Lecture August 25, 2023, FYS4480

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Computational basis

- Example: two-level system

$$|\varphi_0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\varphi_1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

ONB: $\langle\varphi_1|\varphi_0\rangle = 0$

$$\hat{P} = |\varphi_0\rangle\langle\varphi_0| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix}$$

$$\hat{P} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \hat{Q} = |\varphi_1\rangle\langle\varphi_1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\hat{P} \cdot \hat{Q} = 0$$

$$\hat{P} + \hat{Q} = \mathbb{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

in general

$$\hat{P} = \sum_{i=0}^{d-1} \underbrace{|i\rangle\langle i|}_{ONB} \qquad \hat{Q} = \sum_{i=d}^{\infty} |i\rangle\langle i|$$

$$\hat{P}^2 = \hat{P} \qquad \Big| \qquad \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\hat{Q}^2 = \hat{Q} \qquad [\hat{P}, \hat{Q}]$$

computational sp-basis
(single-particle)

Example ; HO in 2 dim

n_x, n_y

$$|n_x\rangle = H_{n_x}(x)\, e^{-x^2\alpha}$$

$$|n_y\rangle = H_{n_y}(y)\, e^{-y^2\alpha}$$

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

$$|n_x\rangle \otimes |n_y\rangle = |n_x n_y\rangle$$

adding spin $s = 1/2$ $m_s = \pm 1/2$

$$|n_x\rangle \otimes |n_y\rangle \otimes |s m_s\rangle$$

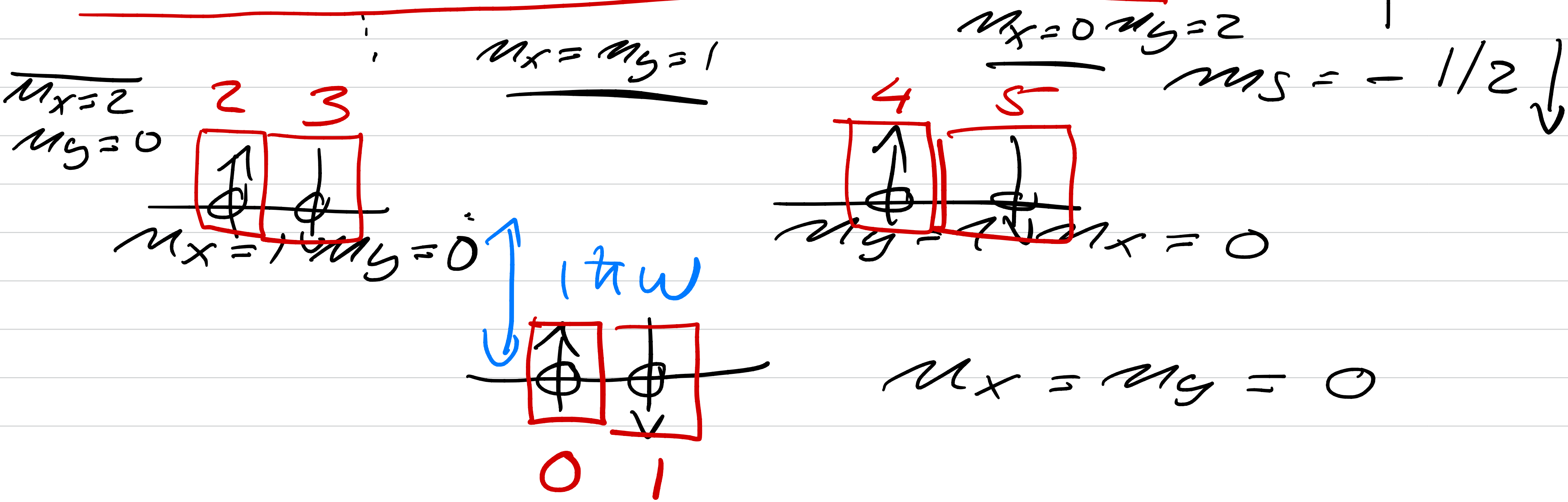
$$= |n_x n_y s m_s\rangle = |a\rangle$$

$$a = \{n_x n_y s m_s\}$$

$$a = 0, 1, 2, \ldots d-1 \quad \infty$$

$$\varepsilon_{n_x n_y} = \hbar\omega(n_x + n_y + 1) \qquad m_s = +1/2$$

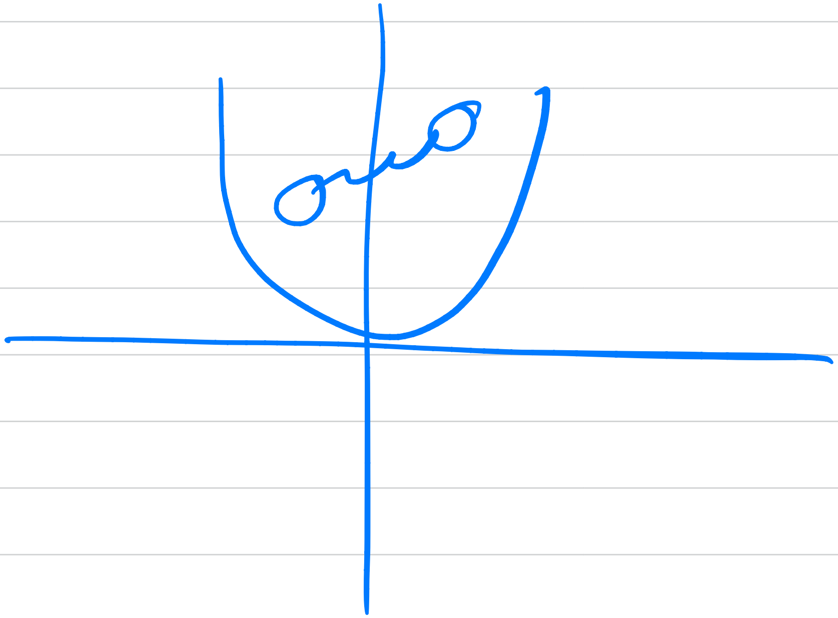
∞



can expand a new state

$$|\psi\rangle = \sum_{i=0}^{\infty} c_i \, |i\rangle$$

2-fermions in a HO potential



Hamiltonian:

interaction

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_0(\vec{x}_i) \qquad N = \text{Number of particles}$$

$$\hat{h}_0(\vec{x}_i) = -\frac{\hbar^2}{2m} \nabla_i^2 + u_{ext}(\vec{x}_i)$$

$$\hat{h}_0 |i\rangle = \varepsilon_i |i\rangle \qquad \langle i|j\rangle = \delta_{ij}$$

assumption made,

$$\hat{H}_I = \sum_{i<j} v(\vec{x}_i, \vec{x}_j)$$

$$v(\vec{x}_i, \vec{x}_j) = v(|\vec{x}_i - \vec{x}_j|)$$

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

ansatz for 2-body state function

$$|ab\rangle = |a\rangle \otimes |b\rangle$$

$$= \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_a(\vec{x}_1) & \varphi_a(\vec{x}_2) \\ \varphi_b(\vec{x}_1) & \varphi_b(\vec{x}_2) \end{vmatrix}$$

$$\varphi_a(\vec{x}_1) = \langle \vec{x}_1 | a \rangle$$

$$\hat{h}_0 \varphi_a(\vec{x}_1) = \varepsilon_a \varphi_a(\vec{x}_1)$$

Example $|a\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $|b\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$$|ab\rangle = |a\rangle \otimes |b\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\langle ab | \hat{H} | ab \rangle$$

$$|ab\rangle = \frac{1}{\sqrt{2}} \left(\varphi_a(x_1)\varphi_b(x_2) - \varphi_a(x_2)\varphi_b(x_1) \right)$$

1)

$$\langle ab | \hat{H}_0 | ab \rangle =$$

$$\frac{1}{2} \iint d\vec{x}_1 \, d\vec{x}_2 \left[\varphi_a^*(x_1)\varphi_b^*(x_2) - \varphi_a^*(x_2)\varphi_b(x_1) \right]$$

$$\times \left[\hat{h}_0(\vec{x}_1) + \hat{h}_0(\vec{x}_2) \right] \left[\varphi_a(x_1)\varphi_b(x_2) - \varphi_a(x_2)\varphi_b(x_1) \right]$$

$$\langle H \rangle = \mathbb{E}[H] = \frac{\int d\tau\, \psi^*(\tau)\, \hat{H}\, \psi(\tau)}{\int d\tau\, |\psi(\tau)|^2}$$

$$d\tau = dx_1 dy_1\, dx_2 dy_2$$

First term:

$$\frac{1}{2} \int d\vec{x}_1 \int d\vec{x}_2\; \varphi_a^*(x_1)\, \varphi_b^*(x_2) \left[\hat{h}_0(x_1) + \hat{h}_0(x_2)\right]$$

$$\times \left[\varphi_a(x_1)\, \varphi_b(x_2)\right]$$

$$= \frac{1}{2}\left(\varepsilon_a + \varepsilon_b\right)$$

second term

$$\frac{1}{2}\iint d\vec{x}_1\, d\vec{x}_2\, \varphi_a^*(x_2)\, \varphi_b^*(x_1)\left[\hat{h}_0(x_1)+\hat{h}_0(x_2)\right]$$

$$\times\ \varphi_a(x_1)\,\varphi_b(x_2) = 0$$

same with the third

last

$$\frac{1}{2}\iint d\vec{x}_1\, d\vec{x}_2\, \varphi_a^*(x_2)\, \varphi_b^*(x_1)\left(\hat{h}_0(x_1)+\hat{h}_0(x_2)\right)$$

$$\times\ \varphi_a(x_2)\,\varphi_b(x_1)$$

$$= \frac{1}{2}\left(\varepsilon_a+\varepsilon_b\right) \Rightarrow$$

$\rightarrow$

$$\langle ab | \hat{H}_0 | ab \rangle = E_a + E_b$$

$$\hat{H}_0 | ab \rangle = (E_a + E_b) | ab \rangle$$

$|ab\rangle$ is an eigenbasis of $\hat{H}_0$

$$\hat{H} | ab \rangle = (H_0 + H_1) | ab \rangle$$

$$\neq E | ab \rangle$$

$$|\Phi_{ab}\rangle = |ab\rangle \qquad \underbrace{ab \rightarrow i}_{\text{configuration}}$$

configuration : way to distribute 1 or more particles in all possible computational basis states (n)

Fermions with n states and N particles $\Rightarrow$

$$\#\text{ possible configs} = \binom{n}{N} \qquad n \geq N$$

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

$$|\Psi_{ab}\rangle = \sum_{i=0}^{d-1} c_i \underbrace{|i\rangle}_{|ab\rangle}$$

Example $n = 100$

$N = 2$

$$\#\ \text{configs} = \frac{100!}{98!\,2!} = 4925$$

$$\langle ab | H_1 | ab \rangle =$$

$$= \frac{1}{2}\iint d\vec{x}_1 d\vec{x}_2 \left[\varphi_a^*(x_1)\,\varphi_b^*(x_2) - \varphi_a^*(x_2)\,\varphi_b^*(x_1)\right] v(\vec{x}_1,\vec{x}_2)\left[\varphi_a(x_1)\,\varphi_b(x_2) - \varphi_a(x_2)\,\varphi_b(x_1)\right]$$

$$v(x_1,x_2) = v(x_2,x_1)$$

1) $\frac{1}{2}\iint d\vec{x}_1 d\vec{x}_2\, \varphi_a^*(x_1)\,\varphi_b^*(x_2)\, v(x_1,x_2)\, \varphi_a(x_1)\,\varphi_b(x_2)$

$$= \frac{1}{2}\langle ab|v|ab\rangle$$

4) Last term

$$\frac{1}{2}\langle ba|v|ba\rangle$$

$$= \frac{1}{2}\langle ab|v|ab\rangle$$

2+3) $-\frac{1}{2}\langle ab|v|ba\rangle$

$$-\frac{1}{2}\langle ab|v|ba\rangle \Rightarrow$$

$$\langle \widetilde{ab}|H_I|\widetilde{ab}\rangle =$$

$$\underbrace{\langle ab|v|ab\rangle}_{\text{Direct}} - \underbrace{\langle ab|v|ba\rangle}_{\text{exchange}}$$