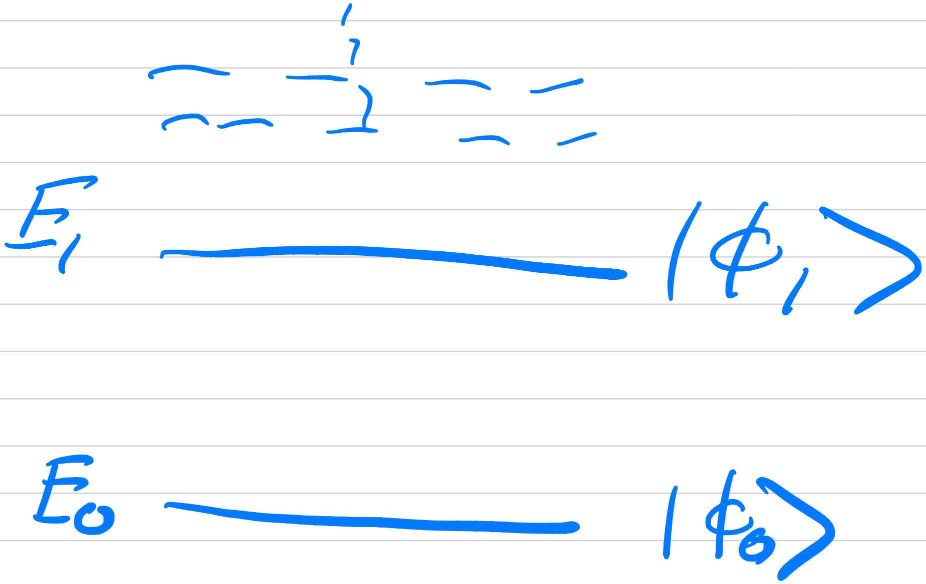
FYS 4480/9480 AUG 22, 2024



$$H|\phi_i\rangle = E_i|\phi_i\rangle$$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}$$

$$|\phi_0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\phi_1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$(\uparrow) \qquad\qquad (\downarrow)$$

computational basis

$|\phi_0\rangle$ and $|\phi_1\rangle$

$$|\Psi_0\rangle = \alpha|\phi_0\rangle + \beta|\phi_1\rangle$$

More general

$$|\Psi_i\rangle = \sum_{j=0}^{\infty} c_{ij}|\phi_j\rangle$$

$$\langle\phi_j|\phi_i\rangle = \delta_{ij}$$

$$\left(\simeq \sum_{j=0}^{D} c_{ij}|\phi_j\rangle \right.$$

Full problem $\quad H|\Psi_i\rangle = E_i|\Psi_i\rangle$

$$H|\phi_j\rangle \neq E_j|\phi_j\rangle$$

why this?

Basic strategy is to find solutions (analytical) for parts of the problem

$$H = H_0 + H_I$$

$$H_0 |\phi_j\rangle = \varepsilon_j |\phi_j\rangle$$

$|\phi_j\rangle$ is an eigenbasis of H_0

ONS $\langle \phi_j | \phi_i \rangle = \delta_{ij}$

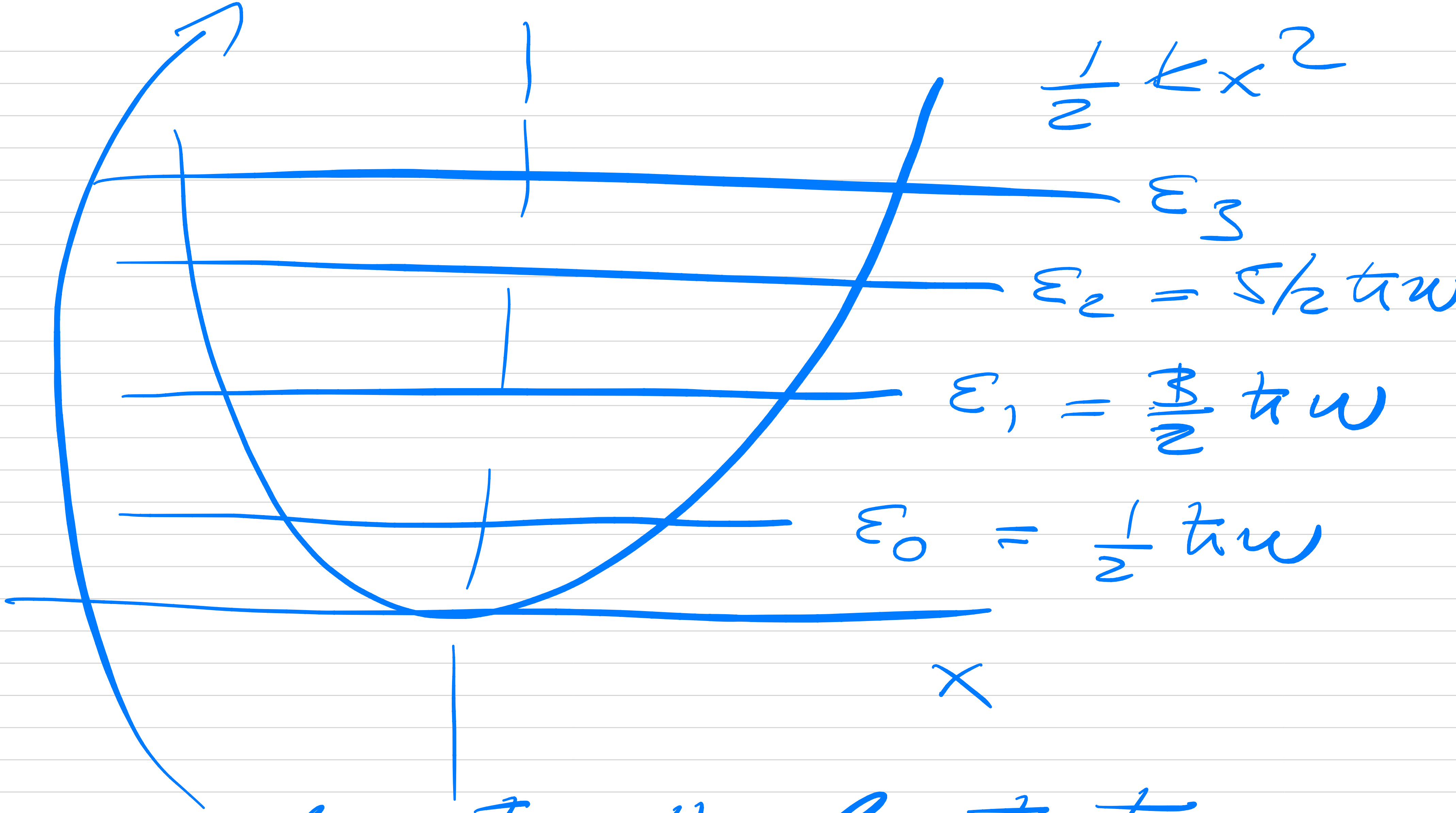
Example : Harmonic oscillator (HO)

1-Dim

$H_0 \to h_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$

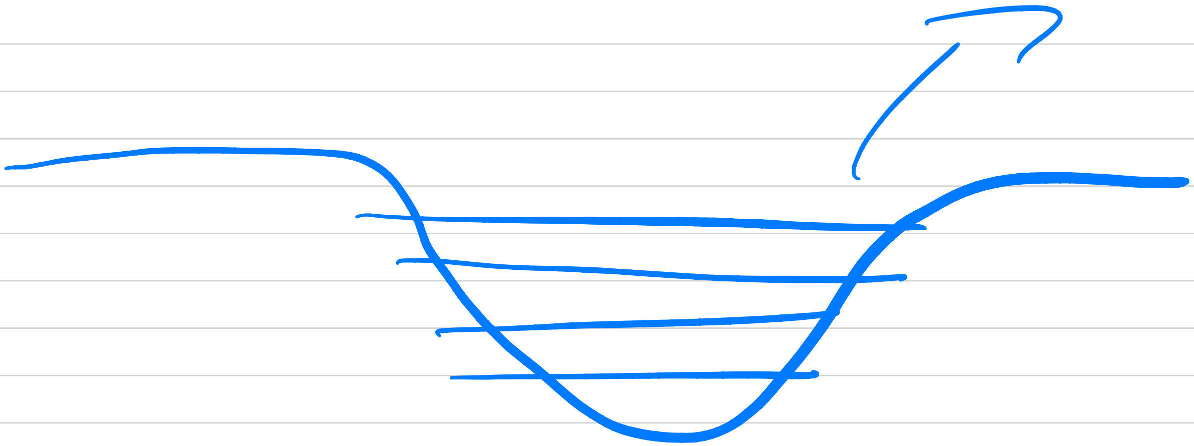
(1-body operator)

$\varepsilon_i = \hbar\omega\left(i + \frac{1}{2}\right)$ $\quad k \propto \omega m$



infinite # of states

real life



$$H|\psi_i\rangle = E_i|\psi_i\rangle$$

$$= H\left(\sum_j c_{ij}|\phi_j\rangle\right)$$

$$c_{ij} = \langle\psi_i|\phi_j\rangle$$

Example :

$$|\phi_0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\phi_1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Completeness

$$I = \sum_{i=0}^{1} |\phi_i\rangle\langle\phi_i| = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$|\psi_0\rangle = \alpha|\phi_0\rangle + \beta|\phi_1\rangle$$

$$P = |\phi_0\rangle\langle\phi_0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$Q = |\phi_1\rangle\langle\phi_1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$P^2 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = P$$

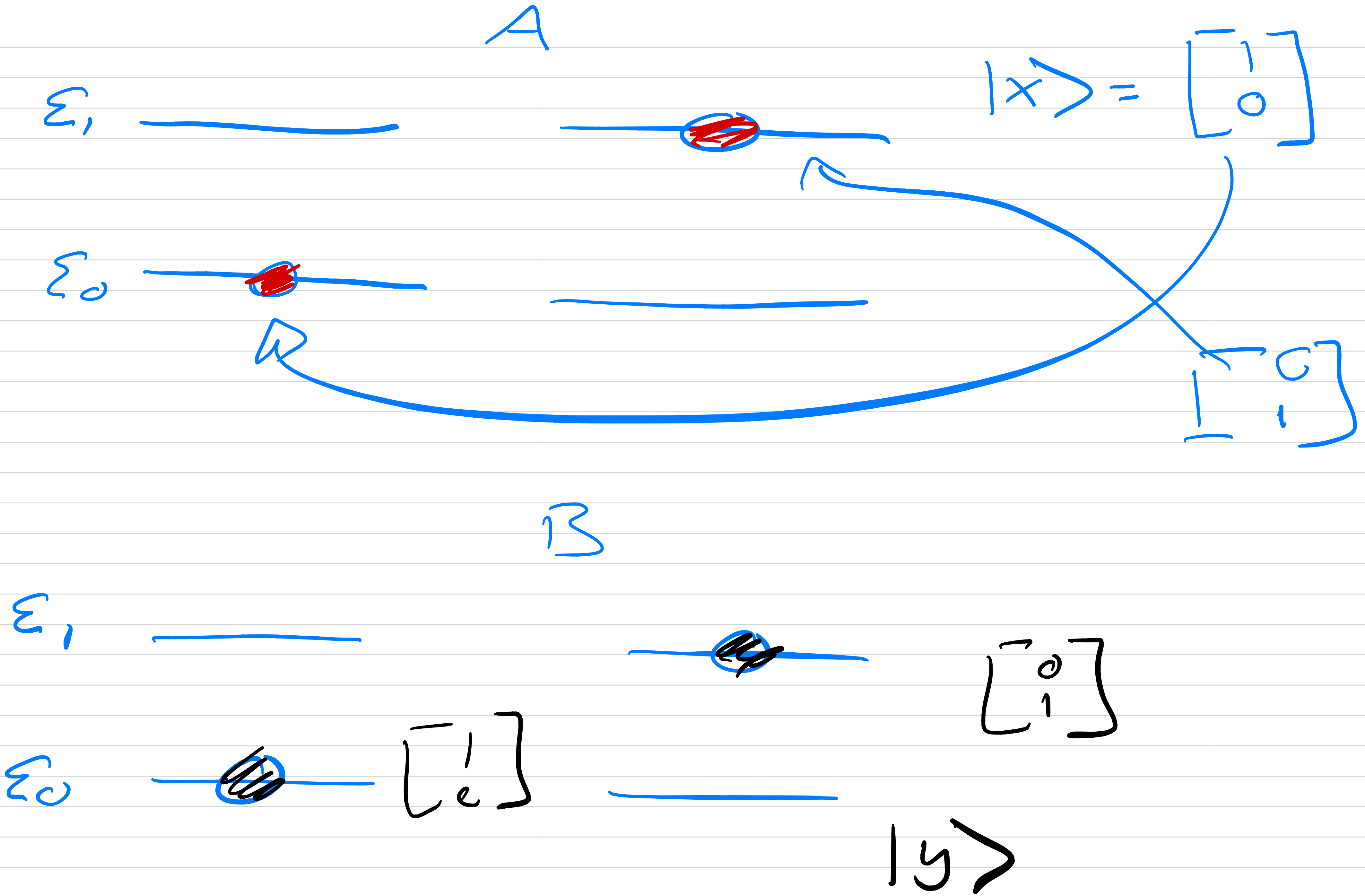
$$Q^2 = Q$$

$$P \cdot Q = 0 \qquad [P, Q] = 0$$

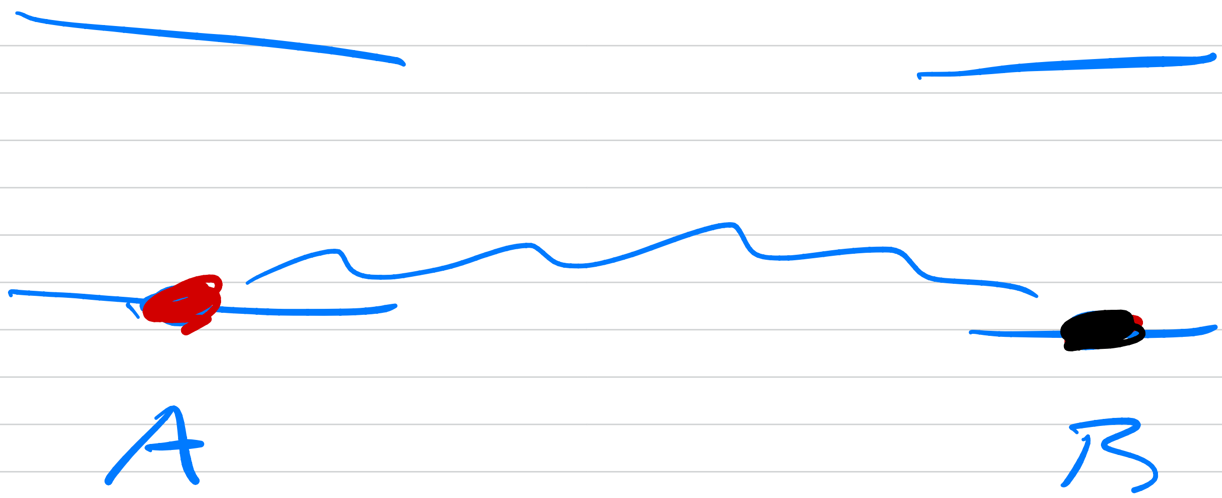
$$P + Q = 1$$

$$P|\psi_0\rangle = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \left(\alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right)$$

$$= \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \alpha |\phi_0\rangle$$


A
ε_1
ε_0
$|x\rangle = \begin{bmatrix}1\\0\end{bmatrix}$
$\begin{bmatrix}0\\1\end{bmatrix}$
B
ε_1
ε_0
$\begin{bmatrix}1\\0\end{bmatrix}$
$\begin{bmatrix}0\\1\end{bmatrix}$
$|y\rangle$

System



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

$$= |xy\rangle_{AB} = |xy\rangle$$

Fermionic systems

$$\Psi(x_1, x_2, \ldots x_N; \alpha, \beta, \ldots)$$

$H\Psi_\lambda = E_\lambda \Psi_\lambda$

positions and other quantum numbers defining a given fermion

$$x_i = (\vec{r}_i, \sigma_i)$$

$$\varphi_i(x_i) = \phi_i(\vec{r}_i) \otimes \xi_{\sigma_i m_{s_i}} \rightarrow |x_i\rangle$$

$$\sigma_i = \frac{1}{2} \quad m_{s_i} = \pm 1/2$$

$$\hat{P}_{ij}\,\Psi_\lambda(x_1 x_2 \ldots x_i x_j \ldots x_N)$$

$$= -\Psi_\lambda(x_1 x_2 \ldots x_j x_i \ldots x_N)$$

Ansatz (Based on a single-particle picture)

$$\Psi_\lambda \rightarrow \Phi_\lambda(x_1 x_2 \ldots x_N; \alpha\beta \ldots)$$

$$H_0 \Phi_\lambda = \varepsilon_\lambda \Phi_\lambda$$

$$H = H_0 + H_I$$

Φ_λ is an ONB

$$\Psi_\lambda = \sum_{\delta=0}^{\infty} c_{\lambda\delta}\, \Phi_\delta$$

$$H_0 = \sum_{i=1}^{N} h_0(x_i)$$

1 Body operator

$$\left(h_0(x_i) = -\frac{\hbar^2}{2m}\frac{d^2}{dx_i^2} + \frac{1}{2}k x_i^2 \right)$$

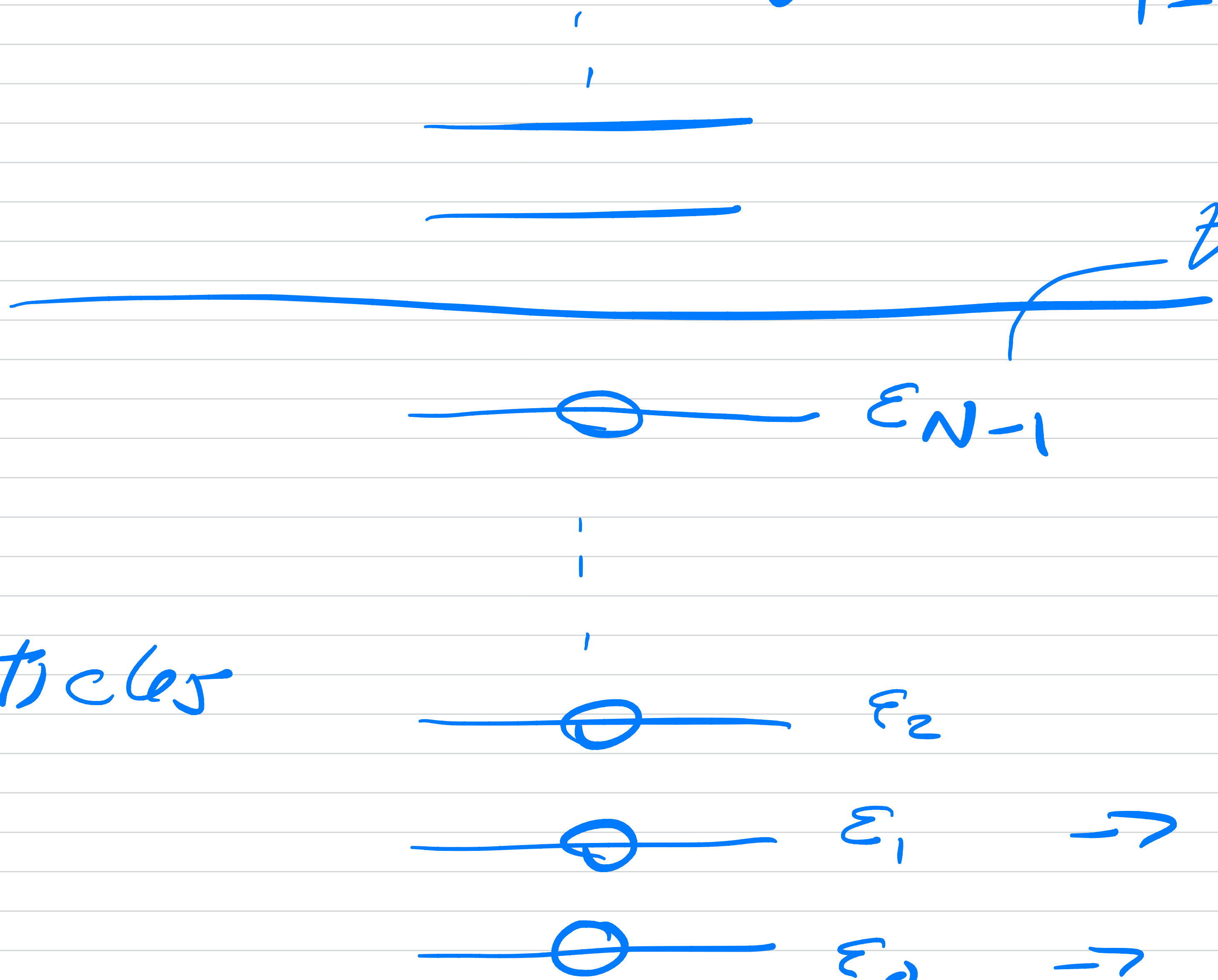
$$h_0 \phi_i = \varepsilon_i \phi_i$$

Ansatz (Slater determinant)

$$\Phi_\lambda(x_1 x_2 \ldots x_N; \alpha \beta \gamma \ldots \lambda) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_\alpha(x_1) & \phi_\alpha(x_2) & \cdots & \phi_\alpha(x_N) \\ \phi_\beta(x_1) & \phi_\beta(x_2) & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \\ \phi_\lambda(x_1) & \phi_\lambda(x_2) & & \phi_\lambda(x_N) \end{vmatrix}$$

we have N SP (single-particle) states with labels $\alpha, \beta, \gamma \ldots \tau$

New labelling (HO example
1-Dim



$\hbar\omega(n_x + 1/2)$

N particles

ε_{N-1} $\quad n_x = N-1$

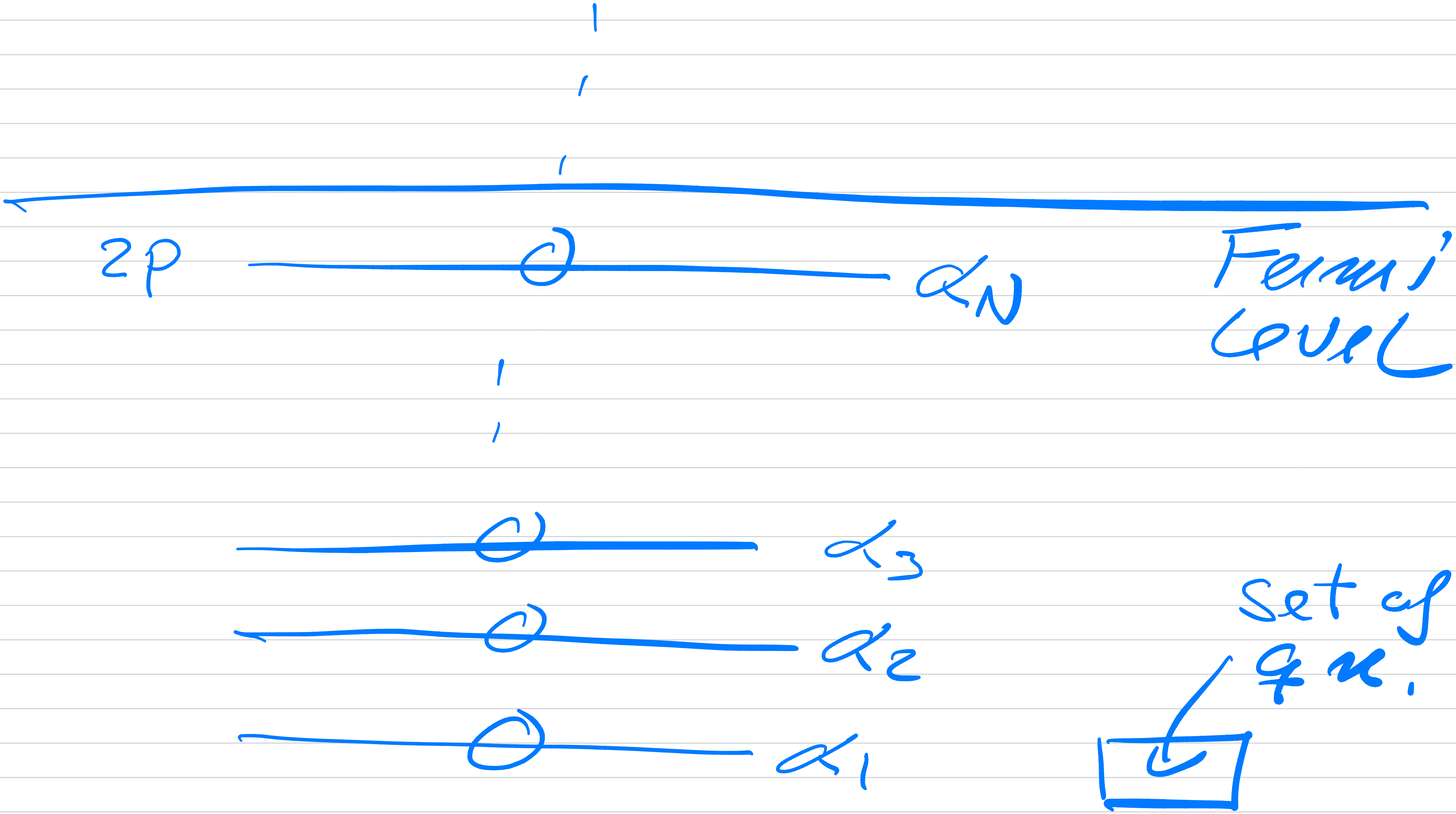
ε_2 $\quad n_x = 2$

$\varepsilon_1 \rightarrow n_x = 1$

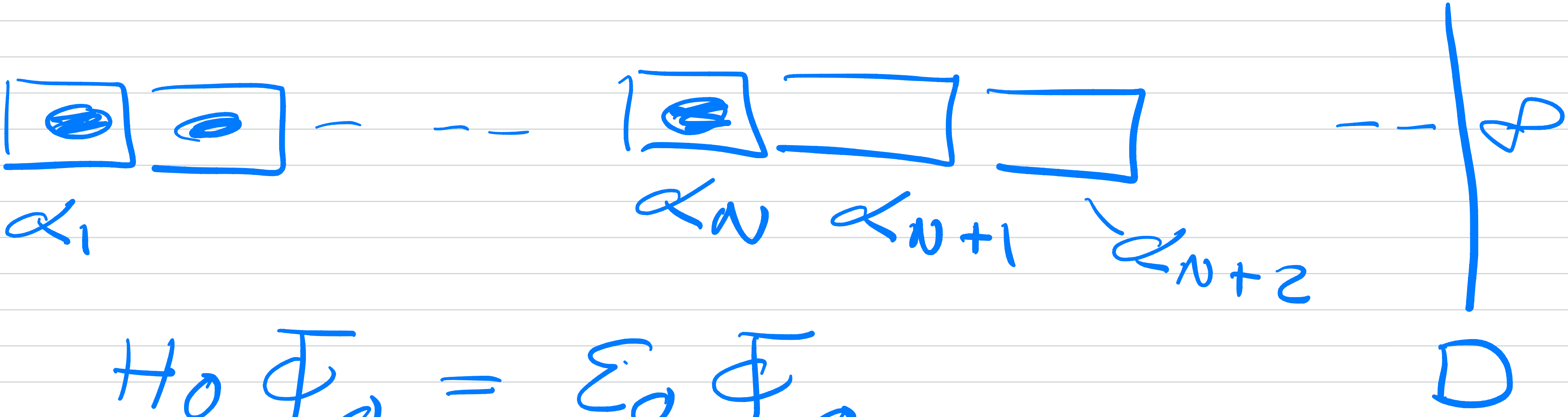
$\varepsilon_0 \rightarrow n_x = 0$

Total Energy $\mathcal{E}_0 = \sum_{i=0}^{N-1} \varepsilon_i$

Ansatz $\Phi_0(x_1 \cdots x_N; \alpha_1, \alpha_2 \cdots \alpha_N)$

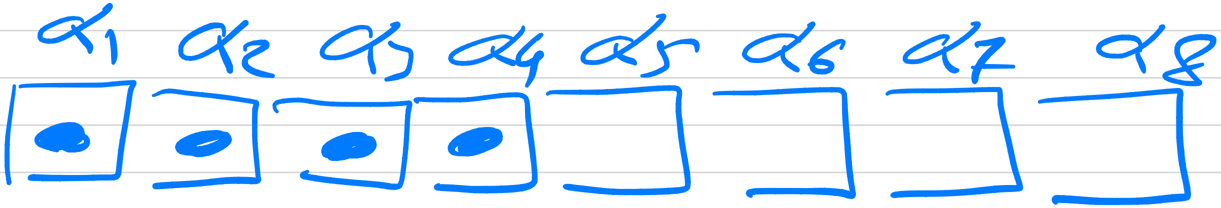


$$\Phi_0(x_1 x_2 \dots x_N;\ \alpha_1 \dots \alpha_N)$$



$$H_0 \Phi_0 = E_0 \Phi_0$$

$N = 4$ $n = 8$ slots



$$|1\ 1\ 1\ 1\ 0\ 0\ 0\ 0\rangle$$

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

$$= a_{11}a_{22} + (-)^{1} a_{12}a_{21}$$

Ordering: here only diag elements

$$= \sum_{P} (-)^{P} P_P \, a_{11}a_{22}$$

P_P = Permutation of two columns

$P = 2 \quad (1,2) \; (2,1)$

3×3 : $3!$ permutations

$(1,2,3)$, $(1,3,2)$, $(2,1,3)$ ...

$$\begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & & & \\ a_{31} & & & \\ \vdots & & & \\ a_{N1} & - & - & a_{NN} \end{vmatrix}$$

$$= \sum_{i=1}^{P!} (-)^i \hat{P}_i \, (a_{11} a_{22} \cdots a_{NN})$$

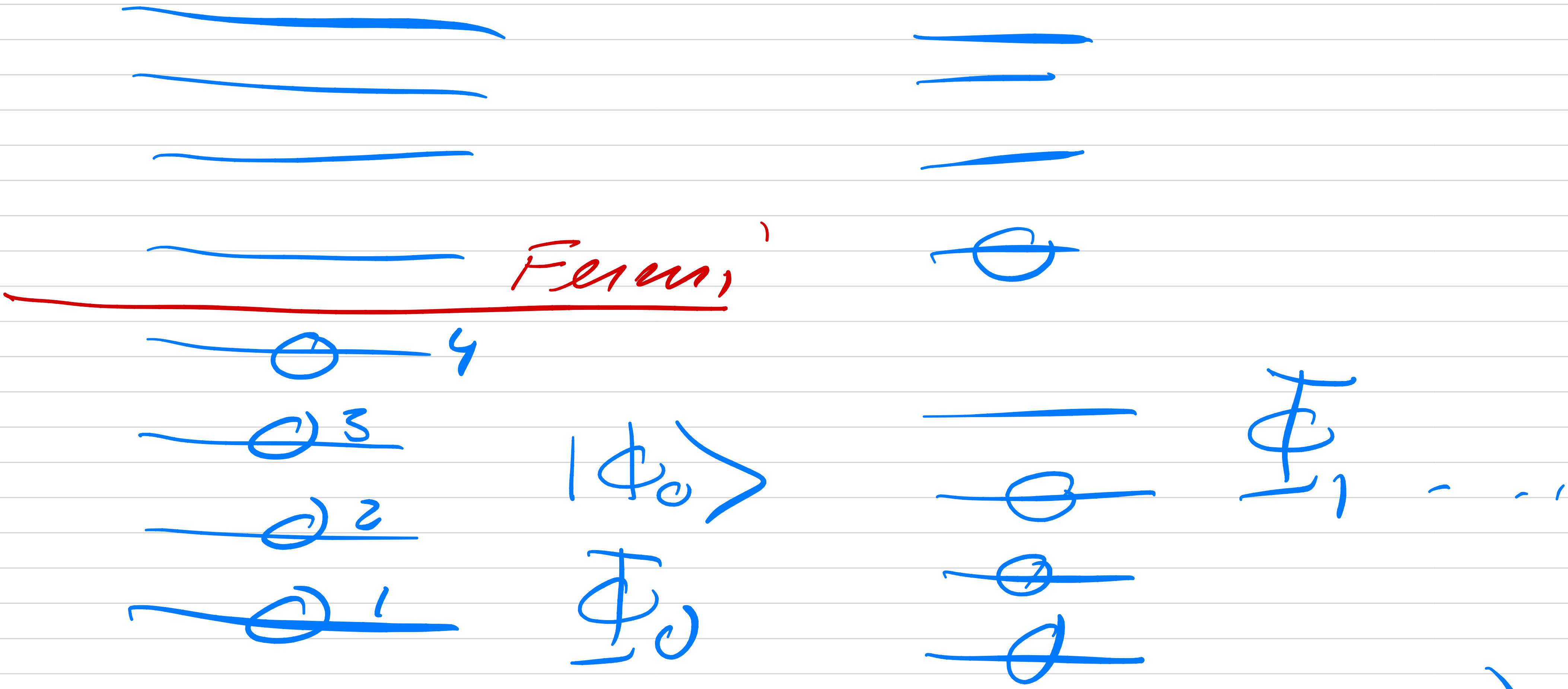
$$[H, \hat{P}] = [H_0, \hat{P}] = [H_I, \hat{P}]$$

$$= 0$$

SD rewritten as

$$\Phi_0 (x_1 x_2 \ldots x_N ; \alpha_1 \alpha_2 \ldots \alpha_N)$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_1}(x_2) & \ldots & \varphi_{\alpha_1}(x_N) \\ \varphi_{\alpha_2}(x_1) & \varphi_{\alpha_2}(x_2) & \ldots & \\ \vdots & & & \vdots \\ \varphi_{\alpha_N}(x_1) & & & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$



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

(N = particles
n = slots)

$$\Phi_0 = \frac{1}{\sqrt{N!}} \sum_P (-)^P \hat{P}\, \Phi_H$$

$$\Phi_H = \phi_{\alpha_1}(x_1)\,\phi_{\alpha_2}(x_2) \cdots \phi_{\alpha_N}(x_N)$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \sum_{\alpha_i} \varepsilon_{\alpha_i}$$

$$\langle \Phi_c | H_1 | \Phi_0 \rangle$$