Density Operator and its significance in Quantum Information

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Working with state-vector notation representation is convenient when dealing with states that can always be expressed as a linear combination of basis states, each with an associated probability amplitude. However, in quantum computation and quantum communication, there are many practical scenarios in which the state of our qubits cannot be written down as linear combinations in a given basis, but instead must be expressed in terms of statistical mixtures of multiple states, each with an associated probability of occurrence. Simply put, the **density matrix is an alternative way of expressing quantum states**. However, unlike the state-vector representation, this formalism allows us to use the same mathematical language to describe both the *pure states*, as well as the *mixed states* that consist of mixtures of pure states.

Pure States: Pure states are those for which we can precisely define their quantum state at every point in time. We understand that if we were to perform a measurement of $|+\rangle$ state, the outcome will be probabilistic. We will measure state $|0\rangle$with 50% probability, state $|1\rangle$ with 50% probability. However, before performing any measurements we can say with 100% certainty that, if our qubit initialization process and our Hadamard gate are ideal, the resulting quantum state will always be $|+\rangle$. We therefore say that, since there is no uncertainty on what this quantum state will be, $|q\rangle$ is a pure state.

Mixed States: Mixed states are those that consist of statistical ensembles of different quantum states. This means that, unlike pure states, mixed states cannot be represented as linear superpositions of normalized state vectors. Consider, once again, the two-qubit entangled state: $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$ we know that since qubits A and B are entangled, measuring a $|0\rangle$ in q1 implies that the quantum state in register q0 will immediately project onto state $|0\rangle$. We know that after a measurement, ψB will be in state $|0B\rangle$ or in state $|1B\rangle$ with probability 1/2; however, ψB is **not** in a linear superposition of $|0B\rangle$ and $|1B\rangle$. In other words, ψB **cannot** be expressed as a state vector of the form (1/√ 2)($|0B\rangle$+$|1B\rangle$). Instead, we have to use a different notation to write down that ψB is rather an ensemble of the states $|0B\rangle$ and $|1B\rangle$.

We then call ψB a mixed state, which can be represented as an ensemble of states: {|ψB0⟩,|ψB1⟩}={|0B⟩,|1B⟩}, each with an associated probability of occurrence: {p0,p1}={1/2,1/2}
In general, a mixed state consisting of an ensemble of n pure states can be expressed in the form of a list of outcome elements: {|ψj⟩}j=1n={|ψ1⟩,|ψ2⟩,...,|ψn⟩}, where each item has a corresponding probability of occurrence given by: {pj}nj=1={p1,p2,...,pn}

Although this way of expressing ψB (or any general mixed state) is perfectly valid, it turns out to be somewhat inconvenient. Since a mixed state can consist of a myriad of pure states, it can be difficult to track how the whole ensemble evolves when, for example, gates are applied to it. It is here that we turn to the density matrix representation. A mixed state, consisting of several possible outcome pure states |ψj⟩, each with probability of occurrence pj, is defined as a density matrix of the form:
ρ≡∑pj|ψj⟩⟨ψj|

Significance in Quantum Information

- **State purity:** A very useful property of the density matrix is that when taking the trace of its square, we obtain a scalar value γ that is good measure of the purity of the state the matrix represents. For normalized states, this value is always less than or equal to 1, with the equality occurring for the case of a pure state.
- **Reduced Density Matrix:** Another advantage of working with the density matrix notation is that, when dealing with composite systems, it provides a practical way to extract the state of each subsystem, even if they are entangled. This is done in the form of what is known as the reduced density matrix.

  Consider a quantum system composed of subsystems A and B , and fully described by the density matrix ρAB . The reduced density matrix of subsystem A is then given by: ρA = Tr B (ρAB). Here, TrB is an operation known as the partial trace, which is defined as:

TrB (| ξu ⟩⟨ ξv |⊗| χu ⟩⟨ χv |) ≡ | ξu ⟩⟨ ξv | Tr (| χu ⟩⟨ χv |), where |ξu⟩ and |ξv⟩ are arbitrary states in the subspace of A , and | χu ⟩ and | χv ⟩ arbitrary states in the subspace of B . Similarly, we can calculate the reduced density matrix of subsystem B using the partial trace over A : Tr A (| ξu ⟩⟨ ξv | ⊗ | χu ⟩⟨ χv |) ≡ Tr(| ξu ⟩⟨ ξv |) |χu ⟩⟨ χv |.

As an example, let's reconsider the pure entangled state:

| ψ A B ⟩ = (1 /√ 2) (| 00 ⟩ + | 11 ⟩)

We know that this system is not separable (i.e.,| χ A B ⟩ ≠ | χ A ⟩ ⊗ | χ B ⟩); however, by using the reduced density matrix, we can find a full description for subsystems A and B.

To calculate the reduced density matrix for, let's say, subsystem B , we have: ρ B = 1 2 [1 0 0 1]. We can then conclude that the reduced density matrix ρB is a way to describe the statistical outcomes of subsystem B , when the measurement outcomes of subsystem A are averaged out. This is in fact what ”tracing out” subsystem A means.

- **Mixed State in Bloch Sphere:**

  | q ⟩ = cos (θ 2) | 0 ⟩ + e i φ sin (θ 2) | 1 ⟩ .

  The qubit can be represented as a vector extending from the origin to the surface of a sphere of unit radius, with its orientation determined by these two angles.

  This geometrical interpretation of states can be generalized to also include mixed states. This is done by relying on the fact that the density matrix of a single-qubit state can be expanded in the form:

$$\rho = \frac{1}{2}\left(\hat{I} + \vec{r}\cdot\hat{\vec{\sigma}}\right)$$

$$\rho = \frac{1}{2}\hat{I} + \frac{1}{2}r_x\hat{\sigma}_x + \frac{1}{2}r_y\hat{\sigma}_y + \frac{1}{2}r_z\hat{\sigma}_z,$$

This is a very convenient way of expressing that this state is not pure because it has been corrupted by noise. Rather than having to use three separate Bloch spheres to represent each of the three possible pure-state outcomes given in the example (ψ_1 , ψ_2 , ψ_3), we now have a single Bloch vector representation for our noisy state.

- **Visualising Multi-Qubit State:** One last scenario we might want to consider is the possibility of visualizing multi-qubit states using multiple Bloch spheres. :

$| \psi_{CD} \rangle = 1/(2\sqrt{2}) (\sqrt{3} | 00 \rangle + | 01 \rangle + | 10 \rangle + \sqrt{3} | 11 \rangle)$.

Here, $| 00 \rangle$ and $| 11 \rangle$ have the same probability of occurrence, but are 3 times more likely to occur than $| 01 \rangle$ and $| 10 \rangle$. Since this is an entangled state, we know that it is not separable (i.e.,
$| \psi_{CD} \rangle \neq | \psi_C \rangle \otimes | \psi_D \rangle$); therefore, this state cannot be represented in terms of unit vectors in two individual Bloch spheres. However, by expressing C and D in terms of their reduced density matrices ρ_C and ρ_D , we can then visualize the composite state as two Bloch vectors, one for each of these matrices.
$\rho_D = [1/2, 0.43301, 0.43301, 1/2]$

$\rho_C = [1/2, 0.43301, 0.43301, 1/2]$

Each of these reduced density matrices has a Bloch vector associated with them, each with components:

$r_x \approx 0.86602$, $r_y = 0$, $r_z = 0$

Understanding the Bloch vector representation for multi-qubit states explains why, when we try to plot a two-qubit maximally entangled state in the Bloch sphere, we get an "empty" plot. Since the reduced density matrices of a state like:

$| \psi_{AB} \rangle = (1/\sqrt{2}) (| 00 \rangle + | 11 \rangle)$ are given by: $\rho_A = \rho_B = 1/2 [1 0 0 1] = 1/2 I$,

we see that the Bloch vector components r_x , r_y , r_z are all 0. Therefore, ρ_A and ρ_B actually have r vector of zero length, represented by points at the origin of the sphere