

Department of Information Engineering
MSc in Computer Engineering (a.y. 2024/2025)
University of Pisa

*Quantum Computing
and
Quantum Internet*

Luciano Lenzini
Full Professor
Department of Information Engineering
School of Engineering
University of Pisa, Italy
e-mail: lenzini44@gmail.com
<http://www.iet.unipi.it/~lenzini/>
<http://www.originiinternetitalia.it/it/>



Mixed States And The Density Operator

Pure States cf. Mixed States

- Thus far, we have represented the state of an *n-qubit quantum system* using state-vector notation
- For this type of system, there is no uncertainty whatsoever regarding its state
- For example, if we initialize the single qubit in state $|0\rangle$, and apply a Hadamard gate, we know our final state will be:

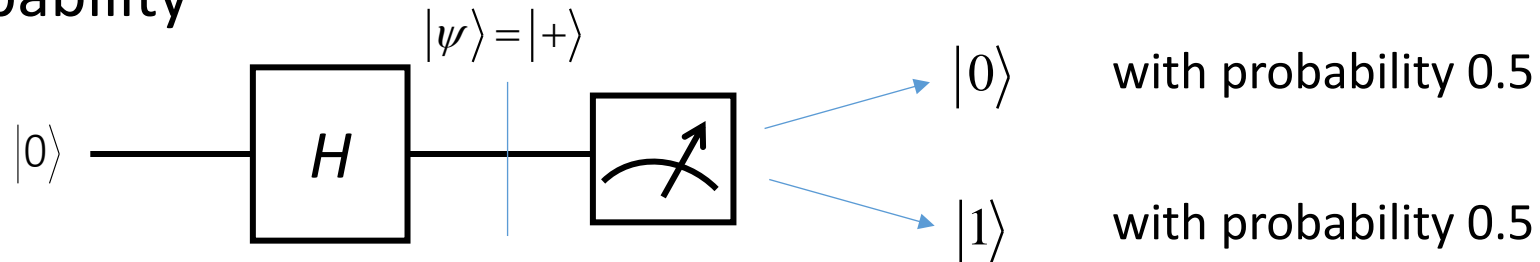
$$|0\rangle \text{ --- } \boxed{H} \text{ --- } |\psi\rangle = H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \equiv |+\rangle$$

- We understand that if we were to perform a measurement of this state, the outcome will be probabilistic

Pure States cf. Mixed States

$$|\psi\rangle = H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

- We will measure state $|0\rangle$ with 50% probability, and 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 $|+\rangle$
- Since there is no uncertainty on what this quantum state will be, we say that $|\psi\rangle$ is a *pure state*

Pure States cf. Mixed States

- Working with this representation is convenient when dealing with states that can always be expressed as a linear combination (superposition) of basis states, each with an associated probability amplitude, e.g.

$$|\psi\rangle = \sum_k a_k |k\rangle$$

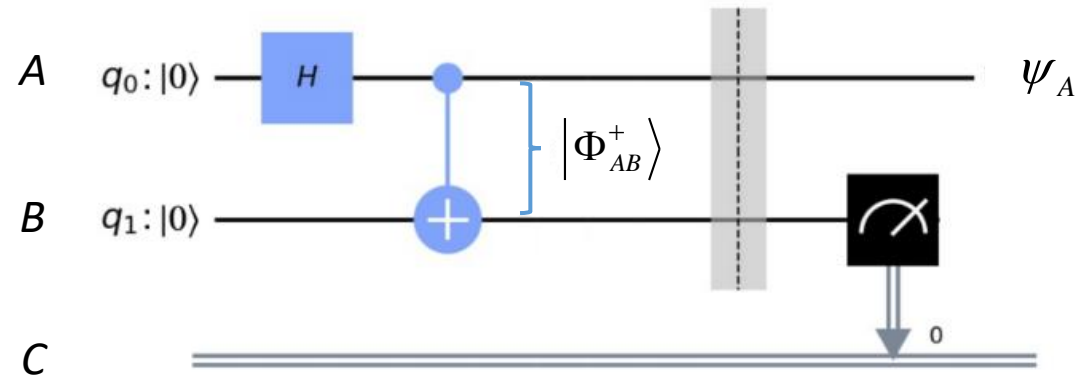
- However, in *quantum computation* and *quantum communication*, there are many practical situations in which the state of our qubits cannot be written down as linear combinations (superposition) in a given basis, but instead must be expressed in terms of *ensembles* (statistical mixtures) of multiple states, each with an associated probability of occurrence

Mixed States: Example #1

- Let's first take a look at a simple example to explain what we mean by this
- Consider the two-qubit entangled state:

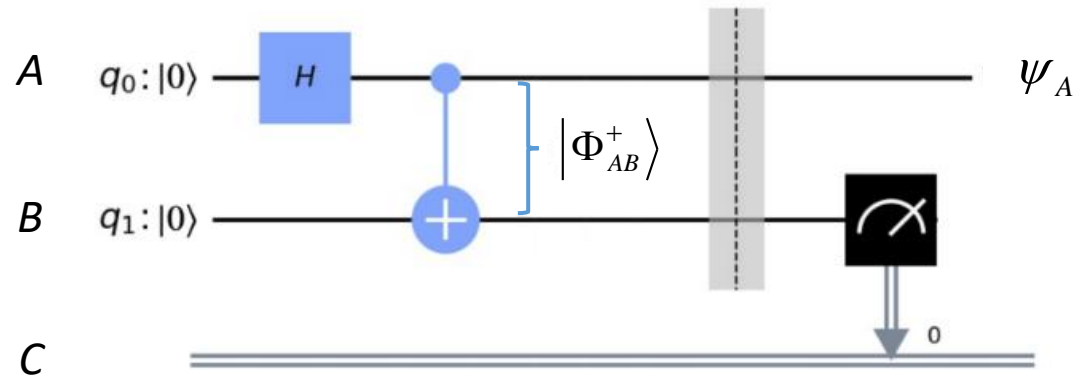
$$|\Phi_{AB}^+\rangle = \frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle)$$

- Here we have explicitly used the subscripts A and B to label the qubits associated with registers q_0 and q_1 , respectively



Mixed States: Example #1

- Now, let's assume that right after preparing our state $|\Phi_{AB}^+\rangle$ we perform a measurement on register q_1 , as shown below:

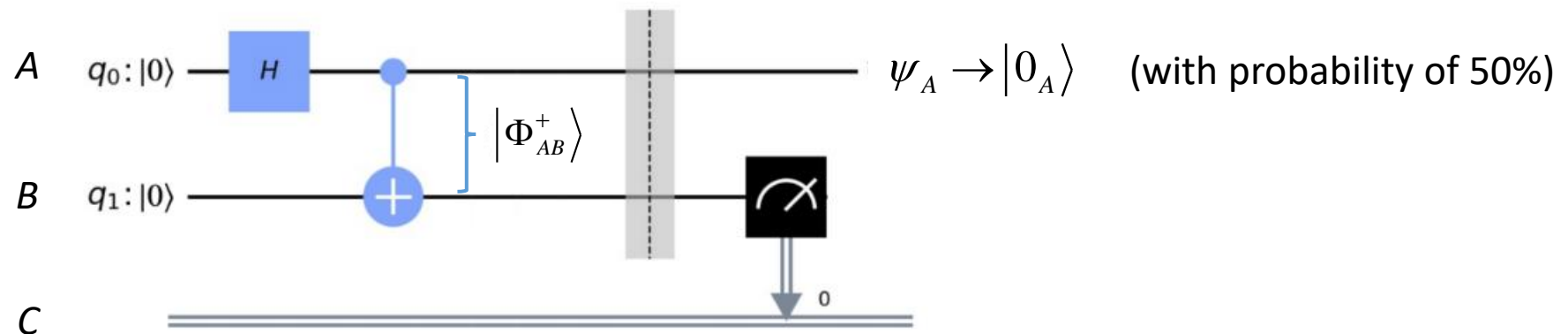


- We can now ask the question: what will the state on register q_0 be right after performing the measurement on register q_1 ?

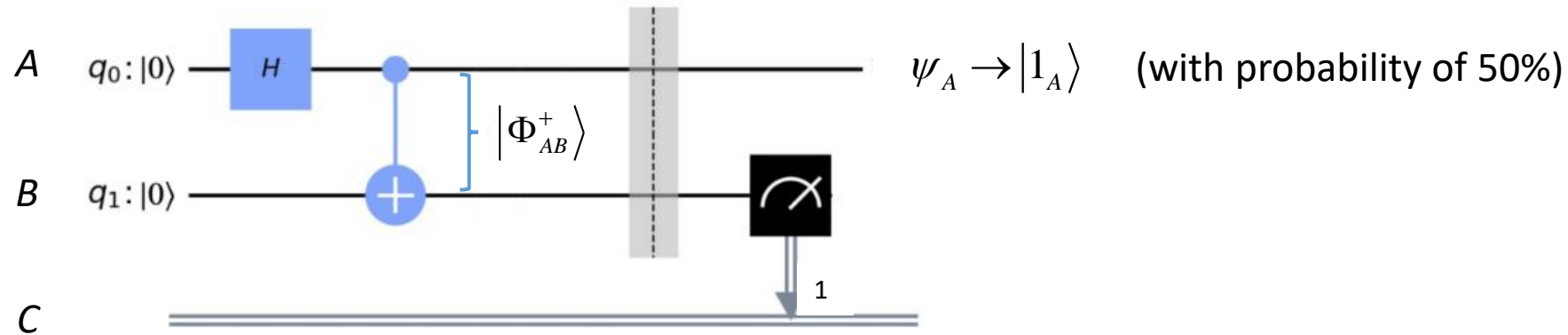
Mixed States: Example #1

- We know that since qubits A and B are entangled, measuring a 0 in register q_1 implies that the quantum state in register q_0 will immediately project onto the state $|0_A\rangle$

$$\frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle) \xrightarrow{\text{measure}} |0_A\rangle|0_B\rangle \quad (\text{with probability of 50\%})$$



Mixed States: Example #1



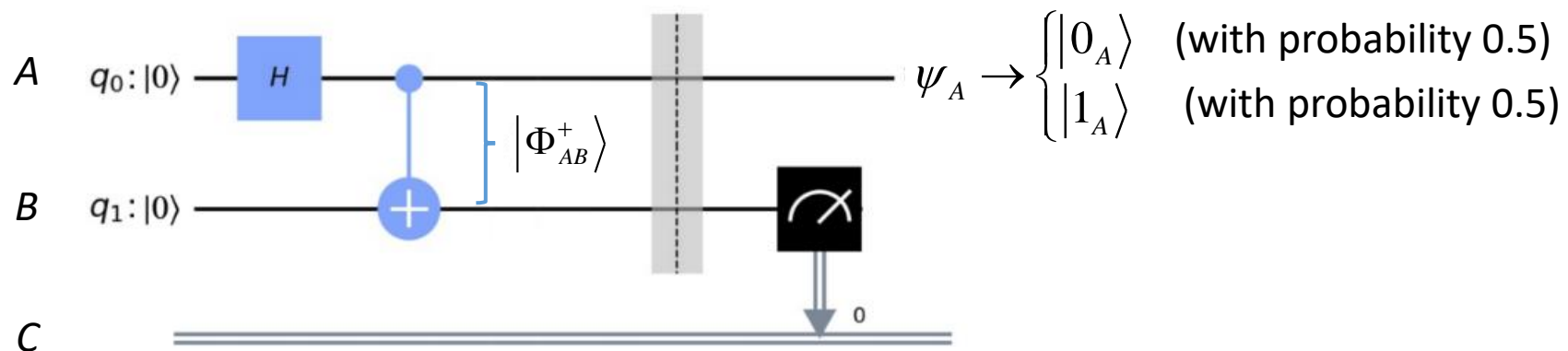
- Similarly, measuring a 1 in register q_1 implies that the quantum state in register q_0 will immediately project onto the state $|1_A\rangle$

$$\frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle) \xrightarrow{\text{measure}} |1_A\rangle |1_B\rangle \quad (\text{with probability of 50\%})$$

- We can now ask the question: what will the state on register q_0 be right after performing the measurement on register q_1 ?

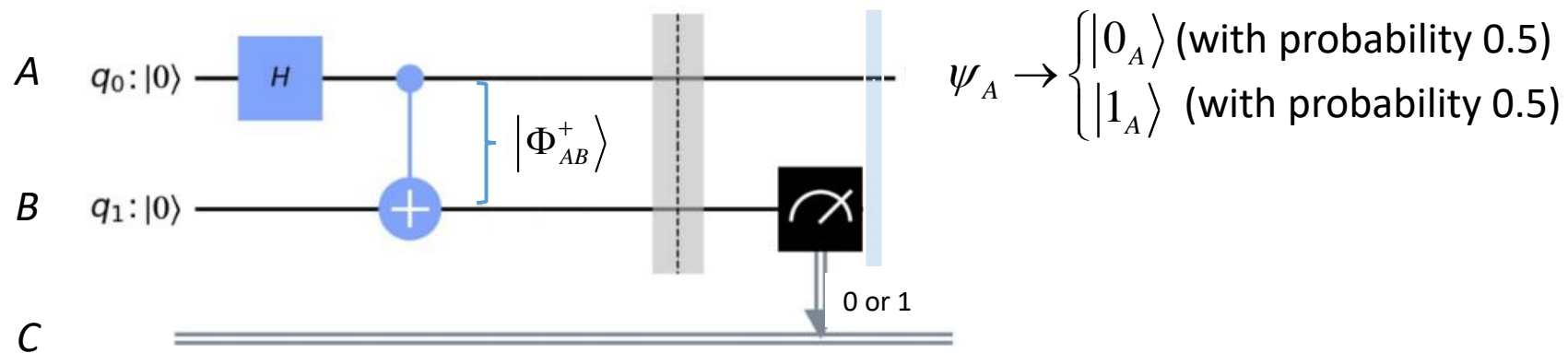
Mixed States: Example #1

- So how do we, in general, represent the final state in register q_0 (labeled as ψ_A in the diagram), *not for a specific measurement outcome in q_1* , but for an *arbitrary result* of this measurement process?
- We know that after a measurement, ψ_A will be in state $|0_A\rangle$ with probability 1/2, or in state $|1_A\rangle$ with probability 1/2; however, ψ_A is **not** in a linear superposition of $|0_A\rangle$ and $|1_A\rangle$



Mixed States: Example #1

- In other words, ψ_A **cannot** be expressed as a state vector of the form $1/\sqrt{2}(|0_A\rangle + |1_A\rangle)$
- Instead, we have to use a different notation to write down that ψ_A is rather an ensemble (not a quantum superposition) of the states $|0_A\rangle$ and $|1_A\rangle$, and whose outcome depends on what we measure on register q_1



Mixed States: Example #1

- We then call ψ_A a *mixed state* which can be represented as an *ensemble of states* each with an associated probability of occurrence

$$\left\{ \frac{1}{2}, |0_A\rangle; \frac{1}{2}, |1_A\rangle \right\}$$

- What this representation shows is that, upon measurement of q_1 , ψ_A will be in *either* state $|0_A\rangle$ *or* state $|1_A\rangle$, each with a *classical probability* of occurrence of 1/2
- We avoided using the ket notation for state ψ_A since we reserve kets only for state vectors that can be written as linear combinations in an orthonormal basis, which ψ_A is not

Mixed States: Example #2

- In an earlier example we considered the following scenario under the assumption that the Hadamard gate was ideal

$$|0\rangle \text{ --- } \boxed{H} \text{ --- } |\psi\rangle = H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \equiv |+\rangle$$

- However, in practice, an Hadamard gate *is not ideal*
- Due to errors in the quantum-computer hardware, only (let's say) 80% of the times the state is prepared, this Hadamard gate produces the desired state (i.e. $|+\rangle$)

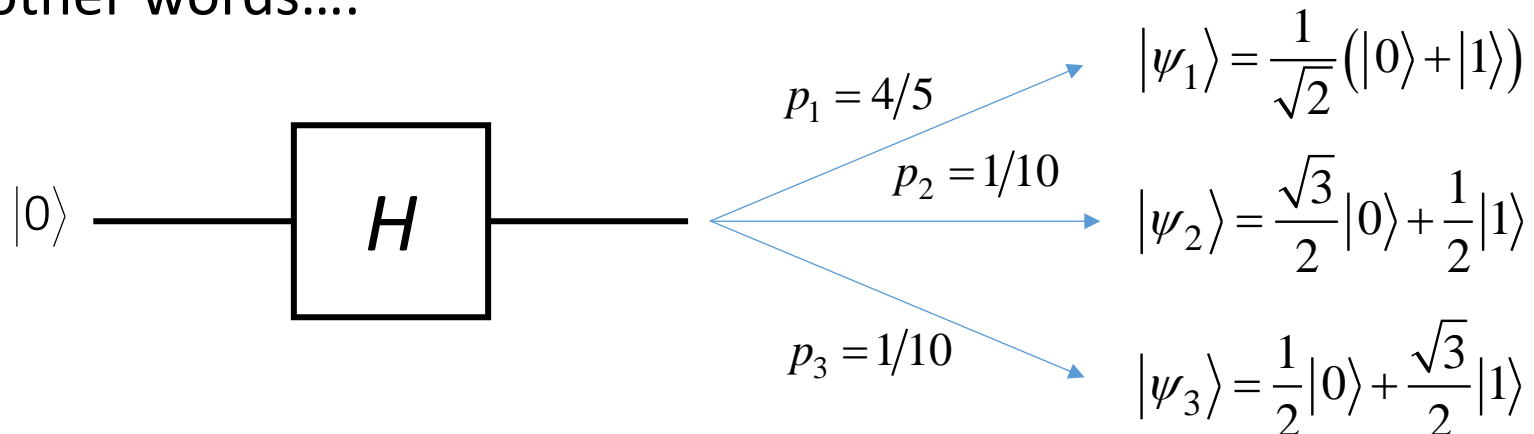
Mixed States: Example #2

- The remaining 20% of the times, when we use this Hadamard gate, we could end up with the same probability (1/10) with one of following two undesired outcome states:

$$|\psi_2\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle = \begin{bmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{bmatrix}$$

$$|\psi_3\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle = \begin{bmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix}$$

- In other words....



Mixed States: Example #2

- Since we do not know the outcome of our qubit every time we prepare it, we can represent it as a *mixed state* characterized by the following *ensemble*

$$\left\{ \frac{4}{5}, |\psi_1\rangle; \frac{1}{10} |\psi_2\rangle; \frac{1}{10} |\psi_3\rangle \right\}$$

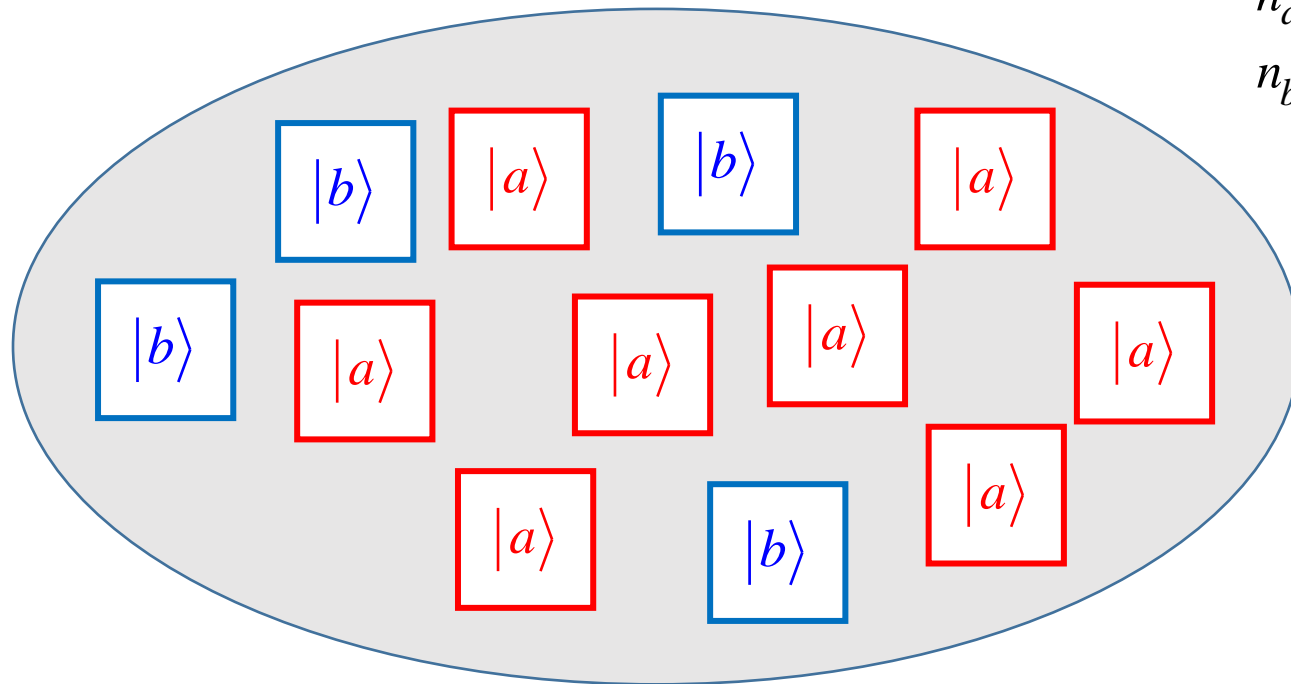
- Here, the factors $4/5$, $1/10$ and $1/10$ correspond to the “*classical*” *probabilities* of obtaining the states $|\psi_1\rangle$, $|\psi_2\rangle$ and $|\psi_3\rangle$, respectively

Mixed States: Example #3

- Consider a two-dimensional Hilbert space with basis vectors $\{|x\rangle, |y\rangle\}$
- We prepare a large number N of quantum systems, where each member of the system can be in one of two state vectors
$$|a\rangle = \alpha|x\rangle + \beta|y\rangle, \quad |b\rangle = \gamma|x\rangle + \delta|y\rangle$$
- These states are normalized, so $|\alpha|^2 + |\beta|^2 = |\gamma|^2 + |\delta|^2 = 1$, and the usual rules of quantum mechanics apply
- For a system in state $|a\rangle$, if a measurement is made, then there is a probability $|\alpha|^2$ of finding $|x\rangle$ while there is a probability $|\beta|^2$ of finding $|y\rangle$, and similarly for state $|b\rangle$

Mixed States: Example #3

- Now suppose that we prepare n_a of these systems in state $|a\rangle$ and n_b of the systems in state $|b\rangle$



$$n_a = 8$$

$$n_b = 4$$

$$n_a + n_b = N = 12$$

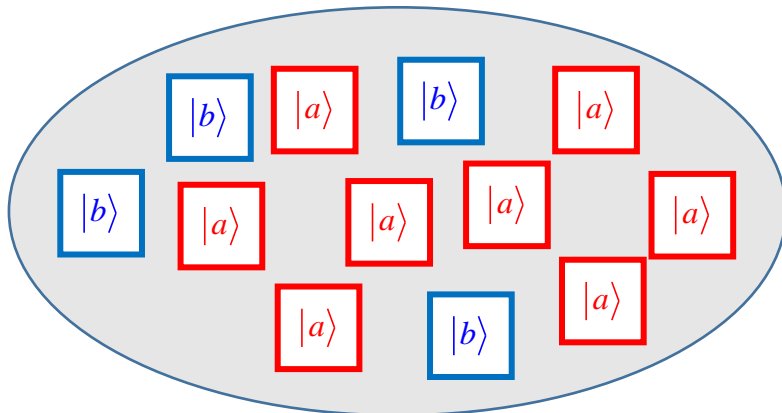
Mixed States: Example #3

– Since we have N total systems, then $n_a + n_b = N$

– If we divide by N ,

$$\frac{n_a}{N} + \frac{n_b}{N} = 1$$

– This relation tells us that if we *randomly select a member of the ensemble*, the probability that it is found in state $|a\rangle$ or $|b\rangle$ is given by $p_a = \frac{n_a}{N}$ or $p_b = \frac{n_b}{N}$ respectively



$$p_a = \frac{n_a}{N} = \frac{8}{12} \simeq 0.66$$

$$p_b = \frac{n_b}{N} = \frac{4}{12} \simeq 0.33$$

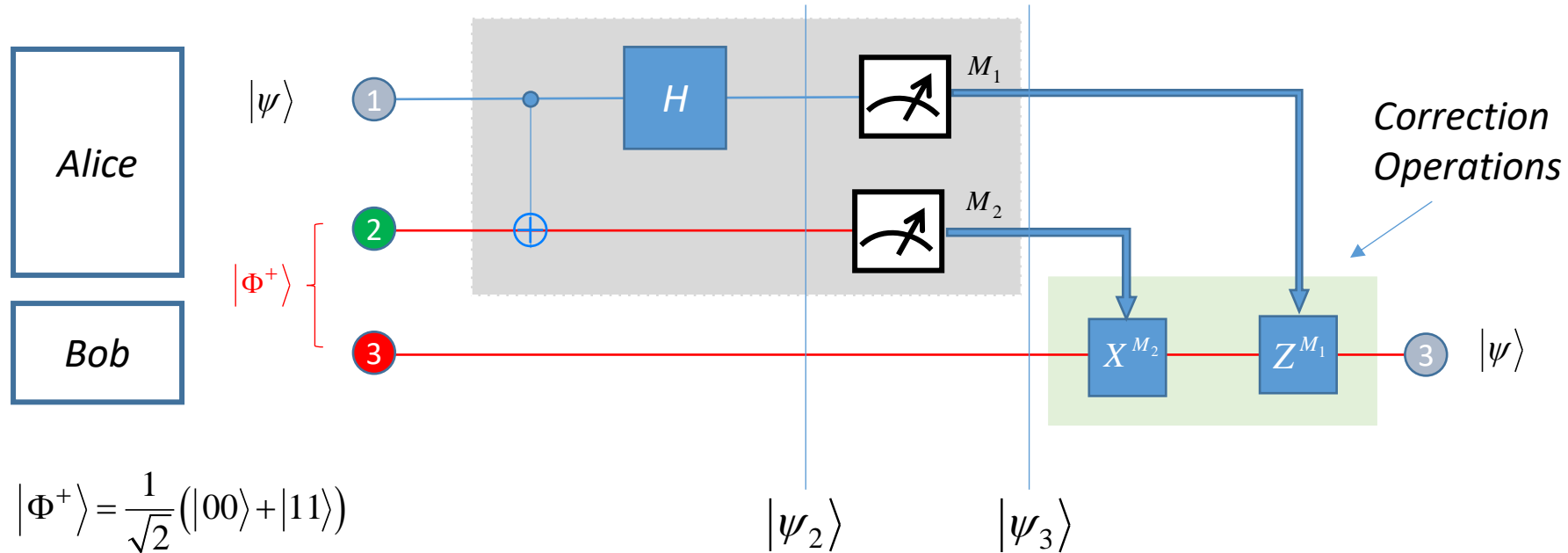
Mixed States: Example #3

- This ensemble comprising N systems is called a *statistical mixture of the pure states* $|a\rangle$ and $|b\rangle$ where each pure state has a corresponding probability of occurrence given by p_a and $p_b = 1 - p_a$ respectively
- Since we do not know the outcome of our quantum system every time we extract it, we can represent it as a *mixed state* characterized by the following *ensemble*

$$\{p_a, |a\rangle; p_b, |b\rangle\}$$

Mixed States: Example #4 - Teleportation

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$



$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$|\psi_2\rangle = \frac{1}{2} \left[|0_1 0_2\rangle (\alpha|0_3\rangle + \beta|1_3\rangle) + |0_1 1_2\rangle (\alpha|1_3\rangle + \beta|0_3\rangle) + |1_1 0_2\rangle (\alpha|0_3\rangle - \beta|1_3\rangle) + |1_1 1_2\rangle (\alpha|1_3\rangle - \beta|0_3\rangle) \right]$$

Mixed States: Example #4 - Teleportation

Depending on Alice's measurement outcome, Bob's qubit will end up in one of these four possible states

$$0_1 0_2 \rightarrow |\psi_3(0_1 0_2)\rangle = [\alpha|0_3\rangle + \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$0_1 1_2 \rightarrow |\psi_3(0_1 1_2)\rangle = [\alpha|1_3\rangle + \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$1_1 0_2 \rightarrow |\psi_3(1_1 0_2)\rangle = [\alpha|0_3\rangle - \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$1_1 1_2 \rightarrow |\psi_3(1_1 1_2)\rangle = [\alpha|1_3\rangle - \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

As a result, Bob's qubit is in a mixed state described by the ensemble:

$$\left\{ \frac{1}{4}, |\psi_3(0_1 0_2)\rangle; \frac{1}{4}, |\psi_3(0_1 1_2)\rangle; \frac{1}{4}, |\psi_3(1_1 0_2)\rangle + \frac{1}{4}, |\psi_3(1_1 1_2)\rangle \right\}$$

Mixed States

- In general, suppose a quantum system is in one of a number n of *pure* states $|\psi_j\rangle$, where j is an index, with respective probabilities p_j
- We shall call $\{p_j, |\psi_j\rangle\}_{j=1}^n$ an *ensemble of pure states*
- At this point, it is important to highlight that the $|\psi_j\rangle$ states that compose an ensemble need not be basis states (like $|0\rangle$ and $|1\rangle$); these states are not necessarily *orthonormal* and can actually be any *arbitrary normalized pure state*

Mixed States

- For an *ensemble of pure states*, the use of probability is operating on *two different levels*:
 - At the *ensemble level*, where p_j corresponds to the *classical* probability of the system being in state $|\psi_j\rangle$
 - At the *level of a single quantum system* $|\psi_j\rangle$, where the Born rule gives us *the probability of obtaining a given measurement result*
- At the *ensemble level* the use of probability is acting in a “*classical*” way

Mixed States

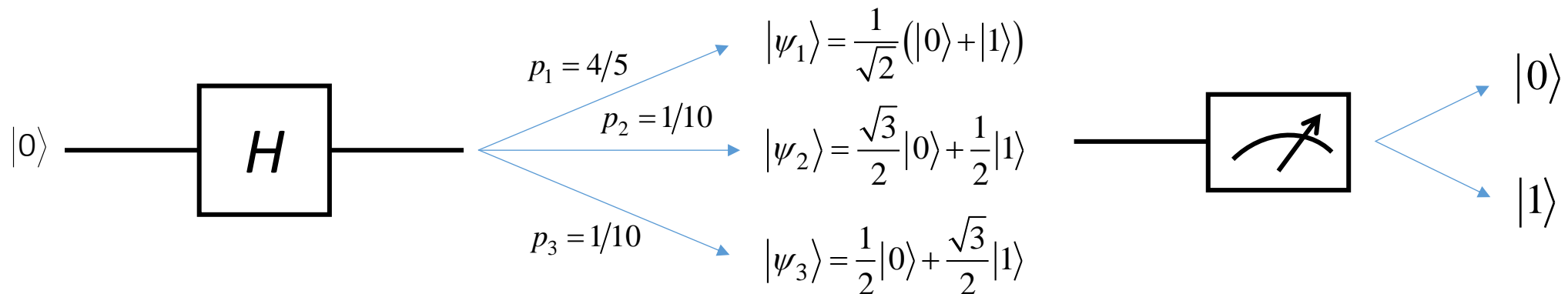
While *superposition* $|\psi_j\rangle = \sum_u \alpha_u^{(j)} |\phi_u\rangle$ is a *quantum linear combination* of *orthonormal basis states* *weighted by probability amplitudes*,

mixed states $\{p_j, |\psi_j\rangle\}_{j=1}^n$ are

a *classical linear combination* of *pure superpositions* (quantum states) *weighted by classical probabilities*

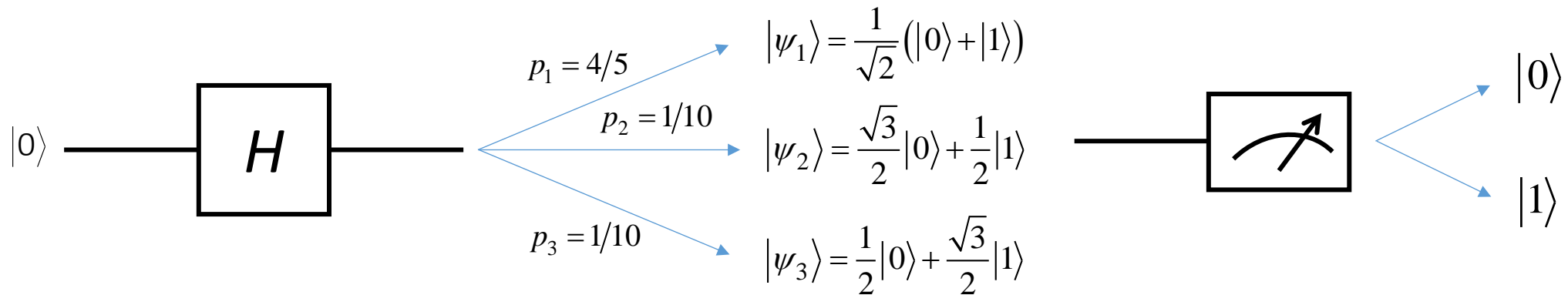
Mixed States

- As we have done for the pure state, we pose the question: If an individual member is drawn from the ensemble and a measurement is made, what are the probabilities of obtaining each possible measurement result?
- Let's focus our attention on Example #2 characterized by the ensemble:
 $\left\{ \frac{4}{5}|\psi_1\rangle; \frac{1}{10}|\psi_2\rangle; \frac{1}{10}|\psi_3\rangle \right\}$ and ask which is, after measuring, the probability to find $|0\rangle$ or $|1\rangle$



Mixed States

- Referring to the previous picture, we can write the probability of observing, after measurement, the state $|0\rangle$ or the state $|1\rangle$

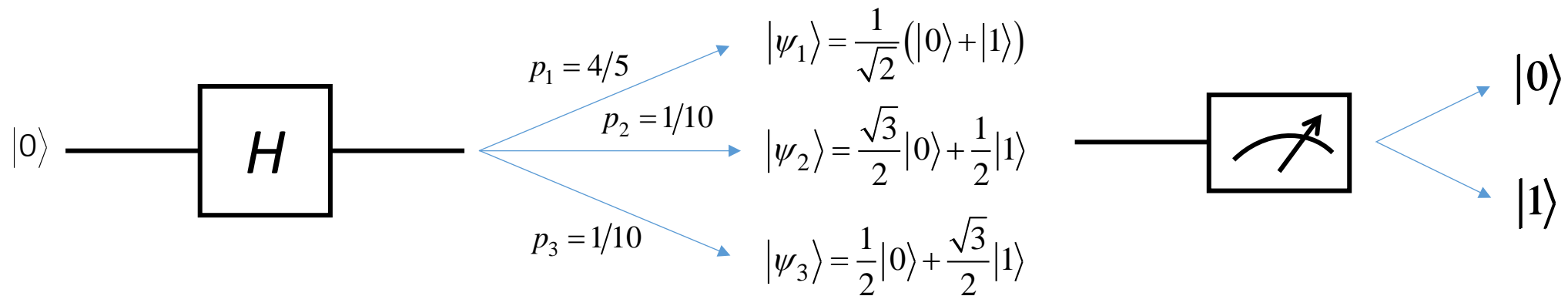


$$P\{0\} = P\{0|\psi_1\} P\{\psi_1\} + P\{0|\psi_2\} P\{\psi_2\} + P\{0|\psi_3\} P\{\psi_3\}$$

$$= |\langle 0|\psi_1\rangle|^2 p_1 + |\langle 0|\psi_2\rangle|^2 p_2 + |\langle 0|\psi_3\rangle|^2 p_3 = \left(\frac{1}{\sqrt{2}}\right)^2 \times \frac{4}{5} + \left(\frac{\sqrt{3}}{2}\right)^2 \times \frac{1}{10} + \left(\frac{1}{2}\right)^2 \times \frac{1}{10} = \frac{1}{2}$$

Mixed States

- By following the same procedure we can calculate $P\{1\}$



$$P\{1\} = P\{1|\psi_1\} P\{\psi_1\} + P\{1|\psi_2\} P\{\psi_2\} + P\{1|\psi_3\} P\{\psi_3\}$$

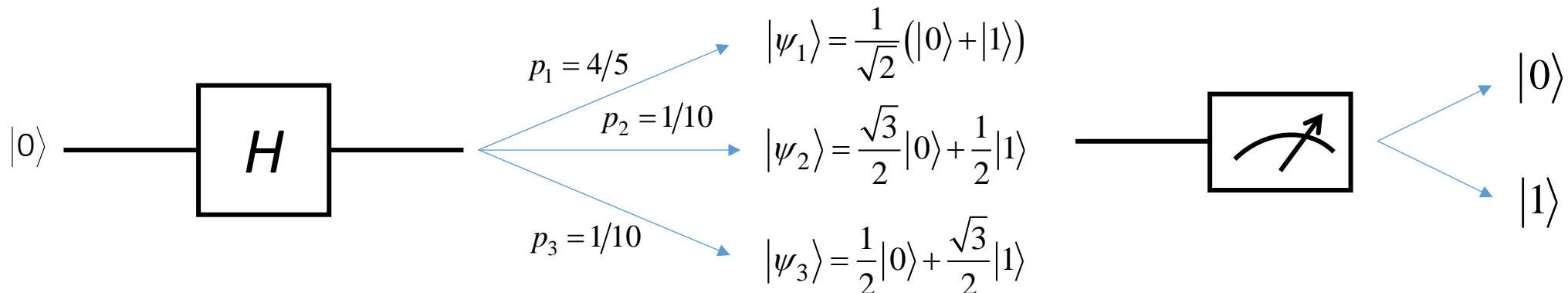
$$= |\langle 1|\psi_1\rangle|^2 p_1 + |\langle 1|\psi_2\rangle|^2 p_2 + |\langle 1|\psi_3\rangle|^2 p_3 = \left(\frac{1}{\sqrt{2}}\right)^2 \times \frac{4}{5} + \left(\frac{1}{2}\right)^2 \times \frac{1}{10} + \left(\frac{\sqrt{3}}{2}\right)^2 \times \frac{1}{10} = \frac{1}{2}$$

Mixed States

- The above calculations boil down to this:

$$P\{0\} = P\{1\} = \frac{1}{2}$$

which means that after the measurement, with the probability 0.5 we observe the state $|0\rangle$ and with the same probability we observe the state $|1\rangle$



Mixed States

- Although this way of expressing 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*
- In the next slide we will formally introduce the **density matrix representation** by looking at how it is used to represent both *pure* and *mixed states*

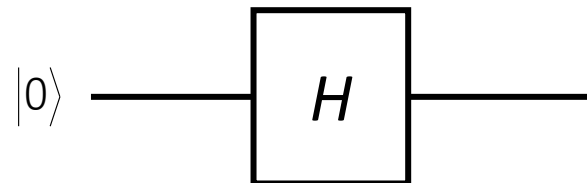
Density Operator for a Pure State

- For a pure state $|\psi\rangle$, the *density operator*, which is denoted by the symbol ρ , is specified as

$$\rho \equiv |\psi\rangle\langle\psi|$$

- For the aforementioned Hadamard in Example #2, the density operator is

$$\rho = |+\rangle\langle+| = \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right) \left(\frac{1}{\sqrt{2}} [1 \quad 1] \right) = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$



The diagram shows a quantum circuit starting with the state $|0\rangle$ on the left. A horizontal line leads to a square box labeled H , representing a Hadamard gate. Another horizontal line leads from the box to the resulting state $|\psi\rangle$.

$$|\psi\rangle = H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \equiv |+\rangle$$

Density Operator for a Pure State

- Now we move on to a more complex two qubits quantum system, in a *maximally-entangled pure state*

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

- The density matrix representation for this state is then given by:

$$\rho = |\Phi^+\rangle\langle\Phi^+| \quad \rightarrow \quad \rho = \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right) \left(\frac{1}{\sqrt{2}} [1 \ 0 \ 0 \ 1] \right) = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

Density Operator for a Mixed State

- For a *mixed state* characterized by an *ensemble of pure states* $\{p_j, |\psi_j\rangle\}_{j=1}^n$ the *density operator* is defined by the expression:

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

- This general definition of the density operator also holds for pure states, for which we will only have one $|\psi_j\rangle$ term with $p_j = 1$, i.e. $\{1, |\psi\rangle\}$

$$\rho = |\psi\rangle\langle\psi|$$

- The output state in the previous examples is a projector $|\psi_j\rangle\langle\psi_j|$ with probability p_j , and the whole output state can be described as a sum of all such projectors

$$\rho = p_1 |\psi_1\rangle\langle\psi_1| + p_2 |\psi_2\rangle\langle\psi_2| + \cdots + p_n |\psi_n\rangle\langle\psi_n|$$

The Density Operator (ρ)

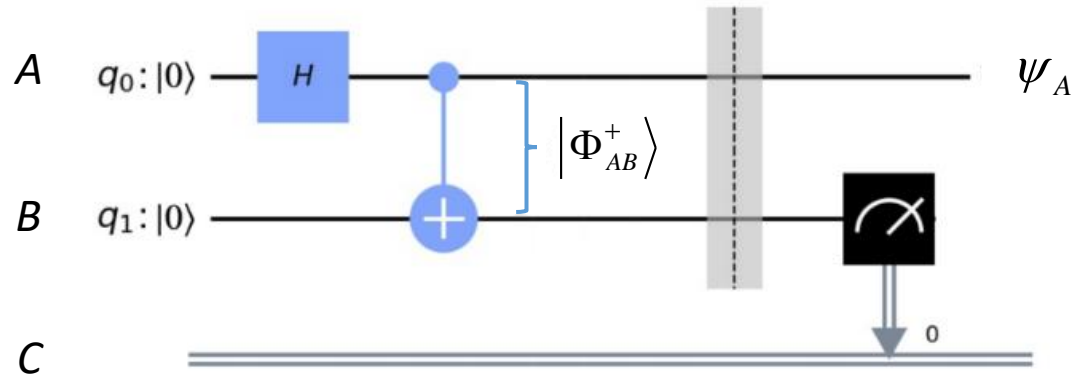
- Thus, the *density matrix* is an alternative way of expressing quantum states
- However, unlike the state-vector representation, this formalism allows us to use the same mathematical language to describe both the *pure states*, as well as the *mixed states* that consist of ensembles of pure states
- The terms *density operator* and *density matrix* are often used interchangeably in quantum mechanics

The Postulates of Quantum Mechanics Using Density Matrices

- This alternative formulation is *mathematically equivalent* to the state vector approach
- It turns out that all the postulates of quantum mechanics can be reformulated in terms of the density operator language
- Whether one uses the *density operator language*, or *the state vector language* is a matter of taste, since both give the same results; however, it is sometimes much easier to approach problems from one point of view rather than the other

Mixed States - Example #1

- Let's go back to the previous Example #1



where the mixed state ψ_A is represented by the following ensemble

$$\left\{ \frac{1}{2}, |0_A\rangle; \frac{1}{2}, |1_A\rangle \right\}$$

Mixed States - Example #1

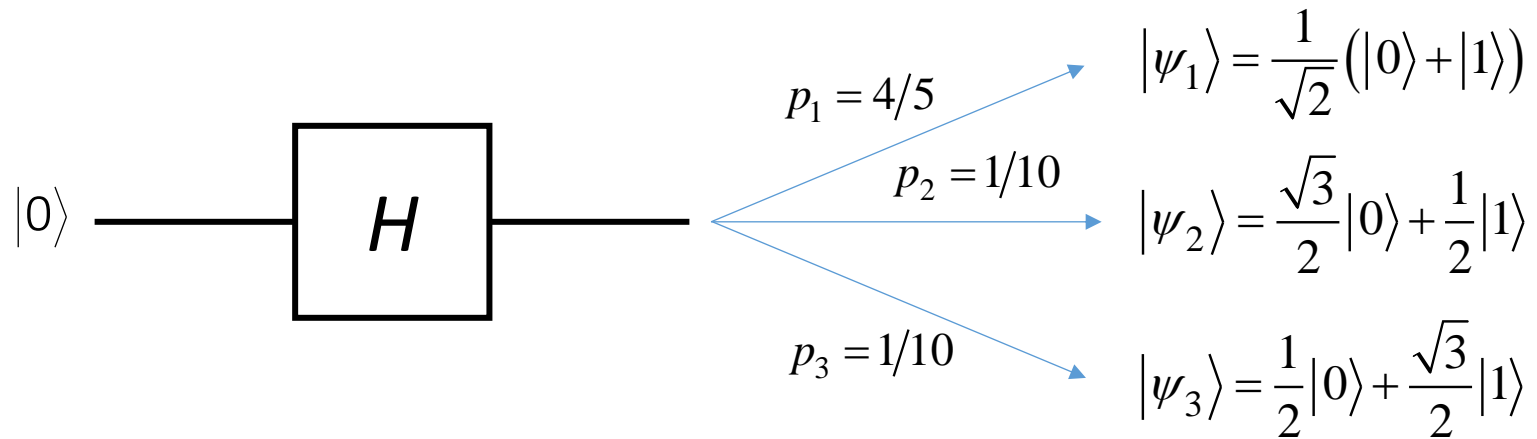
- It's easy to construct the density matrix for this ensemble $\left\{ \frac{1}{2}, |0_A\rangle; \frac{1}{2}, |1_A\rangle \right\}$

$$\begin{aligned}\rho_A &= \frac{1}{2}|0_A\rangle\langle 0_A| + \frac{1}{2}|1_A\rangle\langle 1_A| \\ &= \frac{1}{2}\begin{bmatrix} 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 \\ 1 \end{bmatrix}\begin{bmatrix} 0 & 1 \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \longrightarrow \quad \rho_A = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}\end{aligned}$$

NOTE: I wrote in red the elements on the diagonal since they are numerically equivalent to the probabilities $P\{0\} = P\{1\} = 1/2$ we calculated before

Mixed States - Example #2

- Regarding the previous Example #2 with the *non ideal* Hadamard Gate



the output of the Hadamard state can be represented by the following mixed state

$$\left\{ \frac{4}{5}, |\psi_1\rangle; \frac{1}{10}, |\psi_2\rangle; \frac{1}{10}, |\psi_3\rangle \right\} \rightarrow$$
$$\rho_H = \frac{4}{5} |\psi_1\rangle\langle\psi_1| + \frac{1}{10} |\psi_2\rangle\langle\psi_2| + \frac{1}{10} |\psi_3\rangle\langle\psi_3|$$

Mixed States - Example #2

- Let's start by calculating the outer products

$$|\psi_1\rangle\langle\psi_1| = \left(\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\right)\left(\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \end{bmatrix}\right) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$$|\psi_2\rangle\langle\psi_2| = \begin{bmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{3}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{1}{4} \end{bmatrix}$$

$$|\psi_3\rangle\langle\psi_3| = \begin{bmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} \end{bmatrix}$$

Mixed States - Example #2

- By putting the outer products into the ρ_H expression

$$\begin{aligned}\rho_H &= \frac{4}{5}|\psi_1\rangle\langle\psi_1| + \frac{1}{10}|\psi_2\rangle\langle\psi_2| + \frac{1}{10}|\psi_3\rangle\langle\psi_3| \\ &= \frac{4}{5}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} + \frac{1}{10}\begin{bmatrix} \frac{3}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{1}{4} \end{bmatrix} + \frac{1}{10}\begin{bmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} \end{bmatrix}\end{aligned}$$

$$\rho_H = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{20} + \frac{2}{5} \\ \frac{\sqrt{3}}{20} + \frac{2}{5} & \frac{1}{2} \end{bmatrix}$$

NOTE: I wrote in red the elements on the diagonal since they are numerically equivalent to the probabilities $P\{0\} = P\{1\} = 1/2$ we calculated before

Mixed States - Example #3

- Let's go back to the previous Example #3 with the following *ensemble*

$$\{p_a, |a\rangle; p_b, |b\rangle\} \quad \text{where} \quad |a\rangle = \alpha|x\rangle + \beta|y\rangle, \quad |b\rangle = \gamma|x\rangle + \delta|y\rangle$$

we have

$$\begin{aligned} \rho &= p_a |a\rangle\langle a| + p_b |b\rangle\langle b| = p_a \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \begin{bmatrix} \alpha^* & \beta^* \end{bmatrix} + p_b \begin{bmatrix} \gamma \\ \delta \end{bmatrix} \begin{bmatrix} \gamma^* & \delta^* \end{bmatrix} \\ &= p_a \begin{bmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{bmatrix} + p_b \begin{bmatrix} \gamma\gamma^* & \gamma\delta^* \\ \delta\gamma^* & \delta\delta^* \end{bmatrix} \\ &= \begin{bmatrix} p_a|\alpha|^2 + p_b|\gamma|^2 & p_a\alpha\beta^* + p_b\gamma\delta^* \\ p_a\beta\alpha^* + p_b\delta\gamma^* & p_a|\beta|^2 + p_b|\delta|^2 \end{bmatrix} \end{aligned}$$

Mixed States - Example #4

- Let's go back to the previous Example #4 with the following *ensemble*

$$\left\{ \frac{1}{4} |\psi_3(0_1 0_2)\rangle, \frac{1}{4} |\psi_3(0_1 1_2)\rangle, \frac{1}{4} |\psi_3(1_1 0_2)\rangle, \frac{1}{4} |\psi_3(1_1 1_2)\rangle \right\}$$

where

$$|\psi_3(0_1 0_2)\rangle = \alpha |0_3\rangle + \beta |1_3\rangle, \quad |\psi_3(0_1 1_2)\rangle = \alpha |1_3\rangle + \beta |0_3\rangle, \quad |\psi_3(1_1 0_2)\rangle = \alpha |0_3\rangle - \beta |1_3\rangle, \quad |\psi_3(1_1 1_2)\rangle = \alpha |1_3\rangle - \beta |0_3\rangle$$

- The density matrix of Bob's qubit, after Alice has performed the measurement but before Bob has learned the measurement result is

$$\begin{aligned} \rho = \frac{1}{4} & \left(|\psi_3(0_1 0_2)\rangle \langle \psi_3(0_1 0_2)| + |\psi_3(0_1 1_2)\rangle \langle \psi_3(0_1 1_2)| \right. \\ & \left. + |\psi_3(1_1 0_2)\rangle \langle \psi_3(1_1 0_2)| + |\psi_3(1_1 1_2)\rangle \langle \psi_3(1_1 1_2)| \right) \end{aligned}$$

Mixed States - Example #4

– Continuing...

$$\rho = \frac{1}{4} \left[(\alpha|0_3\rangle + \beta|1_3\rangle)(\alpha^*\langle 0_3| + \beta^*\langle 1_3|) + (\alpha|1_3\rangle + \beta|0_3\rangle)(\alpha^*\langle 1_3| + \beta^*\langle 0_3|) \right. \\ \left. + (\alpha|0_3\rangle - \beta|1_3\rangle)(\alpha^*\langle 0_3| - \beta^*\langle 1_3|) + (\alpha|1_3\rangle - \beta|0_3\rangle)(\alpha^*\langle 1_3| - \beta^*\langle 0_3|) \right]$$

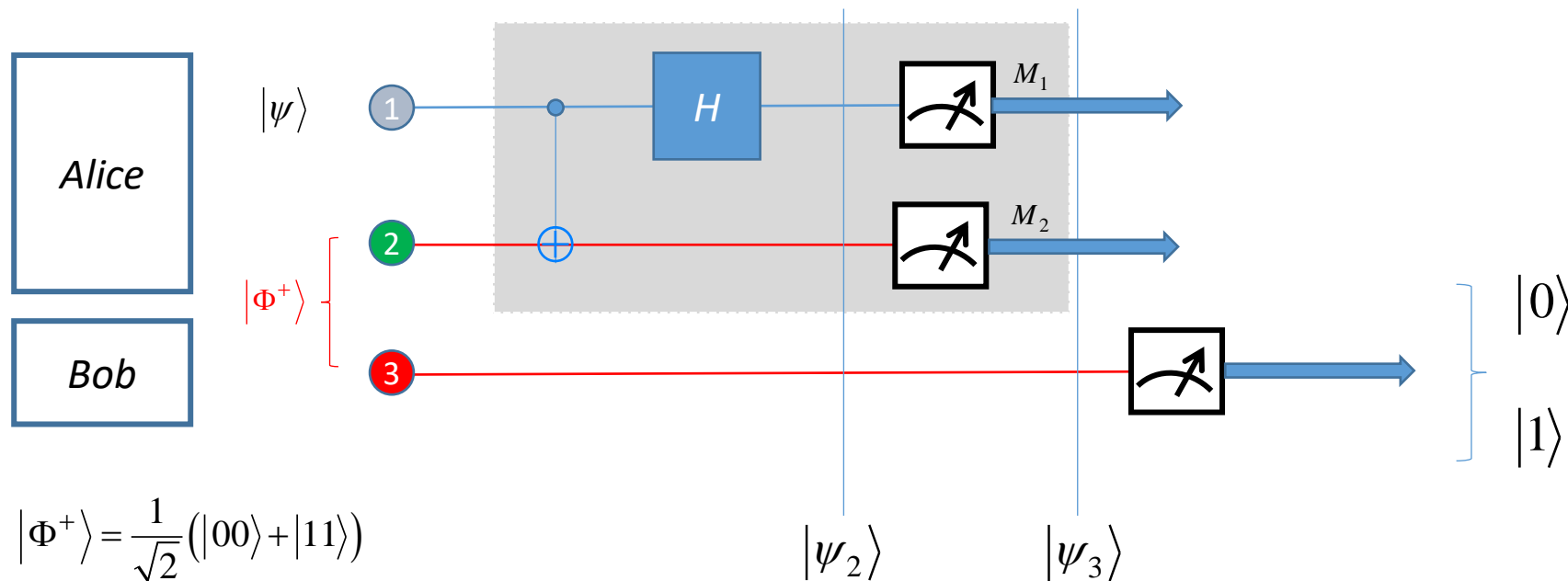
– After some algebraic manipulation we get

$$\rho = \frac{1}{2} (|0_3\rangle\langle 0_3| + |1_3\rangle\langle 1_3|) = \frac{I}{2} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

This state has no dependence upon the state $|\psi\rangle$ being teleported, and thus any measurements performed by Bob will contain no information about $|\psi\rangle$, thus preventing Alice from using teleportation to transmit information to Bob faster than light

Mixed States - Example #4

- Let's now assume, as an exercise, that Bob will make a measurement before the correction operations



Mixed States - Example #4

- Let's now write down the probability that Bob will observe the state $|0\rangle$ or the state $|1\rangle$
- Before the measurement, the state at the Bob's site is a mixed state described by the ensemble

$$\left\{ \frac{1}{4}, |\psi_3(0_1 0_2)\rangle; \frac{1}{4}, |\psi_3(0_1 1_2)\rangle; \frac{1}{4}, |\psi_3(1_1 0_2)\rangle + \frac{1}{4}, |\psi_3(1_1 1_2)\rangle \right\}$$

where $|\psi_3(0_1 0_2)\rangle = [\alpha|0_3\rangle + \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$

$$|\psi_3(0_1 1_2)\rangle = [\alpha|1_3\rangle + \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$|\psi_3(1_1 0_2)\rangle = [\alpha|0_3\rangle - \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$|\psi_3(1_1 1_2)\rangle = [\alpha|1_3\rangle - \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

Mixed States - Example #4

- Following the same procedure set out in Example #2

$$\begin{aligned} P\{0\} &= P\{0|\psi_3(00)\} P\{\psi_3(00)\} + P\{0|\psi_3(01)\} P\{\psi_3(01)\} \\ &\quad + P\{0|\psi_3(10)\} P\{\psi_3(10)\} + P\{0|\psi_3(11)\} P\{\psi_3(11)\} \\ &= \frac{1}{4}(|\alpha|^2 + |\beta|^2 + |\alpha|^2 + |\beta|^2) = \frac{1}{2} \end{aligned}$$

- In the same way, one can calculate $P\{1\}$ and get

$$P\{1\} = \frac{1}{2}$$

$$|\psi_3(0_1 0_2)\rangle = [\alpha|0_3\rangle + \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$|\psi_3(0_1 1_2)\rangle = [\alpha|1_3\rangle + \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$|\psi_3(1_1 0_2)\rangle = [\alpha|0_3\rangle - \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$|\psi_3(1_1 1_2)\rangle = [\alpha|1_3\rangle - \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

Mixed States - Example #4

- In this example, similar to Example #2, we can see that the elements on the diagonal of the density matrix

$$\rho = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

are equal to the probabilities $P\{0\}$ and $P\{1\}$ we have just calculated

Non-Uniqueness

- It is a tempting (and surprisingly common) mistake to suppose that the eigenvalues and eigenvectors of a density matrix have some special significance with regard to the ensemble of quantum states represented by that density matrix
- For example, one might suppose that a quantum system with density matrix

$$\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| = \begin{bmatrix} 3/4 & 0 \\ 0 & 1/4 \end{bmatrix} \quad \text{with eigenvalues} \quad \left\{ \begin{array}{l} 3/4 \rightarrow \text{Eigenvector } |0\rangle \\ 1/4 \rightarrow \text{Eigenvector } |1\rangle \end{array} \right.$$

must be in the state $|0\rangle$ with probability $3/4$ and in the state $|1\rangle$ with probability $1/4$

- Therefore, the above ρ must be associated to the ensemble $ENS_1 = \left\{ \frac{3}{4}, |0\rangle; \frac{1}{4}, |1\rangle \right\}$

Non Uniqueness

- However, this is not necessarily the case. Suppose we define

$$|a\rangle = \sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle, \quad |b\rangle = \sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle$$

and the quantum system is prepared in the state $|a\rangle$ with probability 1/2 and in the state $|b\rangle$ with probability 1/2, giving rise to the following ensemble $ENS_2 = \left\{ \frac{1}{2}, |a\rangle; \frac{1}{2}, |b\rangle \right\}$

- Then it is easily checked that the corresponding density matrix is

$$\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b| = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$$

- That is, these two (ENS_1 and ENS_2) different ensembles of quantum states give rise to the same density matrix

Non Uniqueness

- In general, the **eigenvectors** and **eigenvalues** of a *density matrix* just indicate **one of many possible ensembles** that may give rise to a specific density matrix, and there is no reason to suppose it is an especially privileged ensemble
- A natural question to ask in the light of this discussion is *what class of ensembles does give rise to a particular density matrix?*
- For the solution it is convenient to make use of vectors $|\tilde{\psi}_i\rangle$ which **may not be normalized to unit length**

Non Uniqueness

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

- We say the set $|\tilde{\psi}_i\rangle$ generates the operator $\rho = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|$, and thus the connection to the usual ensemble picture of density operators is expressed by the equation

$$|\tilde{\psi}_i\rangle = \sqrt{p_i} |\psi_i\rangle$$

- When do two sets of vectors, $|\tilde{\psi}_i\rangle$ and $|\tilde{\phi}_j\rangle$ generate the same operator ρ ?
- The solution to this problem will enable us to answer the question of what ensembles give rise to a given density matrix
- Obviously, $|\tilde{\phi}_i\rangle = \sqrt{q_i} |\phi_i\rangle$ where $|\phi_i\rangle \in \left\{q_j, |\phi_j\rangle\right\}_{j=1}^n$

Non Uniqueness

$$\left\{ p_j, |\psi_j\rangle \right\}_{j=1}^n \quad \rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|$$

Theorem: (Unitary freedom in the ensemble for density matrices) The sets $|\tilde{\psi}_i\rangle$ and $|\tilde{\varphi}_j\rangle$ generate the same density matrix if and only if

$$|\tilde{\psi}_i\rangle = \sum_j u_{ij} |\tilde{\varphi}_j\rangle$$

where u_{ij} is a **unitary matrix of complex numbers**, with indices i and j , and we ‘pad’ whichever set of vectors $|\tilde{\psi}_i\rangle$ or $|\tilde{\varphi}_j\rangle$ is smaller with entries having probability 0 so that the two sets have the same size

Non Uniqueness

As a consequence of the theorem, note that

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_j q_j |\varphi_j\rangle\langle\varphi_j|$$

for *normalized* states $|\psi_i\rangle, |\varphi_j\rangle$ and probability distributions p_i and q_j if and only if

$$\sqrt{p_i} |\psi_i\rangle = \sum_j u_{ij} \sqrt{q_j} |\varphi_j\rangle$$

for some **unitary matrix** u_{ij} , and we may pad the smaller ensemble with entries having probability zero in order to make the two ensembles the same size

Thus, the above Theorem characterizes the freedom in ensembles $\{p_i, |\psi_i\rangle\}$ giving rise to a given density matrix ρ

Non Uniqueness

- Indeed, it is easily checked that our earlier example of a density matrix with two different decompositions arises as a special case of this general result

Matrix Elements

- In the case of pure states in the state vector representation, each vector element corresponds to a probability amplitude, i.e., $|\psi_j\rangle = \sum_u \alpha_u^{(j)} |\phi_u\rangle$ in the basis $\{|\phi_u\rangle\}_{u=1}^m$
- But what do the elements of the density matrix represent?
- Consider, once again, a *general mixed state* ρ consisting of an ensemble of pure states

$$\{p_j, |\psi_j\rangle\}_{j=1}^n$$

- Then the density state is

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

Matrix Elements

- We know that each individual **pure state** $|\psi_j\rangle$ can be written as a linear superposition of elements forming a complete **orthonormal basis** $\{|\phi_u\rangle\}_{u=1}^m$

$$|\psi_j\rangle = \sum_u \alpha_u^{(j)} |\phi_u\rangle \quad \rightarrow \quad \langle\psi_j| = \sum_v (\alpha_v^{(j)})^* \langle\phi_v|$$

- We can then replace this expression with our definition of our general mixed state,

$$\rho = \sum_j p_j |\psi_j\rangle \langle\psi_j|$$

and get a density matrix in terms of the orthonormal basis elements:

$$\rho = \sum_j p_j \left(\sum_u \alpha_u^{(j)} |\phi_u\rangle \right) \left(\sum_v (\alpha_v^{(j)})^* \langle\phi_v| \right)$$

Matrix Elements

$$\rho = \sum_j p_j \left(\sum_u \alpha_u^{(j)} |\phi_u\rangle \right) \left(\sum_v (\alpha_v^{(j)})^* \langle \phi_v| \right)$$

- Since the coefficients p_j , $\alpha_u^{(j)}$, $(\alpha_v^{(j)})^*$ are just numbers, we can reorganize the expression as:

$$\rho = \sum_{u,v} \underbrace{\left(\sum_j p_j \alpha_u^{(j)} (\alpha_v^{(j)})^* \right)}_{\rho_{uv}} |\phi_u\rangle \langle \phi_v|$$

$$\rho = \sum_{u,v} \rho_{uv} |\phi_u\rangle \langle \phi_v| \quad \text{where} \quad \rho_{uv} = \sum_j p_j \alpha_u^{(j)} (\alpha_v^{(j)})^*$$

- Thus, ρ_{uv} are the *individual matrix elements* in the $\{|\phi_u\rangle\}_{u=1}^m$ basis

Matrix Elements

- Therefore, the density matrix ρ , in the basis $\{|\phi_u\rangle\}_{u=1}^m$, can be written

$$\rho = \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \cdots & \rho_{1m} \\ \rho_{21} & \rho_{22} & \rho_{23} & \cdots & \rho_{2m} \\ \rho_{31} & \rho_{32} & \rho_{33} & \cdots & \rho_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_{m1} & \rho_{m2} & \rho_{m3} & \cdots & \rho_{mm} \end{bmatrix}$$

- It's worth noticing that, in ρ , the diagonal terms ρ_{kk} actually correspond to the *probability of finding the system* in a particular *basis state* $|\phi_k\rangle$

$$\rho_{kk} = \sum_j p_j \alpha_k^{(j)} \left(\alpha_k^{(j)} \right)^* = \sum_j p_j \left| \alpha_k^{(j)} \right|^2 \quad \left(\text{Keep in mind that } |\psi_j\rangle = \sum_k \alpha_k^{(j)} |\phi_k\rangle \right)$$

Matrix Elements

- In fact, considering that $|\psi_j\rangle = \sum_k \alpha_k^{(j)} |\phi_k\rangle$, $|\alpha_k^{(j)}|^2$ corresponds to the probability of finding the basis state $|\phi_k\rangle$ within a given $|\psi_j\rangle$ state, so summing over all p_j values

$$\rho_{kk} = \sum_j p_j \alpha_k^{(j)} (\alpha_k^{(j)})^* = \sum_j p_j |\alpha_k^{(j)}|^2$$

it gives us the total probability of the whole system being in state $|\phi_k\rangle$

The Density Matrix Is Hermitian

- As we saw before, the density matrix ρ , in the basis $\{|\phi_u\rangle\}_{u=1}^m$, can be written

$$\rho = \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \cdots & \rho_{1m} \\ \rho_{21} & \rho_{22} & \rho_{23} & \cdots & \rho_{2m} \\ \rho_{31} & \rho_{32} & \rho_{33} & \cdots & \rho_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_{m1} & \rho_{m2} & \rho_{m3} & \cdots & \rho_{mm} \end{bmatrix}$$

$$\rho = \sum_{u,v} \rho_{uv} |\phi_u\rangle \langle \phi_v| \quad \text{where} \quad \rho_{uv} = \sum_j p_j \alpha_u^{(j)} \left(\alpha_v^{(j)} \right)^*$$

- The density matrix is *Hermitian*, i.e. $\rho = \rho^\dagger$

- Proof

$$\rho_{uv}^* = \left(\sum_j p_j \alpha_u^{(j)} \left(\alpha_v^{(j)} \right)^* \right)^* = \sum_j p_j \left(\alpha_u^{(j)} \right)^* \alpha_v^{(j)} = \sum_j p_j \alpha_v^{(j)} \left(\alpha_u^{(j)} \right)^* = \rho_{vu}$$

Density Matrix Elements for a Qubit

- Assume that we have a single qubit
- Then it is convenient to write its density matrix in a given basis
- If we choose to compute the density matrix in the $\{|0\rangle, |1\rangle\}$ basis, the matrix will be of the form

$$\rho = \begin{bmatrix} \langle 0 | \rho | 0 \rangle & \langle 0 | \rho | 1 \rangle \\ \langle 1 | \rho | 0 \rangle & \langle 1 | \rho | 1 \rangle \end{bmatrix}$$

Density Matrix Elements For A Qubit

$$\rho_{kk} = \sum_j p_j \alpha_k^{(j)} \left(\alpha_k^{(j)} \right)^* = \sum_j p_j \left| \alpha_k^{(j)} \right|^2$$

$$\rho = \begin{bmatrix} \langle 0 | \rho | 0 \rangle & \langle 0 | \rho | 1 \rangle \\ \langle 1 | \rho | 0 \rangle & \langle 1 | \rho | 1 \rangle \end{bmatrix}$$

- If a measurement on a member of the ensemble is made, then the probability that the qubit is found to be in the state $|0\rangle$ is given by

$$\rho_{00} = \langle 0 | \rho | 0 \rangle \quad (\text{probability a member of the ensemble is found to be in the state } |0\rangle)$$

- If a measurement on a member of the ensemble is made, then the probability the qubit is found to be in the state $|1\rangle$ is

$$\rho_{11} = \langle 1 | \rho | 1 \rangle \quad (\text{probability a member of the ensemble is found to be in the state } |1\rangle)$$

Density Matrix Elements for a Qubit

- For example, let's come back to the ensemble $\left\{\frac{1}{3}, |1\rangle; \frac{2}{3}, |+\rangle\right\}$ and the related density matrix

$$\rho_0 = \begin{bmatrix} 1/3 & 1/3 \\ 1/3 & 2/3 \end{bmatrix}$$

$\langle 0|\rho|0\rangle = 1/3$ is the probability that a measurement found the qubit to be in the state $|0\rangle$

$\langle 1|\rho|1\rangle = 2/3$ is the probability that a measurement found the qubit to be in the state $|1\rangle$

Density Matrix Elements for a Qubit

- We can obtain the same results by using the probability approach already exploited for the Hadamard gate

$$\left\{ \frac{1}{3}, |1\rangle; \frac{2}{3}, |+\rangle \right\} \equiv \left\{ \frac{1}{3}, |1\rangle; \frac{2}{3}, \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right\}$$

$$\begin{aligned} P\{0\} &= P\{0|1\} P\{1\} + P\{0|+\} P\{+\} \\ &= |\langle 0|1\rangle|^2 \times \frac{1}{3} + |\langle 0|+\rangle|^2 \times \frac{2}{3} = 0 \times \frac{1}{3} + \left(\frac{1}{\sqrt{2}} \right)^2 \times \frac{2}{3} = \frac{1}{3} \end{aligned}$$

$$\begin{aligned} P\{1\} &= P\{1|1\} P\{1\} + P\{1|+\} P\{+\} \\ &= |\langle 1|1\rangle|^2 \times \frac{1}{3} + |\langle 1|+\rangle|^2 \times \frac{2}{3} = 1 \times \frac{1}{3} + \left(\frac{1}{\sqrt{2}} \right)^2 \times \frac{2}{3} = \frac{2}{3} \end{aligned}$$

Density Matrix Elements for a Qubit

- On the other hand, the **off-diagonal** terms of the matrix are a measure of the *coherence* between the different basis states of the system
- These terms are a representation of the interference effects among different states, in this case between $|\phi_u\rangle$ and $|\phi_v\rangle$

Math Break

– Important Properties of the Trace

The trace has some important properties that are good to know. These include the following:

- The trace is *cyclic*, meaning that $Tr(ABC) = Tr(CAB) = Tr(BCA)$.
- The trace of an outer product is the inner product $Tr(|\phi\rangle\langle\psi|) = \langle\phi|\phi\rangle$.
- By extension of the above it follows that $Tr(A|\psi\rangle\langle\phi|) = \langle\phi|A|\psi\rangle$.
- The trace is *basis independent*. Let $|u_i\rangle$ and $|v_i\rangle$ be two bases for some Hilbert space. Then $Tr(A) = \sum \langle u_i|A|u_i\rangle = \sum \langle v_i|A|v_i\rangle$.
- The trace of an operator is equal to the sum of its eigenvalues. If the eigenvalues of A are labeled by λ_i , then $Tr(A) = \sum_{i=1}^n \lambda_i$.
- The trace is linear, meaning that $Tr(\alpha A) = \alpha Tr(A)$, $Tr(A+B) = Tr(A) + Tr(B)$.

$$\longrightarrow Tr A \otimes B = Tr A Tr B$$

General Properties of the Density Operator

General Properties of the Density Operator

- The density operator was introduced as a means of **describing** ensembles of quantum states
- In this lecture we move away from this description to develop an intrinsic characterization of density operators that does not rely on an ensemble interpretation
- **This allows us to complete the program of giving a description of quantum mechanics that does not take as its foundation the state vector**
- We also take the opportunity to develop numerous other elementary properties of the density operator

General Properties of the Density Operator

- The class of operators that are density operators are characterized by the following useful theorem:
- Theorem: **(Characterization of density operators)** An operator ρ is the density operator associated to some ensemble $\{p_i, |\psi_i\rangle\}$ *if and only if* it satisfies the conditions:
 1. **(Trace condition)** ρ has trace equal to one.
 2. **(Positivity condition)** ρ is a positive operator, i.e., $\langle\varphi|\rho|\varphi\rangle \geq 0$, where $|\varphi\rangle$ is an arbitrary vector in state space.

Density Matrices and Trace Operator

Proof

- Assume that $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is a density operator. Then

$$\text{tr}(\rho) = \text{tr}\left(\sum_i p_i |\psi_i\rangle\langle\psi_i|\right) = \sum_i \text{tr}(p_i |\psi_i\rangle\langle\psi_i|) = \sum_i \langle\psi_i| p_i |\psi_i\rangle = \sum_i p_i \langle\psi_i|\psi_i\rangle = \sum_i p_i = 1$$

- Therefore, the trace condition $\text{tr}(\rho) = 1$ is satisfied
- Suppose $|\varphi\rangle$ is an arbitrary vector in state space. Then

$$\langle\varphi|\rho|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\psi_i|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\varphi|\psi_i\rangle^* = \sum_i p_i |\langle\varphi|\psi_i\rangle|^2 \geq 0$$

- So, the positivity condition is satisfied

Density Matrices and Trace Operator

- Conversely, suppose ρ is any operator satisfying the **trace** and **positivity** conditions
- Since ρ is positive, it must have a spectral decomposition


$$\rho = \sum_j \lambda_j |j\rangle\langle j|,$$

where the vectors $|j\rangle$ are orthogonal and λ_j are **real, non-negative eigenvalues** (see Unit 2) of ρ

- From the trace condition we see that

$$1 = \text{tr}(\rho) = \text{tr}\left(\sum_j \lambda_j |j\rangle\langle j|\right) = \sum_j \text{tr}(\lambda_j |j\rangle\langle j|) = \sum_j \lambda_j \rightarrow \sum_j \lambda_j = 1$$

Density Matrices and Trace Operator

- Therefore, a system in state $|j\rangle$ with probability λ_j will have density operator ρ
- That is, the ensemble $\{\lambda_j, |j\rangle\}$ is an ensemble of states giving rise to the density operator ρ 
- This theorem provides a characterization of density operators that is intrinsic to the operator itself: we can **define a density operator** to be a **positive operator** ρ which has **trace equal to one**
- Making this definition allows us to reformulate the postulates of quantum mechanics in the density operator picture
- In the following we explain how to perform this reformulation, and explain when it is useful

Reformulation of the Postulates of QM

- Suppose, for example, that the **evolution** of a **closed** quantum system is described by the unitary operator U
- If the system was initially in the state $|\psi_i\rangle$ with probability p_i then after the evolution has occurred the system will be in the state $U|\psi_i\rangle$ with probability p_i

$$p_i, |\psi_i\rangle \xrightarrow{U} p_i, U|\psi_i\rangle$$

Reformulation of the Postulates of QM

- Thus, the evolution of the density operator is described by the equation

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{U} \rho' = \sum_i p_i U |\psi_i\rangle\langle\psi_i| U^\dagger = U \left(\sum_i p_i |\psi_i\rangle\langle\psi_i| \right) U^\dagger = U \rho U^\dagger$$

- Then

$$\rho \xrightarrow{U} \rho' = U \rho U^\dagger$$

Reformulation of the Postulates of QM

- **Measurements** are also easily described in the density operator language
- Suppose we perform a measurement described by measurement operators M_m , which can be, as we saw for pure states, projection operators P_m
- If the initial state was $|\psi_i\rangle$ then the probability of getting result m is

$$p(m|i) = \langle \psi_i | M_m^\dagger M_m | \psi_i \rangle = \text{tr}(M_m^\dagger M_m |\psi_i\rangle \langle \psi_i|) \quad (4)$$

where we have used

$$\text{tr}(A|\psi\rangle \langle \psi|) = \sum_i \langle i | A | \psi \rangle \langle \psi | i \rangle = \sum_i \langle \psi | i \rangle \langle i | A | \psi \rangle = \langle \psi | \left(\sum_i |i\rangle \langle i| \right) A | \psi \rangle = \langle \psi | I A | \psi \rangle = \langle \psi | A | \psi \rangle \quad (5)$$

to obtain the last equality

Reformulation of the Postulates of QM

$$p(m|i) = \text{tr}(M_m^\dagger M_m |\psi_i\rangle\langle\psi_i|)$$

- By the law of total probability, the probability of obtaining result ***m*** is

$$p(m) = \sum_i p(m|i)p_i = \sum_i p_i \text{tr}(M_m^\dagger M_m |\psi_i\rangle\langle\psi_i|) = \text{tr}\left(M_m^\dagger M_m \sum_i p_i |\psi_i\rangle\langle\psi_i|\right) = \text{tr}(M_m^\dagger M_m \rho) \quad (6)$$

- What is the density operator of the system after obtaining the measurement result ***m***?
- If the initial state was $|\psi_i\rangle$ then the state after obtaining the result ***m*** is

$$|\psi_i^m\rangle = \frac{M_m |\psi_i\rangle}{\sqrt{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}} \quad (7)$$

Reformulation of the Postulates of QM

- Thus, after a measurement which yields the result \mathbf{m} , we have an ensemble of states $|\psi_i^m\rangle$ with respective probabilities $p(i|m)$
- The corresponding density operator ρ_m is therefore

$$\rho_m = \sum_i p(i|m) |\psi_i^m\rangle \langle \psi_i^m| = \sum_i p(i|m) \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\langle \psi_i | M_m^\dagger M_m | \psi_i \rangle} \quad (8)$$

- But by elementary probability theory,

$$p(i|m) = \frac{p(m,i)}{p(m)} = \frac{p(m|i)p_i}{p(m)} \quad (9)$$

Reformulation of the Postulates of QM

- Substituting from (9), (4), and (6) we obtain

$$\begin{aligned}
 \rho_m &= \sum_i p(i|m) \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\langle \psi_i | M_m^\dagger M_m | \psi_i \rangle} = \sum_i \frac{p(m|i) p_i}{p(m)} \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\langle \psi_i | M_m^\dagger M_m | \psi_i \rangle} \\
 (4) \quad &= \sum_i \frac{\text{tr}(M_m^\dagger M_m |\psi_i\rangle \langle \psi_i|)}{\text{tr}(M_m^\dagger M_m \rho)} p_i \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\langle \psi_i | M_m^\dagger M_m | \psi_i \rangle} \quad (5) \\
 (6) \quad &= \sum_i \frac{\cancel{\text{tr}(M_m^\dagger M_m |\psi_i\rangle \langle \psi_i|)}}{\text{tr}(M_m^\dagger M_m \rho)} p_i \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\cancel{\text{tr}(M_m^\dagger M_m |\psi_i\rangle \langle \psi_i|)}} \\
 &= \sum_i p_i \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\text{tr}(M_m^\dagger M_m \rho)} = \frac{M_m}{\text{tr}(M_m^\dagger M_m \rho)} \left(\sum_i p_i |\psi_i\rangle \langle \psi_i| \right) M_m^\dagger \\
 &= \frac{M_m \rho M_m^\dagger}{\text{tr}(M_m^\dagger M_m \rho)}
 \end{aligned}$$

Reformulation of the Postulates of QM

- As a conclusion we obtain the following result

$$\rho_m = \frac{M_m \rho M_m^\dagger}{\text{tr}(M_m^\dagger M_m \rho)} \quad (10)$$

with probability

$$p(m) = \text{tr}(M_m^\dagger M_m \rho)$$

Reformulation of the Postulates of QM

- Finally, imagine a quantum system is prepared in the state ρ_i with probability p_i
- It is not difficult to convince yourself that the system may be described by the density matrix $\sum_i p_i \rho_i$
- A proof of this is to suppose that ρ_i arises from some ensemble $\{p_{ij}, |\psi_{ij}\rangle\}$ (note that i is fixed) of pure states, so the probability for being in the state $|\psi_{ij}\rangle$ is $p_i p_{ij}$

Reformulation of the Postulates of QM

- The density matrix for the system is thus

$$\rho = \sum_{ij} p_i p_{ij} |\psi_{ij}\rangle \langle \psi_{ij}| = \sum_i p_i \sum_j p_{ij} |\psi_{ij}\rangle \langle \psi_{ij}| = \sum_i p_i \rho_i$$

where we have used the definition

$$\rho_i = \sum_j p_{ij} |\psi_{ij}\rangle \langle \psi_{ij}|$$

- We say that ρ is a mixture of the states ρ_i with probabilities p_i
- This concept of a mixture comes up repeatedly in the analysis of problems like quantum noise, where the effect of the noise is to introduce ignorance into our knowledge of the quantum state

Reformulation of the Postulates of QM

- For ease of reference, we state all the reformulated postulates in the following slides

Reformulation of the Postulates of QM

- **Postulate 1:** Associated to any *isolated physical system* is a complex vector space with inner product (that is, a Hilbert space) known as the state space of the system.
- The *isolated physical system* is completely described by its **density operator**, which is a **positive operator** ρ with **trace one**, acting on the state space of the system.
- If a quantum system is in the state ρ_i with probability p_i , then the density operator for the system is

$$\sum_i p_i \rho_i$$

Reformulation of the Postulates of QM

- **Postulate 2:** The evolution of a closed quantum system is described by a unitary transformation.
- That is, the state ρ of the system at time t_1 is related to the state ρ of the system at time t_2 by a unitary operator U which depends only on the times t_1 and t_2 ,

$$\rho' = U\rho U^\dagger$$

Reformulation of the Postulates of QM

- **Postulate 3:** Quantum measurements are described by a collection of $\{M_m\}$ measurement operators.
- These operators act on the state space of the system being measured.
- The index ***m*** refers to the measurement outcomes that may occur in the experiment.

Reformulation of the Postulates of QM

- If the state of the quantum system is ρ immediately before the measurement, then the probability that result \mathbf{m} occurs is given by

$$p(m) = \text{tr}(M_m^\dagger M_m \rho) \quad (1)$$

and the state of the system after the measurement is

$$\frac{M_m^\dagger \rho M_m}{\text{tr}(M_m^\dagger M_m \rho)} \quad (2)$$

- The measurement operators satisfy the *completeness equation*

$$\sum_m M_m^\dagger M_m = I \quad (3)$$

Reformulation of the Postulates of QM

- **Postulate 4:** The state space of a composite physical system is the tensor product of the state spaces of the component physical systems.
- Moreover, if we have systems numbered 1 through n , and system number i is prepared in the state ρ_i , then the joint state of the total system is

$$\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_n$$

Reformulation of the Postulates of QM

- These reformulations of the fundamental postulates of quantum mechanics in terms of the density operator are *mathematically equivalent* to the description in terms of the state vector.
- Nevertheless, as a way of thinking about quantum mechanics, the density operator approach really shines for two applications:
 - > the description of quantum systems whose state is not known, and
 - > the description of subsystems of a composite quantum system, as will be described later.
- In the next slides, we flesh out the properties of the density matrix in more detail.

Criterion to Decide if a State is Mixed or Pure

- A very useful property of the density matrix is that when taking the trace **tr** of its square ρ^2 , we obtain a scalar value γ that is a *good metric* 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 in the case of a *pure state*

$$\gamma = \text{Tr}(\rho^2) \leq 1$$

$$\gamma = \text{Tr}(\rho^2) = 1 \quad \text{for pure states only}$$

Criterion to Decide if a State is Mixed or Pure

- We know that, for a *pure state* $|\psi\rangle$, $\rho = |\psi\rangle\langle\psi|$ and for any normalized state $|\psi\rangle$

$$\rho^2 = \rho\rho = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{=1}\langle\psi| = |\psi\rangle\langle\psi| = \rho \quad \rightarrow \quad \rho^2 = \rho$$

- Since we have already proven that $\text{tr}(\rho) = 1$, from $\rho^2 = \rho$ it follows

$$\text{tr}(\rho^2) = \text{tr}(\rho) = 1$$

Criterion to Decide if a State is Mixed or Pure

- Now consider the density matrix describing an ensemble $\{p_j, |\psi_j\rangle\}_{j=1}^n$ and *assume* that, for simplicity's purposes, states $|\psi_j\rangle$ are *orthonormal*. Thus

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \quad \rightarrow$$

$$\rho^2 = \rho\rho = \left(\sum_k p_k |\psi_k\rangle\langle\psi_k| \right) \left(\sum_j p_j |\psi_j\rangle\langle\psi_j| \right) = \sum_k \sum_j p_k p_j |\psi_k\rangle \underbrace{\langle\psi_k|\psi_j\rangle}_{=\delta_{kj}} \langle\psi_j|$$

$$= \sum_k \sum_j p_k p_j |\psi_k\rangle\langle\psi_j| \delta_{kj} = \sum_j p_j^2 |\psi_j\rangle\langle\psi_j|$$

Criterion to Decide if a State is Mixed or Pure

- Therefore

$$\text{tr}(\rho^2) = \text{tr}\left(\sum_j p_j^2 |\psi_j\rangle\langle\psi_j|\right) = \sum_j \text{tr}\left(p_j^2 |\psi_j\rangle\langle\psi_j|\right) = \sum_j \langle\psi_j| p_j^2 |\psi_j\rangle = \sum_j p_j^2 \langle\psi_j|\psi_j\rangle = \sum_j p_j^2$$

- Since $\sum_j p_j = 1$, it follows $\sum_j p_j^2 < 1$ if more than one $p_j \neq 0$

- Thus $\gamma = \text{tr}(\rho^2) \leq 1$

- The *equality* is satisfied if ρ describes a *pure state* and the *inequality* follows if ρ describes a *mixed ensemble*

- Inequality holds even if states $|\psi_j\rangle$ are **not** orthogonal

Maximally Mixed States

- The *maximally mixed state* is a quantum state whose density matrix is **proportional** to the **identity matrix**
- Physically, it may be interpreted as a *uniform mixture* of states in an *orthonormal basis* matrix, e.g.

$$\left\{ \frac{1}{2}, |0\rangle; \frac{1}{2}, |1\rangle \right\} \rightarrow \rho = \frac{1}{2} |0\rangle\langle 0| + \frac{1}{2} |1\rangle\langle 1|$$

$$\rightarrow \rho = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{I}{2}$$

Maximally Mixed States

- If the state space has n dimensions, then

$$\rho = \frac{1}{n} I$$

- Since $I^2 = I$, from $\rho = \frac{1}{n} I$ it follows

$$\rho^2 = \frac{1}{n^2} I$$

- Furthermore, in n dimensions, $\text{tr}(I) = n$
- So, for a *maximally mixed state* we have

$$\text{tr}(\rho^2) = \text{tr}\left(\frac{1}{n^2} I\right) = \frac{1}{n^2} \text{tr}(I) = \frac{1}{n}$$

Maximally Mixed States

- In most if not all cases of interest to us, $n = 2$
- For $n = 2$ the *lower bound*, given by a *maximally mixed state*, is

$$\text{tr}(\rho^2) = \frac{1}{2}$$

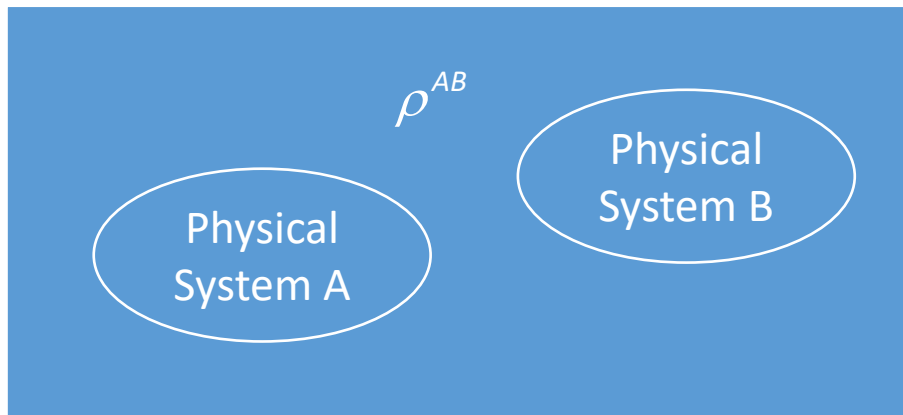
while the *upper bound* for a *pure state* is given by

$$\text{tr}(\rho^2) = 1$$

The Reduced Density Operator

The Reduced Density Operator

- Perhaps the deepest application of the density operator is as a descriptive tool for subsystems of a composite quantum system
- The reduced density operator provides such a description
- Suppose we have physical systems A and B , whose state is described by a density operator ρ^{AB}

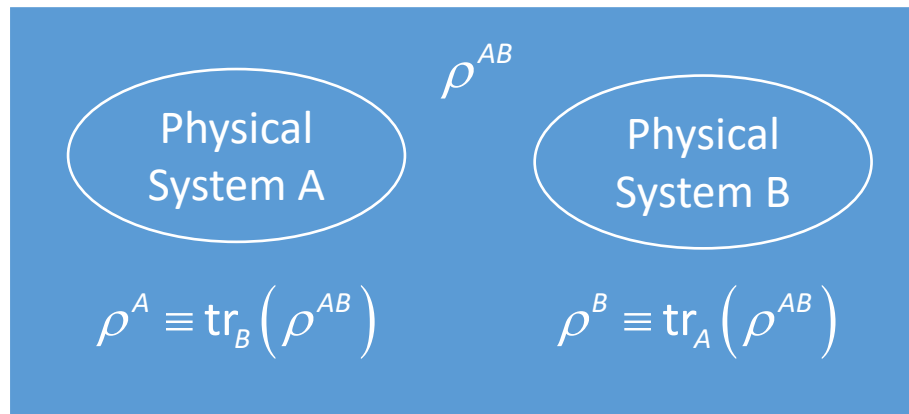


The Reduced Density Operator

- The **reduced density operator** for system A is defined by

$$\rho^A \equiv \text{tr}_B(\rho^{AB})$$

where tr_B is a map of operators known as the *partial trace* over system B



- Similarly, the reduced density operator for system B is defined by

$$\rho^B \equiv \text{tr}_A(\rho^{AB})$$

where tr_A is a map of operators known as the *partial trace* over system A

The Reduced Density Operator

- The partial trace over systems A and B respectively, is defined by

$$\text{tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv |a_1\rangle\langle a_2| \text{tr}(|b_1\rangle\langle b_2|)$$

$$\text{tr}_A(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv (\text{tr}(|a_1\rangle\langle a_2|)) |b_1\rangle\langle b_2|$$

where $|a_1\rangle, |a_2\rangle$ are any two vectors in the state space of A, and $|b_1\rangle, |b_2\rangle$ are any two vectors in the state space of B

- The trace operation appearing on the right-hand side is the usual trace operation for system B, so

$$\text{tr}(|b_1\rangle\langle b_2|) = \langle b_2 | b_1 \rangle$$

The Reduced Density Operator

- It is not obvious that the reduced density operator for system A is in any sense a description for the state of system A
- The physical justification for making this identification is that the reduced density operator provides the correct measurement statistics for measurements made on system A
- This is explained in more detail in Box 2.6 on page 107 of the book *Quantum Computation and Quantum Information* by Michael A. Nielsen and Isaac L. Chuang

The Reduced Density Operator

- The following simple example calculations may also help understand the reduced density operator.
- First, suppose a quantum system is in the product state $\rho^{AB} = \rho \otimes \sigma$, where ρ is a density operator for system A , and σ is a density operator for system B . Then

$$\rho^A \equiv \text{tr}_B(\rho \otimes \sigma) = \rho \text{tr}(\sigma) = \rho,$$

which is the result we intuitively expect.

- Similarly,

$$\rho^B \equiv \text{tr}_A(\rho \otimes \sigma) = [\text{tr}(\rho)]\sigma = \sigma$$

for this state

The Reduced Density Operator

- A less trivial example is the Bell state $|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$

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

$$= \frac{|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|}{2}$$

ρ is obviously a pure state

- Tracing out the second qubit, we find the reduced density operator of the first qubit,

$$\rho^1 \equiv \text{tr}_2(\rho) = \frac{\text{tr}_2(|00\rangle\langle 00|) + \text{tr}_2(|11\rangle\langle 00|) + \text{tr}_2(|00\rangle\langle 11|) + \text{tr}_2(|11\rangle\langle 11|)}{2} \rightarrow$$

linearity of the trace operator

The Reduced Density Operator

$$= \frac{\text{tr}_2(|0\rangle\langle 0| \otimes |0\rangle\langle 0|) + \text{tr}_2(|1\rangle\langle 0| \otimes |1\rangle\langle 0|) + \text{tr}_2(|0\rangle\langle 1| \otimes |0\rangle\langle 1|) + \text{tr}_2(|1\rangle\langle 1| \otimes |1\rangle\langle 1|)}{2}$$

$$= \frac{|0\rangle\langle 0| \text{tr}(|0\rangle\langle 0|) + |1\rangle\langle 0| \text{tr}(|1\rangle\langle 0|) + |0\rangle\langle 1| \text{tr}(|0\rangle\langle 1|) + |1\rangle\langle 1| \text{tr}(|1\rangle\langle 1|)}{2}$$

$$= \frac{|0\rangle\langle 0| \langle 0|0\rangle + |1\rangle\langle 0| \langle 0|1\rangle + |0\rangle\langle 1| \langle 1|0\rangle + |1\rangle\langle 1| \langle 1|1\rangle}{2}$$

$$= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2}$$

$$= \frac{I}{2} \rightarrow$$

$$\rho^1 = \frac{I}{2} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

$$\text{tr}(|b_1\rangle\langle b_2|) = \langle b_2 | b_1 \rangle$$

$$\text{tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv |a_1\rangle\langle a_2| \text{tr}(|b_1\rangle\langle b_2|)$$

Maximally Mixed State

The Reduced Density Operator

- Notice that this state is a mixed state, since:

$$\text{tr}(\rho^1)^2 = \text{tr}\left(\left(\frac{I}{2}\right)^2\right) = \text{tr}\left(\frac{I^2}{4}\right) = \text{tr}\left(\frac{I}{4}\right) = \text{tr}\begin{bmatrix} 1/4 & 0 \\ 0 & 1/4 \end{bmatrix} = \frac{1}{4} + \frac{1}{4} = \frac{1}{2} < 1$$

- This is quite a remarkable result
- The state of the joint system of two qubits is a pure state, that is, it is known exactly; however, the first qubit is in a mixed state, that is, a state about which we apparently do not have maximal knowledge
- This **strange property**, that the joint state of a system can be completely known, yet a subsystem be in mixed states, is another **hallmark** of quantum entanglement

Quantum Teleportation and the Reduced Density Operator

- A useful application of the reduced density operator is to the analysis of quantum teleportation
- Recall from an earlier lecture that quantum teleportation is a procedure for sending quantum information from Alice to Bob, given that Alice and Bob share an EPR pair, and have a classical communications channel
- At first sight it appears as though teleportation can be used to do faster-than-light communication, a contradiction to the theory of relativity

Quantum Teleportation and the Reduced Density Operator

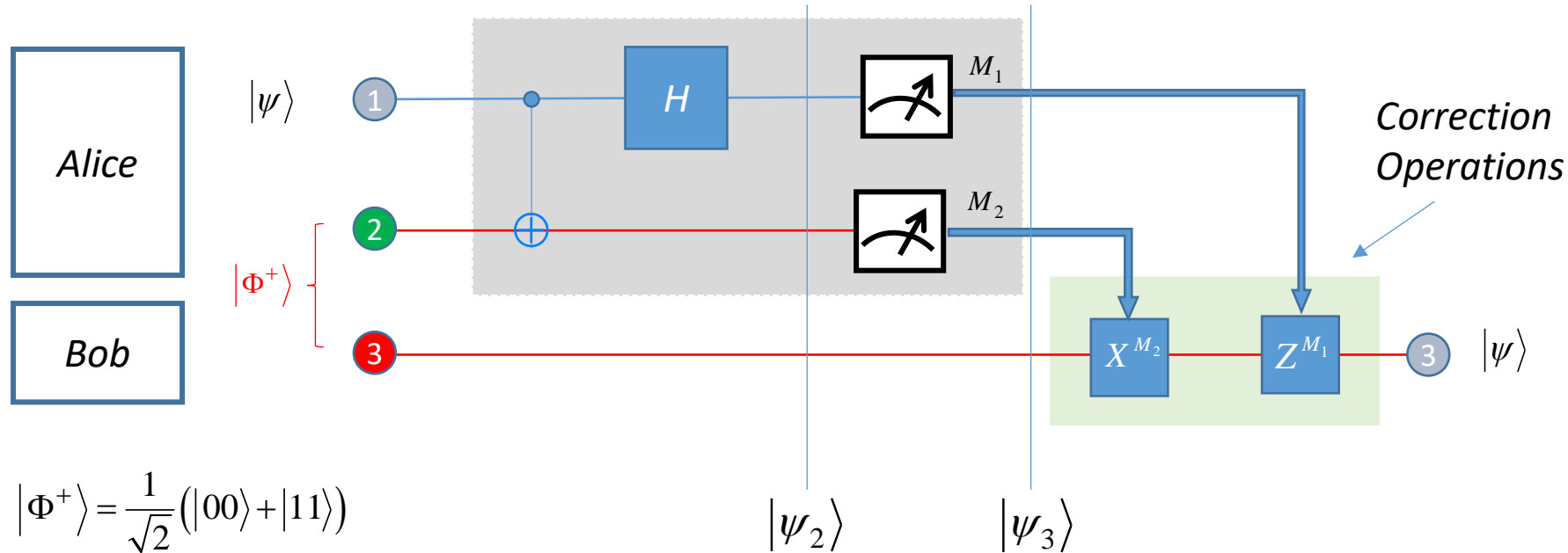
- We surmised that what prevents faster-than-light communication is the need for Alice to communicate her measurement result to Bob
- The reduced density operator allows us to make this rigorous
- Recall that immediately before Alice makes her measurement the quantum state of the three qubits is

$$|\psi_2\rangle = \frac{1}{2} \left[|0_1 0_2\rangle (\alpha |0_3\rangle + \beta |1_3\rangle) + |0_1 1_2\rangle (\alpha |1_3\rangle + \beta |0_3\rangle) + |1_1 0_2\rangle (\alpha |0_3\rangle - \beta |1_3\rangle) + |1_1 1_2\rangle (\alpha |1_3\rangle - \beta |0_3\rangle) \right]$$

- See the next slide

Quantum Teleportation and the Reduced Density Operator

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$



$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$|\psi_2\rangle = \frac{1}{2} \left[|0_1 0_2\rangle (\alpha|0_3\rangle + \beta|1_3\rangle) + |0_1 1_2\rangle (\alpha|1_3\rangle + \beta|0_3\rangle) + |1_1 0_2\rangle (\alpha|0_3\rangle - \beta|1_3\rangle) + |1_1 1_2\rangle (\alpha|1_3\rangle - \beta|0_3\rangle) \right]$$

Quantum Teleportation and the Reduced Density Operator

We have already seen that, depending on Alice's measurement outcome, Bob's qubit will end up in one of these four possible states

$$0_1 0_2 \rightarrow |\psi_3(0_1 0_2)\rangle = [\alpha|0_3\rangle + \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$0_1 1_2 \rightarrow |\psi_3(0_1 1_2)\rangle = [\alpha|1_3\rangle + \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$1_1 0_2 \rightarrow |\psi_3(1_1 0_2)\rangle = [\alpha|0_3\rangle - \beta|1_3\rangle] \rightarrow \text{Prob} = 1/4$$

$$1_1 1_2 \rightarrow |\psi_3(1_1 1_2)\rangle = [\alpha|1_3\rangle - \beta|0_3\rangle] \rightarrow \text{Prob} = 1/4$$

As a result, Bob's qubit is in a mixed state described by the ensemble:

$$\left\{ \frac{1}{4}, |\psi_3(0_1 0_2)\rangle; \frac{1}{4}, |\psi_3(0_1 1_2)\rangle; \frac{1}{4}, |\psi_3(1_1 0_2)\rangle + \frac{1}{4}, |\psi_3(1_1 1_2)\rangle \right\}$$

Quantum Teleportation and the Reduced Density Operator

- From the above ensemble we calculated the density matrix associated to the Bob's qubit

$$\rho = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

- In the following we will derive the same result by calculating the density matrix of the global system (three qubits, two owned by Alice - qubit 1 and qubit 2 - and the other - qubit 3 - owned by Bob) and then tracing out on the Alice's qubits

Quantum Teleportation and the Reduced Density Operator

Again, depending on Alice's measurement outcome, the global system will end up in one of these four possible states

$$\begin{aligned}
 &\text{Alice} \quad \text{Bob} \quad \text{Global System} \\
 &|0_1 0_2\rangle (\alpha |0_3\rangle + \beta |1_3\rangle) = |0_1 0_2\rangle |\psi_3(0_1 0_2)\rangle \rightarrow \text{Prob} = 1/4 \\
 &|0_1 1_2\rangle (\alpha |1_3\rangle + \beta |0_3\rangle) = |0_1 1_2\rangle |\psi_3(0_1 1_2)\rangle \rightarrow \text{Prob} = 1/4 \\
 &|1_1 0_2\rangle (\alpha |0_3\rangle - \beta |1_3\rangle) = |1_1 0_2\rangle |\psi_3(1_1 0_2)\rangle \rightarrow \text{Prob} = 1/4 \\
 &|1_1 1_2\rangle (\alpha |1_3\rangle - \beta |0_3\rangle) = |1_1 1_2\rangle |\psi_3(1_1 1_2)\rangle \rightarrow \text{Prob} = 1/4
 \end{aligned}$$

where

$$|\psi_3(0_1 0_2)\rangle = \alpha |0_3\rangle + \beta |1_3\rangle$$

$$|\psi_3(0_1 1_2)\rangle = \alpha |1_3\rangle + \beta |0_3\rangle$$

$$|\psi_3(1_1 0_2)\rangle = \alpha |0_3\rangle - \beta |1_3\rangle$$

$$|\psi_3(1_1 1_2)\rangle = \alpha |1_3\rangle - \beta |0_3\rangle$$

Quantum Teleportation and the Reduced Density Operator

- As a result, the global system is in a mixed state described by the ensemble:

$$\left\{ \frac{1}{4}, |0_1 0_2\rangle |\psi_3(0_1 0_2)\rangle; \frac{1}{4}, |0_1 1_2\rangle |\psi_3(0_1 1_2)\rangle; \frac{1}{4}, |1_1 0_2\rangle |\psi_3(1_1 0_2)\rangle + \frac{1}{4}, |1_1 1_2\rangle |\psi_3(1_1 1_2)\rangle \right\}$$

- The density operator of the global system is thus

$$\begin{aligned} \rho = \frac{1}{4} & \left[|0_1 0_2\rangle (\alpha |0_3\rangle + \beta |1_3\rangle) \langle 0_1 0_2| (\alpha^* \langle 0_3| + \beta^* \langle 1_3|) + |0_1 1_2\rangle (\alpha |1_3\rangle + \beta |0_3\rangle) \langle 0_1 1_2| (\alpha^* \langle 1_3| + \beta^* \langle 0_3|) \right. \\ & \left. + |1_1 0_2\rangle (\alpha |0_3\rangle - \beta |1_3\rangle) \langle 1_1 0_2| (\alpha^* \langle 0_3| - \beta^* \langle 1_3|) + |1_1 1_2\rangle (\alpha |1_3\rangle - \beta |0_3\rangle) \langle 1_1 1_2| (\alpha^* \langle 1_3| - \beta^* \langle 0_3|) \right] \end{aligned}$$

Quantum Teleportation and the Reduced Density Operator

- Then

$$\rho = \frac{1}{4} \left[|0_1 0_2\rangle \langle 0_1 0_2| (\alpha |0_3\rangle + \beta |1_3\rangle) (\alpha^* \langle 0_3| + \beta^* \langle 1_3|) + |0_1 1_2\rangle \langle 0_1 1_2| (\alpha |1_3\rangle + \beta |0_3\rangle) (\alpha^* \langle 1_3| + \beta^* \langle 0_3|) \right. \\ \left. + |1_1 0_2\rangle \langle 1_1 0_2| (\alpha |0_3\rangle - \beta |1_3\rangle) (\alpha^* \langle 0_3| - \beta^* \langle 1_3|) + |1_1 1_2\rangle \langle 1_1 1_2| (\alpha |1_3\rangle - \beta |0_3\rangle) (\alpha^* \langle 1_3| - \beta^* \langle 0_3|) \right]$$

- Tracing out Alice's system, i.e., qubits 1 and 2, we see that the reduced density operator of Bob's system is

$$\rho^{\text{Bob}} = \text{tr}_{1,2} \left\{ \frac{1}{4} \left[|0_1 0_2\rangle \langle 0_1 0_2| (\alpha |0_3\rangle + \beta |1_3\rangle) (\alpha^* \langle 0_3| + \beta^* \langle 1_3|) + |0_1 1_2\rangle \langle 0_1 1_2| (\alpha |1_3\rangle + \beta |0_3\rangle) (\alpha^* \langle 1_3| + \beta^* \langle 0_3|) \right. \right. \\ \left. \left. + |1_1 0_2\rangle \langle 1_1 0_2| (\alpha |0_3\rangle - \beta |1_3\rangle) (\alpha^* \langle 0_3| - \beta^* \langle 1_3|) + |1_1 1_2\rangle \langle 1_1 1_2| (\alpha |1_3\rangle - \beta |0_3\rangle) (\alpha^* \langle 1_3| - \beta^* \langle 0_3|) \right] \right\}$$

Quantum Teleportation and the Reduced Density Operator

- The density operator of the Bob subsystem is thus

$$\begin{aligned}\rho^{\text{Bob}} = & \left\{ \frac{1}{4} \left[\left(\text{tr}_{1,2} |0_1 0_2\rangle\langle 0_1 0_2| \right) \cdot \left(\alpha |0_3\rangle + \beta |1_3\rangle \right) \left(\alpha^* \langle 0_3| + \beta^* \langle 1_3| \right) \right. \right. \\ & + \left(\text{tr}_{1,2} |0_1 1_2\rangle\langle 0_1 1_2| \right) \cdot \left(\alpha |1_3\rangle + \beta |0_3\rangle \right) \left(\alpha^* \langle 1_3| + \beta^* \langle 0_3| \right) \\ & + \left(\text{tr}_{1,2} |1_1 0_2\rangle\langle 1_1 0_2| \right) \cdot \left(\alpha |0_3\rangle - \beta |1_3\rangle \right) \left(\alpha^* \langle 0_3| - \beta^* \langle 1_3| \right) \\ & \left. \left. + \left(\text{tr}_{1,2} |1_1 1_2\rangle\langle 1_1 1_2| \right) \cdot \left(\alpha |1_3\rangle - \beta |0_3\rangle \right) \left(\alpha^* \langle 1_3| - \beta^* \langle 0_3| \right) \right] \right\}\end{aligned}$$

- Since $\text{tr}_{1,2} |i_1 j_2\rangle\langle i_1 j_2| = \langle i_1 j_2 | i_1 j_2 \rangle = 1, \quad \forall i, j \in \{0, 1\}$

Quantum Teleportation and the Reduced Density Operator

- Then

$$\begin{aligned}\rho^{\text{Bob}} = & \left\{ \frac{1}{4} \left[(\alpha|0_3\rangle + \beta|1_3\rangle)(\alpha^*\langle 0_3| + \beta^*\langle 1_3|) \right. \right. \\ & + (\alpha|1_3\rangle + \beta|0_3\rangle)(\alpha^*\langle 1_3| + \beta^*\langle 0_3|) \\ & + (\alpha|0_3\rangle - \beta|1_3\rangle)(\alpha^*\langle 0_3| - \beta^*\langle 1_3|) \\ & \left. \left. + (\alpha|1_3\rangle - \beta|0_3\rangle)(\alpha^*\langle 1_3| - \beta^*\langle 0_3|) \right] \right\}\end{aligned}$$

- After some algebraic manipulation

$$\rho^{\text{Bob}} = \frac{2(|\alpha|^2 + |\beta|^2)|0_3\rangle\langle 0_3| + 2(|\alpha|^2 + |\beta|^2)|1_3\rangle\langle 1_3|}{4}$$

Quantum Teleportation and the Reduced Density Operator

- Since $|\alpha|^2 + |\beta|^2 = 1$, then:

$$\rho^{\text{Bob}} = \frac{|0_3\rangle\langle 0_3| + |1_3\rangle\langle 1_3|}{2} = \frac{I}{2} = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

where we have used the completeness relation in the last line.

Quantum Teleportation and the Reduced Density Operator

- Thus, the state of Bob's system after Alice has performed the measurement but before Bob has learned the measurement result is $I/2$
- This state has no dependence upon the state $|\psi\rangle$ being teleported, and thus any measurements performed by Bob will contain no information about $|\psi\rangle$, thus preventing Alice from using teleportation to transmit information to Bob faster than light

The Geometry of Single- Qubit Mixed States

The Geometry of Single-Qubit Mixed States

- We introduced earlier the Bloch sphere as a way of visualizing single-qubit *pure states*
- In this picture, the *pure states* are always *points* on the *surface* of the Bloch sphere
- One might wonder where single qubit mixed states would reside in this Bloch sphere picture
- The answer is that single qubit *mixed states* correspond to *points inside* the Bloch sphere, a region we shall henceforth call the *Bloch ball*

The Geometry of Single-Qubit Mixed States

- Mixed states are convex combinations of pure states, linear combinations of pure states with real non-negative coefficients that sum to 1
- The precise connection with the geometry uses the fact that density operators are Hermitian (self-adjoint) operators with trace 1

The Geometry of Single-Qubit Mixed States

- Any self-adjoint 2×2 -matrix is of the form

$$\rho = \begin{bmatrix} a & c - \textcolor{red}{i}d \\ c + \textcolor{red}{i}d & b \end{bmatrix}$$

where a, b, c , and d are **real parameters**

- Requiring that the matrix have *trace* 1 means there are only 3 real parameters. Such matrices can be written as

$$\rho = \frac{1}{2} \begin{bmatrix} 1 + r_z & r_x - \textcolor{red}{i}r_y \\ r_x + \textcolor{red}{i}r_y & 1 - r_z \end{bmatrix} \quad \text{where } r_x, r_y, \text{ and } r_z \text{ are } \mathbf{real} \text{ parameters}$$

The Geometry of Single-Qubit Mixed States

- Thus, any density matrix for a single-qubit system can be written as

$$\rho = \frac{1}{2}(I + \mathbf{r} \cdot \boldsymbol{\sigma}) = \frac{1}{2}(I + r_x \sigma_x + r_y \sigma_y + r_z \sigma_z)$$

where

$$\sigma_x = X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

are the Pauli matrices

The Geometry of Single-Qubit Mixed States

- Math check

$$\begin{aligned} \frac{1}{2} \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + r_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + r_y \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + r_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right) &= \frac{1}{2} \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & r_x \\ r_x & 0 \end{bmatrix} + \begin{bmatrix} 0 & -ir_y \\ ir_y & 0 \end{bmatrix} + \begin{bmatrix} r_z & 0 \\ 0 & -r_z \end{bmatrix} \right) \\ &= \frac{1}{2} \begin{bmatrix} 1+r_z & r_x - \textcolor{red}{i}r_y \\ r_x + \textcolor{red}{i}r_y & 1-r_z \end{bmatrix} = \rho \end{aligned}$$

The Geometry of Single-Qubit Mixed States

- The determinant of a single-qubit density operator

$$\rho = \frac{1}{2} \begin{bmatrix} 1 + r_z & r_x - \textcolor{red}{i}r_y \\ r_x + \textcolor{red}{i}r_y & 1 - r_z \end{bmatrix}$$

has geometric meaning; it is easily computed to be

$$\det(\rho) = \frac{1}{4} \left[(1 + r_z)(1 - r_z) - (r_x - \textcolor{red}{i}r_y)(r_x + \textcolor{red}{i}r_y) \right] = \frac{1}{4} (1 - r^2)$$

where $r = \sqrt{|r_x|^2 + |r_y|^2 + |r_z|^2}$ is the radial distance from the origin in x, y, z coordinates

The Geometry of Single-Qubit Mixed States

- As a conclusion

$$\det(\rho) = \frac{1}{4}(1 - r^2), \quad r = \sqrt{|r_x|^2 + |r_y|^2 + |r_z|^2}$$

- The r_x, r_y , and r_z coefficients correspond to the components of what is known as the Bloch vector \vec{r}
- Since the determinant of ρ is the *product of its eigenvalues*, which for a density operator must be *non-negative*, $\det(\rho) \geq 0$ and therefore $0 \leq r \leq 1$
- Thus, with x, y , and z acting as coordinates, the density matrices of single-qubit mixed states $\rho = (1/2)(I + r_x\sigma_x + r_y\sigma_y + r_z\sigma_z)$ all lie within a sphere of radius 1

Computation of the Eigenvalues of a Density Operator (Exercise)

- Let λ_1 and λ_2 be the eigenvalues of ρ
- Since density operators have trace 1, $\lambda_2 = 1 - \lambda_1$
- Since $\det \rho = \lambda_2 \lambda_1 = (1 - \lambda_1) \lambda_1$, so $\lambda_1^2 - \lambda_1 + \det \rho = 0$ which has solutions

$$\lambda_1 = \frac{1 - \sqrt{1 - 4 \det \rho}}{2}, \quad \lambda_2 = \frac{1 + \sqrt{1 - 4 \det \rho}}{2}$$

- Since $\det(\rho) = \frac{1}{4}(1 - r^2)$, then

$$\lambda_1 = \frac{1 + r}{2}, \quad \lambda_2 = \frac{1 - r}{2}$$

The Geometry of Single-Qubit Mixed States

- The density matrices for states on the boundary of the sphere have $\det(\rho) = 0$; one of their eigenvalues must be 0
- Since density operators have trace 1, the other eigenvalue must be 1
- To find the coordinates (r_x, r_y, r_z) within the Bloch ball corresponding to the mixed state ρ we have

$$\begin{bmatrix} \langle 0|p|0\rangle & \langle 0|p|1\rangle \\ \langle 1|p|0\rangle & \langle 1|p|1\rangle \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1+\mathcal{R}_z & \mathcal{R}_x - i\mathcal{R}_y \\ \mathcal{R}_x + i\mathcal{R}_y & 1-\mathcal{R}_z \end{bmatrix}$$

$$\begin{aligned} \langle 0|p|0\rangle &= \frac{1}{2} (1+\mathcal{R}_z) \\ \langle 1|p|1\rangle &= \frac{1}{2} (1-\mathcal{R}_z) \end{aligned} \Rightarrow$$

$$\langle 0|p|0\rangle - \langle 1|p|1\rangle = \mathcal{R}_z$$

$$\begin{aligned} \langle 0|p|1\rangle &= \frac{1}{2} (\mathcal{R}_x - i\mathcal{R}_y) \\ \langle 1|p|0\rangle &= \frac{1}{2} (\mathcal{R}_x + i\mathcal{R}_y) \end{aligned} \Rightarrow$$

summation

$$\begin{aligned} \langle 0|p|1\rangle + \langle 1|p|0\rangle &= \mathcal{R}_x \\ \langle 0|p|1\rangle - \langle 1|p|0\rangle &= -i\mathcal{R}_y \end{aligned} \Rightarrow$$

$$\begin{cases} \langle 0|p|1\rangle + \langle 1|p|0\rangle = \mathcal{R}_x \\ i\langle 0|p|1\rangle - i\langle 1|p|0\rangle = \mathcal{R}_y \end{cases}$$

Let's consider state $|0\rangle \Rightarrow \rho = |0\rangle\langle 0|$

$$\mathcal{R}_z = \langle 0|\rho|0\rangle - \langle 1|\rho|1\rangle = \underbrace{\langle 0|(10)\langle 01)|0\rangle}_{=1} - \underbrace{\langle 1|(10)\langle 01)|1\rangle}_{=0} = 1$$

$$\mathcal{R}_x = \langle 0|\rho|1\rangle + \langle 1|\rho|0\rangle = \underbrace{\langle 0|(10)\langle 01)|1\rangle}_{=1} + \underbrace{\langle 1|(10)\langle 01)|0\rangle}_{=1} = 0$$

$$\mathcal{R}_y = i\langle 0|\rho|1\rangle - i\langle 1|\rho|0\rangle = i\underbrace{\langle 0|(10)\langle 01)|1\rangle}_{=1} - i\underbrace{\langle 1|(10)\langle 01)|0\rangle}_{=1} = 0$$

Thus, $\rho = |0\rangle\langle 0|$ is characterized by $(0, 0, 1)$ (North Pole)

and therefore

$$\rho = \frac{1}{2} \left(\underbrace{I}_{=0} + \underbrace{\mathcal{R}_x \sigma_x}_{=0} + \underbrace{\mathcal{R}_y \sigma_y}_{=0} + \underbrace{\mathcal{R}_z \sigma_z}_{=1} \right) = \frac{1}{2} (I + \sigma_z) =$$

$$= \frac{1}{2} \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right) = \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$$

The maximally mixed state $\frac{I}{2}$ corresponds to the center of the sphere. In fact, if

$$\rho = \frac{I}{2} \Rightarrow$$

$$\mathcal{I}_z = \langle 0 | \rho | 0 \rangle - \langle 1 | \rho | 1 \rangle = \frac{1}{2} \langle 0 | I | 0 \rangle - \frac{1}{2} \langle 1 | I | 1 \rangle = \frac{1}{2} \underbrace{\langle 0 | 0 \rangle}_{=1} - \frac{1}{2} \underbrace{\langle 1 | 1 \rangle}_{=1} = 0$$

$$\begin{aligned} \mathcal{I}_x &= \langle 0 | \rho | 1 \rangle + \langle 1 | \rho | 0 \rangle = \frac{1}{2} \langle 0 | I | 1 \rangle + \frac{1}{2} \langle 1 | I | 0 \rangle \\ &= \frac{1}{2} \underbrace{\langle 0 | 1 \rangle}_{=0} + \frac{1}{2} \underbrace{\langle 1 | 0 \rangle}_{=0} = 0 \end{aligned}$$

$$\begin{aligned} \mathcal{I}_y &= i \langle 0 | \rho | 1 \rangle - i \langle 1 | \rho | 0 \rangle = i \langle 0 | \frac{I}{2} | 1 \rangle - i \langle 1 | \frac{I}{2} | 0 \rangle \\ &= \frac{i}{2} \underbrace{\langle 0 | 1 \rangle}_{=0} - \frac{i}{2} \underbrace{\langle 1 | 0 \rangle}_{=0} = 0 \end{aligned}$$

Thus, if $\rho = \frac{I}{2} \Rightarrow (\mathcal{I}_x, \mathcal{I}_y, \mathcal{I}_z) = (0, 0, 0)$ i.e., the center of the Bloch sphere.

The Geometry of Single-Qubit Mixed States

- The following table gives the density matrices, in the standard basis, and the Bloch sphere coordinates for some familiar states and mixed states

(x, y, z) coordinate	state vector	density matrix
$(1, 0, 0)$	$ +\rangle$	$\frac{1}{2}(I + \sigma_x) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$
$(0, 1, 0)$	$ i\rangle$	$\frac{1}{2}(I + \sigma_y) = \frac{1}{2} \begin{pmatrix} 1 & -\mathbf{i} \\ \mathbf{i} & 1 \end{pmatrix}$
$(0, 0, 1)$	$ 0\rangle$	$\frac{1}{2}(I + \sigma_z) = \frac{1}{2} \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$
$(0, 0, 0)$		$\rho_0 = \frac{1}{2}I = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

The Geometry of Single-Qubit Mixed States

Example 1

- Let's assume that $\rho = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{20} + \frac{2}{5} \\ \frac{\sqrt{3}}{20} + \frac{2}{5} & \frac{1}{2} \end{bmatrix}$

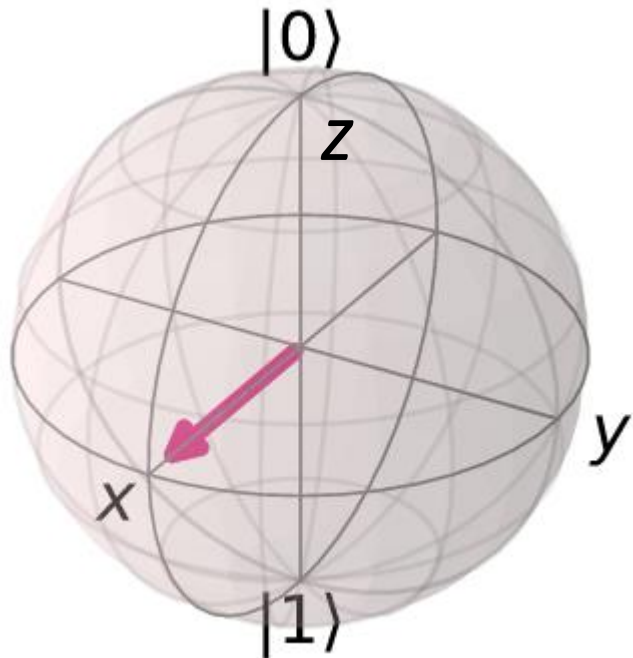
- By comparing the elements of ρ with the elements of

$$\rho = \frac{1}{2} \begin{bmatrix} 1 + r_z & r_x - \textcolor{red}{i}r_y \\ r_x + \textcolor{red}{i}r_y & 1 - r_z \end{bmatrix}$$

we find that: $r_x = 2\left(\frac{\sqrt{3}}{20} + \frac{2}{5}\right)$, $r_y = 0$, $r_z = 0$

The Geometry of Single-Qubit Mixed States

- This means that, in the Bloch sphere, ρ is represented by a vector \vec{r} extending from the origin in the positive x direction, with length $r_x \approx 0.973$



The Geometry of Single-Qubit Mixed States

Example 2

- We have already proved that for a two-qubit maximally entangled state like

$$|\Phi_{AB}^+\rangle = \frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle)$$

its reduced density matrices are

$$\rho_A = \rho_B = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{I}{2}$$

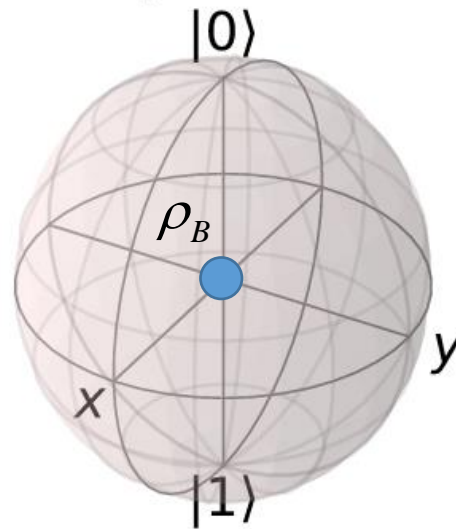
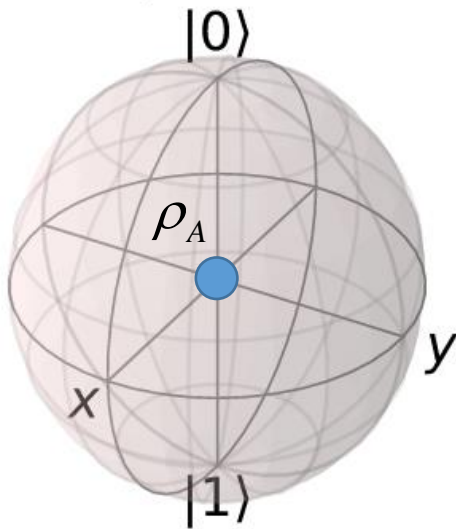
- Comparing ρ_A and ρ_B with the general structure of $\rho = \frac{1}{2} \begin{bmatrix} 1+r_z & r_x - \textcolor{red}{i}r_y \\ r_x + \textcolor{red}{i}r_y & 1-r_z \end{bmatrix}$



$$r_x = r_y = r_z = 0$$

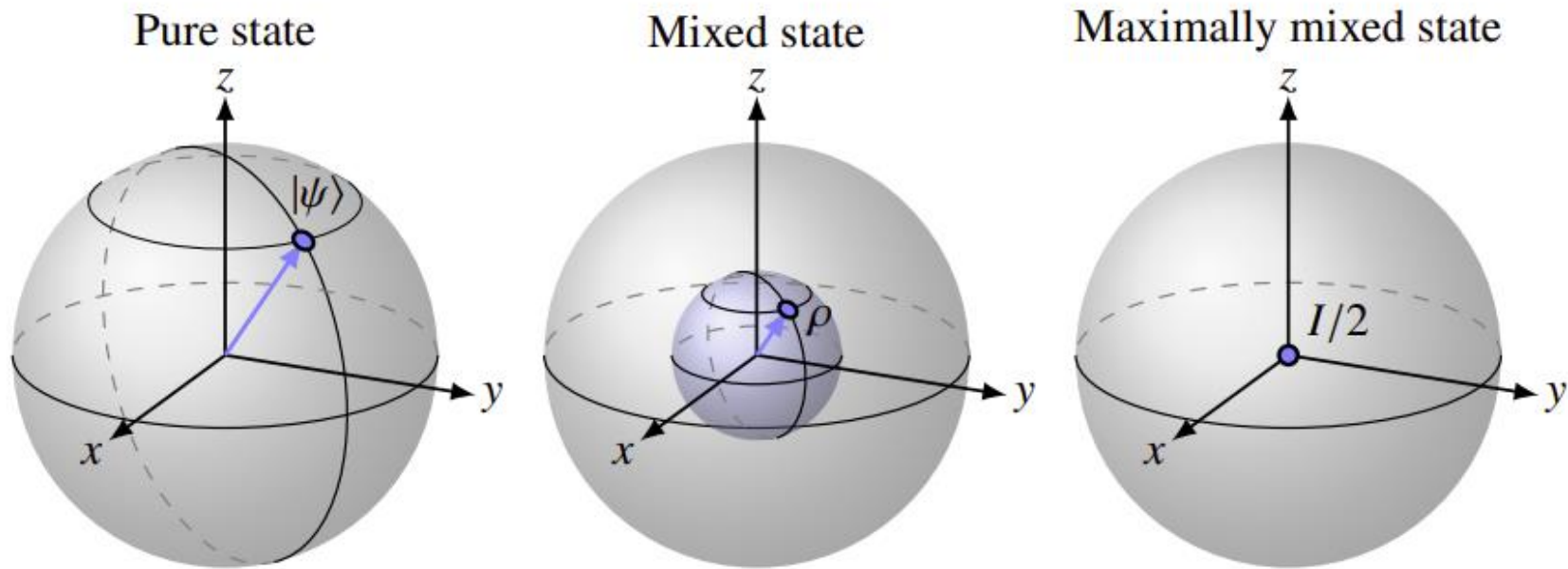
The Geometry of Single-Qubit Mixed States

- Therefore, ρ_A and ρ_B actually have \vec{r} vectors of zero length, represented by points at the origin of the sphere



The Geometry of Single-Qubit Mixed States

- Bloch sphere representation of a pure state $|\psi\rangle$ a mixed state ρ and the maximally mixed state $I/2$



Entanglement in Multipartite Mixed States

- Let's take a brief look at the meaning of entanglement for mixed states
- A mixed state ρ of a quantum system $V_1 \otimes V_2 \otimes \dots \otimes V_n$ **is separable** with respect to this tensor decomposition if it can be written as a probabilistic mixture of **unentangled** states: **ρ is separable** if it can be written as

$$\rho = \sum_{j=1}^m p_j |\phi_j^1\rangle\langle\phi_j^1| \otimes \dots \otimes |\phi_j^n\rangle\langle\phi_j^n|$$

where $|\phi_j^i\rangle \in V_i$ and $p_i \geq 0$ with $\sum_i p_i = 1$

- For a given i , the various $|\phi_j^i\rangle$ need not be orthogonal
- If a mixed state ρ **cannot be written as above**, it is said to be **entangled**