Assignment 6

Density Matrix

November 19th 2024

DENSITY MATRIX

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

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 $\Psi \in \mathscr{H}^{D^N}$;

c) Comment and compare their efficiency;

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

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.$\rho_1 = \mathrm{Tr}_2\rho$.

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 $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$. We can associate each pair of vectors $|\alpha\rangle \in \mathscr{H}_1, \quad |\beta\rangle \in \mathscr{H}_2$ a vector belonging to

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

PROPERTIES OF THE TENSOR PRODUCT

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

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

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

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

DENSITY MATRIX

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

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 $\Psi \in \mathscr{H}^{D^N}$;

c) Comment and compare their efficiency;

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

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.$\rho_1 = \mathrm{Tr}_2\rho$.

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

STATES AND LINEAR OPERATORS

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

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

Linear operators A and B, acting on $\mathscr{H}_1$ and $\mathscr{H}_2$, 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 $\mathscr{H}$ can be written as a linear superposition of tensor products of linear operators A_i acting on $\mathscr{H}_1$ and B_j acting on $\mathscr{H}_2$:

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

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

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

GENERAL QUANTUM STATE

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

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

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

$$|\Psi\rangle = \sum_{\bar{j}} c_{\bar{j}} |j\rangle_1 |j\rangle_2 \ldots |j\rangle_N$$

$$\downarrow$$

$$D^N$$

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 sepable then it can be written as a tensor product of the wave functions relative to each subsystem:

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

$$\downarrow$$

$$DN$$

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 interns of allocated memory and required time to build the vectors

DENSITY MATRIX

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

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 $\Psi \in \mathscr{H}^{D^N}$;

c) Comment and compare their efficiency;

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

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.$\rho_1 = \mathrm{Tr}_2 \rho$.

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

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

$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi| = \sum_{j=1}^{dimB} \langle j|\Psi\rangle\langle\Psi|j\rangle_B$$

Generic subsystems

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

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

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