

February 6-10,2023: Quantum Computing, Quantum Machine Learning and Quantum Information Theories

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Overview, Density matrices, Entropy and Schmidt Decompositions

1. Density matrices and Measurements
2. [Video of lecture](#)
 - [Teaching material in different formats](#)
 - **Reading recommendation:** Scherrer, Mathematics of Quantum Computations, chapters 2 and 3

Introduction

In order to study entanglement and why it is so important for quantum computing, we need to introduce some basic measures and useful quantities. For these endeavors, we will use our two-qubit system from the previous lecture in order to introduce, through examples, density matrices and entropy. These two quantities, together with technicalities like the Schmidt decomposition. The latter is again a linear decompositions which allows us to express a vector in terms of tensor product of two inner product spaces. In quantum information theory and quantum computing it is widely used as a way to define and describe entanglement. The material which follows can thus be seen as a prelude to our discussion of entanglement.

Two-qubit system and definition of density matrices. investigations, we extend the simple two-level system to a four level system. This system can be thought of as composed of two subsystems A and B . Each subsystem has computational basis states

$$|0\rangle_{A,B} = \begin{bmatrix} 1 & 0 \end{bmatrix}^T \quad |1\rangle_{A,B} = \begin{bmatrix} 0 & 1 \end{bmatrix}^T.$$

The subsystems could represent single particles or composite many-particle systems of a given symmetry. This leads to the many-body computational basis states

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^T,$$

and

$$|10\rangle = |1\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^T,$$

and

$$|01\rangle = |0\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}^T,$$

and finally

$$|11\rangle = |1\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}^T.$$

These computational basis states define also the eigenstates of the non-interacting Hamiltonian

$$H_0|00\rangle = \epsilon_{00}|00\rangle,$$

$$H_0|10\rangle = \epsilon_{10}|10\rangle,$$

$$H_0|01\rangle = \epsilon_{01}|01\rangle,$$

and

$$H_0|11\rangle = \epsilon_{11}|11\rangle.$$

The interacting part of the Hamiltonian H_I is given by the tensor product of two σ_x and σ_z matrices, respectively, that is

$$H_I = H_x \sigma_x \otimes \sigma_x + H_z \sigma_z \otimes \sigma_z,$$

where H_x and H_z are interaction strength parameters. Our final Hamiltonian matrix is given by

$$\mathbf{H} = \begin{bmatrix} \epsilon_{00} + H_z & 0 & 0 & H_x \\ 0 & \epsilon_{10} - H_z & H_x & 0 \\ 0 & H_x & \epsilon_{01} + H_z & 0 \\ H_x & 0 & 0 & \epsilon_{11} - H_z \end{bmatrix}.$$

The four eigenstates of the above Hamiltonian matrix can in turn be used to define density matrices. As an example, the density matrix of the first eigenstate (lowest energy E_0) Ψ_0 is

$$\rho_0 = (\alpha_{00}|00\rangle\langle 00| + \alpha_{10}|10\rangle\langle 10| + \alpha_{01}|01\rangle\langle 01| + \alpha_{11}|11\rangle\langle 11|),$$

where the coefficients α_{ij} are the eigenvector coefficients resulting from the solution of the above eigenvalue problem.

Entropy

Define the von Neumann entropy

Schmidt decomposition, density matrices and entropy

The Schmidt decomposition is essentially a restatement of the singular value decomposition in a different context. To see this assume we use the above two-qubit basis states, that is $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. These states define a basis v_0, v_1, v_2, v_3 . We can easily generalize this to a basis with n states v_0, v_1, \dots, v_{n-1} . The basis is assumed to be orthogonal. Similarly we could define another basis w_0, w_1, \dots, w_{m-1} .

We can then in turn define the density matrix for the subsets A or B as

$$\rho_A = \text{Tr}_B(\rho_0) = \langle 0|\rho_0|0\rangle_B + \langle 1|\rho_0|1\rangle_B,$$

or

$$\rho_B = \text{Tr}_A(\rho_{\Psi_0}) = \langle 0|\rho_0|0\rangle_A + \langle 1|\rho_0|1\rangle_A.$$

The density matrices for these subsets can be used to compute the so-called von Neumann entropy, which is one of the possible measures of entanglement. A pure state has entropy equal zero while entangled states have an entropy larger than zero. The von-Neumann entropy is defined as

$$S(A, B) = -\text{Tr}(\rho_{A,B} \log_2(\rho_{A,B})).$$

First entanglement encounter