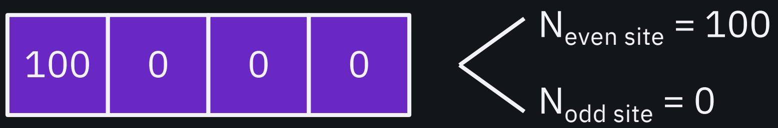
2022 IBM Quantum Challenge
Ex3 Many-body quantum dynamics
Guide Lecture (theories)

Gyeonghun Kim

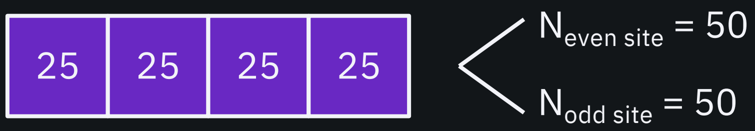
Qiskit Advocate (Republic of Korea)

1. Thermalization

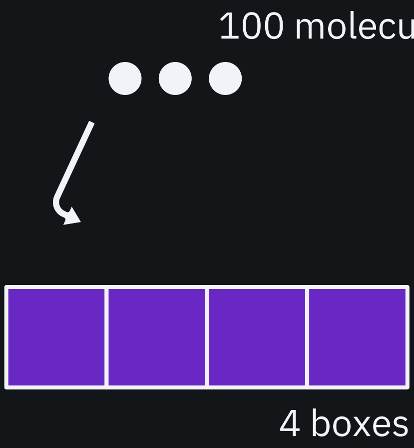
If we put all molecules in the first box,



A few hours later ...



1. Thermalization



Thermalization !

If we put all molecules in the first box,

100	0	0	0

$N_{\text{even site}} = 100$

$N_{\text{odd site}} = 0$

A few hours later ...

25	25	25	25

$N_{\text{even site}} = 50$

$N_{\text{odd site}} = 50$

1. Thermalization

If we put all molecules in the first box,

100	0	0	0

$N_{\text{even site}} = 100$

$N_{\text{odd site}} = 0$

A few hours later …

25	25	25	25

$N_{\text{even site}} = 50$

$N_{\text{odd site}} = 50$

Question: How can we measure the thermalization?

Answer: Imbalance of the system!

$$I = \frac{N_{\text{even site}} - N_{\text{odd site}}}{N_{\text{even site}} + N_{\text{odd site}}}$$

At initial state,

$$I = \frac{100 - 0}{100 + 0} = 1$$

At thermalized state,

$$I = \frac{50 - 50}{50 + 50} = 0$$

1. Thermalization

t = 0

100	0	0	0

$N_{\text{even site}} = 100$

$N_{\text{odd site}} = 0$

→

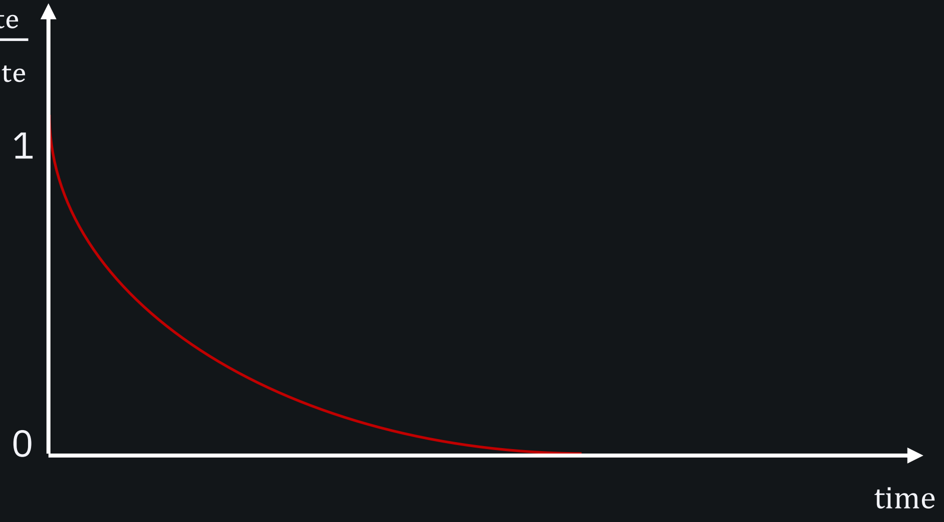
t = 100

25	25	25	25

$N_{\text{even site}} = 50$

$N_{\text{odd site}} = 50$

$$I = \frac{N_{\text{even site}} - N_{\text{even site}}}{N_{\text{even site}} + N_{\text{even site}}}$$



1. Thermalization

For quantum states, we can also define the “Imbalance”.

First, let’s think about some computational basis states with four qubits.

$|\varphi\rangle = |1000\rangle \longrightarrow$ $N_{\text{even site}} = 1$, $N_{\text{odd site}} = 0$ $\longrightarrow I = 1$

$|\varphi\rangle = |1010\rangle \longrightarrow$ $N_{\text{even site}} = 2$, $N_{\text{odd site}} = 0$ $\longrightarrow I = 1$

$|\varphi\rangle = |1110\rangle \longrightarrow$ $N_{\text{even site}} = 2$, $N_{\text{odd site}} = 1$ $\longrightarrow I = 1/3$

1. Thermalization

Qiskit

For quantum states, we can also define the “Imbalance”.

First, let’s think about some computational basis states with four qubits.

$|\varphi\rangle = |1000\rangle \longrightarrow$ $N_{\text{even site}} = 1$, $N_{\text{odd site}} = 0$ $\longrightarrow I = 1$

$|\varphi\rangle = |1010\rangle \longrightarrow$ $N_{\text{even site}} = 2$, $N_{\text{odd site}} = 0$ $\longrightarrow I = 1$

$|\varphi\rangle = |1110\rangle \longrightarrow$ $N_{\text{even site}} = 2$, $N_{\text{odd site}} = 1$ $\longrightarrow I = 1/3$

Imbalance is well-defined for computation basis states.

Can we think imbalance as quantum operator and computational basis as “imbalance eigenstate?”

... Yes!

1. Thermalization

For quantum states, we can also define the “Imbalance”.

First, let’s think about some computational basis states with four qubits.

In same way, we can also define imbalance of the general quantum state!

For $|\varphi\rangle = \frac{1}{\sqrt{2}}|1000\rangle + \frac{1}{\sqrt{2}}|1001\rangle$,

$$I = \left\langle \frac{N_{\text{even site}} - N_{\text{odd site}}}{N_{\text{even site}} + N_{\text{odd site}}} \right\rangle = (\text{imbalance of } |1000\rangle) \times (\text{probability of } |1000\rangle)$$

$$+ (\text{imbalance of } |1001\rangle)(\text{probability of } |1001\rangle)$$

$$= 1\times 0.5 + 0\times 0.5 = 0.5$$

1. Thermalization

For quantum states, we can also define the “Imbalance”.

First, let’s think about some computational basis states with four qubits.

In same way, we can also define imbalance of the general quantum state!

For $|\varphi\rangle = \frac{1}{\sqrt{2}}|1000\rangle + \frac{1}{\sqrt{2}}|1001\rangle$,

$$I = \left\langle \frac{N_{\text{even site}} - N_{\text{odd site}}}{N_{\text{even site}} + N_{\text{odd site}}} \right\rangle = (\text{imbalance of } |1000\rangle) \times (\text{probability of } |1000\rangle)$$

$$+ (\text{imbalance of } |1001\rangle)(\text{probability of } |1001\rangle)$$

$$= 1 \times 0.5 + 0 \times 0.5 = 0.5$$

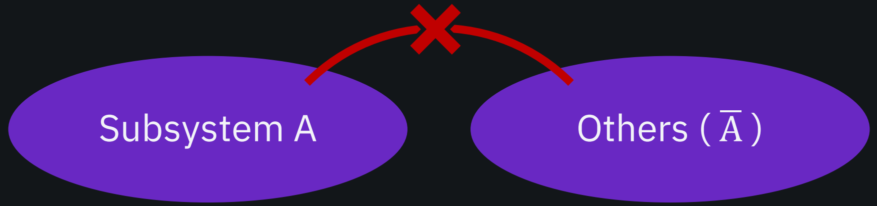
Now you are ready to solve ex3a!!

2. von Neumann Entropy

Before talking about von Neumann entropy, let’s review the concept of partial trace (or trace out) first!

A brief idea of trace out: average out the not-interest part of the system!

Let’s consider product state first.

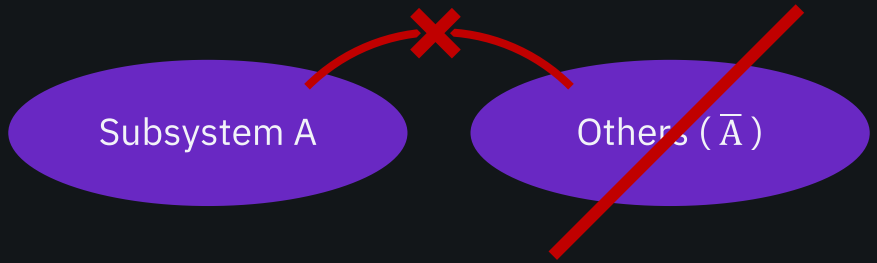


2. von Neumann Entropy

Before talking about von Neumann entropy, let's review the concept of partial trace (or trace out) first!

A brief idea of trace out: average out the not-interest part of the system!

Let's consider product state first.



Averaging (or measuring) $\bar{A}$ does not affect the system A

Subsystem A is "pure state"!

2. von Neumann Entropy

Before talking about von Neumann entropy, let’s review the concept of partial trace (or trace out) first!

A brief idea of trace out: average out the not-interest part of the system!

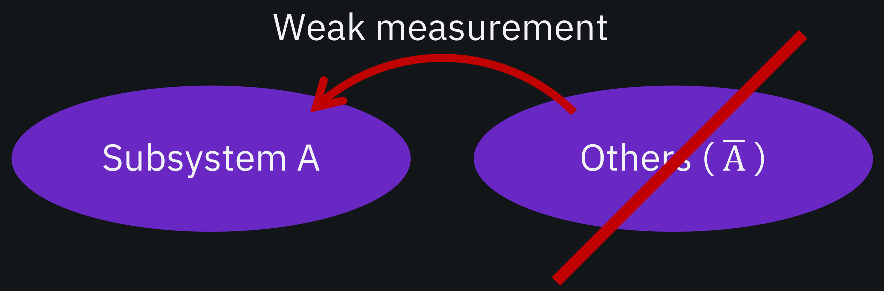
Now, let’s assume that A and $\bar{A}$ have entanglement.

2. von Neumann Entropy

Before talking about von Neumann entropy, let's review the concept of partial trace (or trace out) first!

A brief idea of trace out: average out the not-interest part of the system!

Now, let's assume that A and $\bar{A}$ have entanglement.



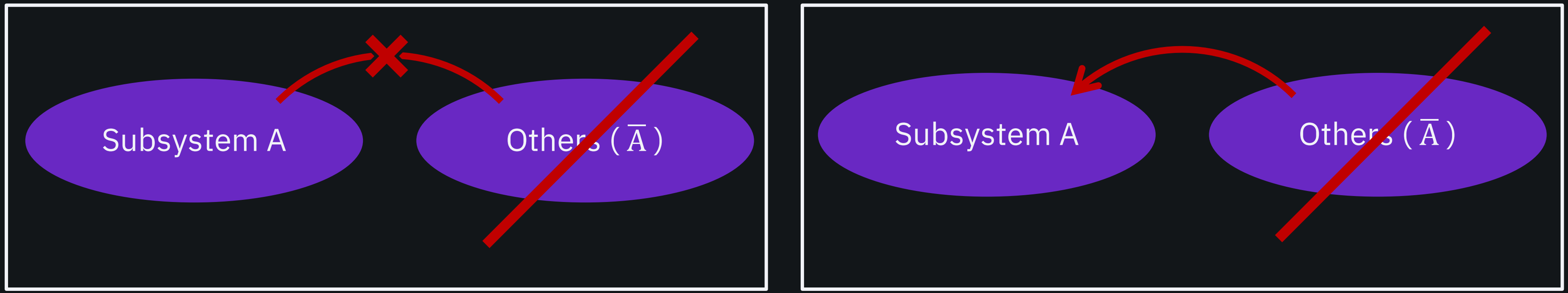
Averaging (or measuring) $\bar{A}$ affect the system A

Subsystem A is "mixed state"!

2. von Neumann Entropy

Before talking about von Neumann entropy, let’s review the concept of partial trace (or trace out) first!

A brief idea of trace out: average out the not-interest part of the system!



von Neumann entropy gives information about “how much our system A is entangled with $\bar{\mathrm{A}}$.

$$S_{\text{von Neumann}}(\rho) = -\mathrm{tr}(\rho_{\mathrm{A}} \ln \rho_{\mathrm{A}}), \qquad \rho_{\mathrm{A}} = \mathrm{tr}_{\bar{\mathrm{A}}}(\rho)$$

2. von Neumann Entropy

Example 1: Maximally entangled case (Bell state)

$$|\varphi\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \longrightarrow \rho_A = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \longrightarrow$$

Question: Can we find $|\varphi\rangle$ where $\rho_A = |\varphi\rangle\langle\varphi|$?

Answer: No! (Mixed state)

$$S_{\text{von Neumann}}(\rho) = \underline{\ln 2}$$

Maximum value of von Neumann entropy

2. von Neumann Entropy

Qiskit

Example 2: Product state (No entanglement!)

$$|\varphi\rangle = |00\rangle$$

$$\rho = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \longrightarrow \rho_A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \longrightarrow$$

Question: Can we find $|\varphi\rangle$ where $\rho_A = |\varphi\rangle\langle\varphi|$?

Answer: Yes! (Pure state)

$$S_{\text{von Neumann}}(\rho) = \underline{0}$$

Minimum value of von Neumann entropy

3. Thermalization, imbalance and von Neumann entropy

$|\varphi(t=0)\rangle = |100010001000\rangle$

Time evolution with

tight-binding Hamiltonian + disorder

$$H = \sum_i (\mathrm{X_i X_{i+1}} + \mathrm{Y_i\, Y_{i+1}}) + \sum_i \epsilon_i\, \mathrm{Z_i}$$

$|\varphi(t)\rangle$

3. Thermalization, imbalance and von Neumann entropy

Qiskit

$|\varphi(t=0)\rangle = |100010001000\rangle$ → Initial state profile:

imbalance = 1 (maximally imbalanced)

von Neumann entropy = 0 (minimum value)

↓ Time evolution with

tight-binding Hamiltonian + disorder

$$H = \sum_i (\mathrm{X_i X_{i+1}} + \mathrm{Y_i\, Y_{i+1}}) + \sum_i \epsilon_i\, \mathrm{Z_i}$$

$|\varphi(t)\rangle$

3. Thermalization, imbalance and von Neumann entropy

Qiskit

$|\varphi(t=0)\rangle = |100010001000\rangle$ → Initial state profile:

imbalance = 1 (maximally imbalanced)

von Neumann entropy = 0 (minimum value)

Time evolution with

tight-binding Hamiltonian + disorder

$$H = \sum_i (\mathrm{X_i X_{i+1}} + \mathrm{Y_i\, Y_{i+1}}) + \sum_i \epsilon_i \, \mathrm{Z_i}$$

$|\varphi(t)\rangle$

Question: How these quantities changes in the case of

(1) Strong localization?
(2) Weak localization?

Keep this question in mind while solving problem ex3b and ex3c!

Enjoy your challenge!!

Gyeonghun Kim
Qiskit Advocate (Republic of Korea)