QUANTUM INFORMATION AND COMPUTING

Assignment 6

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Density matrix for pure states

In this report, we develop a Python class for the representation of N-body quantum states. Each element of such a system resides in a d-dimensional Hilbert space denoted as $\mathcal{H}$. The class is designed to handle a sufficient number of coefficients, facilitating the representation of both separable and general states within the composite Hilbert space $\mathcal{H}^N$.

Theoretical background

Consider a system composed of N particles, each characterized by a d-dimensional Hilbert space $\mathcal{H}$. The composite Hilbert space for the entire system is denoted as $\mathcal{H}^N$, and a basis for it is given by $|k\rangle_{k=1,\ldots,d^N}$.

Any state $|\psi\rangle$ in this composite space can be expressed using d^N complex coefficients, each multiplying a basis vector. However, due to normalization and global phase constraints inherent in quantum states, only $d^N - 1$ complex coefficients are required to fully characterize a generic state.

Now, consider a specific scenario of an N-body non-interacting, separable pure state, represented as:

$$|\psi\rangle = \sum_{j_1=1}^{d} c_{j_1}|j_1\rangle \otimes \sum_{j_2=1}^{d} c_{j_2}|j_2\rangle \otimes \ldots \otimes \sum_{j_N=1}^{d} c_{j_N}|j_N\rangle. \tag{1}$$

Here, $|j_i\rangle_{i=1,\ldots,N}$ denotes the basis vectors for each Hilbert space $\mathcal{H}$ associated with the description of individual particles. Remarkably, to completely characterize such systems, accounting for the normalization and global phase constraints, only $N(d-1)$ complex coefficients are necessary.

Consider the density matrix associated with a generic pure state $|\psi\rangle$, defined as

$$\rho = |\psi\rangle\langle\psi|. \tag{2}$$

Now, imagine this pure state as a 2-body state within a generic Hilbert space $\mathcal{H}^2$, where $\mathcal{H}$ has dimension d. For clarity, let us denote the first subsystem in this system as A and the second as B. In general, associating a pure state directly with the individual components A or B is not straightforward. However, we can define a meaningful quantity known as the *reduced density matrix* ρ_A corresponding to the subsystem A (similar considerations apply to subsystem B). This reduced density matrix is obtained through the partial trace of the density matrix ρ over the basis of system B:

$$\rho_A = \mathrm{Tr}_B\rho = \sum_{j_B=1}^{d} (I_A \otimes \langle j_B|)(|\psi\rangle\langle\psi|)(I_A \otimes |j_B\rangle), \tag{3}$$

where I_A is the identity operator acting on $\mathcal{H}_A$, and $|j_B\rangle$ represents the basis vectors of $\mathcal{H}_B$. Similarly, for subsystem B, the reduced density matrix ρ_B is given by:

$$\rho_B = \mathrm{Tr}_A\rho = \sum_{j_A=1}^{d} (\langle j_A| \otimes I_B)(|\psi\rangle\langle\psi|)(|j_A\rangle \otimes I_B). \tag{4}$$

The reduced density matrix ρ_A captures essential information about subsystem A within the

composite system, offering a more manageable representation. This mathematical construct proves to be a powerful tool for investigating the properties and dynamics of individual components in a multipartite quantum system.

There are three practical methods to compute the reduced density matrix associated with a pure state, each offering distinct computational approaches.

A straightforward method involves direct computation using the equation (3). This method explicitly involves the sum over basis states and operators, providing an intuitive approach to obtain the reduced density matrix.

An alternative strategy is to compute the reduced density matrix from the density matrix of the composite system. This involves reshaping the density matrix into a 4-rank tensor and then contracting it along the appropriate indices, depending on whether subsystem A or B is being traced out.

Another method is to compute the reduced density matrix directly from the state vector. By reshaping the state vector into a 2-rank tensor, one can perform a tensor product with its conjugate, subsequently contracting the product along the relevant indices based on the subsystem being traced out. This method provides a direct route from the state vector to the reduced density matrix.

By implementing and comparing these three methods, we can evaluate how well they perform computationally.

Implementation

We developed a Python class, called *NBodyState*, intended for managing quantum N-body states. Its initialization takes essential parameters: the number of subsystems N, their dimensionality d, complex coefficients for the computational basis (of size $N(d-1)$ for separable state, $d^N - 1$ for non-separable state, as explained before), and a boolean indicating separability.

The class incorporates two key methods. The first computes the density matrix for the quantum N-body state. The second, designed for bipartite systems, calculates the reduced density matrix. This method employs three distinct approaches: direct computation from the equation, reshaping and tensor contraction from the density matrix, and direct computation from the state vector. Users have the flexibility to specify which subsystem to trace out.

This class is finally tested, and the three possible methods are compared.

Results

The implemented class has been successfully tested, demonstrating accurate representation for both separable and non-separable states. It correctly computes the density matrices, and all three methods yield identical reduced density matrices when initialized with the same quantum state. To illustrate this, consider a specific example with two qubits, denoted as A and B, in the following states:

$$|\psi_A\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle \in \mathcal{H}_A, \tag{5}$$

$$|\psi_B\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \in \mathcal{H}_B, \tag{6}$$

where $|0\rangle$ and $|1\rangle$ represent the computational basis for a single qubit. Now, consider the 2-body system described by the following separable state

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B. \tag{7}$$

For this separable state, we only need 2 complex coefficients: those in front of $|0\rangle$ in both equations (5) and (6). The outputs of the class, as shown in Figure 1, align with the expected results. The same holds true if we consider a non-separable state, with the only difference being the requirement for more input coefficients.

```
State
[0.3535    +0.j 0.35360677+0.j 0.61227996+0.j 0.6124649 +0.j]

Density matrix
[[0.12496225+0.j 0.12499999+0.j 0.21644097+0.j 0.21650634+0.j]
 [0.12499999+0.j 0.12503775+0.j 0.21650634+0.j 0.21657174+0.j]
 [0.21644097+0.j 0.21650634+0.j 0.37488675+0.j 0.37499998+0.j]
 [0.21650634+0.j 0.21657174+0.j 0.37499998+0.j 0.37511325+0.j]]

Reduced density matrix of subsystem A

Method 0
[[0.25      +0.j 0.4330127+0.j]
 [0.4330127+0.j 0.75      +0.j]]
Method 1
[[0.25      +0.j 0.4330127+0.j]
 [0.4330127+0.j 0.75      +0.j]]
Method 2
[[0.25      +0.j 0.4330127+0.j]
 [0.4330127+0.j 0.75      +0.j]]

Reduced density matrix of subsystem B

Method 0
[[0.499849  +0.j 0.49999998+0.j]
 [0.49999998+0.j 0.500151  +0.j]]
Method 1
[[0.499849  +0.j 0.49999998+0.j]
 [0.49999998+0.j 0.500151  +0.j]]
Method 2
[[0.499849  +0.j 0.49999998+0.j]
 [0.49999998+0.j 0.500151  +0.j]]
```

Figure 1: Outputs from the class *NBodyState* given the coeffiecients $\{1/2, 1/\sqrt{2}\}$ to represent a separable state with $N = d = 2$.

The advantages of using separable states become evident when considering memory allocation. As illustrated in Figure 2, the number of complex coefficients required to fully describe a N-body quantum state grows linearly with N for separable states. In contrast, for non-separable states, this growth is exponential. This disparity becomes more pronounced when increasing d, limiting our ability to represent composite systems with a higher number of subsystems efficiently when the state is non-separable. This poses a significant constraint on our current approach.
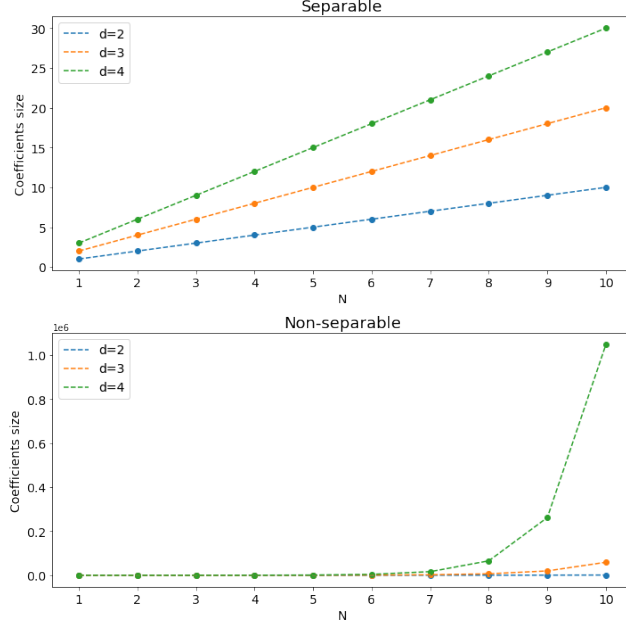
Figure 2: Dependence of the number of complex coefficients needed to represent an N-body quantum state on the value of N.

When considering the computation of the reduced density matrix for a N-body state, Figure 3 depicts the execution times for all the three described methods. For local dimensions to trace out lower than 40 (i.e. where the subsystem to trace out resides in a Hilbert space of dimension 40), the performances of the three methods are nearly identical. Beyond this point, it becomes evident that computing the reduced density matrix directly from the state vectors, without passing through the global density matrix or using the definition in Equation (3), is more advantageous in terms of execution time.
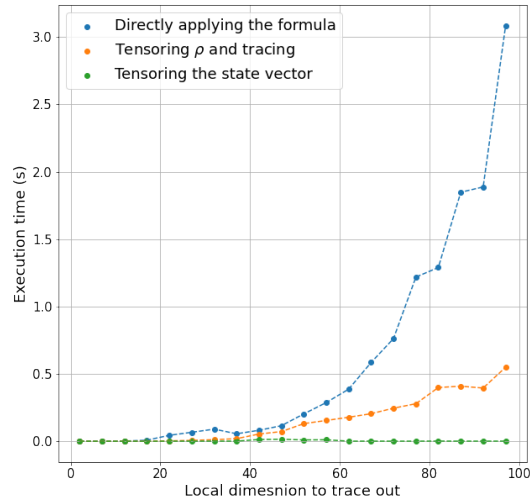

Figure 3: Comparison of the three developed methods for computing the reduced density matrix of a given pure quantum state.