

Density Operators

Ryoichi Kawai

*Department of Physics,
University of Alabama at Birmingham*

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The state of a quantum system is usually expressed with a vector $|\psi\rangle$ in the Hilbert space. Such a state is called pure state. However, in many situations states are not pure and instead they are classical mixtures of many pure states. Such states cannot be expressed as vector. A new mathematical expression, called density operator, can describe any state. In this note, (1) the failure of vector, (2) introduction of density operator and its properties, and (3) applications of density operators are discussed.

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I. $|\psi\rangle$ IS NOT ENOUGH

Consider a qubit (two-dimensional Hilbert space). A general state of the qubit can be written as a superposition of two base kets as

$$|\psi\rangle = c_0 |0\rangle + c_1 |1\rangle, \quad c_i \in \mathbb{C} \quad \& \quad |c_0|^2 + |c_1|^2 = 1. \quad (1)$$

This superposition state suggests that the qubit is partly in state $|0\rangle$ and also in $|1\rangle$. There is uncertainty with respect to $|0\rangle$ and $|1\rangle$. This uncertainty is resolved when measurement is carried out. The outcome is only one of $|0\rangle$ and $|1\rangle$ but we don't know which is precisely observed. the current theory of quantum mechanics cannot predict the outcome. The Born rule tells that the probability of finding $|0\rangle$ is given by $|c_0|^2$. That means we must think of an ensemble of qubits rather than a single qubit. In order to apply this standard interpretation of quantum mechanics, we must have an ensemble of qubits all in the identical state $|\psi\rangle$. Then, $|\psi\rangle$ is no longer a state of the single qubit. It represent the state of all qubits. Since all qubits have the same state $|\psi\rangle$, we call the state of the ensemble *pure state*. However, this is a highly idealized state and we will encounter other kinds of ensembles. In this section, we demonstrate that the pure state $|\psi\rangle$ cannot describe general ensembles.

A. Pure vs Mixed State

Suppose that $N \gg 1$ qubits are all in the same state $|\psi\rangle$ and they are individually stored in an identical box. Since all box contains the identical state $|\psi\rangle$, the ensemble represnets a *pure state*. We can use the same symbol $|\psi\rangle$ for the ensemble. For simplicity, we consider a superposition state $|\psi\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$. Now, we pick one box at random. Since all boxes contain an identical state, it does not matter which one you pick. Then, you open the box and observe if it is $|0\rangle$ or $|1\rangle$. Based on the standard interpretation of quantum mechanics, you will obtain either $|0\rangle$ or $|1\rangle$. However, the quantum mechanics is unable to say which one. After opening all boxes, we obtain a statistical data, $|0\rangle$ is observed from a half of the boxes

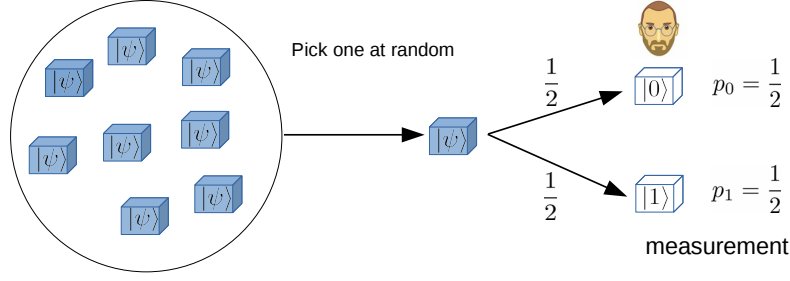


FIG. 1: *Quantum uncertainty*: All qubits are in the same state $|\psi\rangle = \frac{1}{2}|0\rangle + \frac{1}{2}|1\rangle$, hence the box chosen at random always contains $|\psi\rangle$. Upon measurement, $|\psi\rangle$ is transformed to either $|0\rangle$ or $|1\rangle$ with the equal probability. There is no uncertainty in choosing a box. The uncertainty is associated with the superposition of the two states and the quantum measurement resolves the uncertainty.

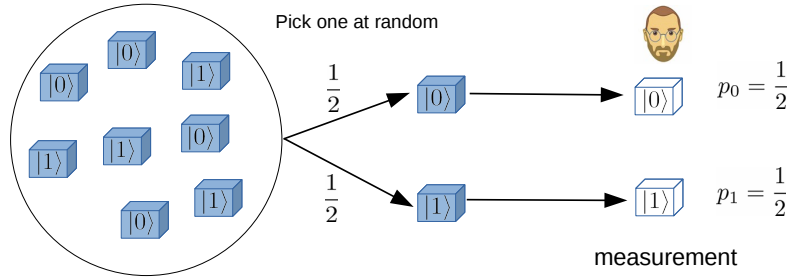


FIG. 2: *Classical uncertainty*: A half of qubits are in $|0\rangle$ and the other half in $|1\rangle$. They are individually stored in an identical box. The box chosen at random contains either $|0\rangle$ or $|1\rangle$ with the equal probability. Upon measurement, the observer has 50% chance to see $|0\rangle$. The observed result is statistically indistinguishable from the uncertainty in case (a). However, in the current situation the state in the box does not change during the measurement. The uncertainty is created when a box is randomly picked without looking into the inside. Hence, this uncertainty is classical.

and $|1\rangle$ from the other half. This situation is illustrated in Figure 1. Note that the random pick does not create uncertainty since all boxes are the same. Uncertainty is associated with the superposition in $|\psi\rangle$ and the uncertainty is resolved by so-called *collapse* of wave function during the quantum measurement.

Now, we consider a different ensemble (Fig. 2) where a half of boxes contain a qubit in state $|0\rangle$ and the remaining boxes contain a qubit in state $|1\rangle$. This ensemble contains two different states and thus we call it *mixed state*. Now you pick a box at random and open it. You will find either $|0\rangle$ or $|1\rangle$. From the observer's point of view, this situation is identical to the previous case. When all the boxes are opened, the statistics tells that a half of boxes show $|0\rangle$ and the other half $|1\rangle$. That is obvious since we prepare the boxes in that way. The uncertainty was created by the construction of the ensemble and has nothing to do with quantum

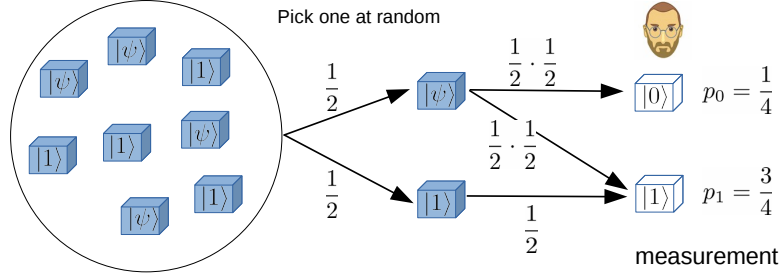


FIG. 3: *Classical and quantum uncertainty*: A half of qubits are in $|\psi\rangle$ and the other half in $|1\rangle$. They are individually stored in an identical box. The box chosen at random contains either $|\psi\rangle$ or $|1\rangle$ with the equal probability. Upon measurement, the observer has 25% chance to see $|0\rangle$ and 75% for $|1\rangle$. The observed result is different from the two previous cases. When a box is selected, classical uncertainty is already generated. If the box with $|\psi\rangle$ were chosen, it contains quantum uncertainty. On the other hand, if the box $|1\rangle$ were picked, there is no quantum uncertainty.

mechanics. Hence, this uncertainty is classical. We say that this ensemble is a classical mixture of $|0\rangle$ and $|1\rangle$. While the outcomes of the previous and current cases are statistically identical, the two ensembles are clearly different. In fact, if $|\pm\rangle = |0\rangle \pm |1\rangle$ are measured, different outcomes are observed from the two ensembles.

In another ensemble (Fig. 3), a half of boxes contain a qubit in state $|\psi\rangle$ and the other half stores a qubit in state $|1\rangle$. The ensemble is a classical mixture of $|\psi\rangle$ and $|1\rangle$ and thus it is a *mixed state*. The measurement of $|0\rangle$ and $|1\rangle$ involves two uncertainty. When a box containing $|1\rangle$, the outcome of measurement is always $|0\rangle$. On the other hand, a box containing $|\psi\rangle$ results in either $|0\rangle$ or $|1\rangle$ with an equal probability. The random choice of boxes creates classical uncertainty and opening boxes with $|\psi\rangle$ generates quantum uncertainty in $|\psi\rangle$.

Homework 1: Find the probability to obtain $|\pm\rangle$ in all three cases.

B. When does a classical mixture appear?

In the previous section, we showed that a state $|\psi\rangle$ of a single system actually describes a state of an ensemble instead of individuals. Then, we showed that an ensemble does not have to be pure. In this section, we show that a classical mixture is more realistic than a pure state. When a system is in a pure state at a certain time, it won't stay pure over a macroscopic time. For example the loss of coherency in light (decoherence) is equivalent to the formation of a classical mixture. Even the whole system remains in a pure state, the subsystems are classical mixtures when they are quantum mechanically entangled. Another example is a composite system consisting of multiple sub systems. The state of the subsystems are classical mixtures when they are quantum mechanically entangled.

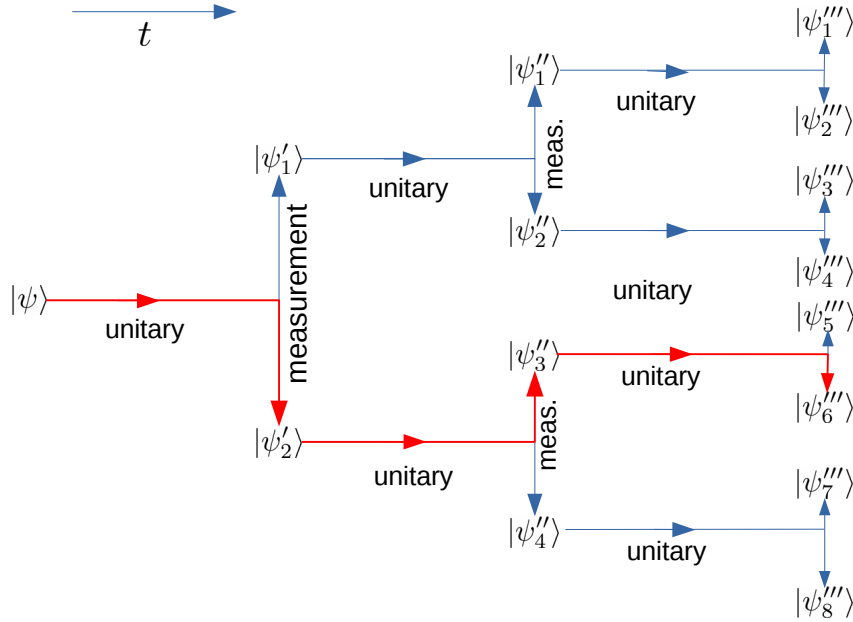


FIG. 4: Initially the system is in a pure state $|\psi\rangle$. The unitary evolution keeps it pure until a measurement is done. Upon the first measurement, the system takes one of two possibilities ($|\psi'_2\rangle$). Then, the unitary evolution is resumed until the second measurement. The measurement picks $|\psi''_3\rangle$ and another unitary evolution follows. The system ended in $|\psi'''_6\rangle$.

1. Realistic time-evolution

Every textbook on quantum mechanics tells that the time evolution of a quantum system is determined by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (2)$$

or equivalently

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} H t} |\psi(0)\rangle = \mathcal{U} |\psi(0)\rangle. \quad (3)$$

where $\mathcal{U} \equiv e^{-\frac{i}{\hbar} H t}$ is a time-evolution operator. We say that the time-evolution is *unitary* since \mathcal{U} is a unitary operator. During the unitary evolution, a pure state remains pure. There is another evolution in quantum mechanics, which happens during measurement. It cannot be described by the Schrödinger equation and it is even not a unitary evolution. At the present we do not know how the measurement happens. The quantum mechanics tells us only the statistics of the measurement outcomes and the ensemble after the measurement is a classical mixture.¹ Figure 4 shows an evolution of a single system. Starting with a pure state $|\psi\rangle$ it repeats unitary evolution between measurements. Upon the measurement, the system picks one outcome at random. For example, the system may take a red path in Fig. 4. However, the principle of quantum mechanics can't predict which path is actually taken. It can predict only the statistics of the outcome based on ensemble. During this evolution, the ensemble also evolves from a pure state to mixed states as

$$\begin{aligned} |\psi\rangle \rightarrow \{|\psi'_1\rangle, |\psi'_2\rangle\} &\rightarrow \{|\psi''_1\rangle, |\psi''_2\rangle, |\psi''_3\rangle, |\psi''_4\rangle\} \\ &\rightarrow \{|\psi'''_1\rangle, |\psi'''_2\rangle, |\psi'''_3\rangle, |\psi'''_4\rangle, |\psi'''_5\rangle, |\psi'''_6\rangle, |\psi'''_7\rangle, |\psi'''_8\rangle\} \end{aligned} \quad (4)$$

After a certain time, this way of writing the ensemble becomes useless since there would be infinitely many outcomes must be taken into account.²

2. Decoherence

When a system is in a superposition state (1), we say that $|0\rangle$ and $|1\rangle$ are *coherent*. For example, we can generate interference between them. However, in a real world, coherence tends to disappear by some processes known as *decoherence*. When the coherence is completely lost, the system must be either in $|0\rangle$ or $|1\rangle$. In other words, it forms a classical mixture of $|0\rangle$ or $|1\rangle$. We also know that the system can have partial coherence. There is no way to describe the partial coherence using a superposition state (1) since it is always perfectly coherent.

¹ If you discard outcomes except for one state, then the result is again pure state but many individuals are lost from the ensemble. This kind of measurement is known as *selective measurement*.

² Many-world theory each elements of the ensemble belongs to a different world.

After quantum measurement, the superposition of eigenstates are not possible and thus the appearance of a classical mixture after quantum measurement must involve decoherence. However, the actual decoherence processes during the measurement is not known. At present, we think that the decoherence is a consequence of quantum entanglement between a system and environments. Understanding decoherence processes is a key to develop quantum technology including quantum computers.

3. Quantum Entanglements

A composite system consists of multiple subsystems. For example, the system of two qubits is a composite system and its Hilbert space is four dimensional ($2 \times 2 = 4$, not $2 + 2 = 4$). Hence, a usual quantum state (pure state) is a four-dimensional ket $|\psi\rangle$. If and only if two qubits are not correlated, the state of the composite system can be expressed as a tensor product of two individual states $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$. Then, we say that the qubit 1 is in state $|\psi_1\rangle$ and the qubit 2 in state $|\psi_2\rangle$ independently.

When the state of the whole system cannot be written as a product of two independent states, the two subsystems are said to be *entangled*. For example,

$$|\psi\rangle = \frac{1}{\sqrt{2}} |0\rangle \otimes |1\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes |0\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \quad (5)$$

is an entangled state. We used a short hand expression $|01\rangle \equiv |0\rangle \otimes |1\rangle$ and similarly $|10\rangle$. When we make a measurement, either $|01\rangle$ or $|10\rangle$ is obtained. That means when qubit 1 is found in state $|0\rangle$, the other qubit must be in state $|1\rangle$. Similarly, when qubit 1 is in $|1\rangle$, the other qubit must be in $|0\rangle$. There is no chance to see that both qubits are in the same state. Hence, they are correlated. If we look at only the qubit 1, it is in $|0\rangle$ with probability $\frac{1}{2}$ 50% and in $|1\rangle$ with 50 %. You might think that the state of qubit 1 can be written as $|\psi_1\rangle = \frac{1}{2} |0\rangle + \frac{1}{2} |1\rangle$, which is a pure state. Similarly for the qubit 2, $|\psi_2\rangle = \frac{1}{2} |0\rangle + \frac{1}{2} |1\rangle$, which is a pure state as well. If they are independently in $|\psi_1\rangle$ and $|\psi_2\rangle$, the state of the whole system is a product state

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = \frac{1}{2} (|00\rangle + |01\rangle + |10\rangle + |11\rangle) \quad (6)$$

which is not an entangled state and different from (5). There is no way to describe the state of the subsystem in a pure form when the system is entangled.

4. Quantum Thermodynamics and Statistical Mechanics

Thermodynamics is explained by statistical mechanics which introduces a concept of ensembles even for classical systems. For example, when a system is in thermal equilibrium, the probability of finding the system with energy E is given by $P(E) \propto e^{-\beta E}$ where $\beta = 1/kT$. To apply the statistical mechanics to quantum systems, we must use a classical mixture of quantum states. It turns out that the concept developed in

classical statistical mechanics, namely phase density and the Liouville equation, give us a hint to construct a mathematical expression of quantum mixed states.

II. DENSITY OPERATORS

As shown in the previous section, $|\psi\rangle$ can describe only a pure state and we need a different mathematical expression for mixed states. In classical mechanics, phase densities are used to describe mixed states. We will develop a similar expression for the quantum mechanics. Comparison between classical and quantum description is given in Table I.

A. Phase Density and Liouville Equation

A state of a classical particle is precisely specified by position q and momentum p , which is a point in the phase space. Its time evolution is a trajectory in the phase space determined by the Newton's equations of motion. This phase point (q, p) is a pure state of the classical system. When we don't know the exact position and momentum at an initial time, the future state is uncertain. To take into account the uncertainty a probability density $\rho(q, p, t)$ is introduced. The probability to find the system in a state (q, p) at time t is given by $\rho(q, p, t) dq dp$. For a pure state, $\rho(q, p, t) = \delta(q - q(t))\delta(p - p(t))$. When there is uncertainty,

$$\rho(q, p, t) = \sum_i P_i \delta(q - q_i(t)) \delta(p - p_i(t)) \quad (7)$$

where P_i is probability to find the system in state (q_i, p_i) . In other words, $\rho(q, p, t)$ represents a mixture of many pure states (q_i, p_i) . This probability density is called *phase density* or simply *density*.

The evolution of a pure state (q, p) is determined by the Hamilton's equation of motion $\frac{dq}{dt} = \frac{\partial H}{\partial p}$, $\frac{dp}{dt} = -\frac{\partial H}{\partial q}$, where H is Hamiltonian of the system. For a mixed state, we are supposed to solve it for all possible state (q_i, p_i) , which is practically impossible. It turns out that we need to find only the evolution of $\rho(q, p, t)$. Using the Liouville theorem, the equation of motion for a density is

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} \quad (8)$$

where $\{\cdot, \cdot\}$ is Poisson bracket. This equation is known as Liouville equation.

B. Density Operator: Definition and basic properties

By analogy from the classical phase density, we want to construct a mathematical expression of classical mixture of quantum states. Suppose that a quantum system is in a mixture of $|\psi_i\rangle$ with the corresponding probability P_i , can we use a linear superposition $|\psi\rangle = \sum_i P_i |\psi_i\rangle$? The principle of quantum mechanics

TABLE I: Comparison between quantum and classical states

	Quantum	Classical
Pure state	$ \psi\rangle$	$\{q, p\}$
Equation of motion for pure state	$i \frac{\partial}{\partial t} \psi\rangle = H \psi\rangle$	$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \frac{dp}{dt} = -\frac{\partial H}{\partial q}$
Mixed State	$\rho = \sum_i P_i \psi_i\rangle\langle\psi_i $	$\rho = \sum_i P_i \delta(q - q_i) \delta(p - p_i)$
Equation of motion for mixed state	$i \frac{\partial \rho}{\partial t} = [H, \rho]$	$\frac{\partial \rho}{\partial t} = \{H, \rho\}$

tells you that any linear superposition of kets is another ket. Hence, we get another pure state. We need to introduce a new mathematical object similar to the phase density, which we shall call *density operator*.

We first express a pure state as $|\psi\rangle\langle\psi|$, a dyadic of $|\psi\rangle$ and $\langle\psi|$ instead of $|\psi\rangle$ itself. Note that the dyadic is a projection operator. Since $|\psi\rangle\langle\psi|$ and $|\psi\rangle$ contain the exactly same information, we can use either of them to describe the pure state. However, their mathematical properties are different.

Using the dyadics, the classical superposition of quantum states can be written in the following form:

$$\rho = \sum_{i=1}^N P_i |\psi_i\rangle\langle\psi_i| = P_1 |\psi_1\rangle\langle\psi_1| + P_2 |\psi_2\rangle\langle\psi_2| + \cdots + P_N |\psi_N\rangle\langle\psi_N| \quad (9)$$

where P_i is classical probability satisfying $P_i \geq 0$ and $\sum_i P_i = 1$. Since it consists of the sum of projection operators, ρ is an operator. We call it *density operator*. It is noted that $|\psi_i\rangle$ must be normalized but they don't have to be orthogonal since $\{|\psi_i\rangle\}$ is not a basis set. N can be any positive integer since we can mix any number of states. It turns out that any operator that satisfies the following two properties is a density operator.

$$\rho^\dagger = \rho \quad (\text{self-adjoint}) \quad (10a)$$

$$\rho \geq 0 \quad (\text{positive semi-definite}) \quad (10b)$$

$$\text{tr } \rho = 1 \quad (\text{normalization}) \quad (10c)$$

Since ρ is a self-adjoint operator in the Hilbert space, it has real eigenvalues λ_i and eigenvectors $|u_i\rangle$ such that $\rho |u_i\rangle = \lambda_i |u_i\rangle$. Then, the spectral representation of the density operator is given by

$$\rho = \sum_{i=1}^D \lambda_i |u_i\rangle\langle u_i| \quad (11)$$

where D is the dimension of the Hilbert space. The requirement (10b) guarantees that $\lambda_i \geq 0$ and (10c) indicates that $\sum_i \lambda_i = 1$. Note that Eq. (11) has the form of Eq (9). It is a classical mixture of $|u_i\rangle$ and the eigenvalues are considered as classical probabilities.

Now we have a little problem. Equations (9) and (11) correspond to the same physical state. There are more than one expression for the same state. This ambiguity causes interpretation problems but it is a property of quantum mechanics. Even $|\psi\rangle$ can be expanded in many different ways.

Like other operators in Hilbert space, the density operator can be expressed as matrix as well, which is known as density matrix. For any basis set $|\phi_i\rangle$, the density matrix is defined as

$$\rho_{ij} = \langle \phi_i | \rho | \phi_j \rangle \quad (12)$$

and

$$\rho = \sum_i \sum_j |\phi_i\rangle \rho_{ij} \langle \phi_j|. \quad (13)$$

C. Pure state

In Eq (9), if $P_1 = 1$ and $P_{i>1} = 0$, then the density operator is simply a projection operator

$$\rho = |\psi_1\rangle\langle\psi_1| \quad (14)$$

Note that the pure state density operator is idempotent, i.e., $\rho^2 = \rho$ since it is a projection operator. Then, we have $\text{tr} \rho^2 = \text{tr} \rho = 1$. This is true only when the system is in a pure state. The quantity $\text{tr} \rho^2$ is called *purity*. If the purity is one, then the system is certainly in a pure state.

As an example, consider pure state (1). The corresponding density operator is $\rho = |\psi\rangle\langle\psi|$, which means that the system is always in $|\psi\rangle$. Note that the $|0\rangle$ and $|1\rangle$ are coherent in this expression. Let us write a density matrix with $|0\rangle$ and $|1\rangle$ as basis.

$$\rho = \begin{pmatrix} |c_0|^2 & c_0 c_1^* \\ c_0^* c_1 & |c_1|^2 \end{pmatrix} = \begin{pmatrix} P_0 & c_0 c_1^* \\ c_0^* c_1 & P_1 \end{pmatrix} \quad (15)$$

Note that the diagonal elements are the probability to find states $|0\rangle$ and $|1\rangle$, $P_0 = |c_0|^2$ and $P_1 = |c_1|^2$, respectively. The presence of non-zero off-diagonal element is a signature of coherency between $|0\rangle$ and $|1\rangle$. You will see in the next example that the off-diagonal elements in the mixed state vanish.

Homework A system is in a pure state $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. Find the density matrix in $|0\rangle$ and $|1\rangle$ as basis.

D. Mixed states

If more than two of P_i are not zero, then the density cannot be written in a form of single projection. It is a combination of multiple projection operators. For simplicity, we consider only the simplest mixed state

$P_1, P_2 > 0$ and $P_{i>2} = 0$.

$$\rho = P_1 |\psi_1\rangle\langle\psi_1| + P_2 |\psi_2\rangle\langle\psi_2| \quad (16)$$

where $|\psi_1\rangle \neq |\psi_2\rangle$. This equation means that the system is in a classical mixture of $|\psi_1\rangle$ and $|\psi_2\rangle$ and the probability to find the system in $|\psi_1\rangle$ and $|\psi_2\rangle$ is P_1 and P_2 , respectively.

Homework 2: Show the purity is less than one, that is $\text{tr } \rho^2 < 1$. [Hint: $\langle\psi_1|\psi_2\rangle < 1$].

Consider a classical mixture of $|0\rangle$ and $|1\rangle$. The corresponding density operator is $\rho = P_0 |0\rangle\langle 0| + P_1 |1\rangle\langle 1|$ where P_0 and P_1 are the probability to find $|0\rangle$ and $|1\rangle$. Its matrix expression is

$$\rho \doteq \begin{pmatrix} P_0 & 0 \\ 0 & P_1 \end{pmatrix} \quad (17)$$

Compare this with (15). Both have the same probability to find 0 and 1. The difference is its off-diagonal elements. The vanishing off-diagonal elements indicate that the coherence is lost. The density matrix (15) corresponds to the situation illustrated in Fig. 1 and the density matrix (17) describes the situation in Fig. 2. After the measurement, two cases end up with the same mixed state (17).

Let us check the 3rd case shown in Fig. 3. The density operator is given by $\rho = \frac{1}{2} |\psi\rangle\langle\psi| + \frac{1}{2} |1\rangle\langle 1|$. Substituting $|\psi\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$, the mid state is expressed as

$$\rho = \frac{1}{4} (|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) + \frac{1}{2} |1\rangle\langle 1| \quad (18)$$

$$= \frac{1}{4} |0\rangle\langle 0| + \frac{1}{4} |0\rangle\langle 1| + \frac{1}{4} |1\rangle\langle 0| + \frac{3}{4} |1\rangle\langle 1| \quad (19)$$

Writing it in a matrix form,

$$\rho \doteq \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} \end{pmatrix} \quad (20)$$

The off-diagonal does not vanish and thus some coherency remains. However, it comes from the coherence in $|\psi\rangle$. Hence, the state is only partially coherent.

E. Unitary Time-evolution

Suppose that a system is initially in a state,

$$\rho(t_0) = \sum_{i=1}^N P_i |\psi_i\rangle\langle\psi_i| \quad (21)$$

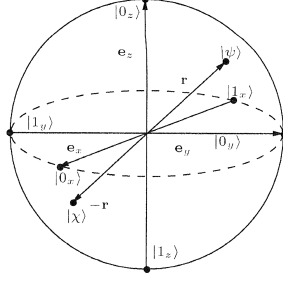


FIG. 5: Bloch sphere

which can be any pure or mixed state. We want to know the state of the system at a later time t . We assume that no measurement is done during the evolution. Hence, the evolution is unitary.

Applying the unitary transformation Eq (3), the density operator at time t is given by

$$\begin{aligned}\rho(t) &= \sum_{i=1}^N P_i e^{-iH(t-t_0)} |\psi_i\rangle\langle\psi_i| e^{iH(t-t_0)} = e^{-iH(t-t_0)} \left(\sum_{i=1}^N P_i |\psi_i\rangle\langle\psi_i| \right) e^{iH(t-t_0)} \\ &= e^{-iH(t-t_0)} \rho(t_0) e^{iH(t-t_0)} = \mathcal{U} \rho(t_0) \mathcal{U}^\dagger\end{aligned}\quad (22)$$

Taking time-derivative of $\rho(t)$, we obtain equation of motion

$$\frac{\partial}{\partial t} \rho(t) = -i[H, \rho(t)] \quad (23)$$

which is known as Liouville–von Neumann equation. Note that this is precisely equivalent to the Schrödinger equation.

Homework: Show that if the initial state is pure, the system remains in pure state all time. Similarly, if the initial state is mixed, it remains in mixed state all time.

F. Single Qubit

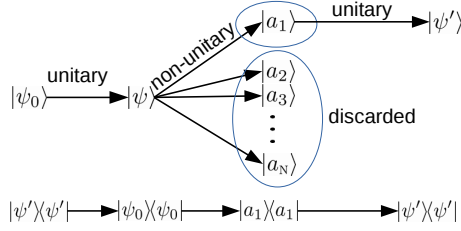
As a simplest example, consider a single qubit. Using $|0\rangle$ and $|1\rangle$ as basis, any pure state of the qubit can be written as

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi} |1\rangle, \quad 0 < \theta < \pi, \quad 0 < \phi < 2\pi \quad (24)$$

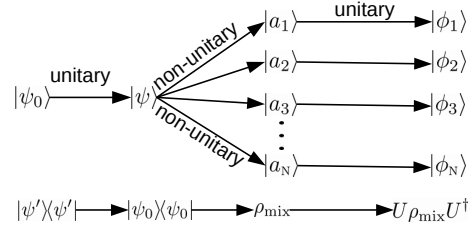
This suggest that any pure state can be mapped to a point on the surface of a unit sphere. For example, the north pole, $\theta = 0$ corresponds to $|0\rangle$ and the south pole $|1\rangle$. This sphere is known as Bloch sphere illustrated in Fig 5.

However about mixed state? Any density operator of 2x2 can be written as

$$\rho = \frac{1}{2} (I + \mathbf{r} \cdot \boldsymbol{\sigma}) \quad (25)$$



(a) Selective measurement



(b) Non-selective measurement

where I is the identity matrix and $\boldsymbol{\sigma}$ the vector form of Pauli matrices $\sigma_x \mathbf{e}_x + \sigma_y \mathbf{e}_y + \sigma_z \mathbf{e}_z$. The radial vector $\mathbf{r} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z$ determines the density operator. The purity

$$\text{tr } \rho^2 = \text{tr} \left[\frac{1}{4} (I + \mathbf{r} \cdot \boldsymbol{\sigma})^2 \right] = \frac{1}{2} (1 + r) \quad (26)$$

suggests that when $r = 1$ the system is in a pure state. This means that every point on the surface of Bloch sphere is a pure state. This also suggests that all mixed states ($r < 1$) are inside the Bloch sphere.

Homework: Show that Eq. (25) satisfies all conditions (10).

Homework: Show that the purity is given by $\text{tr } \rho^2 = \frac{1}{2} (1 + r) \leq 1$.

III. EXAMPLES

A. Quantum Measurement

1. Projective Measurement

A current description of quantum mechanics based on Copenhagen interpretation is the following. If we want to measure a physics observable A , we first find its eigenvalue a_i and the corresponding eigenvector $|a_i\rangle$. If the system is in a pure state $|\psi\rangle$, the Born rule tells that the outcome a_i is obtained with probability

$$P_i = |\langle a_i | \psi \rangle|^2 = \langle a_i | \psi \rangle \langle \psi | a_i \rangle = \langle a_i | \rho_0 | a_i \rangle \quad (27)$$

where $\rho_0 = |\psi\rangle\langle\psi|$ is the density operator just before the measurement. This is called projective measurement. Note that the diagonal element of the density operator is the probability to find the eigenvalue a_i . After the measurement, the system is in $|a_i\rangle$ with the probability (27).

If you keep only the outcome of a particular state $|a_i\rangle$ the state after measurement is a pure state $|a_i\rangle$. Writing it with the density operator

$$\rho_0 = |\psi\rangle\langle\psi| \quad \rightarrow \quad \rho = |a_i\rangle\langle a_i| \quad (28)$$

where ρ_0 and ρ are the density operator before and after measurement, respectively. This type of measurement is called *selective measurement* (see Fig 6a). This transition cannot be described by the Schrödinger equation. At the present, we don't know how it happens. We even don't know how long the transition takes. However, this is a kind of time-evolution of quantum system we need to take into account. After the measurement the evolution of the system again unitary from $|a_i\rangle$.

If we keep all outcomes, the state after the measurement is a classical mixture of $|a_1\rangle, |a_2\rangle, \dots$. Hence, the state after the measurement is a mixed state

$$\rho = \sum_i P_i |a_i\rangle\langle a_i| = \sum_i \langle a_i|\rho_0|a_i\rangle |a_i\rangle\langle a_i| = \sum_i |a_i\rangle\langle a_i| \rho_0 |a_i\rangle\langle a_i| = \sum_i \pi_i \rho_0 \pi_i$$

where we used projection operators $\pi_i = |a_i\rangle\langle a_i|$. This type of measurement is called non-selective measurement (see Fig 6b). Again the physical mechanism of the transition from ρ_0 to ρ remains a major problem with quantum mechanics. We only know that the transition from a pure state ρ_0 to a mixed state $\sum_i P_i |a_i\rangle\langle a_i|$ happens.

In the above description the initial state is assumed to be a pure state. However, the final conclusions are valid even when the initial state is a mixed state. Here is the summary of transition due to measurement.

- The probability of finding a_i is $P_i = \langle a_i|\rho_0|a_i\rangle$.
- After selective measurement, the state of the system is a pure state $\rho = |a_i\rangle\langle a_i|$ and does not depend on the state before the measurement.
- After non-selective measurement, the state of the system is a mixed state $\rho = \sum_i \pi_i \rho_0 \pi_i$.

Now reexamine the case shown in Fig. 4. The system start with a pure state $\rho_0 = |\psi\rangle\langle\psi|$. The evolution (4) can be written as

$$\begin{aligned} \rho_0 &\rightarrow \mathcal{U}\rho_0\mathcal{U}^\dagger \rightarrow \sum_i \Pi_i \mathcal{U}\rho_0\mathcal{U}^\dagger \Pi_i \rightarrow \sum_i \mathcal{U}' \Pi_i \mathcal{U}\rho_0\mathcal{U}^\dagger \Pi_i \mathcal{U}'^\dagger \\ &\rightarrow \sum_j \sum_i \Pi'_j \mathcal{U}' \Pi_i \mathcal{U}\rho_0\mathcal{U}^\dagger \Pi_i \mathcal{U}'^\dagger \Pi'_j \rightarrow \dots \end{aligned} \quad (29)$$

The whole evolution is now expressed as series of unitary operations and projections. This is the full time-evolution of quantum systems. We could not do this without density operators.

2. Expectation Value

In a standard quantum mechanics course, we learned the mean value of physical observable A is given by

$$\langle A \rangle = \langle \psi|A|\psi \rangle = \sum_k |\langle a_k|\psi \rangle|^2 a_k \quad (30)$$

where $|\langle a_k|\psi\rangle|^2$ is the *quantum* probability. Here the observed quantity is averaged over quantum uncertainty.

For mixed state $\rho_0 = \sum_i P_i |\psi_i\rangle\langle\psi_i|$, the expectation value is defined by $\langle A \rangle = \sum_i P_i \langle\psi_i|A|\psi_i\rangle$ which involves two kinds of averaging. One is the averaging over quantum uncertainty taken in the expectation value $\langle\psi_i|A|\psi_i\rangle$ and the other is averaging over classical uncertainty P_i .

In either pure or mixed state, the expectation value can be expressed as

$$\langle A \rangle = \text{tr}(A\rho) \quad (31)$$

and this expression takes into account both classical and quantum uncertainties.

Homework: Prove Eq. (31).

B. Quantum Thermodynamics

1. Gibbs state

An important example of the mixed state is a thermal state. Thermodynamics tells that if the environment is in a thermal equilibrium, the system also eventually reaches to a thermal state with the same temperature as the environment has. The equilibrium state is known as Gibbs state:

$$\rho_G = \frac{1}{Z} e^{-\beta H_s} \quad (32)$$

where H_s is the Hamiltonian of the system, $\beta = 1/k_B T$, and $Z = \text{tr}(e^{-\beta H_s})$ is the partition function of the system.

Using the eigenvalue E_i of H_s and the corresponding eigenket $|u_i\rangle$, the Gibbs state can be written as

$$\rho_G = \sum_i \frac{e^{-\beta E_i}}{Z} |u_i\rangle\langle u_i| = \sum_i P_i |u_i\rangle\langle u_i| \quad (33)$$

where the classical probability is defined as $P_i = \frac{e^{-\beta E_i}}{Z}$. Equation (33) indicates that the thermal equilibrium is a mixed state with so-called Boltzmann distribution $\frac{e^{-\beta E_i}}{Z}$. The transition from a pure state to a thermal state is also induced by the environment.

2. von Neumann Entropy

Entropy is a measure of classical uncertainty. When the system is in a pure state, there is no classical ambiguity and thus it corresponds to the lowest entropy. As you mix states, the entropy increases. To be

more quantitative, we define quantum entropy by

$$S(\rho) = -\text{tr } \rho \ln \rho \quad (34)$$

which is known as von Neumann entropy. In order to see that it is indeed an entropy, we use the spectral decomposition (11). Substituting the decomposition in to the entropy definition, we obtain

$$S(\rho) = -\sum_i \lambda_i \ln \lambda_i \quad (35)$$

Since λ_i is interpreted as probability, $S(\rho)$ is indeed Shannon entropy. The maximum of the entropy is obtained when all eigenvalues are degenerate, that is $\lambda_i = \frac{1}{D}$. Then, $S(\rho) = \ln D$. This is the maximally mixed state. On the other hand, if there is no mixing, $\lambda_1 = 1$ and $\lambda_{i>1} = 0$, we have vanishing entropy $S(\rho_{\text{pure}}) = 0$. Therefore, the von Neumann entropy can be used to determine if the system is pure or mixed. The von Neumann entropy plays essential roles in quantum information theory.

C. Composite Systems

Consider a pair of qubits. As we discussed in the previous section, they can be in a product state like $|00\rangle$ or in an entangled state $\frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|10\rangle$ (known as Bell state). We want to find the state of individual qubits. For the product state, answer is simple, $|00\rangle$ means both qubits are in state $|0\rangle$ and they are independent. On the other hand, when they are entangled, the individual state cannot be expressed as a pure state.

1. Reduced Density

In order to define the state of subsystem and also to understand entanglement, we introduce a mathematical operation called *partial trace* as follows

$$\rho_1 = \text{tr}_2 \rho = \sum_i (I_1 \otimes \langle \phi_i |) \rho (I_1 \otimes | \phi_i \rangle) \quad (36)$$

where I_1 is the identity operator in \mathcal{H}_1 and $|\phi_i\rangle$ orthonormal basis kets in \mathcal{H}_2 . Similarly,

$$\rho_2 = \text{tr}_1 \rho = \sum_i (\langle \phi_i | \otimes I_2) \rho (| \phi_i \rangle \otimes I_2). \quad (37)$$

ρ_1 and ρ_2 satisfy the definition of density operator (10) and thus are called *reduced density*. We interpret the reduced densities ρ_1 and ρ_2 as the state of subsystem 1 and 2, respectively.

Example of Partial Trace

Consider a pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. The corresponding density operator is

$$\rho = \frac{1}{2}(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|) \quad (38)$$

Then, the reduced density can be calculated as

$$\rho_1 = \text{tr}_2 \rho = (I \otimes \langle 0|)\rho(I \otimes |0\rangle) + (I \otimes \langle 1|)\rho(I \otimes |1\rangle) \quad (39)$$

Actual computing involves

$$(I \otimes \langle 1|)|00\rangle = (I|0\rangle)\langle 1|0\rangle = 0 \quad (40a)$$

$$(I \otimes \langle 1|)|01\rangle = (I|0\rangle)\langle 1|1\rangle = |1\rangle \quad (40b)$$

Now we can calculate Eq (46) and the result is

$$\rho_1 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \quad (41)$$

which is a mixed state. Note that the total density is a pure state but the reduced density is a mixed state. In other words, if you look at only a subsystem, its state is a mixed state. even when the whole system is in a pure state

2. Product States

When the whole system, regardless of pure or mixed, can be written as

$$\rho = \rho_1 \otimes \rho_2 \quad (42)$$

we say that the system is in a *product state*. In this case, the two subsystems are independent and there is no correlation between them. In this case the calculation of partial trace is trivial. $\text{tr}_2 \rho_1 \otimes \rho_2 = \rho_1 \text{tr}_2 \rho_2 = \rho_1$.

D. Separable States

If the two subsystems are classically correlated but not quantum mechanically, the total density operator can be written in a *separable* form

$$\rho = \sum_i P_i \rho_1^i \otimes \rho_2^i \quad (43)$$

where P_i is classical probability. This expression means that when the subsystem \mathcal{S}_1 is in ρ_1^i then, the other system \mathcal{S}_2 must be in ρ_2^i . Hence, there is correlation between \mathcal{S}_1 and \mathcal{S}_2 . However, this correlation is classical. The product state is a special case of separable states.

The state of the subsystem can be computed easily.

$$\rho_1 = \text{tr}_2 \sum_i P_i \rho_1^i \otimes \rho_2^i = \sum_i P_i \rho_1^i (\text{tr}_2 \rho_2^i) = \sum_i P_i \rho_1^i \quad (44)$$

and thus the subsystem 1 is in a mix state.

E. Entangled States and Decoherence

When the total density operator cannot be written in a product nor separable form, \mathcal{S}_1 and \mathcal{S}_2 are quantum mechanically correlated, which is now known as *quantum entanglement*. Consider a pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. The corresponding density operator is

$$\rho = \frac{1}{2}(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|) \quad (45)$$

which cannot be written in a separable form. Now we calculate the reduced density for the subsystem 1.

$$\rho_1 = \text{tr}_2 \rho = (I \otimes \langle 0|)\rho(I \otimes |0\rangle) + (I \otimes \langle 1|)\rho(I \otimes |1\rangle) \quad (46)$$

Actual computing involves

$$(I \otimes \langle 1|)|00\rangle = (I|0\rangle)\langle 1|0\rangle = 0 \quad (47a)$$

$$(I \otimes \langle 1|)|01\rangle = (I|0\rangle)\langle 1|1\rangle = |1\rangle \quad (47b)$$

Now we can calculate Eq (46) and the result is

$$\rho_1 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \quad (48)$$

which is a mixed state. Note that the total density is a pure state but the reduced density is a mixed state. In other words, if you look at only a subsystem, its state is a mixed state, even when the whole system is in a pure state. This result is very significant. When the system is entangled, the subsystem does not have coherence!

Consider a system of interest \mathcal{S} and the surrounding environment \mathcal{E} . The total system $\mathcal{S} + \mathcal{E}$ is assumed to be in a pure state $\rho_{\text{SB}}(t) = |\psi_{\text{SB}}(t)\rangle\langle\psi_{\text{SB}}(t)|$ and its evolution is unitary. We are not interested in the environment. We want to know how the system evolves in time. This is known as the problem of open quantum system. How can we describe the state of the system? This is not a trivial question especially when the system and the environment are quantum mechanically entangled. The time evolution of the subsystem is not unitary in general. In other words, the equation of motion for the total system is the Schrödinger equation but the equation of motion for the subsystem cannot be written in the form of Schrödinger equation. At

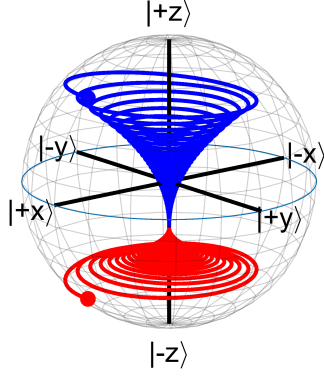


FIG. 7: Dynamics of a qubit interacting with environments.

the present we don't know any universal equation of motion for the subsystem. However, in certain cases, we can develop an approximated equation of motion. A popular one is known as quantum master equation in the Lindblad form. Figure 7 shows that the exact evolution of qubit interacting with bosonic environments. Starting with a pure state $\rho(t_0) = |\psi\rangle\langle\psi|$, as the system evolves, decoherence between $|0\rangle$ and $|1\rangle$ takes place. The final state is a Gibbs state $P_0 |0\rangle\langle 0| + P_1 |1\rangle\langle 1|$ where $P_i = e^{-\beta E_i} / (\sum_j e^{-\beta E_j})$ which lost coherence entirely.