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A Density Matrix Approach Towards Quantum Computing

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Abstract:
In this article, the authors start with a discussion of various quantum states and their associated density matrices. The evaluation of the density matrices for pure, mixed, and entangled states is done elaborately. The concept of the trace of the density matrices is then explored and its relation with the purity of any state is discussed. The mathematical process of diagonalization of a matrix is studied for pure, mixed, and entangled states.

***Key Word**: Quantum states; Pure state; Mixed states; Entangled states; Density matrix; Purity of state*

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I. Introduction

Quantum states for any quantum system can be classified as pure, mixed, and entangled. The simplest example of understanding the **pure** quantum states is to solve Schrodinger's equation for the Hydrogen atom. The mixed states are composed of pure states with their classical probability amplitudes of occurrences (*e.g.*, mixing of the pure states due to measurements and/or the environmental interactions including noise, or due to faulty operators/gates/observables, all these resulting in the loss of quantum-ness of the system). Whereas the mixed states are separable, the entangled states cannot be separated. The purity of the density matrix is maximum for a pure and an entangled state, and it reduces for the mixed states. Any unitary operation performed on a quantum state alters its density matrix.

II. Quantum States: Pure, Mixed, and Entangled

A Hydrogen atom defines a single qubit system. The solution of the Schrodinger's equation for a Hydrogen atom yields Eigen values which are the various Quantum numbers (abbreviated in this paper as QN), namely the Principal QN, the Orbital QN, the Magnetic QN, and the Spin QN) (Griffiths 2003). The corresponding wave functions give the Eigen Vectors corresponding to each 'pure Quantum state' belonging to a separable complex Hilbert space (vector space). In a single Qubit system, we define just the two basis quantum states represented as the state vectors in bra-ket notation: $|0\rangle$ and $|1\rangle$. The pure Quantum states in a Hydrogen atom are the two energy levels, *i.e.*, an electron in the ground state denotes a pure Quantum state designated as $|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ in the matrix notation (Aitken 2017). Similarly, an electron in 1st excited energy level (state) denotes another pure Quantum state designated as $|1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$ in the matrix representation. Linear Algebra tells us that a linear combination (superposition) of these two pure states is also a valid solution of the Schrodinger's equation and hence represents a legitimate superposition state (which is a pure quantum phenomenon) of a single qubit quantum system, denoted as: $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle = \alpha\begin{bmatrix}1\\0\end{bmatrix} + \beta\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}\alpha\\\beta\end{bmatrix}$. Here α and β are the complex numbers from where the quantum probabilities of the electron to be in pure state $|0\rangle$ and $|1\rangle$ respectively can be extracted by computing their absolute square values. An electron in this superposition state can be viewed as making a transition between the ground state and the 1st excited state. Any measurement on this electron will collapse this superposition state into one of the basis states yielding the classical information of either $|0\rangle$ or $|1\rangle$, along with release of a photon of energy equal to the difference of the excited state energy and the ground state energy, or absorption of a photon of energy equal to the difference of the excited state energy and the ground state energy, respectively. An observable (a mathematical operator) is needed to extract the classical information from the pure states, *e.g.*, the energy operator, the angular momentum operator.

A mixed quantum state is obtained by classical probabilistic mixing of the pure quantum states of one or more sub-quantum systems. Whereas a pure state and entangled state are represented as points on the Bloch sphere, a mixed state is represented by a point inside the Bloch sphere. The authors would like to emphasize that a mixed state is not to be compared with a superposition state, a superposition state carries the quantum probability amplitudes of its constituent pure states, while a mixed state carries the classical amplitudes of the constituent pure/sub-system states. Pure states do not have any uncertainty outcome when an operator is operated upon it. A mixed state has uncertainty in the outcome when a certain operator is applied on it, and this uncertainty is given by the classical probability associated with its constituent pure states. When in a superposition state, the particle is present in all the constituent states at the same time, which has been proven by the interference experiments. Although the act of measurement on the particle in the superposition state, gradually pushes the particle out of the superposition state into one of its constituent states due to de-coherence (Schlosshauer 2007).

We now discuss the density matrices defined for pure, and mixed states (Blum 2012; Peres 1996). By definition, the density matrix for a quantum state $|\psi\rangle$ is evaluates as the outer product of $|\psi\rangle$ with itself:

$$\boldsymbol{\rho} = |\psi\rangle\langle\psi| \qquad (1)$$

For a pure state, the density matrix is an idempotent matrix, *i.e.*, $\boldsymbol{\rho}^2 = \boldsymbol{\rho}$. It is a projection operator, with its Trace =Rank=1=sum of its Eigen values=sum of all the diagonal terms. It implies that it has only one Eigen value as 1 and all other Eigen values as 0. Studying some of the examples of pure vector states to compute:

$$\text{Let} \quad |\psi_0\rangle = |0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \qquad (2)$$

$$\boldsymbol{\rho_0} = |\psi_0\rangle\langle\psi_0| = |0\rangle\langle 0| = \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \qquad (3)$$

Considering a superposition state (which is also a pure state) $|\psi_+\rangle$ which lies on the positive x −axis on the Bloch Sphere:

$$|\psi_+\rangle = \frac{(|0\rangle+|1\rangle)}{\sqrt{2}} = |+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\end{bmatrix} + \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \qquad (4)$$

$$\boldsymbol{\rho}_+ = |\psi_+\rangle\langle\psi_+| = |+\rangle\langle +| = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} \qquad (5)$$

As another example, consider $|\psi_\ell\rangle$ which lies on the negative y −axis on the Bloch sphere:

$$|\psi_\ell\rangle = \frac{(|0\rangle-i|1\rangle)}{\sqrt{2}} = |\ell\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\end{bmatrix} - \frac{i}{\sqrt{2}}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-i\end{bmatrix} \qquad (5)$$

$$\boldsymbol{\rho}_\ell = |\psi_\ell\rangle\langle\psi_\ell| = |\ell\rangle\langle\ell| = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-i\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & +i\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & +i\\-i & 1\end{bmatrix} \qquad (6)$$

Generalizing for n-qubits, we have $N = 2^n$ state vectors:

$$|\psi_N\rangle = \begin{bmatrix}\alpha_0\\\alpha_1\\\alpha_2\\\alpha_3\\\vdots\\\alpha_{N-1}\end{bmatrix} \qquad (7)$$

$$\boldsymbol{\rho_N} = |\psi_N\rangle\langle\psi_N| = \begin{bmatrix}\alpha_0\\\alpha_1\\\alpha_2\\\alpha_3\\\vdots\\\alpha_{N-1}\end{bmatrix}\begin{bmatrix}\alpha_0^* & \alpha_1^* & \alpha_2^* & \alpha_3^* & \dots & \alpha_{N-1}^*\end{bmatrix} = \begin{bmatrix}\alpha_0\alpha_0^* & \cdots & \alpha_0\alpha_{N-1}^*\\\vdots & \ddots & \vdots\\\alpha_{N-1}\alpha_0^* & \cdots & \alpha_{N-1}\alpha_{N-1}^*\end{bmatrix} \qquad (8)$$

From Eqn. (8), we notice that the diagonal terms of the $N \times N$ density matrix are of the form $\alpha_i\alpha_i^* = |\alpha_i|^2$, which give us the probability of finding a state vector (basis vector) in a particular Eigen state. The off-diagonal terms give the information about the coherence of these states, *i.e.*, whether the states are pure or mixed states.

An example of $n = 2$ qubits, implying the number of state vectors is $N = 2^2 = 4$, a superposition state denoted as $|\psi_4\rangle$ (which is a pure state) with equal quantum probability of all the 4 state vectors is written as:

$$|\psi_4\rangle = \frac{(|00\rangle+|01\rangle+|10\rangle+|11\rangle)}{2} = \frac{1}{2}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \frac{1}{2}\begin{bmatrix}0\\1\\0\\0\end{bmatrix} + \frac{1}{2}\begin{bmatrix}0\\0\\1\\0\end{bmatrix} + \frac{1}{2}\begin{bmatrix}0\\0\\0\\1\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1\\1\\1\\1\end{bmatrix} \quad (9)$$

$$\boldsymbol{\rho}_4 = |\psi_4\rangle\langle\psi_4| = \frac{1}{2}\begin{bmatrix}1\\1\\1\\1\end{bmatrix}\frac{1}{2}\begin{bmatrix}1 & 1 & 1 & 1\end{bmatrix} = \frac{1}{4}\begin{bmatrix}1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\end{bmatrix} \quad (10)$$

Eqns. (9) and (10) represent a pure state (in superposition of all 4 state vector for a 2-qubit system) and its corresponding density matrix showcasing maximum off-diagonal terms signifying maximum coherence, and the diagonal terms summing up to unity probability (*i.e.*, trace=1 for a pure state) (Luo and Sun 2017; Schlosshauer 2007; Schlosshauer 2019).

Considering now an example of evaluating the density matrix of a mixed state: Let a pure 1-qubit superposition state $|\psi_+\rangle = |+\rangle = \frac{(|0\rangle+|1\rangle)}{\sqrt{2}} = |+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\end{bmatrix} + \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$ be transmitted from location A to B. Due to environmental factors the transmitted qubit $|+\rangle$ gets flipped to qubit $|-\rangle$ by a 25% probability (this is classical probability), with the result that the qubit received at B is either $|+\rangle$ or $|-\rangle$ with 75 % and 25% probability respectively. Hence the qubit received and '*measured*' at B is in a mixed state represented as: $|\psi_\pm\rangle = \begin{Bmatrix}|+\rangle & , & |-\rangle\\ \frac{3}{4}(\boldsymbol{P}_+) & , & \frac{1}{4}(\boldsymbol{P}_-)\end{Bmatrix} = \begin{Bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}, & \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}\\ \frac{3}{4} \quad , & \frac{1}{4}\end{Bmatrix}$; In this representation, the upper row tells the constituents of the measured mixed state at location B, and the bottom row tells the corresponding classical probability of measurement ($\boldsymbol{P}$). The individual states of a mixed state need not be the Eigen states of the computational basis. The density matrix can be evaluated as

$$\boldsymbol{\rho}_\pm = \boldsymbol{P}_\pm|\psi_\pm\rangle\langle\psi_\pm| = \frac{3}{4}(|+\rangle\langle+|) + \frac{1}{4}(|-\rangle\langle-|) \quad (11)$$

$$\boldsymbol{\rho}_\pm = \frac{3}{4}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\end{bmatrix} + \frac{1}{4}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1\end{bmatrix} \quad (12)$$

$$\boldsymbol{\rho}_\pm = \frac{3}{8}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} + \frac{1}{8}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix} \quad (13)$$

$$\boldsymbol{\rho}_\pm = \frac{1}{8}\begin{bmatrix}4 & 0\\0 & 4\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \quad (14)$$

The density matrix of the considered mixed state shows zero off-diagonal terms, meaning that there is no coherence in the mixed state measured at B (Luo and Sun 2017). The density matrix for a mixed state of an n −qubit system ($N = 2^n$) can in general be written as:

$$\boldsymbol{\rho} = \sum_{i=0}^{N-1} \boldsymbol{P}_i\,|\psi_i\rangle\langle\psi_i| \quad (15)$$

Where $\boldsymbol{P}_i$ is the classical probability of i^{th} constituent vector state of the mixed state. Eqn. (15) also signifies the post-measurement density matrix of the ensemble of the quantum states at destination B in this example. And the density matrix of the corresponding pure quantum state $|\psi_+\rangle$ transmitted from point A being given by Eqn. (5) above. Comparing Eqns. (5) and (14), we can state that the process of measurement (of an observable) leads to interaction with the environment and hence erases the off-diagonal elements that carry the superposition/entanglement information, hence converting the density matrix towards a diagonal matrix. A completely de-coherent state has a density matrix with only finite diagonal elements.

Mathematically a matrix A can be diagonalized as

$$\mathbb{P}^{-1}A\mathbb{P} = D \tag{16}$$

Where $\mathbb{P}$ is a matrix consisting of Eigen vectors of matrix A and D is the corresponding diagonal matrix of matrix A.

Computing the Eigen values (λ), Eigen vectors (υ), and the corresponding diagonal matrix (D) for a pure state vector $|+\rangle$ as follows: Starting from Eqn. (5), we calculate the two Eigen values of $\boldsymbol{\rho}_+ = \frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}$ by solving the determinant

$$|\boldsymbol{\rho}_+ - \lambda \mathrm{I}| = 0 \tag{17}$$

We get $\lambda_{1,2} = 0, 1$ and corresponding $\upsilon_{1,2} = \begin{bmatrix}a\\ -a\end{bmatrix}, \begin{bmatrix}b\\ b\end{bmatrix}$ where a, b are complex constants. Diagonalization of $\boldsymbol{\rho}_+$ as per Eqn. (16) yields $D = \begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}$, which has Trace= rank=1.

We will now consider maximally entangled states, *e.g.*, the four Bell states (Bell 1964):

$$|\beta_{00}\rangle = \frac{(|00\rangle+|11\rangle)}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\1\end{bmatrix} \tag{18}$$

The density matrix for $|\beta_{00}\rangle$ can be evaluated as:

$$\boldsymbol{\rho}_{\beta_{00}} = |\beta_{00}\rangle\langle\beta_{00}| = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & 0 & 1\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 1\end{bmatrix} \tag{19}$$

$$|\beta_{01}\rangle = \frac{(|01\rangle+|10\rangle)}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\0\\0\end{bmatrix} + \frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\1\\0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\1\\0\end{bmatrix} \tag{20}$$

The density matrix for $|\beta_{01}\rangle$ can be evaluated as:

$$\boldsymbol{\rho}_{\beta_{01}} = |\beta_{01}\rangle\langle\beta_{01}| = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\1\\0\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}0 & 1 & 1 & 0\end{bmatrix} = \frac{1}{2}\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 1 & 1 & 0\\ 0 & 1 & 1 & 0\\ 0 & 0 & 0 & 0\end{bmatrix} \tag{21}$$

$$|\beta_{10}\rangle = \frac{(|01\rangle-|10\rangle)}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\0\\0\end{bmatrix} - \frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\1\\0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\-1\\0\end{bmatrix} \tag{22}$$

The density matrix for $|\beta_{10}\rangle$ can be evaluated as:

$$\boldsymbol{\rho}_{\beta_{10}} = |\beta_{10}\rangle\langle\beta_{10}| = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\-1\\0\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}0 & 1 & -1 & 0\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & 0 & 0 & 1\\ 0 & 1 & -1 & 0\\ 0 & -1 & 1 & 0\\ 1 & 0 & 0 & 1\end{bmatrix} \tag{23}$$

$$|\beta_{11}\rangle = \frac{(|00\rangle-|11\rangle)}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} - \frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\-1\end{bmatrix} \tag{24}$$

The density matrix for $|\beta_{00}\rangle$ can be evaluated as:

$$\boldsymbol{\rho}_{\beta_{11}} = |\beta_{11}\rangle\langle\beta_{11}| = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 0 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \tag{25}$$

Eqns. (19), (21), (23), and (25) show that the density matrices corresponding to the maximally entangled Bell states have Trace=Ranks=1. The off-diagonal terms are finite (unity) only along the other diagonal (not the main diagonal) of these density matrices and are symmetrically placed with respect to the diagonal terms, showing maximum coherence.

Another term to find the purity (γ) of a quantum state is defined as

$$\gamma = Tr(\boldsymbol{\rho}^2) \tag{26}$$

For pure and completely entangled states, $\boldsymbol{\rho} = \boldsymbol{\rho}^2$, *i.e.*, the density matrix is idempotent, but for mixed states, this does not hold true. The value of purity (γ) lies in the range $\frac{1}{2^n} \leq \gamma \leq 1$ where n is the number of qubits in the quantum system under consideration. For pure states, $\gamma = 1$ because $Tr(\boldsymbol{\rho}) = Tr(\boldsymbol{\rho}^2) = 1$. Whereas for completely mixed states, it can be shown that $\gamma = \frac{1}{2^n}$ (Blum 2012).

For the sake of completeness, when a unitary operator is applied on a vector state, *e.g.*,

$$|\psi_{in}\rangle \xrightarrow{U} |\psi_{out}\rangle \tag{27}$$

Then it can be proved that the evolution of the corresponding density matrix $\boldsymbol{\rho}_{in}$ through the same unitary operation yields $\boldsymbol{\rho}_{out}$ which is the density matrix for $|\psi_{out}\rangle$:

$$\boldsymbol{\rho}_{in} \xrightarrow{U} \boldsymbol{\rho}_{out} = U\boldsymbol{\rho}_{in}U^{\dagger} \tag{28}$$

Where the symbol † signifies conjugate transpose.

III. Discussion

The authors have analyzed the density matrices for pure, mixed, and entangled quantum states and shown that the Trace for all these cases is one. The concept of purity of a quantum state is discussed.

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