Mixed States

A **pure state** of n qubits is one denoted by a unit vector in $\mathbb{C}^{2^n}$. A **mixed state** is any linear combination of pure states by non-negative weights that sum to 1. That is, a mixed state is a classical probability distribution over pure states. Whether "mixed state" includes pure states depends on context; one can say "properly mixed" to exclude pure states.

For one qubit, every properly mixed state maps to a point interior to the Bloch Sphere. This also holds for generalizations of the Bloch Sphere to higher dimensions for more qubits. So let us have pure states $|\phi_1\rangle, \dots, |\phi_m\rangle$ and probabilities $p_1, \dots, p_m$ summing to 1. Then

$$p_1|\phi_1\rangle \; + \; \cdots \; + p_m|\phi_m\rangle$$

is the "standard" representation of the mixed state. We will see momentarily that, like writing $|\phi_k\rangle$ to begin with, it may presume more than we can directly sense. A philosophical question that comes first is whether a mixed state is a "thing", or just our lack of full knowledge about the state. I will try to convey a *yes*-and-*no* answer along lines of the parable of the blind men and the elephant: the mixed state is like a leg or trunk or tusk attached to a larger pure state, but can be operated on apart from it.

Both of these require taking a second look at measurements-in-any-basis.

General Measurements and Operators

The **triple product** of a row-vector x, a matrix A, and a column vector y is just xAy. We will care about the case where x is the "bra" dual of y. Let's write $y = |\kappa\rangle$, where κ (kappa) could be any meaningful label, and further put $|\kappa\rangle = [a,b]^T$ where a and b are complex numbers such that $|a|^2 + |b|^2 = 1$.

Now when we measure in the standard basis, the probability of getting $|0\rangle$ as the outcome is $|a|^2$, which we can also get as a^*a, and the probability of $|1\rangle$ is $b^*b = |b|^2$. Note that

$$\langle\kappa|\kappa\rangle \;=\; \left[a^*, b^*\right] \cdot [a,b]^T \;=\; \left[a^*, b^*\right] \cdot \begin{bmatrix} a \\ b \end{bmatrix} = \; a^*a + b^*b \;=\; 1 \,,$$

but that didn't finally tell us about the individual outcomes---it just gave us 1, "big whoop". Moreover, the triple product with the identity $\langle\kappa|\mathbf{I}|\kappa\rangle$ just comes out to the same thing. But now let's try a different triple product:

$$\left\langle\kappa\left|\begin{bmatrix}1&0\\0&0\end{bmatrix}\right|\kappa\right\rangle = \left[a^*,b^*\right]\cdot\begin{bmatrix}1&0\\0&0\end{bmatrix}\cdot[a,b]^T = \left[a^*,0\right]\cdot[a,b]^T = a^*a = |a|^2 .$$

Weird that the matrix in the middle is not invertible, but the end result was the probability of $|0\rangle$ separately. And for the probability of $|1\rangle$, we get

$$\left\langle\kappa\left|\begin{bmatrix}0&0\\0&1\end{bmatrix}\right|\kappa\right\rangle = \left[a^*,b^*\right]\cdot\begin{bmatrix}0&0\\0&1\end{bmatrix}\cdot[a,b]^T = \left[0,b^*\right]\cdot[a,b]^T = b^*b = |b|^2 .$$

How can we associate the matrices $\begin{bmatrix}1&0\\0&0\end{bmatrix}$ and $\begin{bmatrix}0&0\\0&1\end{bmatrix}$ to the basis vectors $|0\rangle = [1,0]^T$ and $|1\rangle = [0,1]^T$? The answer is that they are the **outer product** of each vector *with itself*.

$$|0\rangle\langle 0| = \begin{bmatrix}1\\0\end{bmatrix}\cdot[1,0] = \begin{bmatrix}1\cdot 1 & 1\cdot 0\\0\cdot 1 & 0\cdot 0\end{bmatrix} = \begin{bmatrix}1&0\\0&0\end{bmatrix}$$

$$|1\rangle\langle 1| = \begin{bmatrix}0\\1\end{bmatrix}\cdot[0,1] = \begin{bmatrix}0\cdot 0 & 0\cdot 1\\1\cdot 0 & 1\cdot 1\end{bmatrix} = \begin{bmatrix}0&0\\0&1\end{bmatrix}.$$

So we get that $a^*a = \langle\kappa|\cdot|0\rangle\langle 0|\cdot|\kappa\rangle = \left\langle\kappa\middle|\left(|0\rangle\langle 0|\right)\middle|\kappa\right\rangle$ as the first triple product and $b^*b = \langle\kappa|\cdot|1\rangle\langle 1|\cdot|\kappa\rangle$ as the second. The point of going to this trouble is that the outer-product representation *will generalize straightforwardly to any basis*.

Now we will understand this yet another way:

$$a^*a = \langle\kappa|\cdot|0\rangle\langle 0|\cdot|\kappa\rangle = \langle\kappa|0\rangle\cdot\langle 0|\kappa\rangle = |\langle\kappa|0\rangle|^2 = |a|^2 .$$

What this says is that we **projected** the vector denoted by κ **onto** the basis vector $|0\rangle$, and then took the magnitude of that projection. Thus $|0\rangle\langle 0|$ represents the operation of **projecting onto the $|0\rangle$ vector**. Moreover, look how it transforms the $|\kappa\rangle$ vector:

$$\left(|0\rangle\langle 0|\right)\cdot|\kappa\rangle = |0\rangle\cdot\langle 0|\kappa\rangle = |0\rangle(1\cdot a+0\cdot b) = a|0\rangle .$$

If we let $p_0 = |a|^2$ stand for the probability of $|0\rangle$ and divide through by $\sqrt{p_0}$ then we get just $|0\rangle$. Oh wait, what we actually get is

$$\frac{1}{\sqrt{p_0}}\left(|0\rangle\langle 0|\right)\cdot|\kappa\rangle = \frac{1}{\sqrt{p_0}}a|0\rangle = \frac{a}{|a|}|0\rangle.$$

This might not be exactly $|0\rangle$, but it is **equivalent** to it since $\dfrac{a}{|a|}$ is always a unit complex scalar. That's good enough. Thus $\frac{1}{\sqrt{p_0}}\left(|0\rangle\langle 0|\right)$ updates the state when outcome $|0\rangle$ happens. Similarly, $\frac{1}{\sqrt{p_1}}\left(|1\rangle\langle 1|\right)$ faithfully updates the state when outcome $|1\rangle$ happens. Again, the point is how this works for any basis state, not just the standard basis. Let's trot out the general definitions first, then do the example within the $|+\rangle, |-\rangle$ basis, then use $|+\rangle, |-\rangle$ to measure κ as originally defined as $a|0\rangle + b|1\rangle$.

Definition: The **projection operator** associated to a pure state $|\phi\rangle$ is $\mathbf{P}_\phi \;=\; |\phi\rangle\langle\phi|$.

Note that $\mathbf{P}_\phi^* \;=\; \left(|\phi\rangle \cdot \langle\phi|\right)^* \;=\; \langle\phi|^* \cdot |\phi\rangle^* \;=\; |\phi\rangle \cdot \langle\phi| \;=\; \mathbf{P}_\phi$, so every projection operator is Hermitian. More generally, we define:

Definition: A matrix B is **positive semidefinite** (PSD) if there is a matrix A such that $B \;=\; AA^*$.

Definition: A matrix P computes a **projection** if it is PSD and $P^2 = P$.

By $\mathbf{P}_\phi^* = \mathbf{P}_\phi$ we also have

$$\mathbf{P}_\phi \mathbf{P}_\phi^* \;=\mathbf{P}_\phi^2 = |\phi\rangle\langle\phi| \cdot |\phi\rangle\langle\phi| \;=\; |\phi\rangle \cdot \langle\phi|\phi\rangle \cdot \langle\phi| \;=\; |\phi\rangle \cdot 1 \cdot \langle\phi| \;=\; \mathbf{P}_\phi \;,$$

since $|\phi\rangle$ is a unit vector. So $\mathbf{P}_\phi$ is indeed a projection and is PSD.

Definition: A **projective measurement** is given by a set $\{\mathbf{P}_1, \ldots, \mathbf{P}_m\}$ of projections such that

$$\sum_{i=1}^{m} \mathbf{P}_i \;=\; \mathbf{I}.$$

From above, $\left\{|0\rangle\langle 0|, |1\rangle\langle 1|\right\}$ is a projective measurement. How about the $\mathbf{X}$ basis $\left\{|+\rangle\langle +|, |-\rangle\langle -|\right\}$? Using the numerics of the standard basis, we get:

$$|+\rangle\langle +| \;=\; \left[\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right]^T \left[\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right] = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$|-\rangle\langle -| \;=\; \left[\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}\right]^T \left[\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}\right] = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$|+\rangle\langle +| \;+\; |-\rangle\langle -| \;=\; \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \;=\; \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \;=\; \mathbf{I}.$$

So $\{|+\rangle\langle+|, |-\rangle\langle-|\}$ is a projective measurement. Note that if we used the $|+\rangle, |-\rangle$ coordinates to begin with, then the numerics would be $|+\rangle\langle+| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and would come out literally identical, likewise if we apply the measurement to $|\kappa'\rangle = a|+\rangle + b|-\rangle$. (Note: the third from last line on page 145 would be less confusing if it defined $|\kappa'\rangle$ this way rather than say $|\kappa\rangle$ again.) Using the standard-basis numerics:

$$|\kappa'\rangle = \left[\frac{a}{\sqrt{2}}, \frac{a}{\sqrt{2}}\right]^T + \left[\frac{b}{\sqrt{2}}, \frac{-b}{\sqrt{2}}\right]^T = \frac{1}{\sqrt{2}}[a+b, a-b]^T .$$

The triple product with $|+\rangle\langle+|$ is:

$$\langle\kappa'|\cdot|+\rangle\langle+|\cdot|\kappa'\rangle = \frac{1}{4}\left[a^*+b^*, a^*-b^*\right]\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}[a+b, a-b]^T = \frac{1}{4}\left[2a^*, 2a^*\right]\begin{bmatrix} a+b \\ a-b \end{bmatrix}$$
$$= \frac{1}{4}\left(2a^*a + 2a^*b + 2a^*a - 2a^*b\right) = \frac{1}{4}\left(4a^*a\right) = a^*a = |a|^2.$$

Similarly, we get $\langle\kappa'|\cdot|-\rangle\langle-|\cdot|\kappa'\rangle = |b|^2$. That is a lot of rigamarole to replicate the answer we got for measuring the original $|\kappa\rangle$ in the standard basis. The larger point is that the $|\kappa'\rangle$ vector with regard to the $\mathbf{X}$ basis has the same relation to it as $|\kappa\rangle$ did to the standard basis.

However, when we expressly write $|\kappa\rangle = a|0\rangle + b|1\rangle$ rather than $|\kappa\rangle = [a, b]^T$, then we are defining it in a way that is independent of a particular coordinate notation, and so it really is a different physical vector from $|\kappa'\rangle = a|+\rangle + b|-\rangle$. To underscore the point (this is an example that should be on page 146), let us measure $|\kappa\rangle$ not $|\kappa'\rangle$ in the $\mathbf{X}$ basis.

$$\langle\kappa|\cdot|+\rangle\langle+|\cdot|\kappa\rangle = \left[a^*, b^*\right]\frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}[a, b]^T = \frac{1}{2}\left[a^*+b^*, a^*+b^*\right]\begin{bmatrix} a \\ b \end{bmatrix}$$
$$= \frac{1}{2}\left(a^*a + a^*b + b^*a + b^*b\right) = \frac{1}{2}\left(|a|^2 + |b|^2 + a^*b + b^*a\right) = \frac{1}{2} + \frac{c+c^*}{2}$$

where $c = a^*b$. What happened? The first thing to note is that the sum of a unit complex number c and its conjugate is always a real number because the imaginary parts cancel. Although in general the sum could be as big as 2 (or as low as -2), because c arises as a^*b where $|a|^2 + |b|^2 = 1$, the maximum magnitude of $c + c^*$ is 1. Hence the probability of getting the outcome $|+\rangle$ stays within the range $[0, 1]$ as required for a probability.

In fact, if $\kappa = |+\rangle$ then $a = b = \frac{1}{\sqrt{2}}$ so $c = \frac{1}{2}$ and $c + c^* = 1$, finally giving that the probability of getting the outcome $|+\rangle$ is 1. And the probability of getting the outcome $|-\rangle$ is:

$$\langle\kappa|\cdot|-\rangle\langle-|\cdot|\kappa\rangle = [a^*, b^*]\frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}[a,b]^T = \frac{1}{2}[a^*-b^*, -a^*+b^*]\begin{bmatrix} a \\ b \end{bmatrix}$$

$$= \frac{1}{2}\left(a^*a - b^*a - a^*b + b^*b\right) = \frac{1}{2}\left(|a|^2+|b|^2-a^*b-b^*a\right) = \frac{1}{2} - \frac{c+c^*}{2}$$

with $c = a^*b$ as before. This ensures that the probabilities sum to 1, regardless of what c is. It is a nice self-study exercise to repeat this with the example $|\kappa\rangle = \left[\frac{1}{2}, \frac{\sqrt{3}}{2}\right]$ from the beginning of Tuesday's lecture.

There is an essential symmetry of measurement as well. If we instead did $\langle-|\cdot|\kappa\rangle\langle\kappa|\cdot|-\rangle$ then we would get the same answer. Indeed, for a general other pure state $|\phi\rangle$, the **double action**

$$P_{|\kappa\rangle}(|\phi\rangle) = \langle\phi|\cdot|\kappa\rangle\langle\kappa|\cdot|\phi\rangle$$

is a product of the form cc^* where $c = \langle\phi|\kappa\rangle$. And $(cc^*)^* = (c^*)^*(c)^* = cc^*$ back again, so the *product* of a complex number and its conjugate is always a real number too. (More simply put, the phase angles add and cancel.) This feeds into some notable philosophy:

- The only knowledge we can *gain* about a quantum state $|\kappa\rangle$ (relative to any prior knowledge about how it was prepared) is by *measuring* it.
- All measurements of κ go through the outer product $|\kappa\rangle\langle\kappa|$.
- Hence $|\kappa\rangle\langle\kappa|$, not $|\kappa\rangle$, is the "unit of epistemology" (the origin of "episte-" is the idea of sending a message, i.e., an *epistle*). This is a Hermitian operator and a PSD matrix with real entries and a projection. All complex numbers have vamoosed.

This carries through when $|\kappa\rangle$ is a state of multiple qubits, or of multiple **qutrits**, **quarts**, **qudits** (meaning d-ary, as with card ranks where $d = 13$), **quopits** (meaning qudits with $d = p$ standing for a prime number), etc. (in infinite-dimensional Hilbert spaces). The "real proof" of the principle, IMHO, comes from the extension to mixed states.

Mixed States Again (Decoherence later...)

Consider a mixed state represented as $p_1|\phi_1\rangle + p_2|\phi_2\rangle + \cdots + p_m|\phi_m\rangle$ where the p_i are nonnegative and sum to 1.

Definition: The corresponding **density matrix** is

$$\rho = p_1|\phi_1\rangle\langle\phi_1| + p_2|\phi_2\rangle\langle\phi_2| + \cdots + p_m|\phi_m\rangle\langle\phi_m|.$$

Per above philosophy, ρ is all we can know about the mixed state (aside from any prior knowledge from having prepared it). The letter ρ tends to be used, without a ket or bra around it. Some more facts:

1. A density matrix is always Hermitian: $\rho^* = \rho$.
2. The matrix designates a pure state if and only if $\rho^2 = \rho$; note that this is automatic as shown above when $m = 1$.
3. The results of measuring a mixed state can be computed by applying ρ as an operator to update the state, or with the double action to compute a probability of getting a given state. By linearity, this gives the same results as working with each individual term and taking the linear combination.

Example: The density matrix of the mixed state $p|0\rangle + (1-p)|1\rangle$ is

$$\rho_p \;=\; p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1| \;=\; p\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + (1-p)\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix}.$$

Note that $\rho_p^2 = \begin{bmatrix} p^2 & 0 \\ 0 & (1-p)^2 \end{bmatrix} \neq \rho_p$ unless $p = 1$ or $p = 0$, so this is generally not a pure state.

How about $p|+\rangle\langle +| \;+\; (1-p)|-\rangle\langle -|$? We get

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

In general, this is different. But for the equal mixture $p = \frac{1}{2}$, both density matrices are the same: $\rho_{1/2} = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$. In terms of the Bloch sphere, both mixtures map to the exact center of the sphere, which is halfway down the axis between $|0\rangle$ and $|1\rangle$ at the poles, and also halfway along the equatorial axis between $|+\rangle$ and $|-\rangle$. In physical terms, that means they are *the same state*. That might come as a surprise, because:

> One is defined as a spread between the outcomes $|0\rangle$ and $|1\rangle$, the other between the outcomes $|+\rangle$ and $|-\rangle$. Isn't that like saying one is a choice between an apple and a pear, the other between an orange and a grapefruit?

The ultimate point is that to probe the state, we have to choose a basis to measure against in advance. If we choose the standard basis, then to measure the probability for the outcome $|0\rangle$, even if we use the $|+\rangle$ and $|-\rangle$ mixture, we still get

$$P_{|0\rangle}(\rho_{1/2}) \;=\; \langle 0|\big(0.5|+\rangle\langle +| \;+\; 0.5|-\rangle\langle -|\big)|0\rangle \;\;=\;\; 0.5\langle 0|+\rangle\langle +|0\rangle \;\;+\; 0.5\langle 0|-\rangle\langle -|0\rangle$$

$$= \; 0.5\frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}} \; + \; 0.5\frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}} \; = \; 0.5.$$

Note that this associated the terms so that the fact that the $|0\rangle$ and $|+\rangle$ vectors are 45° aligned to each other in Cartesian coordinates, likewise $|0\rangle$ and $|-\rangle$, came out as an idea. But we can get the point much more succinctly upon measuring any outcome $|\kappa\rangle$ for $\boldsymbol{\rho}_{1/2}$:

$$\langle\kappa|\boldsymbol{\rho}_{1/2}|\kappa\rangle \; = \; \left\langle\kappa\left|\begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}\right|\kappa\right\rangle \; = \; \langle\kappa|0.5\mathbf{I}|\kappa\rangle \; = \; 0.5\langle\kappa|\mathbf{I}|\kappa\rangle \; = \; 0.5\langle\kappa|\kappa\rangle \; = \; 0.5.$$

That's it. However we try to probe the **completely mixed state** $\rho_{1/2}$, it just behaves like a perfect unbiased classical coin. Regardless of the past history of what we mixed to make it, there is nothing else that it is now.

There is an especially meaningful way of decomposing a density matrix, indeed any Hermitian matrix. This is the **spectral decomposition**, given by the **spectral theorem** on page 149. We will pause here and go back to chapters 5--7 to do more with quantum operations on multiple qubits first, however.