

# Assignment 6

## Density Matrix

November 28th 2023

## DENSITY MATRIX

Consider a quantum system composed by  $N$  subsystems (spins, atoms, particles etc..) each described by a wave function  $\psi_i \in \mathcal{H}^D$  where  $\mathcal{H}^D$  is  $D$ -dimensional Hilbert space. How do you write the total wave function of the system  $\Psi(\psi_1, \psi_2, \dots, \psi_N)$ ?

a) Write a code to describe the composite system in the case of  $N$ -body non interacting, separable pure state;

b) and in the case of a general  $N$ -body pure wave function  $\Psi \in \mathcal{H}^{D^N}$ ;

c) Comment and compare their efficiency;

d) Given  $N=2$ , write the density matrix of a general pure state  $\Psi$ ,  $\rho = |\Psi\rangle\langle\Psi|$ ;

e) Given a generic density matrix of dimension  $D^N \times D^N$  compute the reduced density matrix of either the left or the right system, e.g.  $\rho_1 = \text{Tr}_2 \rho$ .

f) Test the functions described before (and all others needed) on two-spin one-half (qubits) with different states.

## HILBERT SPACE OF COMPOSITE SYSTEMS

Given two Hilbert spaces of dimension  $m$  and  $n$ , the composite Hilbert space is  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ . We can associate each pair of vectors  $|\alpha\rangle \in \mathcal{H}_1$ ,  $|\beta\rangle \in \mathcal{H}_2$  a vector belonging to

$$\mathcal{H}, \quad |\alpha\rangle \otimes |\beta\rangle = |\alpha, \beta\rangle \quad \dim \mathcal{H} = mn$$

## PROPERTIES OF THE TENSOR PRODUCT

Vectors in  $\mathcal{H}$  are linear superposition of the above one and satisfy the following properties:

$$1) \forall |\alpha\rangle \in \mathcal{H}_1, |\beta\rangle \in \mathcal{H}_2, c \in \mathbb{C} \quad c(|\alpha\rangle \otimes |\beta\rangle) = (c|\alpha\rangle) \otimes |\beta\rangle = (|\alpha\rangle \otimes c|\beta\rangle)$$

$$2) \forall |\alpha_1\rangle, |\alpha_2\rangle \in \mathcal{H}_1, |\beta\rangle \in \mathcal{H}_2 \quad (|\alpha_1\rangle + |\alpha_2\rangle) \otimes |\beta\rangle = (|\alpha_1\rangle \otimes |\beta\rangle) + (|\alpha_2\rangle \otimes |\beta\rangle)$$

$$3) \forall |\alpha\rangle \in \mathcal{H}_1, |\beta_1\rangle, |\beta_2\rangle \in \mathcal{H}_2 \quad |\alpha\rangle \otimes (|\beta_1\rangle + |\beta_2\rangle) = (|\alpha\rangle \otimes |\beta_1\rangle) + (|\alpha\rangle \otimes |\beta_2\rangle)$$

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## STATES AND LINEAR OPERATORS

two dimensional Hilbert spaces, basis vector:  $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

General state:  $|\Psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle$

Linear operators  $A$  and  $B$ , acting on  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , respectively :

$$(A \otimes B) \sum_{i,j} c_{i,j} |i\rangle \otimes |j\rangle = \sum_{i,j} c_{i,j} A|i\rangle \otimes B|j\rangle$$

A generic operator  $O$  acting on  $\mathcal{H}$  can be written as a linear superposition of tensor products of linear operators  $A_i$  acting on  $\mathcal{H}_1$  and  $B_j$  acting on  $\mathcal{H}_2$ :

$$O = \sum_{i,j} \gamma_{i,j} A_i \otimes B_j$$

Matrix representation of the operator  $A \otimes B$  in the basis  $|k\rangle = |ij\rangle$  labeled by a single index  $k=1, \dots, mn$  with  $k = (i-1)n + j$  with  $i=1, m$  and  $j=1, n$ .

$$A \otimes B = \begin{bmatrix} A_{11}B & A_{12}B & \dots & A_{1m}B \\ A_{21}B & A_{22}B & \dots & A_{2m}B \\ \vdots & \vdots & \dots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mm}B \end{bmatrix}$$

## GENERAL QUANTUM STATE

Consider  $N$  subsystems each described by a wave function  $|\psi_i\rangle \in \mathcal{H}_i$  with  $\dim=D$ . Basis vectors are built from the tensor product of each subsystem basis vector:

$$\{ |j\rangle_i \}_{i=1,\dots,N}^{j=1,\dots,D}$$

The general form of a state  $|\Psi\rangle \in \mathcal{H}$  with  $\dim = D^N$

$$|\Psi\rangle = \sum_{\vec{j}} c_{\vec{j}} |j\rangle_1 |j\rangle_2 \dots |j\rangle_N$$



$D^N$

How many real parameters are needed to describe a general quantum state:  $2(D^N - 2)$  (global phase and normalization)

## SEPARABLE QUANTUM STATE

If the state is separable then it can be written as a tensor product of the wave functions relative to each subsystem:

$$|\Psi\rangle_S = \sum_{j_1} c_{j_1} |j_1\rangle \otimes \sum_{j_2} c_{j_2} |j_2\rangle \otimes \dots \otimes \sum_{j_N} c_{j_N} |j_N\rangle$$



$DN$

How many real parameters are needed to describe a separable quantum state:  $N(2D - 2)$  (global phase and normalization)

c) Comment and compare their efficiency;

Look at these two different representations of quantum state both in terms of allocated memory and required time to build the vectors



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$$\rho = |\Psi\rangle\langle\Psi|$$

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi| = \sum_{j=1}^{\dim B} \langle j | \Psi \rangle \langle \Psi | j \rangle_B$$

Generic subsystems

$$\{S_1, S_2, \dots, S_N\} \longrightarrow \{\tilde{A}, \tilde{B}\}$$

$$\tilde{A} = \{S_1, \dots, S_i\} \in \mathcal{H}^{D^i}, \tilde{B} = \{S_i, \dots, S_N\} \in \mathcal{H}^{D^{(N-i)}}$$

$$[\rho_A]_{ij} = \sum_{k=1}^{D_B} \rho[(i-1)D_B + k, (j-1)D_B + k]$$