Quantum Information and Computing- II Density Matrix Formulation of Quantum Mechanics

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1 Introduction

Earlier, we have discussed the postulates of quantum mechanics. However, under many situations, we find these axioms to be violated. This happens because most of the time, the system that we wish to study, is a part of a much larger system. In such a case, it is found that (i) the states may not be represented by rays in their own Hilbert space, (ii) measurements may not be orthogonal projections and the evolution may not be unitary. To illustrate this consider the following two examples:

Consider a two dimensional Hilbert space with basis vectors $\{\mid x\rangle, \mid y\rangle\}$. Suppose we prepare a large number of such systems, where each of the members is prepared in one of the two states,

$$
\mid a\rangle = \alpha \mid x\rangle + \beta \mid y\rangle
$$
$$
\mid b\rangle = \gamma \mid x\rangle + \delta \mid y\rangle \tag{1}
$$

where $\mid \alpha \mid^2 + \mid \beta \mid^2 = \mid \gamma \mid^2 + \mid \delta \mid^2 = 1$. Thus, if we select a system in state $\mid a\rangle$ and make a measurement in the basis $\{\mid x\rangle, \mid y\rangle\}$, we would get the state $\mid x\rangle$ with a probability $\mid \alpha \mid^2$ and likewise for the result $\mid y\rangle$.

Suppose now, that out of the N systems prepared by us n_a systems are in the state $\mid a\rangle$ and n_b number of the systems are in the state $\mid b\rangle$, such that $n_a + n_b = N$. If we pick a random system from this ensemble of N systems, the probability that the selected system is in the state $\mid a\rangle$ has a probability $p_a = n_a/N$ and the probability it it has the state $\mid b\rangle$ has a probability $n_b/N = 1 - p$. These probabilities are just the classical probability which works at the ensemble level. However, once the system is selected, the measurement probabilities are determined by Born interpretation of quantum mechanics. This is an

example of an open system in which we need to modify our rules of quantum mechanise, as discussed earlier.

Consider a second example. Suppose we call our system of interest as system A which interacts with its environment, which we call as system B. If the state of the combined system factorises into a product of a state of system A with that of system B,i.e. if

$$| \psi_{AB} \rangle = | \psi_A \rangle \otimes | \psi_B \rangle$$

the effect of the environment can be neglected because given any operator $\mathcal{O}_A$, which only acts on the system A but not on B, we have

$$\langle \psi_{AB} | \mathcal{O}_A | \psi_{AB} \rangle = \langle \psi_A | \mathcal{O}_A | \psi_A \rangle$$

In such a situation, the system A is said to be in a **pure state**. However, if the state of system of interest is not disentangled from the environment, the effect of the environment cannot be factored out. The word "environment" need not be a big system, one could consider a two bit system, with one of the qubits belonging to the Hilbert space $\mathcal{H}_A$ and the other (the "environment") belonging to the Hilbert space $\mathcal{H}_B$. Consider a state in the composite space $\mathcal{H}_A \otimes \mathcal{H}_B$,

$$| \psi \rangle = a | 0 \rangle_A \otimes | 0 \rangle_B + b | 1 \rangle_A \otimes | 1 \rangle_B$$

Note that the qubits A and B are correlated in that when we measure the qubit A, we would project it to $\{| 0 \rangle, | 1 \rangle\}$ basis of system A. The probability with which we will find it is state $| 0 \rangle$ is $| a |^2$. In this case, the state would collapse to $| 0 \rangle_A \otimes | 0 \rangle_B$. Note that the system B is in a definite state. Same is true of the measurement $| 1 \rangle_A$. The system A is said to be in a **mixed state**. In dealing with mixed state (as also with pure state) a more appropriate formalism is provided by **Density Matrix**.

2   Density Matrix

Let us look at a general measurement of the system A irrespective of its effect on B. Such a measurement operator is $M_A \otimes I_B$. We then have,

$$\begin{aligned}
_{AB}\langle \psi | M_A \otimes I_B | \psi \rangle_{AB} &= [a^*{}_A\langle 0 | \otimes {}_B\langle 0 | + b^*{}_A\langle 1 | \otimes {}_B\langle 1 | (M_A \otimes I_B)[a | 0 \rangle_A \otimes | 0 \rangle_B + b | 1 \rangle_A \otimes | 1 \rangle_B \\
&= | a |^2 {}_A\langle 0 | M_A | 0 \rangle_A + | b |^2 {}_A\langle 1 | M_A | 1 \rangle_A \\
&= \langle M_A \rangle = \text{tr}(M_A \rho_A)
\end{aligned} \tag{2}$$

where the operator ρ_A is the density operator or the density matrix,

$$\rho_A = | a |^2 | 0 \rangle_A {}_A\langle 0 | + | b |^2 | 1 \rangle_B {}_B\langle 1 |$$

and the operator M_A acts on qubit A only. We can interpret ρ_A as an ensemble of possible quantum states each of which occur with a specified probability, $P_0 = | a |^2, P_a = | b |^2$. Thus, in the above, we have talked about two distinct type of states:

1. A coherent superposition of states $| 0 \rangle_A$ and $| 1 \rangle_A$

2. a probabilistic superposition in which the states $| 0 \rangle$ and $| 1 \rangle$ occur with a predetermined and specified probability.

To see the distinction consider measurement of σ_x in these two types of states. Consider a coherent superposition $\frac{1}{\sqrt{2}}(| 0 \rangle + | 1 \rangle)$. The expectation value of σ_x in this state is given by

$$
\begin{aligned}
\langle \sigma_x \rangle &= \frac{1}{2} \left(\langle 0 | + \langle 1 | \right) X \left(| 0 \rangle + | 1 \rangle \right) \\
&= \frac{1}{2} \left(\langle 0 | + \langle 1 | \right) \left[| 0 \rangle \langle 1 | + | 1 \rangle \langle 0 | \right] \left(| 0 \rangle + | 1 \rangle \right) \\
&= \frac{1}{2} \left(\langle 0 | + \langle 1 | \right) \left(\langle 1 | + \langle 0 | \right) \\
&= 1
\end{aligned}
$$

On the other hand, if we consider an ensemble in which the state $| 0 \rangle$ and $| 1 \rangle$ occur with a probability of 1/2 each, we get $\langle \sigma_x \rangle = \frac{1}{2} \left(\langle \alpha | X | \alpha \rangle + \langle \beta | X | \alpha \rangle \right) = 0$. In this case the density matrix is

$$
\rho = \frac{1}{2} \left(| \alpha \rangle \langle \alpha | + | \beta \rangle \langle \beta | \right) = \frac{I}{2}
$$

so that

$$
\langle \sigma_x \rangle = \text{tr}(\sigma_x \rho) = \frac{1}{2} \text{tr}(\sigma_x) = 0
$$

Thus the density operator is an average operator which allows us to describe a system which is not necessarily in a pure state but may be a statistical mixture of pure states. we first start with the case where the system is in a pure state. Let $\{ | e_i \rangle \}$ be a basis in the Hilbert space of the system in terms of which the state $| \psi \rangle$ is given by $| \psi \rangle = \sum_i c_i | e_i \rangle$. Note that this is not a mixture but is a pure state. The expectation value of an operator $\hat{A}$ in this state is given by

$$
\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_{i,j} c_i^* c_j A_{i,j}
$$

where $A_{i,j} = \langle e_i | \hat{A} | e_j \rangle$, $c_j = \langle e_j | \psi \rangle$ and $c_i^* = \langle \psi | e_i \rangle$. We have

$$
\begin{aligned}
c_i^* c_j &= \langle \psi | e_i \rangle \langle e_j | \psi \rangle \\
&= \langle e_j | \psi \rangle \langle \psi | e_i \rangle \\
&= \langle e_j | \left(| \psi \rangle \langle \psi | \right) | e_i \rangle \\
&= \langle e_j | \hat{\rho} | e_i \rangle
\end{aligned}
$$

where

$$
\hat{\rho} = | \psi \rangle \langle \psi | \tag{3}
$$

is the density matrix for the pure state, which is just the projection operator for the state $|\psi\rangle$. In terms of the density matrix, the expectation value of $\hat{A}$ can be written as

$$\langle \hat{A} \rangle = \sum_{i,j} \langle e_j \, |\hat{\rho}| \, e_i \rangle A_{i,j}$$

. We can rewrite the above expectation value as follows:

$$\langle \hat{A} \rangle = \sum_{i,j} \langle e_j \, |\psi\rangle\langle\psi \, |e_i\rangle\langle e_i \, |\hat{A}| \, e_j\rangle$$

$$= \sum_{i,j} \langle e_j \, |\hat{\rho}| \, e_i\rangle\langle e_i \, |\hat{A}| \, e_j\rangle$$

$$= \sum_{j} \langle e_j \, |\hat{\rho}\hat{A}| \, e_j\rangle$$

$$= \operatorname{tr} \hat{\rho}\hat{A} \tag{4}$$

In the last but one step, we have used the completeness relation to perform the sum over i. Note that the trace of $\hat{\rho}$ itself can be calculated as follows, since trace can be calculated in any basis,

$$\operatorname{tr} \rho = \sum_{i} \langle e_i \, |\hat{\rho}| \, e_i\rangle = \sum_{i} \langle e_i \, |\psi\rangle\langle\psi \, |e_i\rangle$$

$$= \sum_{i} c_i^* c_i = \sum_{i} |\, c_i \,|^2 = 1$$

Example:

A system is in the state $|\psi\rangle = \dfrac{1}{\sqrt{3}} \, |e_1\rangle + i\sqrt{\dfrac{2}{3}} \, |e_2\rangle$. Determine the density operator and find its trace.

Solution:

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

$$= \left(\frac{1}{\sqrt{3}} \, |e_1\rangle + i\sqrt{\frac{2}{3}} \, |e_2\rangle\right)\left(\frac{1}{\sqrt{3}}\langle e_1| - i\sqrt{\frac{2}{3}}\langle e_2|\right)$$

$$= \frac{1}{3} \, |e_i\rangle\langle e_1| + \frac{2}{3} \, |e_2\rangle\langle e_2| - \frac{i}{3}\sqrt{2} \, |e_1\rangle\langle e_2| + i\frac{\sqrt{2}}{3} \, |e_2\rangle\langle e_1|$$

The trace is easy to calculate

$$\operatorname{tr} \hat{\rho} = \langle e_1 \, |\hat{\rho}| \, e_2\rangle + \langle e_2 \, |\hat{\rho}| \, e_2\rangle = \frac{1}{3} + \frac{2}{3} = 1$$

How does the density operator evolve with time? As the state $|\psi\rangle$ satisfies the Schrödinger equation, we have

$$i\hbar\frac{d}{dt} \, |\psi\rangle = \mathcal{H} \, |\psi\rangle \tag{5a}$$

$$-i\hbar\frac{d}{dt}\langle\psi| = \langle\psi| \, \mathcal{H} \tag{5b}$$

We thus have

$$i\hbar \mid \psi\rangle\langle\psi \mid = \left(i\hbar\frac{d}{dt} \mid \psi\rangle\right)\langle\psi \mid + \mid \psi\rangle\left(i\hbar\frac{d}{dt}\langle\psi \mid\right)$$
$$= \mathcal{H} \mid \psi\rangle\langle\psi \mid - \mid \psi\rangle\langle\psi \mid \mathcal{H}$$
$$= [\mathcal{H}, \rho]$$

where we have use (**??**) and (**??**). Thus the density matrix satisfies Liouville equation,

$$i\hbar\frac{d}{dt}\hat{\rho} = [\mathcal{H}, \hat{\rho}] \tag{6}$$

Note that though ρ is an operator, it does not satisfy the quantum mechanical Heisenberg equation of motion. This is because the density operator does not represent any observable and simply has the mathematical structure of an operator.

The density operator is clearly hermitian as $\rho^\dagger = \mid \psi\rangle\langle\psi \mid$. Further,

$$\rho^2 = (\mid \psi\rangle\langle\psi \mid)(\mid \psi\rangle\langle\psi \mid) = \mid \psi\rangle\hat{I}\langle\psi \mid = \rho$$

This is true of pure states only, for which we have,

$$\operatorname{tr}\rho^2 = \operatorname{tr}\rho = 1$$

Not also that ρ is a **positive operator**, because for an arbitrary state $\mid \phi\rangle$, we have

$$\langle\phi \mid\rho\mid \phi\rangle = \langle\phi \mid\psi\rangle\langle\psi \mid\phi\rangle = \mid \langle\phi \mid\psi\rangle \mid^2$$

Since ρ is self adjoint (hence normal) we can use a spectral decomposition for the operator

$$\rho = \sum_n \lambda_n \mid n\rangle\langle n \mid$$

As ρ is a positive operator, the eigenvalues are nonnegative. This along with $\operatorname{tr}\rho = 1$ gives $\sum_n \lambda_n = 1$,

3   Mixed State Density Matrix

If instead of a pure state, we have an ensemble in which systems could be in various states $\mid \psi\rangle$ with classical probability p_i, we define the density operator by the relation

$$\rho = \sum_i p_i\rho_i = \sum_i p_i \mid \psi_i\rangle\langle\psi_i \mid \tag{7}$$

The states $\mid \psi_i\rangle$ s need not be orthogonal.The properties of the density operator are as follows:

(i) $\rho^\dagger = \rho$

(ii) ρ is a positive operator

(iii) $\text{tr}(\rho) = 1$

(iv) $\langle A \rangle = \text{tr}(\rho A)$

(v) It satisfies Liouville equation $i\hbar \dfrac{d}{dt}\rho = [\mathcal{H}, \rho]$

3.1 Density Matrix and Bloch Sphere

Consider the density matrix corresponding to spin $1/2$. Recall that a point on the Bloch sphere is associated with the state of a qubit. Naturally, for every point on the Bloch sphere, we can associate a density matrix as well. One can see it directly by considering the eigenstates of σ_n, where the unit vector $\hat{n}$ has coordinates $(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. The eigenstates are given by

$$| \psi \rangle = \begin{pmatrix} \cos\dfrac{\theta}{2} \\ e^{i\varphi}\sin\dfrac{\theta}{2} \end{pmatrix}$$

The corresponding density matrix can be calculated using $\rho = | \psi \rangle \langle \psi |$, so that

$$
\begin{aligned}
\rho &= | \psi \rangle \langle \psi | \\
&= \begin{pmatrix} \cos^2\dfrac{\theta}{2} & e^{-i\varphi}\sin\dfrac{\theta}{2}\cos\dfrac{\theta}{2} \\ e^{i\varphi}\sin\dfrac{\theta}{2}\cos\dfrac{\theta}{2} & \sin^2\theta \end{pmatrix} \\
&= \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \\
&= \dfrac{1}{2}I + \dfrac{1}{2}\sin\theta\cos\varphi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \dfrac{1}{2}\sin\theta\sin\varphi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \dfrac{1}{2}\cos\theta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= \dfrac{1}{2}(1 + \hat{n} \cdot \vec{\sigma})
\end{aligned}
$$

It is possible to associate a density matrix for the mixed state with the Bloch sphere, only that such points lie inside the sphere and not on it as is the case for the pure states.

Since any 2×2 matrix can be written in terms of a unit matrix and the three Pauli matrices σ_x, σ_y and σ_z , we can write

$$\rho = \dfrac{1}{2}(1 + \vec{a} \cdot \vec{\sigma})$$

Since $\text{tr}(\sigma_i) = 0$ and $\text{tr}(I) = 2$ for a 2×2 identity matrix, we have $\text{tr}(\rho) = 1$. the vector $\vec{a}$ is called the Bloch vector. Note that

$$
\begin{aligned}
\sigma_x &= \text{tr}(\sigma_x \rho) \\
&= \frac{1}{2} \text{tr} \left(\sigma_x (1 + a_x \sigma_x + a_y \sigma_y + a_z \sigma_z) \right) \\
&= \frac{a_x}{2} \text{tr}(\sigma_x^2) \\
&= \frac{a_x}{2} \times 2 = a_x
\end{aligned}
$$

In the above we have used the properties of the Pauli matrices such as $\sigma_x \sigma_y = i\sigma_z$, $\sigma_i^2 = I$ and the fact that the trace of σ_i is zero. The above result shows that a_x, a_y and a_z are respectively the expectation values of σ_x, σ_y and σ_z. Let us calculate the trace of ρ^2. We have,

$$
\begin{aligned}
\text{tr}(\rho^2) &= \text{tr}[\frac{1}{4}(I + \vec{a} \cdot \sigma)^2] \\
&= \frac{1}{4} \text{tr}[I^2 + a_x^2 \sigma_x^2 + a_y^2 \sigma_y^2 + a_z^2 \sigma_z^2 + 2a_x \sigma_x + 2a_y \sigma_y + 2a - z\sigma_z] \\
&= \frac{1}{2}[1 + a_x^2 + a_y^2 + a_z^2] \\
&= \frac{1 + |a|^2}{2}
\end{aligned}
$$

In the above, we have used $\text{tr}(\sigma_i) = 0$ and $\text{tr}(\sigma_i^2) \equiv \text{tr}(I) = 2$. Thus for mixed states, we require the distance from the centre $|a|$ to be less than 1 and hence they lie *inside* the Bloch sphere.

What is the difference between a pure state $|\psi\rangle = \frac{1}{2}(|0\rangle + |1\rangle)$ and a system which is a statistical mixture of 50% in $|0\rangle$ and another 50% in $|1\rangle$ state? For the pure state, the state $|\psi\rangle$ is on the Bloch sphere with $\theta = \pi/2, \varphi = 0$, because the state has a matrix representation

$$
\psi(\frac{\pi}{2}, 0) = \begin{pmatrix} \cos(\frac{\pi}{4}) \\ e^{i \times 0} \sin(\frac{\pi}{4}) \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)
$$

If we rotate this state on the Bloch sphere by $-\pi/2$ about the y-axis, the state would go to the north pole, i.e. to the state $|0\rangle$. On measurement, we would get the state $|0\rangle$ with unit probability. Consider now what would happen if we had a mixture given above. Rotating the Bloch sphere by $-\pi/2$ about the y-axis would take $|0\rangle$ to the equator, to the state $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Similarly the state $|1\rangle$ would go to $\frac{1}{2}(|0\rangle + |1\rangle)$. Hence we would, on measurement, get the state $|0\rangle$ with 50% probability and the state $|1\rangle$ with 50% probability, the same as was the case before rotation. The mixed state lies at the origin of the Bloch sphere and hence does not change on rotation described above.

Does density matrix uniquely represent a physical system? For a mixed system, the answer is no. Consider the 50-50 mixture given above. The density matrix is

$$\rho = \frac{1}{2}(|\,0\rangle\langle 0\,| + |\,1\rangle\langle 1\,|) = \frac{I}{2}$$

Consider a different mixture consisting of 50% in the state $|\,+\rangle = \frac{1}{2}(|\,0\rangle + |\,1\rangle)$ and another 50% in the state $|\,-\rangle = \frac{1}{2}(|\,0\rangle - |\,1\rangle)$. The density matrix works out to be same as in the previous case!

The elements of the density matrix are interpreted as follows. If a system is described by a density matrix ρ, the probability of of finding it in a state $|\,\psi\rangle$ is given by $\langle P_\psi\rangle$, where $P_\psi = |\,\psi\rangle\langle\psi\,|$ is the projection operator for the state $|\,\psi\rangle$. Consider a pure state $|\,\psi\rangle = a\,|\,0\rangle + b\,|\,1\rangle$. The probability of finding this state in the state $|\,0\rangle$ is $\langle\psi\,|P_0|\,\psi\rangle = |\,a\,|^2$. For an arbitrary state described by a density matrix,

$$P_0 = \text{tr}(P_0\rho)$$

$$= \text{tr}\left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}\right]$$

$$= \text{tr}\begin{pmatrix} \rho_{00} & \rho_{01} \\ 0 & 0 \end{pmatrix} = \rho_{00} = \frac{1 + a_z}{2}$$

Likewise, the probability to find it in state $|\,1\rangle$ is given by

$$P_1 = \rho_{11} = \frac{1 - a_z}{2}$$

The probability of find the system in a certain state is given by the diagonal element of the density matrix. The off-diagonal elements give the coherence between the states.

Note that for a pure state $\rho^2 = \rho$. Using the spectral theorem, $\rho = \sum_i \lambda_i\,|\,\lambda_i\rangle\langle\lambda_i\,|$ in which case $\rho^2 = \sum_i \lambda_i^2\,|\,\lambda_i\rangle\langle\lambda_i\,|$. Since $\rho^2 = \rho$ we have $\lambda_i^2 = \lambda_i$, so that $\lambda_i = 0$ or 1 (ρ being Hermitian λ_i are real). Since $\text{tr}(\rho) = 1$ we have $\lambda_p = 1$ for some $i = p$ and is zero for $i \neq p$. For a mixed state, however, let us write $\rho = p_i\rho_i$ with ρ_i being a pure state density matrix, we have $\rho^2 = \sum_{i,j} p_i p_j \rho_i \rho_j$. The trace of ρ is still 1 as (trace can be calculated in any basis)

$$\text{tr}(\rho) = \sum_j \sum_i p_i\langle e_j\,|\psi_i\rangle\langle\psi_i\,|e_j\rangle$$

$$= \sum_{i,j} p_i\langle\psi_i\,|e_j\rangle\langle e_j\,|\psi_i\rangle$$

$$= \sum_i p_i\langle\psi_i\,|\psi_i\rangle = \sum_i p_i = 1$$

where, in the last but one step we have used the completeness relation. However, for a mixed state the trace of ρ^2 is always less than one, as can be seen in the following:

$$\begin{aligned}
\text{tr}(\rho^2) &= \sum_k \sum_{i,j} p_i p_j \langle e_k \, |\rho_i \rho_j| \, e_k \rangle \\
&= \sum_{i,j,k} p_i p_j \langle e_k \, |\psi_i\rangle \langle \psi_i \, |\psi_j\rangle \langle \psi_j \, |e_k\rangle \\
&= \sum_{i,k} p_i^2 \langle \psi_i \, |e_k\rangle \langle e_k \, |\psi_i\rangle \\
&= \sum_i p_i^2 \leq 1
\end{aligned}$$

where the equality is applicable only when one of the p_is is equal to one and the others zero, i.e. a pure state. Thus for mixed states $\text{tr}(\rho^2) \leq \text{tr}(\rho)$.

4 Postulates of Quantum Mechanics - in Density Matrix Language

We have seen that the advantage of the density matrix formulation over the state vector description lies in the former's ability to provide a description of open systems. This is because our system of interest is usually a sub-system which interacts with the environment. In such situations, it is not possible to associate a ray with the system under investigation. The density matrix, on the other hand, can take care of both open systems or closed systems. It is therefore, necessary to reformulate the quantum postulates in terms of the density matrix.

1. A quantum system is completely described by a density operator (matrix) ρ which is a **positive operator with unit trace**, which acts on the state space of the system.

2. A closed system evolves unitarily,

$$\rho(t) = U(t, t_0) \rho(t_0) U^\dagger(t, t_0)$$

3. Outcome of a measurement is probabilistic, the only possible outcomes are eigenvalues λ_m of the operator representing the observable and the probability of this measurement is given by

$$P(m) = \langle \phi_m \, |\rho| \, \phi_m \rangle$$

where $| \phi_m \rangle$ is the eigenstate corresponding to the eigenvalue λ_m. Note that in case of a pure system, this boils down to the Born postulate, since

$$P(m) = \text{tr}\left(\langle \phi_m \, |\psi\rangle \langle \psi \, |\phi\rangle \right) = | \, \langle \phi_m \, |\psi\rangle \, |^2$$

For a mixed state with $\rho = \sum_i p_i \mid \psi \rangle \langle \psi_i \mid$, we obviously can generalise this to

$$P(m) = \sum_i p_i \mid \langle \phi_m \mid \psi \rangle \mid^2 = \sum_i p_i \langle \phi_m \mid \psi_i \rangle \langle \psi_i \mid \phi_m \rangle = \langle \phi_m \mid \rho \mid \phi_m \rangle$$

However, the last expression is equal to $\mathrm{tr}(\rho \mid \phi_m \rangle \langle \phi_m \mid \equiv \mathrm{tr}(\rho P_m)$, where $P_m = \mid \phi_m \rangle \phi_m$ is the projection operator for the eigenstate $\mid \phi_m \rangle$. Later, we will rewrite this postulate in terms of the measurement operators.

4. The post measurement state of the system is given by

$$\rho(\lambda_m) = \frac{1}{p(\lambda_m)} \mid \phi_m \rangle \langle \phi_m \mid \langle \phi_m \mid \rho \mid \phi_m \rangle \langle \phi_m \mid \tag{8}$$

Note that as per the state postulate, the post measurement state is given by

$$\frac{P_m \mid \psi \rangle}{\sqrt{\langle \psi \mid P_m^2 \mid \psi \rangle}} = \frac{P_m \mid \psi \rangle}{[\langle \psi \mid P_m \mid \psi \rangle]^{1/2}} = \frac{P_m \mid \psi \rangle}{\sqrt{p_m}}$$

Clearly, the density matrix corresponding to the above is given by (**??**).

5 Reduced Density Matrix

As we have mentioned earlier, frequently, our system of interest A is a part of a larger system with which it interacts. The quantum coo relations that exist within our system of interest would decohere as a result of interaction with the environment. If the entire system (A+ the environment, which we label as B). is described by a density matrix, the properties of A is obtained by taking partial trace (i.e. averaging) over the trace of the environment. We will illustrate the basic concept of the reduced density matrix by considering A to be a one bit system and B also to be a one bit system. Since we would like to make our measurements only on the system A, it is of interest to see, how things change if we were to make a measurement on the composite system (A+B) described by a single density matrix ρ^{AB}. We define the **reduced density matrix** for the system A by

$$\rho^A = \mathrm{tr}_B(\rho^{AB})$$

where tr_B is the partial trace over B, defined by

$$\mathrm{tr}\left(\mid a_1 \rangle \langle a_2 \mid \otimes \mid b_1 \rangle \langle b_2 \mid\right) = \mid a_1 \rangle \langle a_2 \mid \mathrm{tr}(\mid b_1 \rangle \langle b_2 \mid)$$

where $\{b_1, b_2\}$ are the (pure) states of B. Now,

$$\mathrm{tr} \mid b_1 \rangle \langle b_2 \mid = \sum_i \langle i \mid b_1 \rangle \langle b_2 \mid i \rangle = \langle b_2 \mid b_1 \rangle$$

We will see that the reduced density matrix provides proper measurement statistic for the system A. Why do we need partial trace in dealing with composite system?

Let M be an observable on system A while $\tilde{M}$ be the same measurement done on system AB. We need to show that $\tilde{M} = M \otimes I_B$. Let our composite system is prepared in the state $| m \rangle \otimes | \psi \rangle$, where $| m \rangle$ is an eigenstate of A and $| \psi \rangle$ is an arbitrary state of B. Suppose we perform a measurement on the composite system. If P_m is the projector for $| m \rangle$ on the eigenspace of M, the projector for $\tilde{M}$ s $P_m \otimes I_B$. Hence

$$\tilde{M} = \sum_m m P_m \otimes I_B = M \times I_B$$

We should get the same result whether we calculate the result of measurement through ρ_A or ρ_{AB}, we must have

$$\text{tr}(\rho_A M) = \text{tr}(\rho_{AB} \tilde{M}) = \text{tr}\left((M \otimes I_B)\rho_{AB}\right)$$

One can see that if we take $\rho_A = \text{tr}_B(\rho_{AB})$, above equation is satisfied.

Example 1:

Let $\rho_{AB} = \rho \otimes \sigma$ where ρ is the density operator for A and σ for B. We can see that

$$\rho_A = \text{tr}_B(\rho \otimes \sigma) = \rho \, \text{tr}(\sigma) = \rho$$

(as $\text{tr}(\sigma) = 1$. Likewise, we can show that $\rho_B = \text{tr}_A(\rho_{AB})$).

Example 2:

Consider the density matrix corresponding to the Bell state $\dfrac{| 00 \rangle + | 11 \rangle}{\sqrt{2}}$ which is a two qubit entangled state.

$$\rho = \frac{1}{2}\left(| 00 \rangle \langle 00 | + | 11 \rangle \langle 00 | + | 00 \rangle | 11 \rangle + | 11 \rangle \langle 11 |\right)$$

Let us trace over the second qubit

$$\begin{aligned}
\rho_1 &= \text{tr}_2 \rho \\
&= {}_2\langle 0 | \rho | 0 \rangle_2 + {}_2\langle 1 | \rho | 1 \rangle_2 \\
&= \frac{1}{2}\left[(| 0 \rangle \langle 0 | [\langle 0 | 0 \rangle \langle 0 | 0 \rangle + \langle 1 | 0 \rangle \langle 0 | 1 \rangle] + | 1 \rangle \langle 0 | [\langle 0 | 1 \rangle \langle 0 | 0 \rangle + \langle 1 | 1 \rangle \langle 0 | 1 \rangle] \right. \\
&\quad \left. + | 0 \rangle \langle 1 | [\langle 0 | 0 \rangle \langle 1 | 0 \rangle + \langle 1 | 0 \rangle \langle 1 | 1 \rangle] + | 1 \rangle \langle 1 | [\langle 0 | 1 \rangle \langle 1 | 0 \rangle + \langle 1 | 1 \rangle \langle 1 | 1 \rangle]]\right) \\
&= \frac{1}{2}[| 0 \rangle \langle 0 | + | 1 \rangle \langle 1 |] = \frac{I}{2}
\end{aligned}$$

Note that $\text{tr}\,\rho_1 = 1$ but $\text{tr}(\rho_1^2) = \text{tr}(I^2/4) = 1/2$, i.e. it is a mixed state!. It may be noted that the original two qubit state is a pure state but the reduced density matrix corresponds to a mixed state. This is a consequence of quantum entanglement.

6 Schmidt Decomposition and Schmidt Number

An arbitrary vector in the composite space $\mathcal{H}_A \otimes \mathcal{H}_B$ can obviously be expressed in terms of an orthonormal basis $\{| \phi_i^A \rangle\}$ for $\mathcal{H}_A$ and an orthonormal basis $\{| \phi_\mu^B \rangle\}$ for $\mathcal{H}_B$,

$$| \psi \rangle = \sum_{i,\mu} C_{i,\mu} | \phi_i^B \rangle \otimes | \phi_\mu^B \rangle$$

The coefficients $C_{i,\mu}$ are, in general, complex and has the form $\sqrt{p_{i,\mu}} e^{i\varphi_{i\mu}}$. If $\mathcal{H}_A$ has the dimension m and $\mathcal{H}_B$ has dimension n, the composite system has dimension mn.

The Schmidt decomposition tells us that we can always find a pair of basis $\{| \tilde{\phi}_i^A \rangle\}$ and $\{| \tilde{\phi}_i^B \rangle\}$ such that all the cross terms in the expansion of $| \psi \rangle$ vanish and we have

$$| \psi \rangle = \sum_{i} \sqrt{p_i} | \tilde{\phi}_i^A \rangle \otimes | \tilde{\phi}_i^B \rangle$$

such that all coefficients $\sqrt{p_i}$ are real and the dimension of the space is $\min(m, n)$.

Example:

Express $| \psi \rangle = \dfrac{1}{2}(| 00 \rangle + | 01 \rangle + | 10 \rangle + | 11 \rangle)$ in Schmidt basis.

Note that the computational basis for $\mathcal{H}_A$ and $\mathcal{H}_B$ are not Schmidt basis because of presence of cross terms like $| 01 \rangle$ and $| 10 \rangle$. However, if we choose

$$| \tilde{\phi}_0^A \rangle = \frac{1}{\sqrt{2}}(| 0 \rangle + | 1 \rangle); \quad | \tilde{\phi}_1^A \rangle = \frac{1}{\sqrt{2}}(| 0 \rangle - | 1 \rangle)$$
$$| \tilde{\phi}_0^B \rangle = \frac{1}{\sqrt{2}}(| 0 \rangle + | 1 \rangle); \quad | \tilde{\phi}_1^B \rangle = \frac{1}{\sqrt{2}}(| 0 \rangle - | 1 \rangle)$$

We can write $| \psi \rangle = | \tilde{\phi}_0^A \rangle \otimes | \tilde{\phi}_0^B \rangle$, which does not have any cross term.

Define $| \tilde{\phi}_i^B \rangle = \sum_\mu C_{i,\mu} | \phi_\mu^B \rangle$ so that $| \psi \rangle = \sum_i | \phi_i^A \rangle \otimes | \tilde{\phi}_i^B \rangle$. Note that the set $\{| \tilde{\phi}_i^B \rangle\}$ may be neither normalised nor orthogonal. However, we could, without loss of generalty choose the basis $\{| \phi_i^A \rangle\}$ such that ρ_A is orthogonal in this basis. Thus

$$\rho_A = \sum_i p_i | \phi_i^A \rangle \langle \phi_i^A | \tag{9}$$

However, we can calculate ρ_A as a reduced density matrix from the expression for the density matrix of the composite system.

$$\begin{aligned}
\rho_A &= \mathrm{tr}_B \, \rho_{AB} \\
&= \mathrm{tr}_B(| \psi \rangle_{AB} \, {}_{AB}\langle \psi |) \\
&= \mathrm{tr}_B \left[\sum_{i,j} \left(| \phi_i^A \rangle \otimes | \tilde{\phi}_i^B \rangle \right) \left(\langle \phi_j^A | \otimes \langle \tilde{\phi}_j^B | \right) \right] \\
&= \sum_{i,j} (| \phi_i^A \rangle \langle \phi_j^A |) \, \mathrm{tr}((| \tilde{\phi}_i^B \rangle \langle \tilde{\phi}_j^B |)) \\
&= \sum_{i,j} (| \phi_i^A \rangle \langle \phi_j^A |) \langle \tilde{\phi}_j^B | \tilde{\phi}_i^B \rangle \tag{10}
\end{aligned}$$

where we have used $\text{tr}((| \tilde{\phi}_i^B\rangle\langle\tilde{\phi}_j^B |) = \langle\tilde{\phi}_j^B |\tilde{\phi}_i^B\rangle$. However, we have also obtained (**??**) for ρ_A. Thus, on comparing (**??**) and (**??**), we get

$$\sum_i p_i \mid \phi_i^A\rangle\langle\phi_i^A \mid = \sum_{i,j}(\mid \phi_i^A\rangle\langle\phi_j^A \mid)\langle\tilde{\phi}_j^B |\tilde{\phi}_i^B\rangle$$

This shows that $\langle\tilde{\phi}_j^B |\tilde{\phi}_i^B\rangle = p_i\delta_{i,j}$, i.e., the new basis is orthogonal. Assuming $\pi \neq 0$, we can normalise it so that

$$| \tilde{\phi}_i^B\rangle \rightarrow \frac{1}{\sqrt{p_i}} | \tilde{\phi}_i^B\rangle$$

Thus

$$| \psi\rangle_{AB} = \sum_i \sqrt{p_i} | \phi\rangle_A \otimes | \tilde{\phi}_i^B\rangle$$

We can take partial trace over A to get ρ_B

$$\rho_B = \text{tr}_A(| \psi_{AB}\rangle\langle\psi_{AB} |)$$

$$= \text{tr}_A \left(\sum_{i,j} \sqrt{p_i p_j} | \phi_i^A\rangle\langle\phi_j^A | \otimes | \tilde{\phi}_i^B\rangle\langle\tilde{\phi}_j^B | \right)$$

$$= \sum_i p_i | \tilde{\phi}_i^B\rangle\langle\tilde{\phi}_i^B |$$

which shows that ρ_A and ρ_B have the same non-zero eigenvalues. This does not imply that $\mathcal{H}_A$ and $\mathcal{H}_B$ have the same dimension as the number of zero eigenvalues may differ. The number of non-zero eigenvalues of ρ_A and ρ_B is known as the **Schmidt Number**. If a state is separable, the Schmidt number is 1.

Example 1:

Let $| \psi\rangle = \frac{| 01\rangle - | 10\rangle}{\sqrt{2}}$. Is this state separable?

$$\rho = | \psi\rangle\langle\psi | = \frac{1}{2}[| 01\rangle\langle01 | - | 01\rangle\langle10 | - | 10\rangle\langle01 | + | 10\rangle\langle10 |]$$

Taking partial trace, we get $\rho_A = \text{tr}_B \rho = \frac{1}{2}I$ which has two eigenvalues $\lambda_1 = \lambda_2 = \frac{1}{2}$. Since there are two non-zero eigenvalues, the state is not separable and is entangled.

Example 2:

Check the separability of the state

$$| \psi\rangle = \frac{1}{2} | 00\rangle + \frac{1}{2} | 01\rangle + \frac{i}{2} | 20\rangle + \frac{i}{2} | 21\rangle$$

where $| 0\rangle, | 1\rangle$ and $| 2\rangle$ constitute an orthonormal set in $\mathcal{H}_A$ and $| 0\rangle$ and $| 1\rangle$ form a set on $\mathcal{H}_B$.

It is easy to check that taking partial trace over B, gives us ρ_A to be

$$\rho_A = \text{tr}_B\,\rho = \frac{1}{2}\mid 0\rangle\langle 0\mid + \frac{1}{2}\mid 2\rangle\langle 2\mid -\frac{i}{2}\mid 0\rangle\langle 2\mid +\frac{i}{2}\mid 2\rangle\langle 0\mid$$

$$= \begin{pmatrix} \dfrac{1}{2} & -\dfrac{i}{2} \\ \dfrac{i}{2} & \dfrac{1}{2} \end{pmatrix}$$

which has eigenvalues 1 or 0. The non-zero eigenvalue is only 1. Hence the state is separable. One can directly check that

$$\mid \psi\rangle = \left(\frac{\mid 0\rangle + i\mid 2\rangle}{\sqrt{2}}\right) \otimes \left(\frac{\mid 0\rangle + \mid 1\rangle}{\sqrt{2}}\right)$$

7   Purification

We have seen that taking partial trace of a pure state gives us a mixed state. Is the converse true? Is it possible to to find a pure state density matrix, whose partial trace yields a given mixed state density matrix? The answer is yes. The process is called **purification**.

Let $\rho_a = \sum_k p_k\mid \psi_k\rangle\langle\psi_k\mid$ be a density matrix of A in the Hilbert space $\mathcal{H}_A$. Introduce a second Hilbert space $\mathcal{H}_B$ which has the same dimension as that of $\mathcal{H}_A$. Define

$$\mid \psi\rangle = \sum_k \sqrt{p_k}\mid \psi_k\rangle \otimes\mid \phi_k\rangle$$

where $\{\mid \phi_k\rangle\}$ is an orthonormal basis in $\mathcal{H}_B$. Now,

$$\text{tr}_B\mid \psi\rangle\langle\psi\mid = \text{tr}_B\sum_{k,l}\sqrt{p_k p_l}\mid \psi_k\rangle_A\,{}_A\langle\psi_l\mid\otimes\mid \phi_k\rangle_B\,{}_B\langle\phi_l\mid$$

$$= \sum_{k,l}\sqrt{p_k p_l}\mid \psi_k\rangle_A\,{}_A\langle\psi_l\mid\langle\phi_k\mid\phi_m\rangle$$

$$= \sum_{k,l}\sqrt{p_k p_l}\mid \psi_k\rangle_A\,{}_A\langle\psi_l\mid\delta_{k,l}$$

$$= \sum_k p_k\mid \psi_k\rangle_A\,{}_A =\rho_A$$

Example:

Let $\rho_A = \dfrac{1}{4}(\mid 0\rangle\langle 0\mid +3\mid 1\rangle\langle 1\mid)$. Find a purification.

Now,

$$\rho_A = \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$$

Let $\mid 0\rangle$ and $\mid 1\rangle$ be a basis for B. Define

$$\mid \psi\rangle = \frac{1}{2}\mid 0\rangle_A \times\mid 0\rangle_B + \frac{\sqrt{3}}{2}\mid 1\rangle_A \otimes\mid 1\rangle_B$$

The tensor product matrix can be seen to be

$$
\begin{aligned}
\mid \psi \rangle &= \frac{1}{2}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} + \frac{\sqrt{3}}{2}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + \frac{\sqrt{3}}{2}\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix}1 & 0\\0 & \sqrt{3}\end{pmatrix}
\end{aligned}
$$

Thus

$$
\begin{aligned}
\mid \psi \rangle \langle \psi \mid &= \frac{1}{4}\begin{pmatrix}1 & 0\\0 & \sqrt{3}\end{pmatrix}\begin{pmatrix}1 & 0\\0 & \sqrt{3}\end{pmatrix} \\
&= \frac{1}{4}\begin{pmatrix}1 & 0 & 0 & 0\\0 & \sqrt{3} & 0 & 0\\0 & 0 & \sqrt{3} & 0\\0 & 0 & 0 & 3\end{pmatrix}
\end{aligned}
$$