$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle = \mathrm{Tr}(\rho\hat{O})$$

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

$$|\psi\rangle = \sum_{s_1\cdots s_N} \psi_{s_1\cdots s_N}|s_1\cdots s_N\rangle$$

$$\langle\psi| = \sum_{s_1'\cdots s_N'} \langle s_1'\cdots s_N'|\psi^*_{s_1'\cdots s_N'}$$

$$\rho = |\psi\rangle\langle\psi| = \sum \psi_{s_1\cdots s_N}\psi^*_{s_1'\cdots s_N'}|\quad\rangle\langle\quad|$$

$$\Downarrow$$

$$\rho_{(s_1\cdots s_N),(s_1',\cdots s_N')} = \begin{bmatrix} \quad \end{bmatrix}$$

density matrix

state $|\psi\rangle \Rightarrow \hat{O} \Rightarrow \langle\psi|\hat{O}|\psi\rangle$

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} \vdots \\ \vdots \end{bmatrix}_{N\times 1} \begin{bmatrix} \cdots\cdots \end{bmatrix}_{1\times N} = \begin{bmatrix} & & \\ & \rho & \\ & & \end{bmatrix}_{N\times N}$$

$$\langle\psi|\hat{O}|\psi\rangle = \mathrm{tr}(\hat{O}\hat{\rho})$$

$$\mathrm{tr}\Big(\begin{bmatrix} O \end{bmatrix}\begin{bmatrix} \rho \end{bmatrix}\Big) = \langle\psi|\hat{O}|\psi\rangle$$

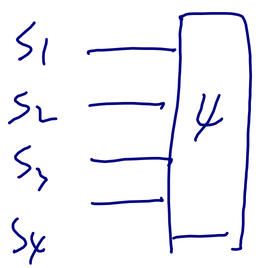
$$|\psi\rangle = \sum_{s_1\cdots s_N} \psi_{s_1\cdots s_N} |s_1\cdots s_N\rangle$$

$$\langle\psi| = \sum_{s_1'\cdots s_N'} \psi^*_{s_1'\cdots s_N'} \langle s_1'\cdots s_N'|$$

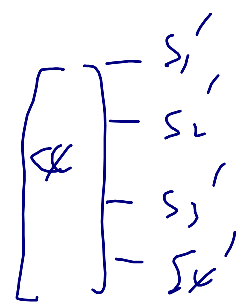
$$\Rightarrow \rho = |\psi\rangle\langle\psi| = \sum_{s}\sum_{s'} |s\cdots s_N\rangle\langle s_1'\cdots s_N'| \underbrace{\psi_{s_1\cdots s_N}\psi^*_{s_1'\cdots s_N'}}_{\rho_{(s_1\cdots s_N),(s_1'\cdots s_N')}}$$

$$[\rho], \quad \rho_{(s_1\cdots s_N),(s_1'\cdots s_N')} \equiv \psi_{s_1\cdots s_N}\psi^*_{s_1'\cdots s_N'}$$

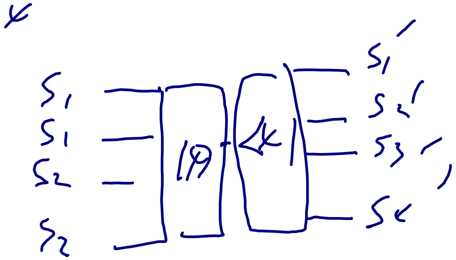
$|\psi\rangle =$



$\langle\psi| =$



$[\rho] =$



$T = 0$

$\hat{H} = \quad \varepsilon_0 < \varepsilon_1 < \varepsilon_2 \cdots$

$\quad\quad |\phi_0\rangle \quad |\phi_1\rangle \quad |\phi_2\rangle \cdots$

$\langle \hat{O} \rangle = \langle \phi_0 | \hat{O} | \phi_0 \rangle$

$e^{-\frac{\varepsilon}{T}} \quad T \to 0$

$\frac{P_1}{P_0} = e^{-\frac{(\varepsilon_1 - \varepsilon_0)}{T}} \xrightarrow{T \to 0} 0$

$\varepsilon_1 - \varepsilon_0 > 0$

$T \neq 0$

$\langle \hat{O} \rangle = e^{-\frac{\varepsilon_0}{T}} \langle \phi_0 | \hat{O} | \phi_0 \rangle + \cancel{e^{-\frac{\varepsilon_1}{T}} \langle \phi_1 | \hat{O} | \phi_1 \rangle} + \cancel{e^{-\frac{\varepsilon_2}{T}} \langle \phi_2 | \hat{O} | \phi_2 \rangle} + \cdots$

$T = 0 \quad \langle \hat{O} \rangle = \langle \phi_0 | \hat{O} | \phi_0 \rangle$

Tr

$T \neq 0 \quad \rho(T \neq 0) = e^{-\frac{\varepsilon_0}{T}} |\phi_0\rangle\langle\phi_0| + e^{-\frac{\varepsilon_1}{T}} |\phi_1\rangle\langle\phi_1| + e^{-\frac{\varepsilon_2}{T}} \cdots$

$= \mathrm{tr}(\hat{\rho} \hat{O})$

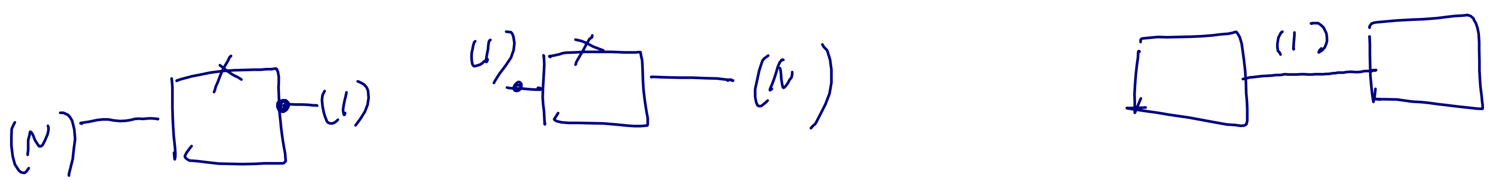
ρ

$\psi(\vec{r})$

$\rho(\vec{r}, \vec{r}') = \psi(r)\,\psi^*(r')$

diag $\rho(\vec{r}, \vec{r}) = \psi(r)\,\psi^*(r) =$

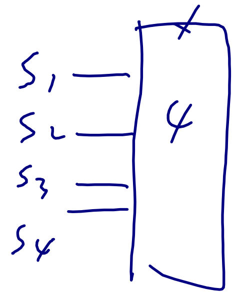
$$\begin{bmatrix} \\ \\ \\ \end{bmatrix}_{N\times 1} \begin{bmatrix} \quad \end{bmatrix}_{1\times N} = \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}_{N,N}$$

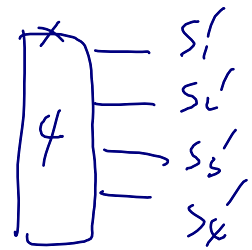


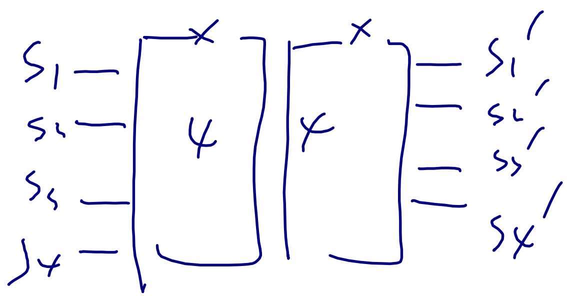
$a_i \quad b_j$

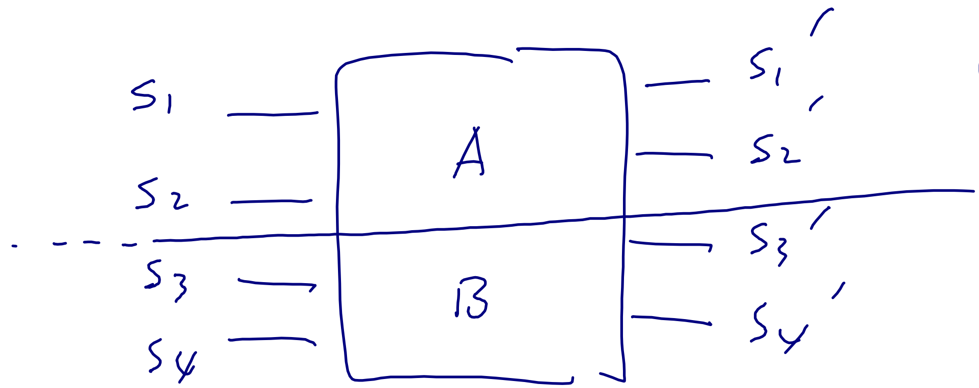
$a_{ik} \quad b_{kj}$ $\quad k=1$

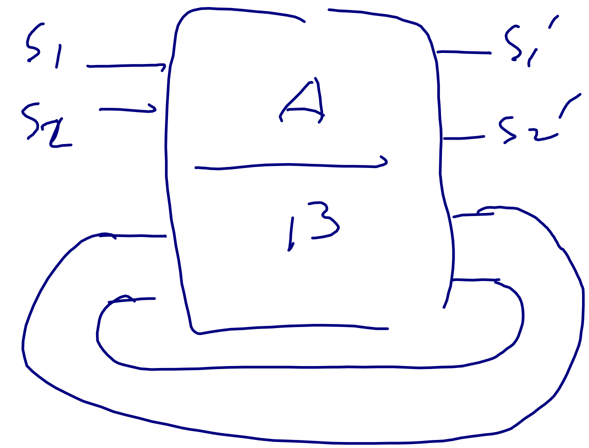
$$\sum_{k=1}^{1} a_{ik}\, b_{kj} = a_i b_j$$

$|\psi\rangle \leftrightarrow \psi_{s_1 \cdots s_N} \leftrightarrow$ 

$\langle\psi| \leftrightarrow \psi^*_{s_1' \cdots s_N'}$ 

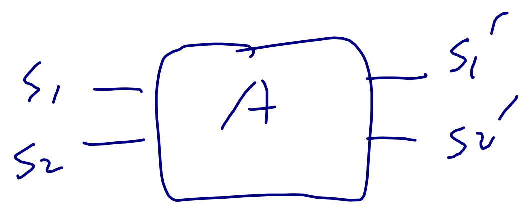
$\rho =$ 

$\rho =$ 

$\rho_A :$ 

reduced density matrix

$$\rho_A = \sum_{\alpha\beta} \rho_{s_1 s_2 \underbrace{s_3 s_4}_{\alpha\ \beta},\ s_1' s_2' \underbrace{s_3 s_4}_{\alpha\ \beta}} = \rho^A_{(s_1 s_2),(s_1' s_2')}$$

$=$ 

$$\hat{O} \longrightarrow \langle \hat{O} \rangle = \mathrm{tr}(\hat{O}\hat{\rho})$$

$$\hat{O}_A \qquad \langle \hat{O}_A \rangle = \mathrm{tr}(\hat{O}_A \hat{\rho}) \overset{\text{Math}}{=\!=} \mathrm{tr}(\hat{O}_A \hat{\rho}_A)$$

$$S_{A,B} = -\operatorname{tr}\left[(\rho_A)\ln(\rho_A)\right] = -\operatorname{tr}\left[(\rho_B)\ln(\rho_B)\right]$$

$$\rho_A = \begin{bmatrix} w_1 & & \\ & w_2 & \\ & & \ddots\, w_N \end{bmatrix} \qquad \ln(\rho_A) = \begin{bmatrix} \ln(w_1) & & \\ & \ddots & \\ & & \end{bmatrix}$$

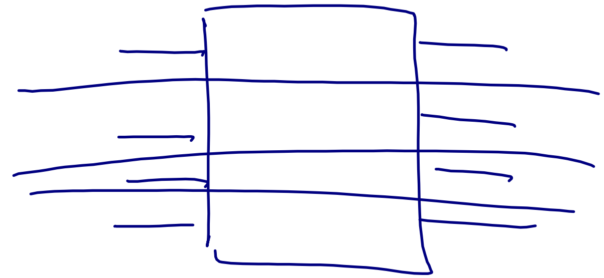
$\rho_A \longrightarrow$ eigenvalues w_i

$$-\sum_i w_i \ln(w_i)$$

$$w_i = \lambda_i^2$$

$\hat{H} \xrightarrow{\text{diag}} |\psi_i\rangle$ ground state

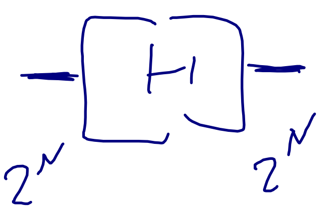
$\rho = |\psi_0\rangle\langle\psi_0|$

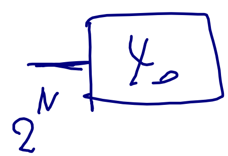


1 + 3

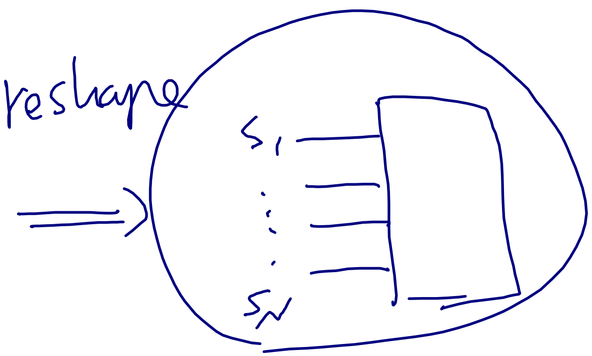
2 + 2

3 + 1





reshape



ρ, 1, 2, 3

0, 1, 2, 3

$N = 4$

2 + 2

$\psi_{s_1, s_2 \dots \boxed{. \ s_N}}$

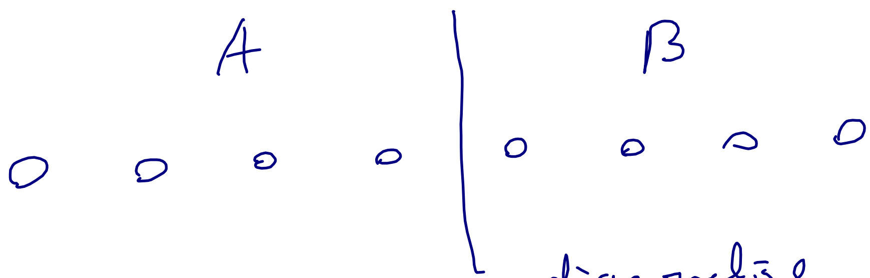
$\psi^*_{s_1', s_2' \boxed{\dots s_N'}}$

numpy.tensordot(psi, psi, axes = ([2, 3], [2, 3]))

$H \xrightarrow{\text{diag}} |\psi_i\rangle \qquad \rho = |\psi_0\rangle\langle\psi_0|$

give $A|B \qquad \rho_A = \mathrm{tr}_B(\rho)$

$$\rho_A \xrightarrow{\text{diag}} w_i \longrightarrow S_{A|B} = -\sum_i (w_i)\ln(w_i)$$



$$\rho \longrightarrow [\rho_A]_{2^{N_A},\,2^{N_A}} \xrightarrow{\text{diagonalize}} \text{eigenvalues } w_i$$

$$w_i = \lambda_i^2$$

$$S = -\sum \lambda_i^2 \ln(\lambda_i^2)$$

$$\sum_{s_1} \sum_{s_2} \sum_{s_3} \sum_{s_4} \psi_{s_1 s_2 s_3 s_4}$$

$$\binom{2^N}{} \longrightarrow \left([2, 2, 2, \ldots, 2] \right)$$

$\sim$

$$[2] \times N = [2, 2, \ldots\ldots, 2]$$

$$[2] \times 3 = [2, 2, 2]$$

$$[2] \times 4$$

$$\hat{H}|R\rangle = \varepsilon |R\rangle$$

$$\Rightarrow \langle R|\hat{H}^{+} = \varepsilon^{*}\langle R| = \varepsilon \langle R|$$

if ε real

$$= \langle R|\hat{H}$$ if Hermitian

$$\Rightarrow \langle R|\hat{H} = \langle R|\varepsilon$$

$$\hat{H}^{+} = \hat{H}$$

$$\hat{H}|R\rangle = \varepsilon |R\rangle$$

assume ε real

$$\langle L|\hat{H} = \langle L|\varepsilon$$

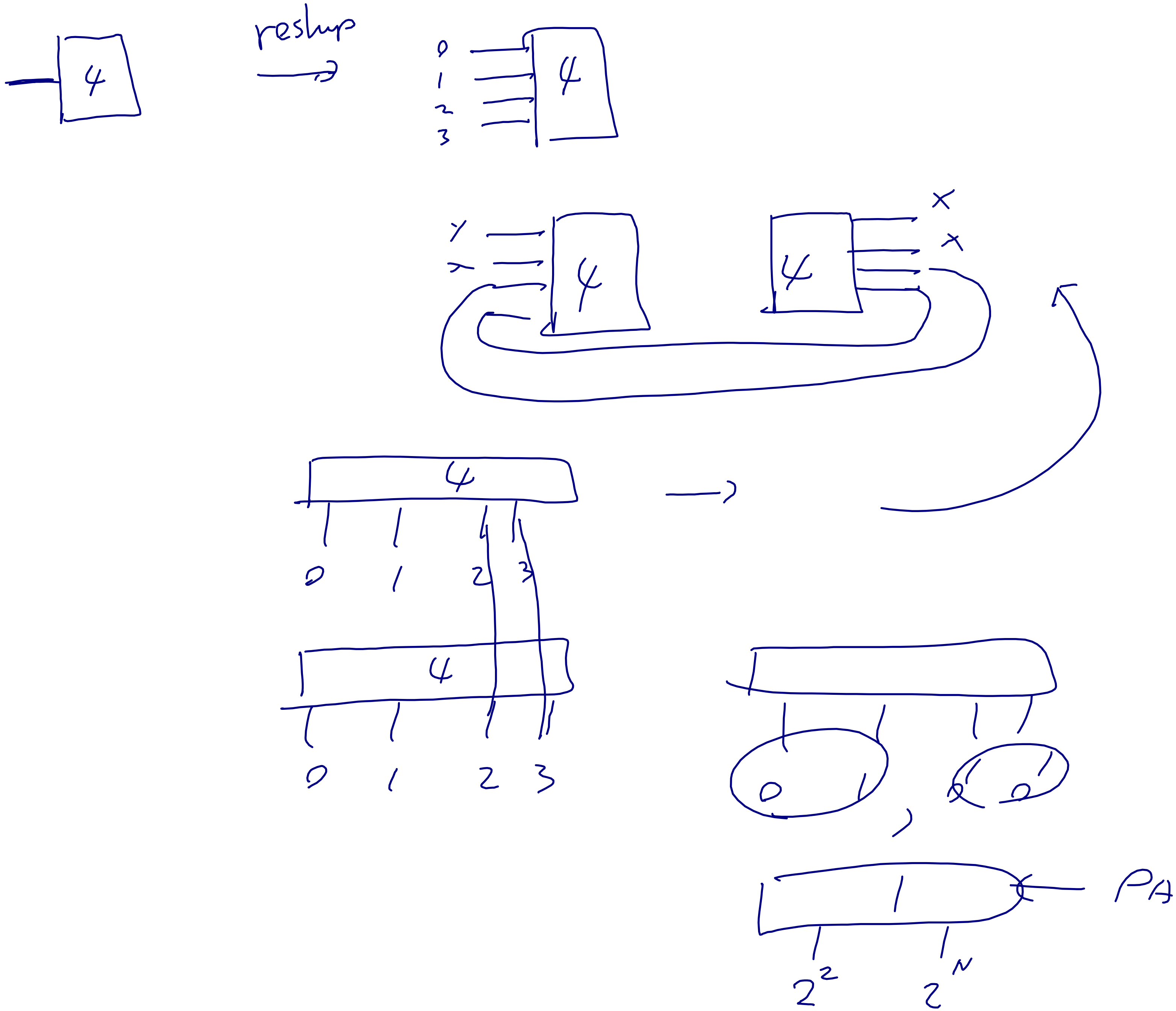
$$\hat{H}^{+}|L\rangle = \varepsilon |L\rangle$$

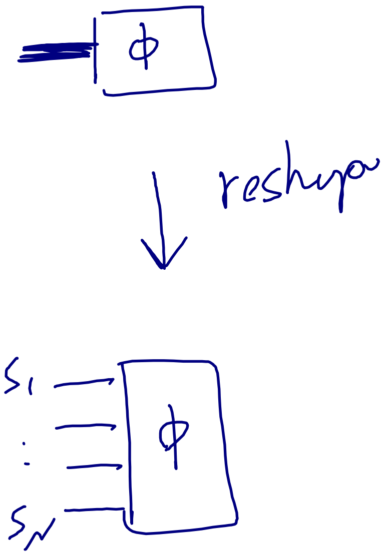
$$\Rightarrow \begin{cases} \hat{H}|R_i\rangle = \varepsilon_i |R_i\rangle \\ \hat{H}^{+}|L_i\rangle = \varepsilon_i |L_i\rangle \end{cases}$$

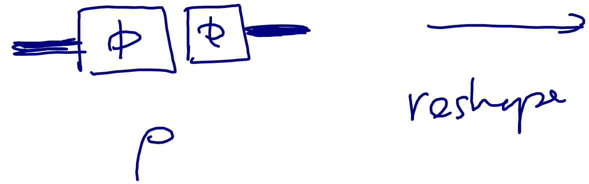
if $\quad |L_i\rangle = e^{i\phi} |R_i\rangle$

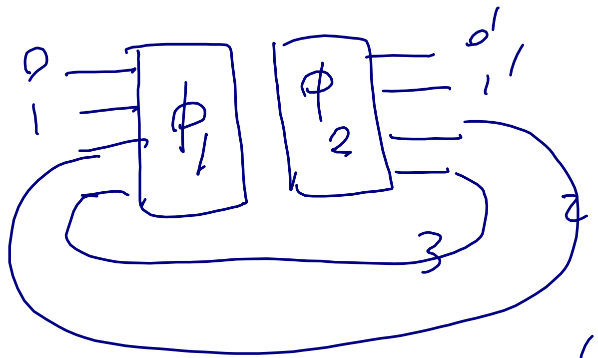
then $\quad \langle L_i|R_i\rangle = e^{-i\phi}\langle R_i|R_i\rangle = e^{-i\phi}$

$$|\tilde{L}_i\rangle = \frac{|L_i\rangle}{\langle R_i|L_i\rangle}$$

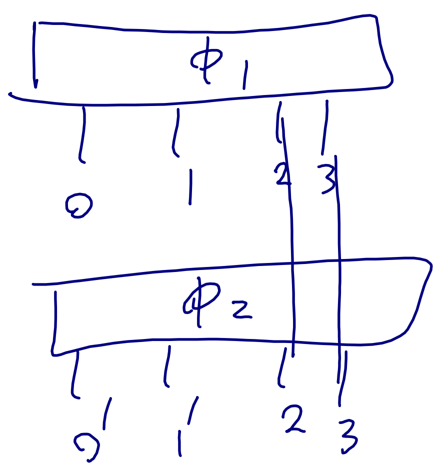

4
reshp
0
1
2
3
4
4
4
4
0 1 2 3
4
0 1 2 3
0
0
PA
2^2
2^N

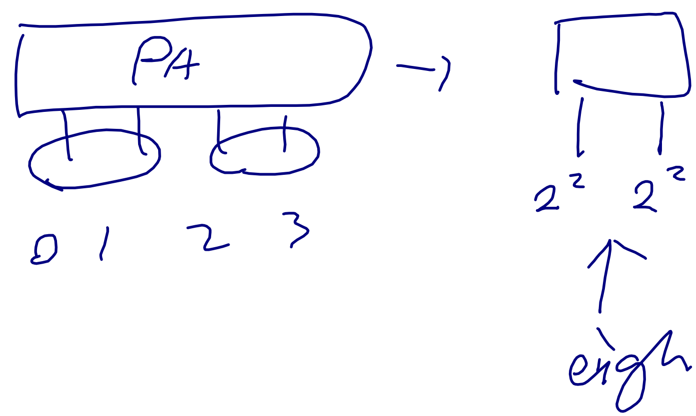






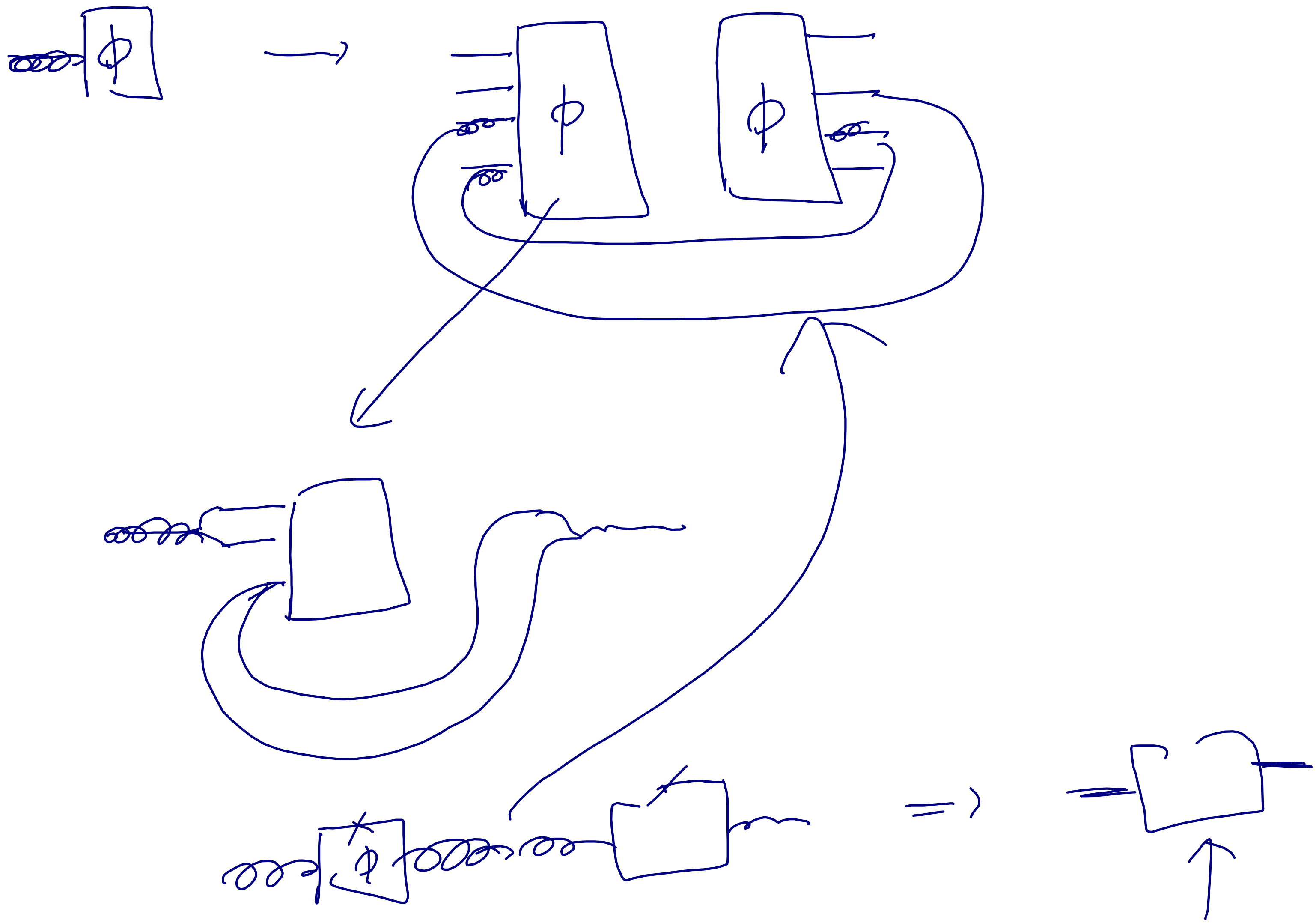
numpy.tensordot(ϕ, ϕ, axes = ([2, 3], [2, 3]))





RR [. _ _ _ _]

LL^* [. _ _ _ _ .]


ϕ
ϕ
ϕ
ϕ

$$H|R\rangle = \varepsilon |R\rangle \qquad \varepsilon \text{ real}$$

$$\langle L|H = \langle L|\varepsilon$$

if $H = H^{+}$

$$H^{+}|L\rangle = \varepsilon |L\rangle$$

if $\Rightarrow H^{+} = H \Rightarrow H|L\rangle = \varepsilon |L\rangle$

$$|L\rangle = e^{i\phi} |R\rangle$$

$$H \neq H^{+}$$

$$H\,|R\rangle = \varepsilon\,|R\rangle$$

$$\begin{cases} H^{+}\,|L\rangle = \varepsilon\,|L\rangle \\ \langle L|\,H^{+} = \langle L|\,\varepsilon \end{cases}$$

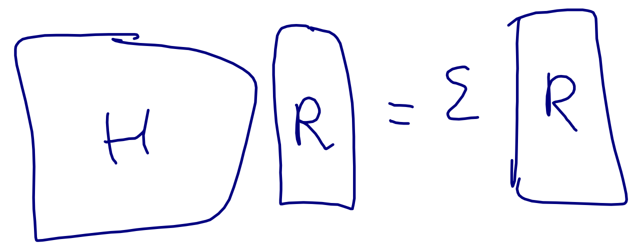
def

$$H|R\rangle = \varepsilon|R\rangle \quad ①$$

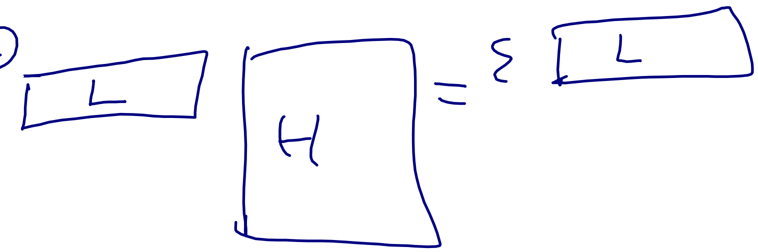
$$\langle L|H = \langle L|\varepsilon \quad ②$$

---

①



②



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②' $\Rightarrow$ $H^\dagger|L\rangle = \varepsilon|L\rangle$

$\dagger$ = transpose + conj()

$$\begin{cases} H|R\rangle = \varepsilon|R\rangle \\ H^\dagger|L\rangle = \varepsilon|L\rangle \end{cases}$$

if $H^\dagger = H$ $\Rightarrow$ $H|L\rangle = \varepsilon|L\rangle$

$$|L\rangle = e^{i\phi}|R\rangle$$

$$\left(\boxed{L} \; \boxed{H} \right)^{T\#} = \left(\boxed{L} \cdot \varepsilon \right)^{T\#}$$

$$= \boxed{H^T} \; \boxed{L} = \varepsilon \; \boxed{L}$$

$H = H^\dagger$

$|L\rangle = e^{i\phi} |R\rangle$

$H \to |R\rangle$

$H^\dagger \to |L\rangle$

$\rho = |R\rangle\langle R|$

$\langle L|R\rangle = e^{i\phi} \neq 0$

$|\tilde{L}\rangle = \dfrac{|L\rangle}{\langle R|L\rangle}$

$H \neq H^\dagger$

$\boxed{\rho = |R\rangle\langle L|}$

$\langle L|R\rangle = 1$

$\Rightarrow \langle \tilde{L}|R\rangle = 1$

$\rho = |R\rangle\langle \tilde{L}|$

$$H = H^{+} \qquad |L\rangle = |R\rangle$$

$$\rho = |R\rangle\langle R| = |R\rangle\langle L|$$

$$|\tilde{L}\rangle = e^{i\phi}|L\rangle = e^{i\phi}|R\rangle$$

$$\begin{cases} \rho = |R\rangle\langle\tilde{L}| \\ \langle\tilde{L}|R\rangle = 1 \end{cases}$$

$$H = H^{+}$$

$$\rho = |R\rangle\langle R|$$

$$H\,|R\rangle = \varepsilon|R\rangle$$

$$\rho = |R\rangle\langle L|\,e^{-i\phi}$$

$$= |R\rangle\langle\tilde{L}|$$

$$\left\{\begin{array}{l} \rho = |R\rangle\langle L| \\ \langle L|R\rangle = 1 \end{array}\right.$$

$$\langle L|H = \langle L|\,\varepsilon$$

$$|L\rangle = e^{i\phi}|R\rangle$$

$$\langle R| = \langle L|\,e^{-i\phi}$$

def $|\tilde{L}\rangle = |L\rangle e^{i\phi}$

$$\langle\tilde{L}| = \langle L|\,e^{-i\phi}$$

$$\langle\tilde{L}|R\rangle = 1$$

$$\langle L | R \rangle = e^{i\phi}$$

$$\langle \tilde{L} | = \frac{\langle L |}{e^{i\phi}} \implies \langle \tilde{L} | R \rangle = \frac{e^{i\phi}}{e^{i\phi}} = 1$$

$$\begin{cases} H|R\rangle = \varepsilon_0 |R\rangle \\ H^\dagger |L\rangle = \varepsilon_0 |L\rangle \\ \langle L|R\rangle = 1 \end{cases} \implies \rho = |R\rangle\langle L|$$