# FYS4480 AUGUST 25

## Basic Definitions

a vector with $n$ elements

$$|x\rangle = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{bmatrix} \qquad x_i \in \mathbb{R}^n, \mathbb{C}^n$$

$$\langle x| = \begin{bmatrix} x_0^* & x_1^* & \cdots & x_{n-1}^* \end{bmatrix}$$

$$= |x\rangle^\dagger$$

orthonormal basis

$$\langle x|x\rangle = 1$$

$$\langle y|x\rangle = \sum_{i=0}^{n-1} y_i^* x_i$$

outer product

$$|x\rangle\langle x| = \begin{bmatrix} x_0 x_0^* & x_0 x_1^* & \cdots & x_0 x_{n-1}^* \\ \vdots & & & \\ x_{n-1} x_0^* & & \cdots & x_{n-1} x_{n-1}^* \end{bmatrix}$$

Tensor products

$$|x\rangle \otimes |y\rangle = |xy\rangle$$

$$|x\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad (|0\rangle)$$

$$|y\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad (|1\rangle)$$

(computational basis)

$$\langle y|x\rangle = 0 \qquad \langle x|x\rangle = \underline{1}$$

$$\langle y|y\rangle = \underline{1}$$

$$|x\rangle \otimes |x\rangle = \begin{bmatrix} 1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ 0 \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= |xx\rangle = |00\rangle$$

$(|0\rangle)$

single-particle state function

$$\varphi_\alpha(\vec{r}) \otimes \xi_{m_s} = |\vec{r}\alpha\, m_s\rangle$$

$$\rightarrow |\alpha\, m_s\rangle$$

$n\,l\,m_l$ (hydrogen atom)

$$|x\rangle \otimes |x\rangle = |0\rangle \otimes |0\rangle = |00\rangle$$

$$= \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$|0\rangle \otimes |1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle$$

$$|1\rangle \otimes |0\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle$$

$$|1\rangle \otimes |1\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |11\rangle$$

$$\langle 11|00\rangle = 0$$

$$\langle 00|00\rangle = 1$$

$$\langle 11|11\rangle = 1$$

$$\langle 01|01\rangle = 1$$

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

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

$$\mathbb{1} = \sum_{i=0}^{n-1\,(\infty)} |i\rangle\langle i|$$

$i=0 \; : \; |0\rangle$

$i=1 \; : \; |1\rangle$

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

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

$$= |0\rangle\langle 0| \qquad\qquad |1\rangle\langle 1|$$

$\hat{P}^2 = \hat{P}$ idempotent operator

$\hat{Q}^2 = \hat{Q}$ projection

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

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

if our computational basis

is $|0\rangle$ and $|1\rangle$

$$|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$\Big( |\psi\rangle = \sum^{\infty} c_i |i\rangle \Big)$

$$\left( |\varphi\rangle = \sum_{i=0} c_{\varphi i} |i\rangle \right)$$

$$\hat{P}|\varphi\rangle = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \left( \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right)$$

$$= \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \alpha |0\rangle$$

$$\hat{Q}|\varphi\rangle = \beta |1\rangle$$

Density matrix

$$\rho = |\varphi\rangle\langle\varphi| = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \begin{bmatrix} \alpha^* & \beta^* \end{bmatrix}$$

$$= \begin{bmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{bmatrix}$$

$$\mathrm{Tr}(\rho) = |\alpha|^2 + |\beta|^2 = \underline{1}$$

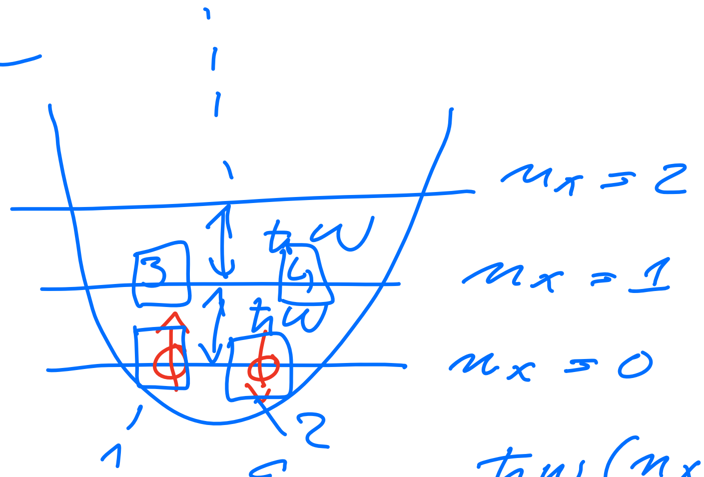
= sum of all probabilities

Computational basis

– Harmonic oscillator
(quantum dots,
Bose-Einstein condensation)

nuclear physics

1-Dim




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

Hamiltonian (1-particle)

$$\hat{h}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

computational basis

$$\varphi_{n_x}(x) = \langle x | n_x \rangle$$

$$n_x \to i$$

Basis : $i = 0, 1, 2, \cancel{A}, \ldots \infty$

First truncation in the computational basis

$$\varphi_i(x)$$

$$\hat{h}_0 \varphi_i(x) = \varepsilon_i \varphi_i(x)$$

$$\boxed{\hat{h}_0 |i\rangle = \varepsilon_i |i\rangle}$$

one-body operator

$$\hat{H} = \underbrace{\sum_{i=1}^{N = \#\text{ particles}} -\frac{\hbar^2 \nabla_i^2}{2m_i} + \sum_{i=1}^{N} V_{ext}(\vec{x}_i)}_{H_0}$$

$$+ \underbrace{\sum_{i<j}^{N} v(\underbrace{|\vec{x}_i - \vec{x}_j|}_{x_{ij}})}_{H_I} \quad \{ v(\vec{x}_i, \vec{x}_j)$$

construct many body ansatz $|\Phi_i\rangle$ based on the single-particle computational basis

$$|\Phi_i\rangle = \cancel{\prod_{j=0}^{d} \varphi_j(x_j)}$$

$$\propto \prod_{j}^{d} \varphi_j(x_j)$$

$H\,|\Phi\rangle$

$$H_0 |\Phi_i\rangle \qquad j=0$$

$$= E_i |\Phi_i\rangle$$

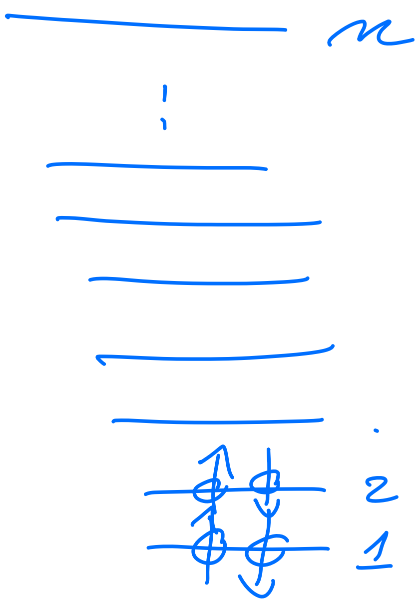
$$h_0 |\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$

Exact state function

$$H|\Psi_k\rangle = \mathcal{E}_k |\Psi_k\rangle$$

$$|\Psi_k\rangle = \sum_{j=0}^{d} C_{kj} |\Phi_j\rangle$$

comp. many-body basis




$N = 4$

$\sim 2n$ single particle states

# fermionic states

$$= \binom{2n}{N}$$

$$= \frac{2n!}{(2n-N)!\,N!}$$