Assignment 6

Density matrices

Quantum Information and Computing

Giacomo Gasparotto

23 December 2025, A.Y. 2025/2026

Theory and complexity

N-bodies composite system

The purpose is to simulate a system of N particles of dimension D each.

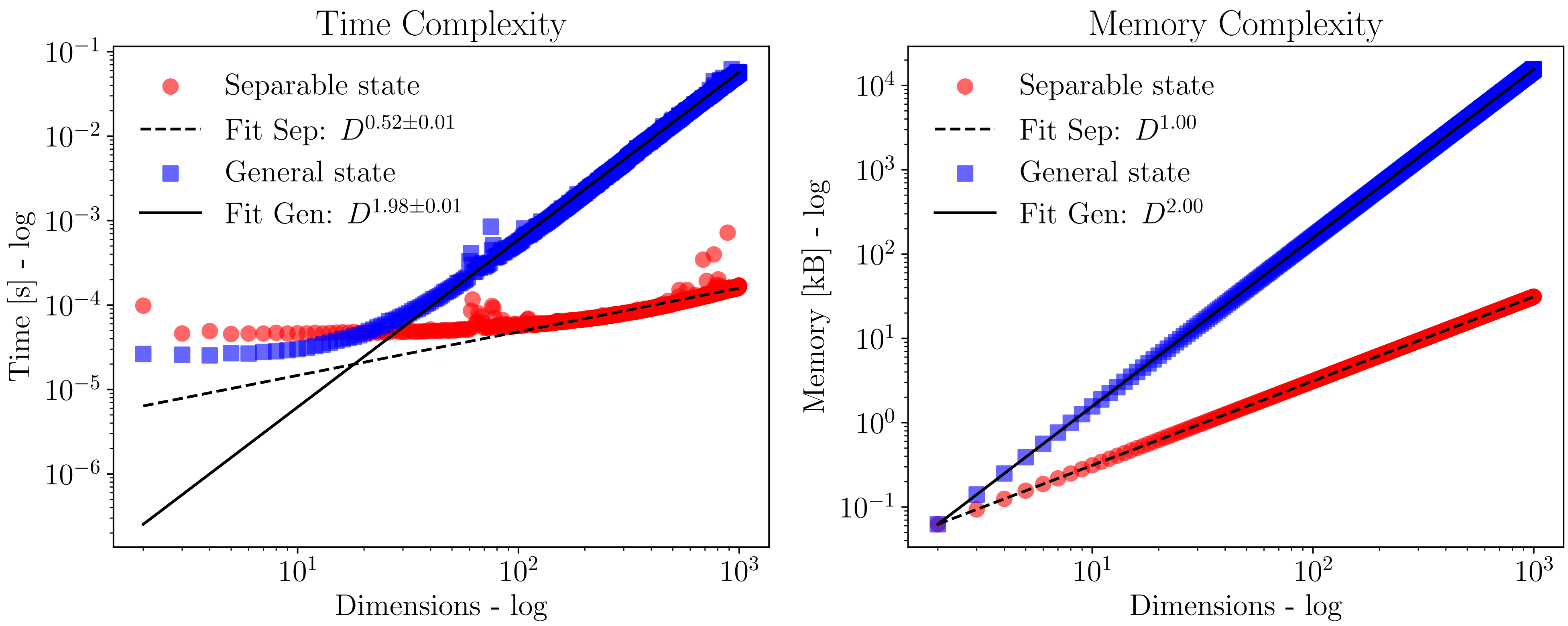
It can be described by $\Psi(\psi_1, \psi_2, \ldots, \psi_N)$, where: $\psi_i = \sum_{j=1}^{D} j_i \left| j_i \right\rangle \in \mathscr{H}^D$

We inspected two cases:

1. **Separable pure state**:
    - Tensor product of local states: $|\Psi\rangle_S = \sum_{j_1} c_{j_1} |j_1\rangle \otimes \sum_{j_2} c_{j_2} |j_2\rangle \otimes \cdots \otimes \sum_{j_N} c_{j_N} |j_N\rangle$
    - Expected complexity: $O(ND)$
2. **General pure state**:
    - Superposition of all basis states: $|\Psi\rangle = \sum_{\bar{j}} c_{\bar{j}} |j\rangle_1 |j\rangle_2 \cdots |j\rangle_N$
    - Expected complexity: $O(N^D)$

Computational complexity

Bipartite system ($N = 2$) with subsystem dimensions D



For both time and memory allocation:

Separable states ($|\psi_A\rangle \otimes |\psi_B\rangle$): *Linear scaling,* as expected $N(2D-2) \propto D$ parameters to store

General states ($\sum \psi_{A,B} |\psi_A\rangle |\psi_B\rangle$): *Quadratic scaling,* as expected $2(D^N - 1) \propto D^2$ parameters to store

Density matrix representation

- A generic state Ψ can also be described via a density matrix defined as:
  - $\rho = |\Psi\rangle\langle\Psi|$ if it is a **pure state**
  - $\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|$ if it is a **mixed state**

Properties:
- $\rho = \rho^\dagger$
- $Tr(\rho) = 1$
- $\rho \geq 0$
- $Tr(\rho^2) \leq 1$

- If our state represent two subsystems ($N = 2$) we can get information about one of the two by performing the **partial trace** on the total system:

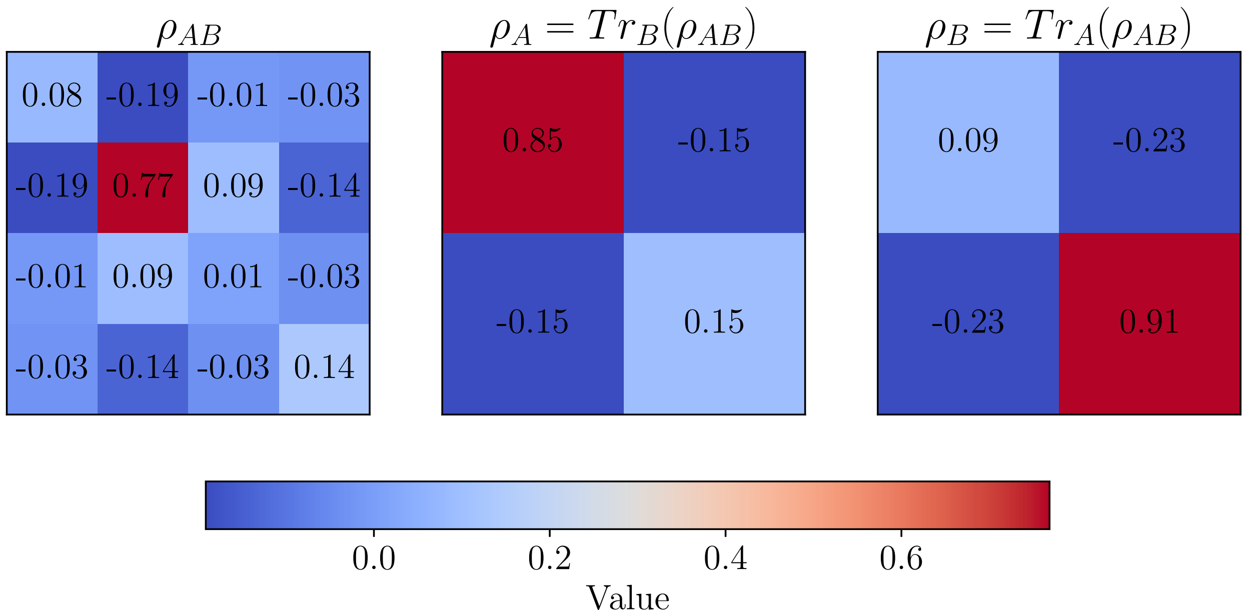
$$\rho_A = Tr_B|\Psi\rangle\langle\Psi|, \ \rho_B = Tr_A|\Psi\rangle\langle\Psi|$$

Example:

Generate a pure random state Ψ ($N = 2$, $D = 2$).

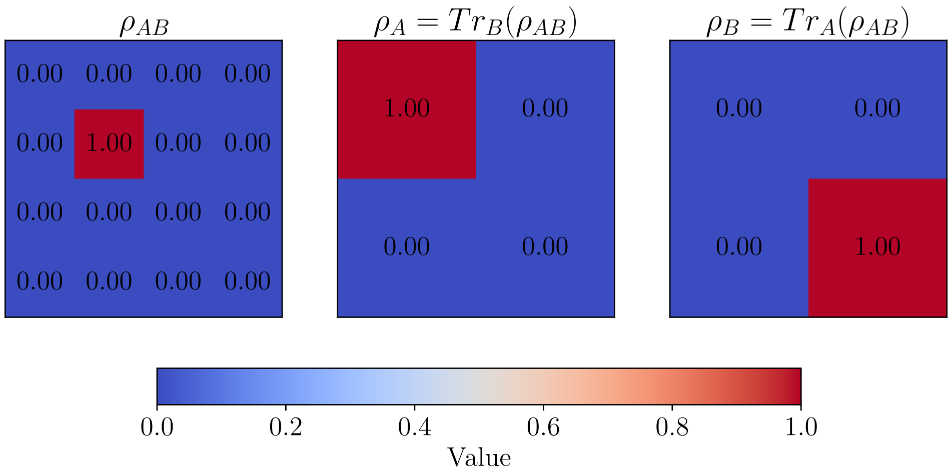
We can recognise that all the properties have been respected.

```
Purity of rho2:
1.0000000000000004+1.38777878
07814457e-17j
```



Check for analytical states

Consider the computational basis: $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and generate two states.



Separable state: $|\chi\rangle = |0\rangle_A \otimes |1\rangle_B = |01\rangle$

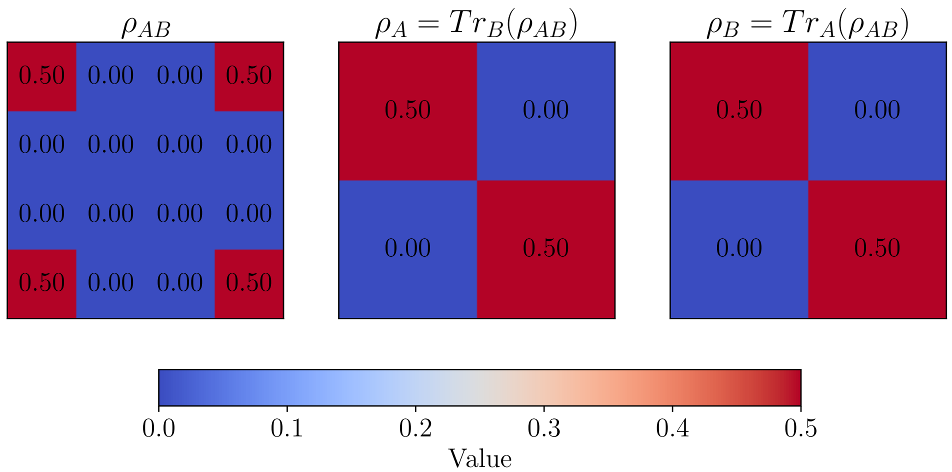
- $\rho_{AB} = |\chi\rangle\langle\chi| = |01\rangle\langle 01|$
- $\rho_A = |0\rangle\langle 0|_A \cdot \underbrace{\mathrm{Tr}(|1\rangle\langle 1|_B)}_{=1} = |0\rangle\langle 0|$
- $\rho_B = |1\rangle\langle 1|$

```
Trace(rho^2) = 1.0000
Trace(rhoA^2) = 1.0000+0.0000j
Trace(rhoB^2) = 1.0000+0.0000j
```

Bell (entangled) state: $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

- $\rho_{AB} = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|)$
- $\rho_A = \rho_B = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$

```
Trace(rho^2) = 1.0000+0.0000j
Trace(rhoA^2) = 0.5000+0.0000j
Trace(rhoB^2) = 0.5000+0.0000j
```



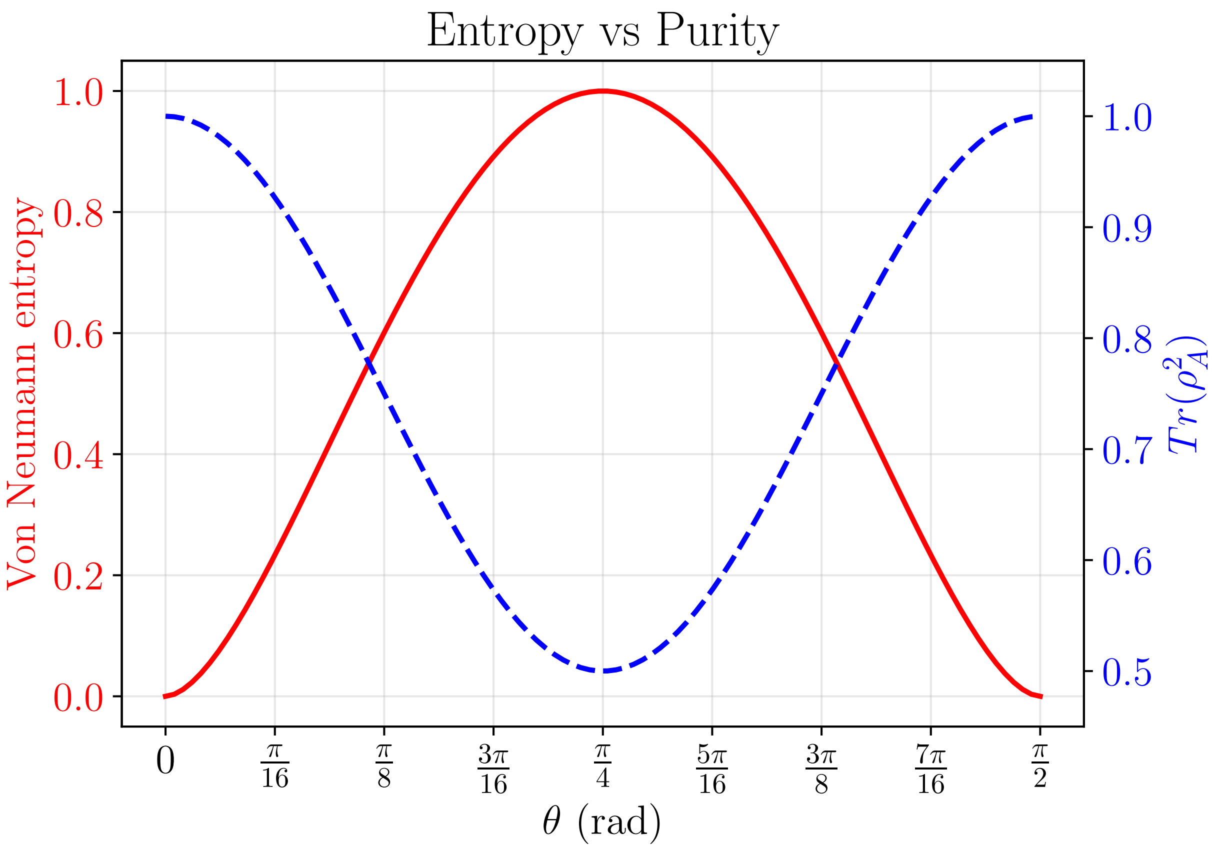
Von Neumann entropy

Transition from separable to entangled

Prepare a generic state $|\psi(\theta)\rangle = \cos(\theta)|01\rangle + e^{i\phi}\sin(\theta)|10\rangle$

Change θ to inspect:

- The **Entanglement sweep** (purity of one subsystem) changing
- The **Von Neumann entropy**: $S(\rho_A) = -Tr[\rho_A \log \rho_A]$



“Critical” angles:

- $\theta = 0, \frac{\pi}{2}$: no entropy, pure states
- $\theta = \frac{\pi}{4}$: max entropy, maximally entangled states

As expected from the theory