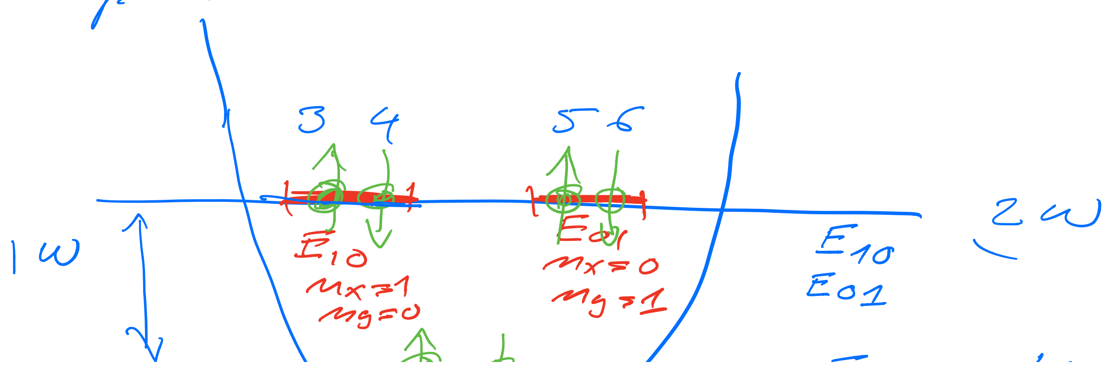
$\hbar = m = c = e = 1$

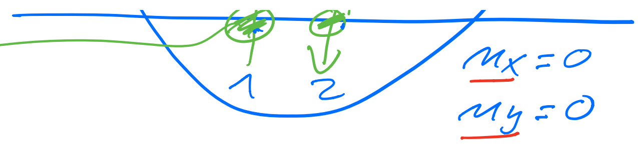
$\boxed{N = 6}$ HO system

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

2-dim

HO-potential





$E_{00} = \hbar \omega$

$m_x = 0$ $\quad \hbar = 1$

$m_y = 0$ $\quad E_0 = \omega$

$m_s = +1/2$
$S = 1/2$

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \chi_{s m_s} = \chi_{1/2\,1/2}$$

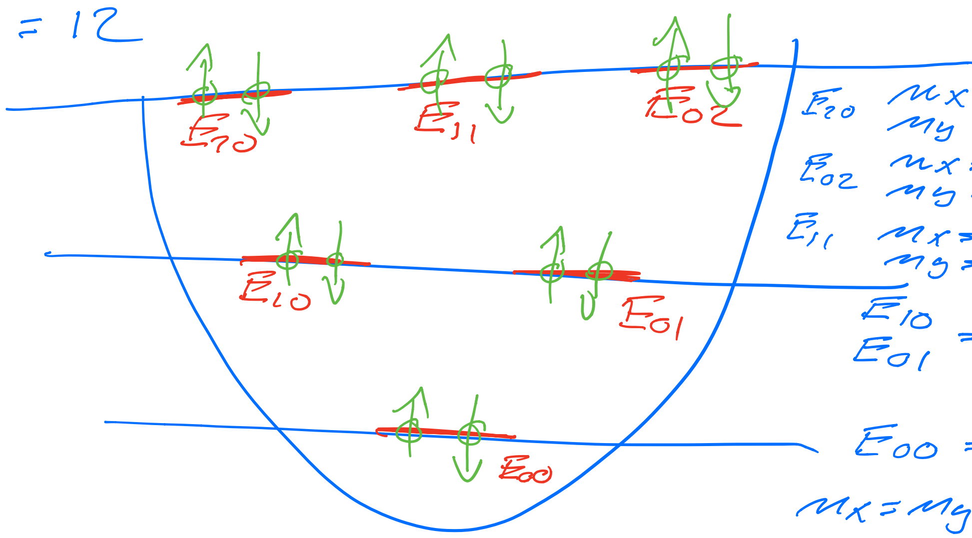
$m_s = -1/2$
$S = 1/2$

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \chi_{s m_s} = \chi_{1/2\,-1/2}$$

Single-particle HO wf

$$\psi_i = \underbrace{\varphi_{m_{x_i} m_{y_i}}}_{\text{HO wf}} \; \chi_{s_i m_{s_i}}, \qquad s_i = 1/2$$

$N = 12$



3ω

E_{20} $\quad m_x = 2$, $m_y = 0$

E_{02} $\quad m_x = 0$, $m_y = 2$

E_{11} $\quad m_x = 1$, $m_y = 1$

E_{10}, E_{01} $= 2\omega$

$E_{00} = \omega$

$m_x = m_y = 0$

E_0 total energy for N particles

$\underline{N = 6}$

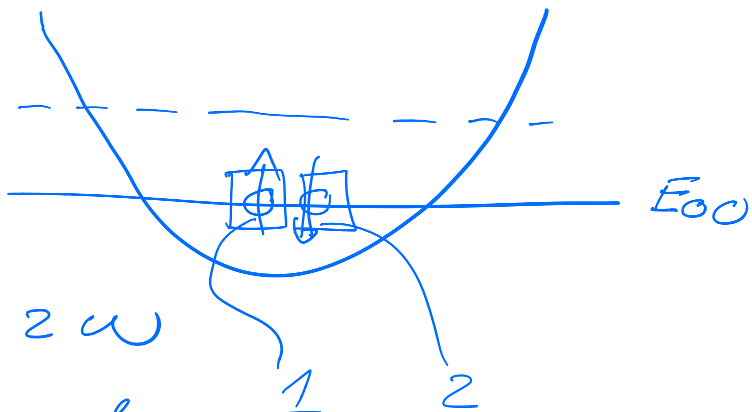
$$E_0 = \underset{(E_{00} \times 2)}{2\omega} + 4 \times 2\omega = 10\omega$$

Useful test for our code with fermions:

$N=12$

$$E_0 = 2\omega + 8\omega + 18\omega = 28\omega$$

<u>$N=2$</u>



$$E_0 = 2\omega$$

<u>Trial wf</u>

$$\psi_1(\vec{r}_i, s_i) = \underline{\varphi_{00}(\vec{r}_i)}\, \chi_{1/2\,1/2}(s_i) \qquad \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$r_i = \sqrt{x_i^2 + y_i^2} \qquad \vec{r}_i = x_i \vec{e}_x + y_i \vec{e}_y$$

$$\psi_2(\vec{r}_i, s_i) = \varphi_{00}(\vec{r}_i)\, \chi_{1/2\,-1/2}(s_i)$$

$$\Psi(\vec{r}_1, \vec{r}_2; s_1 s_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix} \psi_1(1) & \psi_1(2) \\ \psi_2(1) & \psi_2(2) \end{vmatrix}$$

Slater determinant

$$\frac{1}{\sqrt{2}}\left(\psi_1(1)\psi_2(2) - \psi_1(2)\psi_2(1) \right)$$

$$\psi(\vec{r}_2\vec{r}_1; s_2 s_1) = \boxed{\psi(2,1) = -\psi(1,2)}$$

our ansatz

$$\frac{1}{\sqrt{2}}\Big(\underbrace{\varphi_{00}(1)}_{HO}\varphi_{00}(2)\chi_\uparrow(1)\chi_\downarrow(2) - \varphi_{00}(2)\varphi_{00}(1) \times \chi_\uparrow(2)\chi_\downarrow(1)\Big)$$

$$= \varphi_{00}(1)\varphi_{00}(2)\frac{1}{\sqrt{2}}\left[\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\uparrow(2)\chi_\downarrow(1)\right]$$

$S=0$

6 electrons 6×6 det,

12 — " — 12×12 det

Trial function $\varphi_{00}(i) \propto e^{-\frac{1}{2}\alpha^2(x_i^2+y_i^2)}$

Hermite polynomial

$H_{n_{x_i}}(x_i) H_{n_{y_i}}(y_i)$

$n_{x_i} = n_{y_i} = 0 \Rightarrow H_0(i) = \underline{1}$

- spatial part $(\varphi_{00}(1)\varphi_{00}(2))$ is symmetric
- spin part is antisymmetric

$S=0 \quad M_S = m_{s_1} + m_{s_2} = 0$

- Hamiltonian is spin independent.

$$\langle \Psi' | H | \Psi \rangle = 0$$

$$S' \neq S$$

$$H = H_0 + H_1$$

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

$$\chi_\uparrow = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \chi_\downarrow = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\frac{1}{2} \left[\underline{\chi_\uparrow^*(1) \chi_\downarrow^*(2)} - \underline{\chi_\uparrow^*(2) \chi_\downarrow^*(1)} \right]$$

$$\times H_0 \left[\underline{\chi_\uparrow(1) \chi_\downarrow(2)} - \underline{\chi_\uparrow(2) \chi_\downarrow(1)} \right]$$

$$\frac{1}{2} \left[\underbrace{\begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{1} \underbrace{\begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{2} - \underbrace{\begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{1} \underbrace{\begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{2} \right.$$

$$= 0$$

$$- \underbrace{\cdots}_{= 0} + \underbrace{\begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}}_{2} \underbrace{\begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{1}$$

$$\frac{1}{2} \cdot 2 = \underline{1}$$

How to deal with a determinant efficiently in our VMC code?

$$\Psi_{T...} = \Psi_D \times \Psi_J$$

$$\underbrace{\quad D \quad}_{\text{anti symmetry}} \quad J$$

two body correlation

$$D = \begin{vmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ d_{21} & & & \\ \vdots & & d_{ij} & \\ d_{N1} & \cdots & \cdots & d_{NN} \end{vmatrix}$$

$D \in \mathbb{R}^{N \times N}$ to obtain the determinant $O(N^3)$ FLOPs

when moving N-particles

$\sim O(N^4)$ FLOPS

- Metropolis ratio

$$\frac{|\psi_D(r^{new})\psi_J(r^{new})|^2}{|\psi_D(r^{old})\psi_J(r^{old})|^2}$$

Slater determinant = SD

$$\psi_{SD}(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots \vec{r}_N; s_1 s_2 s_3 \ldots s_N)$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(1) & \cdots & \varphi_1(N) \\ \varphi_2(1) & & \varphi_2(N) \\ \vdots & \varphi_i(j) & \vdots \\ \varphi_N(1) & & \varphi_N(N) \end{vmatrix}$$

columns = given particle

rows = given single particle quantum state.

$$d_{ij} = \varphi_i(\vec{r}_j, s_j)$$

$\underline{3\times 3}$ det:

$$\begin{vmatrix} \boxed{\begin{matrix} d_{11} \\ d_{21} \\ d_{31} \end{matrix}} & \begin{matrix} d_{12} \\ d_{22} \\ d_{32} \end{matrix} & \begin{matrix} d_{13} \\ d_{23} \\ d_{33} \end{matrix} \end{vmatrix}$$

$$= d_{11} \underline{\begin{vmatrix} d_{22} & d_{23} \\ d_{32} & d_{33} \end{vmatrix}} - d_{21} \underline{\begin{vmatrix} d_{12} & d_{13} \\ d_{32} & d_{33} \end{vmatrix}}$$

move particle $\underline{1}$

$$+ \; d_{31} \underline{\begin{vmatrix} d_{12} & d_{13} \\ d_{22} & d_{23} \end{vmatrix}}$$

C_{23} C_{13} C_{12} and

$$= \sum_{i=1}^{n} d_{ij} \cdot C_{ij}$$

$$C_{ij} = (-1)^{i+j} M_{ij}$$

Minor

$$D^{-1} D = \underline{\mathbb{1}}$$

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

$$d^{-1}_{ij} = \frac{C_{ji}}{|D|}$$

Metropolis test

$$R = \frac{\Psi_{SD}(r^{new})}{\Psi_{SD}(r^{old})}$$

$$= \frac{\sum_{j=1}^{n} d_{ij}(r^{new})\, C_{ij}(r^{new})}{\sum_{j=1}^{n} d_{ij}(r^{old})\, C_{ij}(r^{old})}$$

moving particle j from r_j^{old} to r_j^{new} leaves C_{ij} unchanged.

$$C_{ij}(r^{old}) = C_{ij}(r^{new})$$

$$\frac{C_{ij}}{|D|} = d^{-1}_{ji}$$

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

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

<u>Next simplification</u>

$$\frac{\nabla_i |\Psi_{SD}|}{|\Psi_{SD}|} = \sum_{j=1}^{N} \nabla_i \psi_j(\vec{r}_i) \cdot d_{ji}^{-1}(\vec{r}_i)$$

Final simplification

$$\frac{\nabla_i^2 |\Psi_{SD}|}{|\Psi_{SD}|}$$